Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 05:03 PM JST

PDB ID	:	7YMM / pdb_00007ymm
EMDB ID	:	EMD-33933
Title	:	PSII-Pcb Tetramer of Acaryochloris Marina
Authors	:	Shen, L.L.; Gao, Y.Z.; Wang, W.D.; Zhang, X.; Shen, J.R.; Wang, P.Y.; Han, G.Y.
Deposited on	:	2022-07-28
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

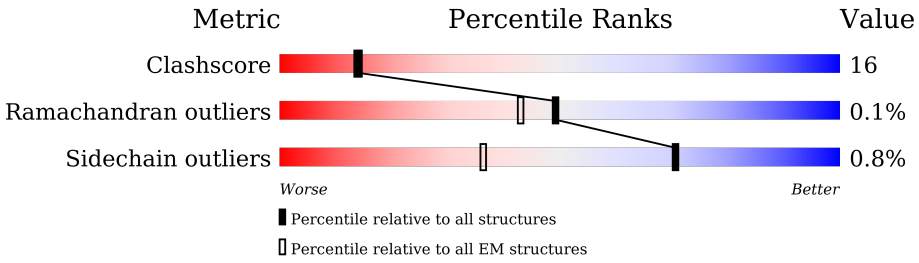
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

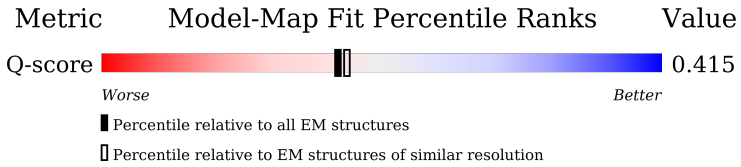
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	360	21% 61% 18% 21%
1	2A	360	12% 60% 19% 21%
1	3A	360	12% 61% 18% 21%
1	4A	360	22% 59% 19% 21%

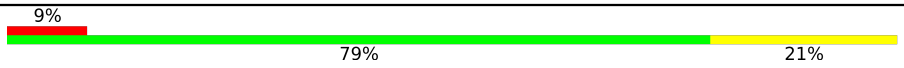
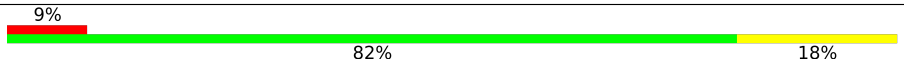
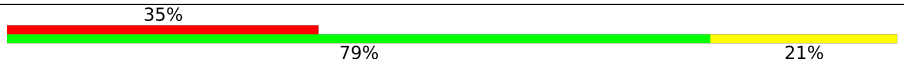
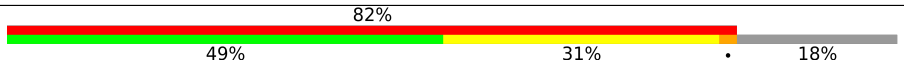
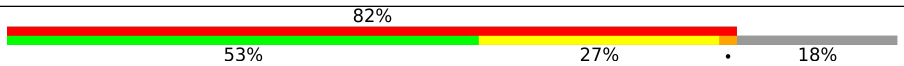
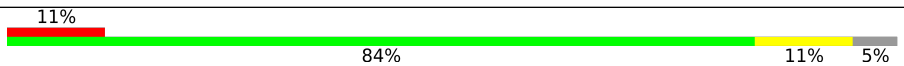
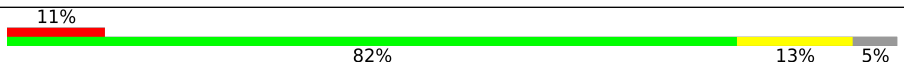
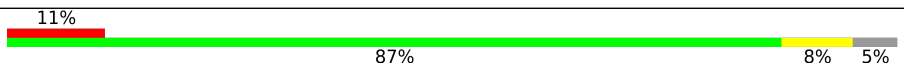
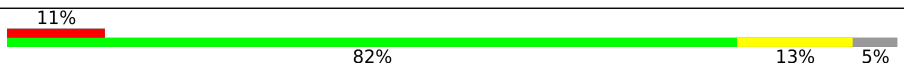
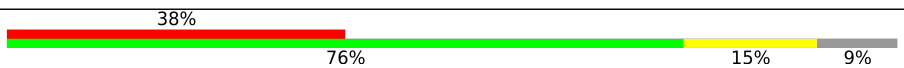
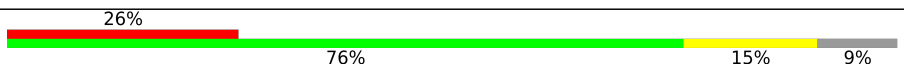
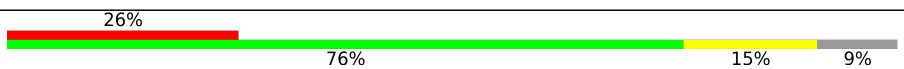
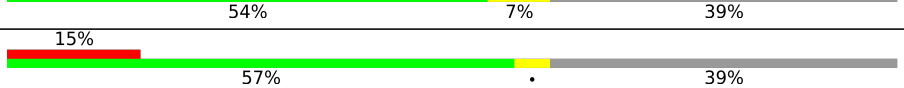
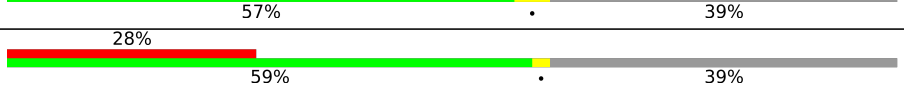
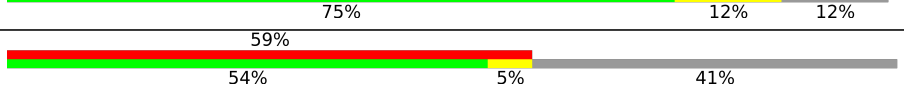
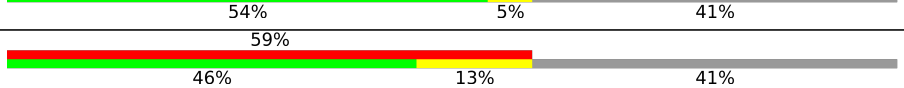
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1B	506	34% 77% 18% 5%
2	2B	506	19% 77% 17% 5%
2	3B	506	19% 78% 17% 5%
2	4B	506	34% 77% 17% 5%
3	1C	490	53% 69% 17% 14%
3	2C	490	25% 68% 17% 14%
3	3C	490	25% 69% 17% 14%
3	4C	490	53% 69% 17% 14%
4	1D	351	30% 72% 20% 8%
4	2D	351	13% 73% 19% 8%
4	3D	351	13% 73% 19% 8%
4	4D	351	30% 73% 19% 8%
5	1E	83	73% 60% 18% 22%
5	2E	83	52% 64% 14% 22%
5	3E	83	52% 60% 18% 22%
5	4E	83	73% 60% 18% 22%
6	1F	99	28% 28% 70%
6	2F	99	14% 27% 70%
6	3F	99	14% 27% 70%
6	4F	99	28% 27% 70%
7	1H	71	56% 79% 17%
7	2H	71	25% 79% 17%
7	3H	71	25% 79% 17%
7	4H	71	56% 79% 17%
8	1I	34	35% 76% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	2I	34	
8	3I	34	
8	4I	34	
9	1K	45	
9	2K	45	
9	3K	45	
9	4K	45	
10	1L	38	
10	2L	38	
10	3L	38	
10	4L	38	
11	1M	34	
11	2M	34	
11	3M	34	
11	4M	34	
12	1T	46	
12	2T	46	
12	3T	46	
12	4T	46	
13	1X	40	
13	2X	40	
13	3X	40	
13	4X	40	
14	1Y	39	
14	2Y	39	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	3Y	39	59% 51% 8% 41%
14	4Y	39	59% 49% 10% 41%
15	1Z	62	95% 85% 10% 5%
15	2Z	62	85% 84% 11% 5%
15	3Z	62	85% 84% 11% 5%
15	4Z	62	95% 85% 10% 5%
16	12	352	57% 69% 30%
16	22	352	33% 70% 29%
16	32	352	32% 69% 30%
16	42	352	58% 69% 30%
17	1G	41	61% 93% 7%
17	2G	41	51% 93% 7%
17	3G	41	51% 93% 7%
17	4G	41	63% 93% 7%
18	11	356	83% 64% 28% 8%
18	21	356	43% 63% 29% 8%
18	31	356	43% 63% 29% 8%
18	41	356	83% 63% 29% 8%
19	13	349	42% 77% 21%
19	23	349	38% 76% 22%
19	33	349	38% 77% 21%
19	43	349	42% 76% 22%
20	14	353	71% 68% 25% 6%
20	24	353	36% 69% 25% 6%
20	34	353	37% 68% 25% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	44	353	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	11	402	X	-	-	-
21	CL7	11	403	X	-	-	-
21	CL7	11	404	X	-	-	-
21	CL7	11	405	X	-	-	-
21	CL7	11	406	X	-	-	-
21	CL7	11	407	X	-	-	-
21	CL7	11	408	X	-	-	-
21	CL7	11	409	X	-	-	-
21	CL7	11	410	X	-	-	-
21	CL7	11	411	X	-	-	-
21	CL7	11	412	X	-	-	-
21	CL7	11	413	X	-	-	-
21	CL7	11	414	X	-	-	-
21	CL7	11	415	X	-	-	-
21	CL7	11	416	X	-	-	-
21	CL7	11	417	X	-	-	-
21	CL7	11	418	X	-	-	-
21	CL7	11	419	X	-	-	-
21	CL7	11	420	X	-	-	-
21	CL7	12	501	X	-	-	-
21	CL7	12	502	X	-	-	-
21	CL7	12	503	X	-	-	-
21	CL7	12	504	X	-	-	-
21	CL7	12	505	X	-	-	-
21	CL7	12	506	X	-	-	-
21	CL7	12	507	X	-	-	-
21	CL7	12	508	X	-	-	-
21	CL7	12	509	X	-	-	-
21	CL7	12	510	X	-	-	-
21	CL7	12	511	X	-	-	-
21	CL7	12	512	X	-	-	-
21	CL7	12	513	X	-	-	-
21	CL7	12	514	X	-	-	-
21	CL7	12	515	X	-	-	-
21	CL7	12	516	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	12	517	X	-	-	-
21	CL7	12	518	X	-	-	-
21	CL7	13	501	X	-	-	-
21	CL7	13	502	X	-	-	-
21	CL7	13	503	X	-	-	-
21	CL7	13	504	X	-	-	-
21	CL7	13	505	X	-	-	-
21	CL7	13	506	X	-	-	-
21	CL7	13	507	X	-	-	-
21	CL7	13	508	X	-	-	-
21	CL7	13	509	X	-	-	-
21	CL7	13	510	X	-	-	-
21	CL7	13	511	X	-	-	-
21	CL7	13	512	X	-	-	-
21	CL7	13	513	X	-	-	-
21	CL7	13	514	X	-	-	-
21	CL7	13	515	X	-	-	-
21	CL7	13	516	X	-	-	-
21	CL7	13	517	X	-	-	-
21	CL7	13	518	X	-	-	-
21	CL7	14	404	X	-	-	-
21	CL7	14	405	X	-	-	-
21	CL7	14	406	X	-	-	-
21	CL7	14	407	X	-	-	-
21	CL7	14	408	X	-	-	-
21	CL7	14	409	X	-	-	-
21	CL7	14	410	X	-	-	-
21	CL7	14	411	X	-	-	-
21	CL7	14	412	X	-	-	-
21	CL7	14	413	X	-	-	-
21	CL7	14	414	X	-	-	-
21	CL7	14	415	X	-	-	-
21	CL7	14	416	X	-	-	-
21	CL7	14	417	X	-	-	-
21	CL7	1A	401	X	-	-	-
21	CL7	1A	403	X	-	-	-
21	CL7	1A	407	X	-	-	-
21	CL7	1B	601	X	-	-	-
21	CL7	1B	602	X	-	-	-
21	CL7	1B	603	X	-	-	-
21	CL7	1B	604	X	-	-	-
21	CL7	1B	605	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	1B	606	X	-	-	-
21	CL7	1B	607	X	-	-	-
21	CL7	1B	608	X	-	-	-
21	CL7	1B	609	X	-	-	-
21	CL7	1B	610	X	-	-	-
21	CL7	1B	611	X	-	-	-
21	CL7	1B	612	X	-	-	-
21	CL7	1B	613	X	-	-	-
21	CL7	1B	614	X	-	-	-
21	CL7	1B	615	X	-	-	-
21	CL7	1B	616	X	-	-	-
21	CL7	1B	622	X	-	-	-
21	CL7	1C	501	X	-	-	-
21	CL7	1C	502	X	-	-	-
21	CL7	1C	503	X	-	-	-
21	CL7	1C	504	X	-	-	-
21	CL7	1C	505	X	-	-	-
21	CL7	1C	506	X	-	-	-
21	CL7	1C	507	X	-	-	-
21	CL7	1C	508	X	-	-	-
21	CL7	1C	509	X	-	-	-
21	CL7	1C	510	X	-	-	-
21	CL7	1C	511	X	-	-	-
21	CL7	1C	512	X	-	-	-
21	CL7	1C	513	X	-	-	-
21	CL7	1C	517	X	-	-	-
21	CL7	1D	402	X	-	-	-
21	CL7	1D	404	X	-	-	-
21	CL7	1D	405	X	-	-	-
21	CL7	21	402	X	-	-	-
21	CL7	21	403	X	-	-	-
21	CL7	21	404	X	-	-	-
21	CL7	21	405	X	-	-	-
21	CL7	21	406	X	-	-	-
21	CL7	21	407	X	-	-	-
21	CL7	21	408	X	-	-	-
21	CL7	21	409	X	-	-	-
21	CL7	21	410	X	-	-	-
21	CL7	21	411	X	-	-	-
21	CL7	21	412	X	-	-	-
21	CL7	21	413	X	-	-	-
21	CL7	21	414	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	21	415	X	-	-	-
21	CL7	21	416	X	-	-	-
21	CL7	21	417	X	-	-	-
21	CL7	21	418	X	-	-	-
21	CL7	21	419	X	-	-	-
21	CL7	21	420	X	-	-	-
21	CL7	22	501	X	-	-	-
21	CL7	22	502	X	-	-	-
21	CL7	22	503	X	-	-	-
21	CL7	22	504	X	-	-	-
21	CL7	22	505	X	-	-	-
21	CL7	22	506	X	-	-	-
21	CL7	22	507	X	-	-	-
21	CL7	22	508	X	-	-	-
21	CL7	22	509	X	-	-	-
21	CL7	22	510	X	-	-	-
21	CL7	22	511	X	-	-	-
21	CL7	22	512	X	-	-	-
21	CL7	22	513	X	-	-	-
21	CL7	22	514	X	-	-	-
21	CL7	22	515	X	-	-	-
21	CL7	22	516	X	-	-	-
21	CL7	22	517	X	-	-	-
21	CL7	22	518	X	-	-	-
21	CL7	23	402	X	-	-	-
21	CL7	23	403	X	-	-	-
21	CL7	23	404	X	-	-	-
21	CL7	23	405	X	-	-	-
21	CL7	23	406	X	-	-	-
21	CL7	23	407	X	-	-	-
21	CL7	23	408	X	-	-	-
21	CL7	23	409	X	-	-	-
21	CL7	23	410	X	-	-	-
21	CL7	23	411	X	-	-	-
21	CL7	23	412	X	-	-	-
21	CL7	23	413	X	-	-	-
21	CL7	23	414	X	-	-	-
21	CL7	23	415	X	-	-	-
21	CL7	23	416	X	-	-	-
21	CL7	23	417	X	-	-	-
21	CL7	23	418	X	-	-	-
21	CL7	23	419	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	24	404	X	-	-	-
21	CL7	24	405	X	-	-	-
21	CL7	24	406	X	-	-	-
21	CL7	24	407	X	-	-	-
21	CL7	24	408	X	-	-	-
21	CL7	24	409	X	-	-	-
21	CL7	24	410	X	-	-	-
21	CL7	24	411	X	-	-	-
21	CL7	24	412	X	-	-	-
21	CL7	24	413	X	-	-	-
21	CL7	24	414	X	-	-	-
21	CL7	24	415	X	-	-	-
21	CL7	24	416	X	-	-	-
21	CL7	24	417	X	-	-	-
21	CL7	2A	401	X	-	-	-
21	CL7	2A	403	X	-	-	-
21	CL7	2A	407	X	-	-	-
21	CL7	2B	602	X	-	-	-
21	CL7	2B	603	X	-	-	-
21	CL7	2B	604	X	-	-	-
21	CL7	2B	605	X	-	-	-
21	CL7	2B	606	X	-	-	-
21	CL7	2B	607	X	-	-	-
21	CL7	2B	608	X	-	-	-
21	CL7	2B	609	X	-	-	-
21	CL7	2B	610	X	-	-	-
21	CL7	2B	611	X	-	-	-
21	CL7	2B	612	X	-	-	-
21	CL7	2B	613	X	-	-	-
21	CL7	2B	614	X	-	-	-
21	CL7	2B	615	X	-	-	-
21	CL7	2B	616	X	-	-	-
21	CL7	2B	617	X	-	-	-
21	CL7	2B	623	X	-	-	-
21	CL7	2C	501	X	-	-	-
21	CL7	2C	502	X	-	-	-
21	CL7	2C	503	X	-	-	-
21	CL7	2C	504	X	-	-	-
21	CL7	2C	505	X	-	-	-
21	CL7	2C	506	X	-	-	-
21	CL7	2C	507	X	-	-	-
21	CL7	2C	508	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	2C	509	X	-	-	-
21	CL7	2C	510	X	-	-	-
21	CL7	2C	511	X	-	-	-
21	CL7	2C	512	X	-	-	-
21	CL7	2C	513	X	-	-	-
21	CL7	2C	517	X	-	-	-
21	CL7	2D	402	X	-	-	-
21	CL7	2D	404	X	-	-	-
21	CL7	2D	405	X	-	-	-
21	CL7	31	402	X	-	-	-
21	CL7	31	403	X	-	-	-
21	CL7	31	404	X	-	-	-
21	CL7	31	405	X	-	-	-
21	CL7	31	406	X	-	-	-
21	CL7	31	407	X	-	-	-
21	CL7	31	408	X	-	-	-
21	CL7	31	409	X	-	-	-
21	CL7	31	410	X	-	-	-
21	CL7	31	411	X	-	-	-
21	CL7	31	412	X	-	-	-
21	CL7	31	413	X	-	-	-
21	CL7	31	414	X	-	-	-
21	CL7	31	415	X	-	-	-
21	CL7	31	416	X	-	-	-
21	CL7	31	417	X	-	-	-
21	CL7	31	418	X	-	-	-
21	CL7	31	419	X	-	-	-
21	CL7	31	420	X	-	-	-
21	CL7	32	501	X	-	-	-
21	CL7	32	502	X	-	-	-
21	CL7	32	503	X	-	-	-
21	CL7	32	504	X	-	-	-
21	CL7	32	505	X	-	-	-
21	CL7	32	506	X	-	-	-
21	CL7	32	507	X	-	-	-
21	CL7	32	508	X	-	-	-
21	CL7	32	509	X	-	-	-
21	CL7	32	510	X	-	-	-
21	CL7	32	511	X	-	-	-
21	CL7	32	512	X	-	-	-
21	CL7	32	513	X	-	-	-
21	CL7	32	514	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	32	515	X	-	-	-
21	CL7	32	516	X	-	-	-
21	CL7	32	517	X	-	-	-
21	CL7	32	518	X	-	-	-
21	CL7	33	501	X	-	-	-
21	CL7	33	502	X	-	-	-
21	CL7	33	503	X	-	-	-
21	CL7	33	504	X	-	-	-
21	CL7	33	505	X	-	-	-
21	CL7	33	506	X	-	-	-
21	CL7	33	507	X	-	-	-
21	CL7	33	508	X	-	-	-
21	CL7	33	509	X	-	-	-
21	CL7	33	510	X	-	-	-
21	CL7	33	511	X	-	-	-
21	CL7	33	512	X	-	-	-
21	CL7	33	513	X	-	-	-
21	CL7	33	514	X	-	-	-
21	CL7	33	515	X	-	-	-
21	CL7	33	516	X	-	-	-
21	CL7	33	517	X	-	-	-
21	CL7	33	518	X	-	-	-
21	CL7	34	404	X	-	-	-
21	CL7	34	405	X	-	-	-
21	CL7	34	406	X	-	-	-
21	CL7	34	407	X	-	-	-
21	CL7	34	408	X	-	-	-
21	CL7	34	409	X	-	-	-
21	CL7	34	410	X	-	-	-
21	CL7	34	411	X	-	-	-
21	CL7	34	412	X	-	-	-
21	CL7	34	413	X	-	-	-
21	CL7	34	414	X	-	-	-
21	CL7	34	415	X	-	-	-
21	CL7	34	416	X	-	-	-
21	CL7	34	417	X	-	-	-
21	CL7	3A	401	X	-	-	-
21	CL7	3A	403	X	-	-	-
21	CL7	3A	407	X	-	-	-
21	CL7	3B	601	X	-	-	-
21	CL7	3B	602	X	-	-	-
21	CL7	3B	603	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	3B	604	X	-	-	-
21	CL7	3B	605	X	-	-	-
21	CL7	3B	606	X	-	-	-
21	CL7	3B	607	X	-	-	-
21	CL7	3B	608	X	-	-	-
21	CL7	3B	609	X	-	-	-
21	CL7	3B	610	X	-	-	-
21	CL7	3B	611	X	-	-	-
21	CL7	3B	612	X	-	-	-
21	CL7	3B	613	X	-	-	-
21	CL7	3B	614	X	-	-	-
21	CL7	3B	615	X	-	-	-
21	CL7	3B	616	X	-	-	-
21	CL7	3B	622	X	-	-	-
21	CL7	3C	501	X	-	-	-
21	CL7	3C	502	X	-	-	-
21	CL7	3C	503	X	-	-	-
21	CL7	3C	504	X	-	-	-
21	CL7	3C	505	X	-	-	-
21	CL7	3C	506	X	-	-	-
21	CL7	3C	507	X	-	-	-
21	CL7	3C	508	X	-	-	-
21	CL7	3C	509	X	-	-	-
21	CL7	3C	510	X	-	-	-
21	CL7	3C	511	X	-	-	-
21	CL7	3C	512	X	-	-	-
21	CL7	3C	513	X	-	-	-
21	CL7	3C	517	X	-	-	-
21	CL7	3D	402	X	-	-	-
21	CL7	3D	404	X	-	-	-
21	CL7	3D	405	X	-	-	-
21	CL7	41	402	X	-	-	-
21	CL7	41	403	X	-	-	-
21	CL7	41	404	X	-	-	-
21	CL7	41	405	X	-	-	-
21	CL7	41	406	X	-	-	-
21	CL7	41	407	X	-	-	-
21	CL7	41	408	X	-	-	-
21	CL7	41	409	X	-	-	-
21	CL7	41	410	X	-	-	-
21	CL7	41	411	X	-	-	-
21	CL7	41	412	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	41	413	X	-	-	-
21	CL7	41	414	X	-	-	-
21	CL7	41	415	X	-	-	-
21	CL7	41	416	X	-	-	-
21	CL7	41	417	X	-	-	-
21	CL7	41	418	X	-	-	-
21	CL7	41	419	X	-	-	-
21	CL7	41	420	X	-	-	-
21	CL7	42	501	X	-	-	-
21	CL7	42	502	X	-	-	-
21	CL7	42	503	X	-	-	-
21	CL7	42	504	X	-	-	-
21	CL7	42	505	X	-	-	-
21	CL7	42	506	X	-	-	-
21	CL7	42	507	X	-	-	-
21	CL7	42	508	X	-	-	-
21	CL7	42	509	X	-	-	-
21	CL7	42	510	X	-	-	-
21	CL7	42	511	X	-	-	-
21	CL7	42	512	X	-	-	-
21	CL7	42	513	X	-	-	-
21	CL7	42	514	X	-	-	-
21	CL7	42	515	X	-	-	-
21	CL7	42	516	X	-	-	-
21	CL7	42	517	X	-	-	-
21	CL7	42	518	X	-	-	-
21	CL7	43	402	X	-	-	-
21	CL7	43	403	X	-	-	-
21	CL7	43	404	X	-	-	-
21	CL7	43	405	X	-	-	-
21	CL7	43	406	X	-	-	-
21	CL7	43	407	X	-	-	-
21	CL7	43	408	X	-	-	-
21	CL7	43	409	X	-	-	-
21	CL7	43	410	X	-	-	-
21	CL7	43	411	X	-	-	-
21	CL7	43	412	X	-	-	-
21	CL7	43	413	X	-	-	-
21	CL7	43	414	X	-	-	-
21	CL7	43	415	X	-	-	-
21	CL7	43	416	X	-	-	-
21	CL7	43	417	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	43	418	X	-	-	-
21	CL7	43	419	X	-	-	-
21	CL7	44	404	X	-	-	-
21	CL7	44	405	X	-	-	-
21	CL7	44	406	X	-	-	-
21	CL7	44	407	X	-	-	-
21	CL7	44	408	X	-	-	-
21	CL7	44	409	X	-	-	-
21	CL7	44	410	X	-	-	-
21	CL7	44	411	X	-	-	-
21	CL7	44	412	X	-	-	-
21	CL7	44	413	X	-	-	-
21	CL7	44	414	X	-	-	-
21	CL7	44	415	X	-	-	-
21	CL7	44	416	X	-	-	-
21	CL7	44	417	X	-	-	-
21	CL7	4A	401	X	-	-	-
21	CL7	4A	403	X	-	-	-
21	CL7	4A	407	X	-	-	-
21	CL7	4B	602	X	-	-	-
21	CL7	4B	603	X	-	-	-
21	CL7	4B	604	X	-	-	-
21	CL7	4B	605	X	-	-	-
21	CL7	4B	606	X	-	-	-
21	CL7	4B	607	X	-	-	-
21	CL7	4B	608	X	-	-	-
21	CL7	4B	609	X	-	-	-
21	CL7	4B	610	X	-	-	-
21	CL7	4B	611	X	-	-	-
21	CL7	4B	612	X	-	-	-
21	CL7	4B	613	X	-	-	-
21	CL7	4B	614	X	-	-	-
21	CL7	4B	615	X	-	-	-
21	CL7	4B	616	X	-	-	-
21	CL7	4B	617	X	-	-	-
21	CL7	4B	623	X	-	-	-
21	CL7	4C	501	X	-	-	-
21	CL7	4C	502	X	-	-	-
21	CL7	4C	503	X	-	-	-
21	CL7	4C	504	X	-	-	-
21	CL7	4C	505	X	-	-	-
21	CL7	4C	506	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	4C	507	X	-	-	-
21	CL7	4C	508	X	-	-	-
21	CL7	4C	509	X	-	-	-
21	CL7	4C	510	X	-	-	-
21	CL7	4C	511	X	-	-	-
21	CL7	4C	512	X	-	-	-
21	CL7	4C	513	X	-	-	-
21	CL7	4C	517	X	-	-	-
21	CL7	4D	402	X	-	-	-
21	CL7	4D	404	X	-	-	-
21	CL7	4D	405	X	-	-	-
22	PHO	1D	408	X	-	-	-
22	PHO	2D	408	X	-	-	-
22	PHO	3D	408	X	-	-	-
22	PHO	4D	408	X	-	-	-
24	LMG	1A	405	X	-	-	-
24	LMG	2A	405	X	-	-	-
24	LMG	3A	405	X	-	-	-
24	LMG	4A	405	X	-	-	-
32	ZEX	11	422	-	-	X	-
32	ZEX	12	520	-	-	X	-
32	ZEX	13	522	-	-	X	-
32	ZEX	13	525	-	-	X	-
32	ZEX	14	403	-	-	X	-
32	ZEX	21	422	-	-	X	-
32	ZEX	22	520	-	-	X	-
32	ZEX	23	401	-	-	X	-
32	ZEX	23	423	-	-	X	-
32	ZEX	24	403	-	-	X	-
32	ZEX	31	422	-	-	X	-
32	ZEX	32	520	-	-	X	-
32	ZEX	33	522	-	-	X	-
32	ZEX	33	525	-	-	X	-
32	ZEX	34	403	-	-	X	-
32	ZEX	41	422	-	-	X	-
32	ZEX	42	520	-	-	X	-
32	ZEX	43	401	-	-	X	-
32	ZEX	43	423	-	-	X	-
32	ZEX	44	403	-	-	X	-

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 136856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	2A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	3A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	4A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	2B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	3B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	4B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	2C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	3C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	4C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		

- Molecule 4 is a protein called Photosystem II D2 protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	2D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	3D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	4D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	2E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	3E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	4E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		

- Molecule 6 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	2F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	3F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	4F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		

- Molecule 7 is a protein called Photosystem II 10 kDa phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	2H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	3H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

- Molecule 8 is a protein called Photosystem II protein PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	2I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	3I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	4I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	2K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	3K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	4K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	1L	36	Total	C	N	O	0	0
			288	194	45	49		
10	2L	36	Total	C	N	O	0	0
			288	194	45	49		
10	3L	36	Total	C	N	O	0	0
			288	194	45	49		
10	4L	36	Total	C	N	O	0	0
			288	194	45	49		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	2M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	3M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		
11	4M	31	Total	C	N	O	S	0	0
			232	156	36	39	1		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	2T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	3T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		
12	4T	28	Total	C	N	O	S	0	0
			231	163	32	34	2		

- Molecule 13 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	1X	35	Total	C	N	O	0	0
			269	185	39	45		
13	2X	35	Total	C	N	O	0	0
			269	185	39	45		
13	3X	35	Total	C	N	O	0	0
			269	185	39	45		
13	4X	35	Total	C	N	O	0	0
			269	185	39	45		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		
14	2Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		
14	3Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4Y	23	Total	C	N	O	S	0	0
			164	111	27	25	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	2Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	3Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		
15	4Z	59	Total	C	N	O	S	0	0
			429	290	64	73	2		

- Molecule 16 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	12	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	22	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	32	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	42	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1G	41	Total	C	N	O	0	0
			205	123	41	41		
17	2G	41	Total	C	N	O	0	0
			205	123	41	41		
17	3G	41	Total	C	N	O	0	0
			205	123	41	41		
17	4G	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 18 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	11	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	21	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	31	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	41	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		

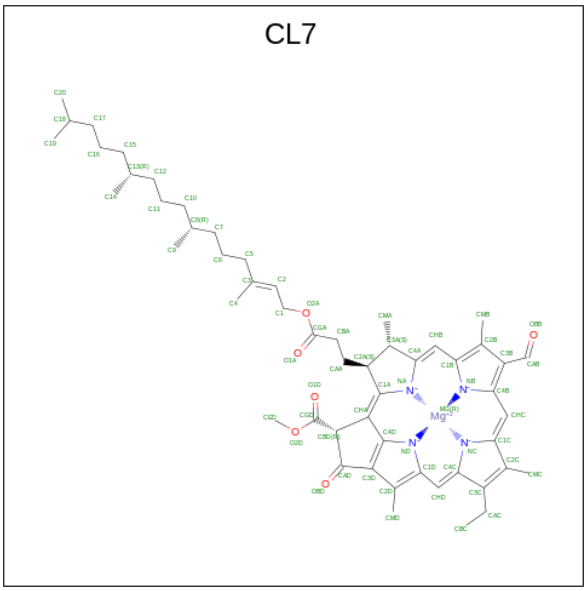
- Molecule 19 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	13	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	23	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	33	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	43	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		

- Molecule 20 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	14	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	24	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	34	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	44	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		

- Molecule 21 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	1B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	1C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	1C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	1D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	1D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	1D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	12	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	11	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	11	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	11	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	13	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	13	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	14	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	14	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	14	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	14	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	2A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	2C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	2C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	2C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	2D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	2D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	22	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	21	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	21	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	21	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			58	47	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	23	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	23	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	24	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	24	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	24	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	24	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	3A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	3C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	3C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	3D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	32	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	31	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	31	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	33	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	33	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	33	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	34	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	34	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	34	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	4A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4A	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4B	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	4C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	4C	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4C	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4D	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	4D	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	4D	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	42	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	41	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	41	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

Continued on next page...

Continued from previous page...

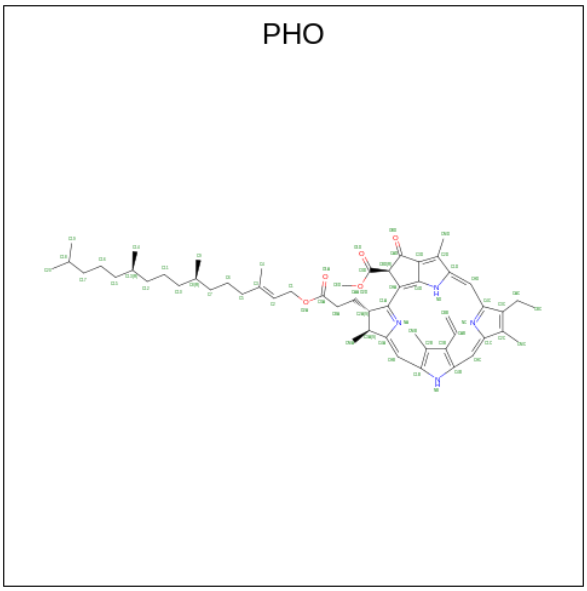
Mol	Chain	Residues	Atoms					AltConf
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	43	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	43	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

Continued on next page...

Continued from previous page...

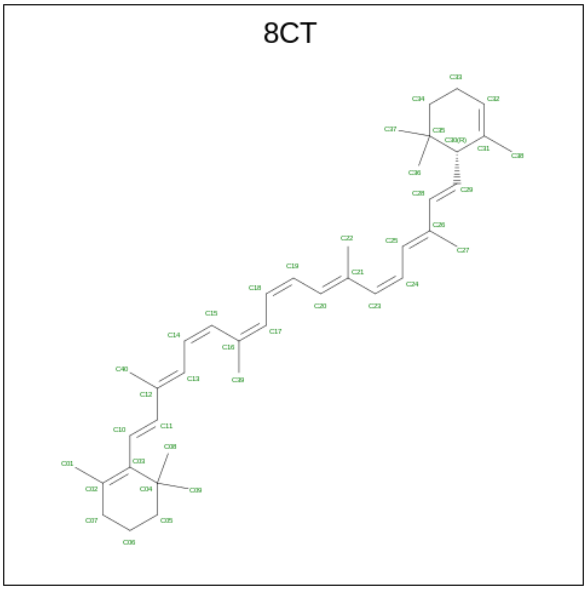
Mol	Chain	Residues	Atoms					AltConf
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	44	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	44	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
22	1A	1	Total C N O 64 55 4 5	0
22	1D	1	Total C N O 64 55 4 5	0
22	2A	1	Total C N O 64 55 4 5	0
22	2D	1	Total C N O 64 55 4 5	0
22	3A	1	Total C N O 64 55 4 5	0
22	3D	1	Total C N O 64 55 4 5	0
22	4A	1	Total C N O 64 55 4 5	0
22	4D	1	Total C N O 64 55 4 5	0

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
23	1A	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

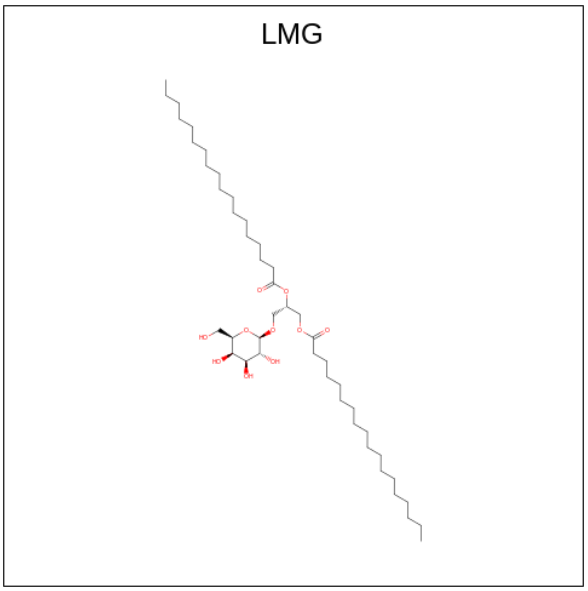
Mol	Chain	Residues	Atoms	AltConf
23	1B	1	Total C 40 40	0
23	1B	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1C	1	Total C 40 40	0
23	1D	1	Total C 40 40	0
23	1K	1	Total C 40 40	0
23	14	1	Total C 40 40	0
23	2A	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2B	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2C	1	Total C 40 40	0
23	2D	1	Total C 40 40	0
23	2K	1	Total C 40 40	0
23	24	1	Total C 40 40	0
23	3A	1	Total C 40 40	0
23	3B	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
23	3B	1	Total C 40 40	0
23	3B	1	Total C 40 40	0
23	3B	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3C	1	Total C 40 40	0
23	3D	1	Total C 40 40	0
23	3K	1	Total C 40 40	0
23	34	1	Total C 40 40	0
23	4A	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4B	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4C	1	Total C 40 40	0
23	4D	1	Total C 40 40	0
23	4K	1	Total C 40 40	0
23	44	1	Total C 40 40	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



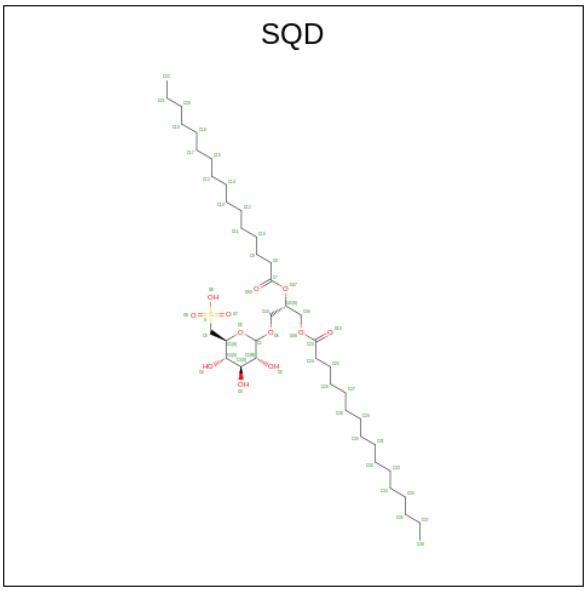
Mol	Chain	Residues	Atoms			AltConf
24	1A	1	Total	C	O	0
			50	40	10	
24	1B	1	Total	C	O	0
			51	41	10	
24	1D	1	Total	C	O	0
			33	23	10	
24	11	1	Total	C	O	0
			51	41	10	
24	2A	1	Total	C	O	0
			50	40	10	
24	2B	1	Total	C	O	0
			51	41	10	
24	2D	1	Total	C	O	0
			33	23	10	
24	21	1	Total	C	O	0
			51	41	10	
24	3A	1	Total	C	O	0
			50	40	10	
24	3B	1	Total	C	O	0
			51	41	10	
24	3D	1	Total	C	O	0
			33	23	10	
24	31	1	Total	C	O	0
			51	41	10	
24	4A	1	Total	C	O	0
			50	40	10	
24	4B	1	Total	C	O	0
			51	41	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
24	4D	1	Total C O 33 23 10	0
24	41	1	Total C O 51 41 10	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



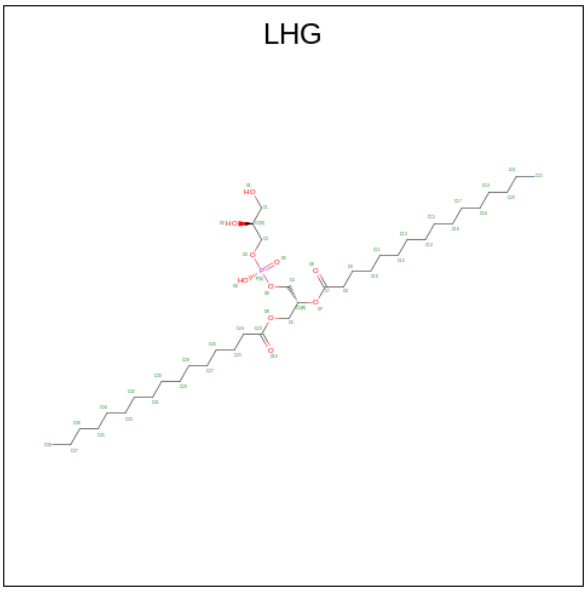
Mol	Chain	Residues	Atoms	AltConf
25	1A	1	Total C O S 34 21 12 1	0
25	1B	1	Total C O S 54 41 12 1	0
25	12	1	Total C O S 50 37 12 1	0
25	12	1	Total C O S 41 28 12 1	0
25	11	1	Total C O S 32 19 12 1	0
25	13	1	Total C O S 46 33 12 1	0
25	13	1	Total C O S 50 37 12 1	0
25	2A	1	Total C O S 34 21 12 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
25	2B	1	Total	C	O	S	0
			54	41	12	1	
25	22	1	Total	C	O	S	0
			50	37	12	1	
25	22	1	Total	C	O	S	0
			41	28	12	1	
25	21	1	Total	C	O	S	0
			32	19	12	1	
25	23	1	Total	C	O	S	0
			46	33	12	1	
25	23	1	Total	C	O	S	0
			50	37	12	1	
25	3A	1	Total	C	O	S	0
			34	21	12	1	
25	3B	1	Total	C	O	S	0
			54	41	12	1	
25	32	1	Total	C	O	S	0
			50	37	12	1	
25	32	1	Total	C	O	S	0
			41	28	12	1	
25	31	1	Total	C	O	S	0
			32	19	12	1	
25	33	1	Total	C	O	S	0
			46	33	12	1	
25	33	1	Total	C	O	S	0
			50	37	12	1	
25	4A	1	Total	C	O	S	0
			34	21	12	1	
25	4B	1	Total	C	O	S	0
			54	41	12	1	
25	42	1	Total	C	O	S	0
			50	37	12	1	
25	42	1	Total	C	O	S	0
			41	28	12	1	
25	41	1	Total	C	O	S	0
			32	19	12	1	
25	43	1	Total	C	O	S	0
			46	33	12	1	
25	43	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



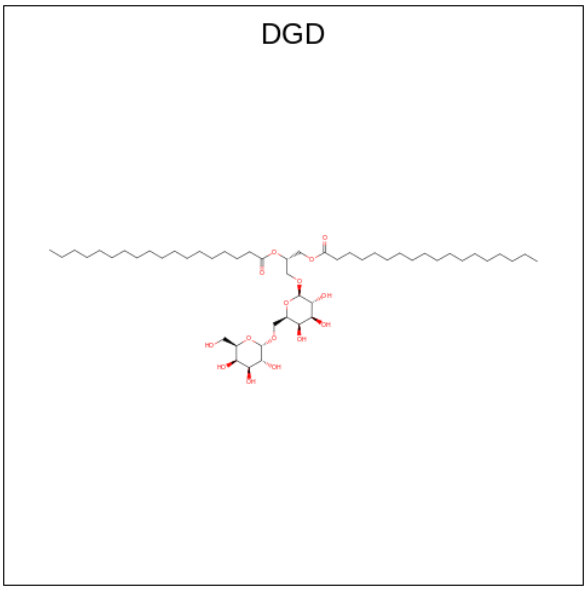
Mol	Chain	Residues	Atoms				AltConf
26	1A	1	Total	C	O	P	0
			46	35	10	1	
26	1B	1	Total	C	O	P	0
			45	34	10	1	
26	1B	1	Total	C	O	P	0
			49	38	10	1	
26	1D	1	Total	C	O	P	0
			49	38	10	1	
26	13	1	Total	C	O	P	0
			36	25	10	1	
26	14	1	Total	C	O	P	0
			49	38	10	1	
26	2A	1	Total	C	O	P	0
			46	35	10	1	
26	2B	1	Total	C	O	P	0
			45	34	10	1	
26	2B	1	Total	C	O	P	0
			49	38	10	1	
26	2D	1	Total	C	O	P	0
			49	38	10	1	
26	23	1	Total	C	O	P	0
			36	25	10	1	
26	24	1	Total	C	O	P	0
			49	38	10	1	
26	3A	1	Total	C	O	P	0
			46	35	10	1	
26	3B	1	Total	C	O	P	0
			45	34	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
26	3B	1	Total	C	O	P	0
			49	38	10	1	
26	3D	1	Total	C	O	P	0
			49	38	10	1	
26	33	1	Total	C	O	P	0
			36	25	10	1	
26	34	1	Total	C	O	P	0
			49	38	10	1	
26	4A	1	Total	C	O	P	0
			46	35	10	1	
26	4B	1	Total	C	O	P	0
			45	34	10	1	
26	4B	1	Total	C	O	P	0
			49	38	10	1	
26	4D	1	Total	C	O	P	0
			49	38	10	1	
26	43	1	Total	C	O	P	0
			36	25	10	1	
26	44	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	1B	1	Total	C	O	0
			62	47	15	

Continued on next page...

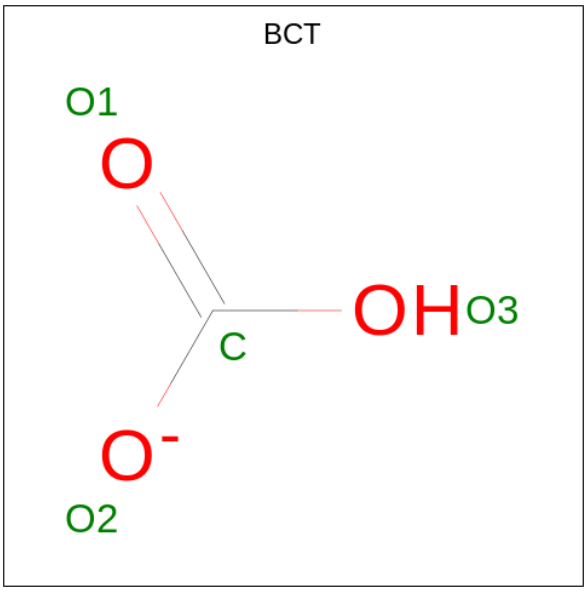
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
27	1C	1	Total C O 62 47 15	0
27	2B	1	Total C O 62 47 15	0
27	2C	1	Total C O 62 47 15	0
27	3B	1	Total C O 62 47 15	0
27	3C	1	Total C O 62 47 15	0
27	4B	1	Total C O 62 47 15	0
27	4C	1	Total C O 62 47 15	0

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

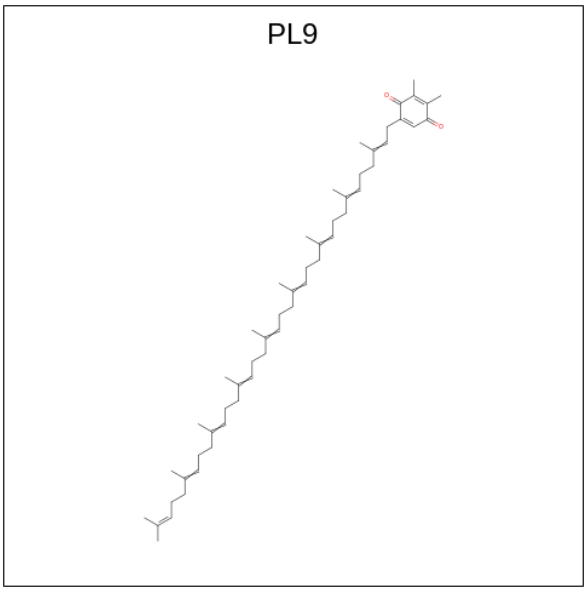
Mol	Chain	Residues	Atoms	AltConf
28	1D	1	Total Fe 1 1	0
28	2D	1	Total Fe 1 1	0
28	3D	1	Total Fe 1 1	0
28	4D	1	Total Fe 1 1	0

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



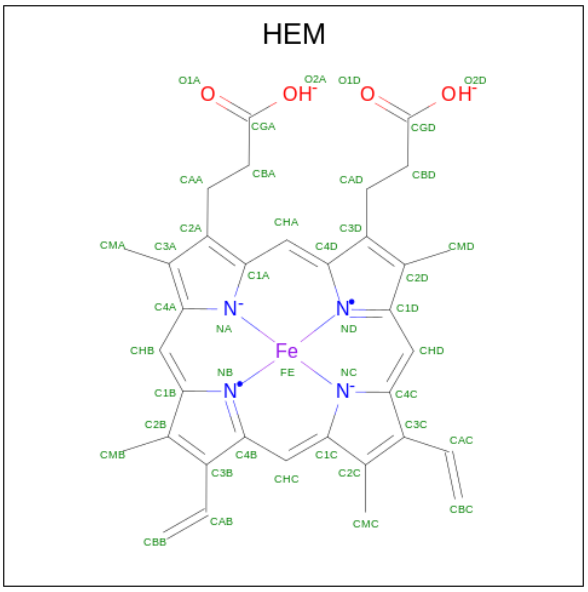
Mol	Chain	Residues	Atoms			AltConf
29	1D	1	Total	C	O	0
			4	1	3	
29	2D	1	Total	C	O	0
			4	1	3	
29	3D	1	Total	C	O	0
			4	1	3	
29	4D	1	Total	C	O	0
			4	1	3	

- Molecule 30 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



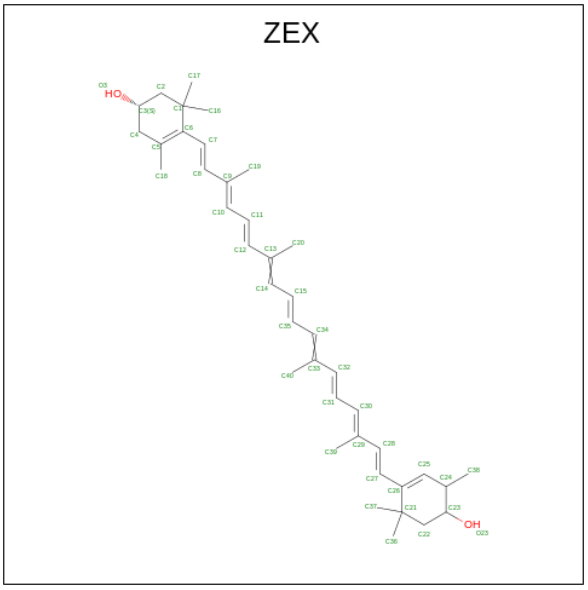
Mol	Chain	Residues	Atoms	AltConf
30	1D	1	Total C O 55 53 2	0
30	2D	1	Total C O 55 53 2	0
30	3D	1	Total C O 55 53 2	0
30	4D	1	Total C O 55 53 2	0

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	2F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	3F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	4F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 32 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	12	1	Total	C	O	0
			42	40	2	
32	11	1	Total	C	O	0
			42	40	2	
32	11	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	13	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	14	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	22	1	Total	C	O	0
			42	40	2	
32	21	1	Total	C	O	0
			42	40	2	
32	21	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	23	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	
32	24	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
32	24	1	Total	C	O	0
			42	40	2	
32	32	1	Total	C	O	0
			42	40	2	
32	32	1	Total	C	O	0
			42	40	2	
32	32	1	Total	C	O	0
			42	40	2	
32	32	1	Total	C	O	0
			42	40	2	
32	31	1	Total	C	O	0
			42	40	2	
32	31	1	Total	C	O	0
			42	40	2	
32	33	1	Total	C	O	0
			42	40	2	
32	33	1	Total	C	O	0
			42	40	2	
32	33	1	Total	C	O	0
			42	40	2	
32	33	1	Total	C	O	0
			42	40	2	
32	34	1	Total	C	O	0
			42	40	2	
32	34	1	Total	C	O	0
			42	40	2	
32	34	1	Total	C	O	0
			42	40	2	
32	34	1	Total	C	O	0
			42	40	2	
32	42	1	Total	C	O	0
			42	40	2	
32	42	1	Total	C	O	0
			42	40	2	
32	42	1	Total	C	O	0
			42	40	2	
32	42	1	Total	C	O	0
			42	40	2	
32	41	1	Total	C	O	0
			42	40	2	
32	41	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	43	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	
32	44	1	Total	C	O	0
			42	40	2	

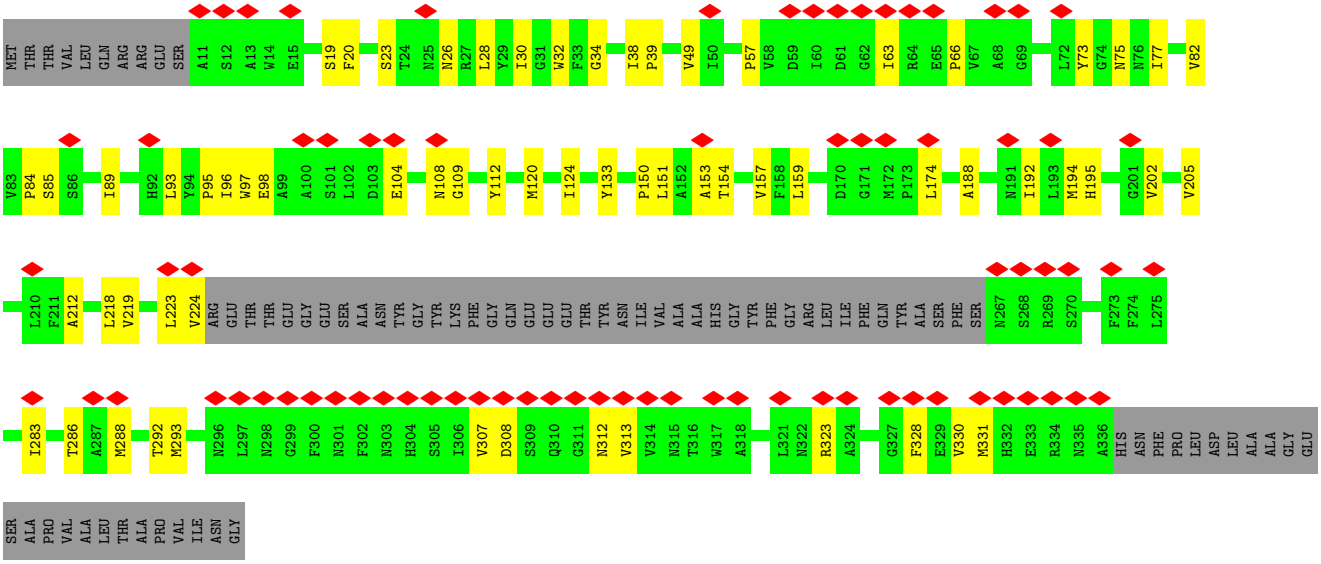
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem II protein D1 2

Chain 1A:

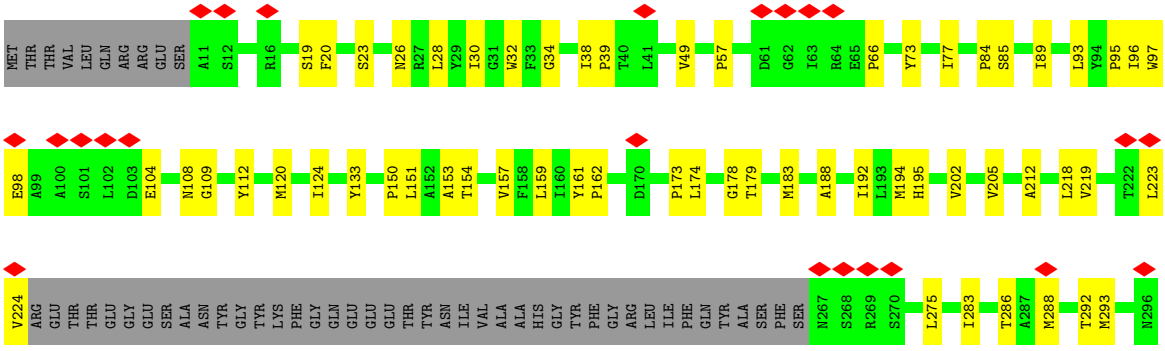


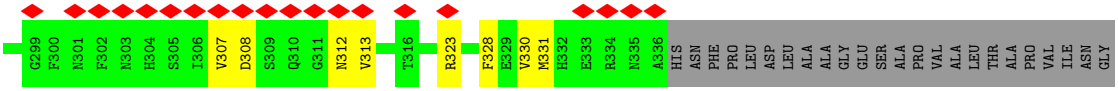


• Molecule 1: Photosystem II protein D1 2

Chain 2A:



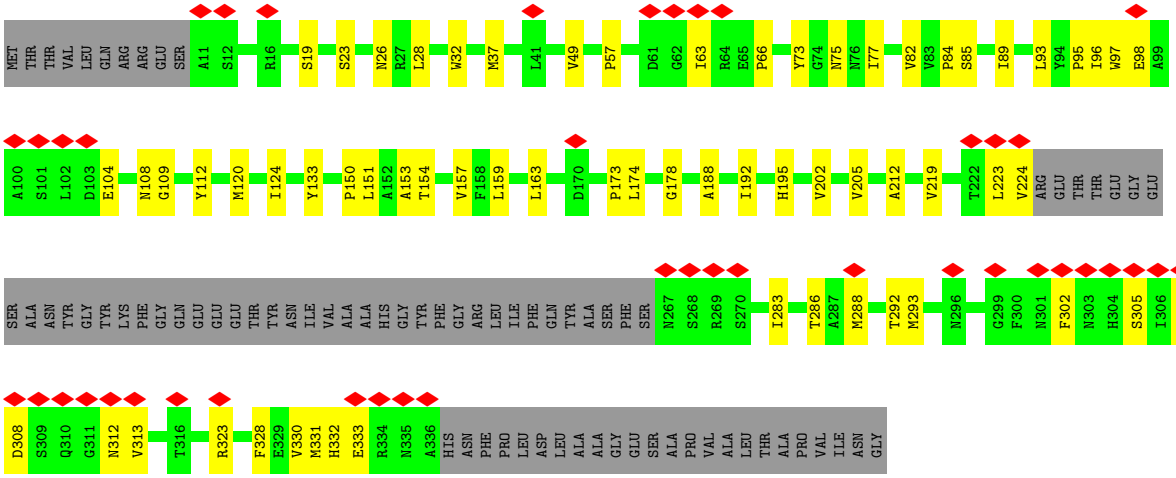




• Molecule 1: Photosystem II protein D1 2

Chain 3A:

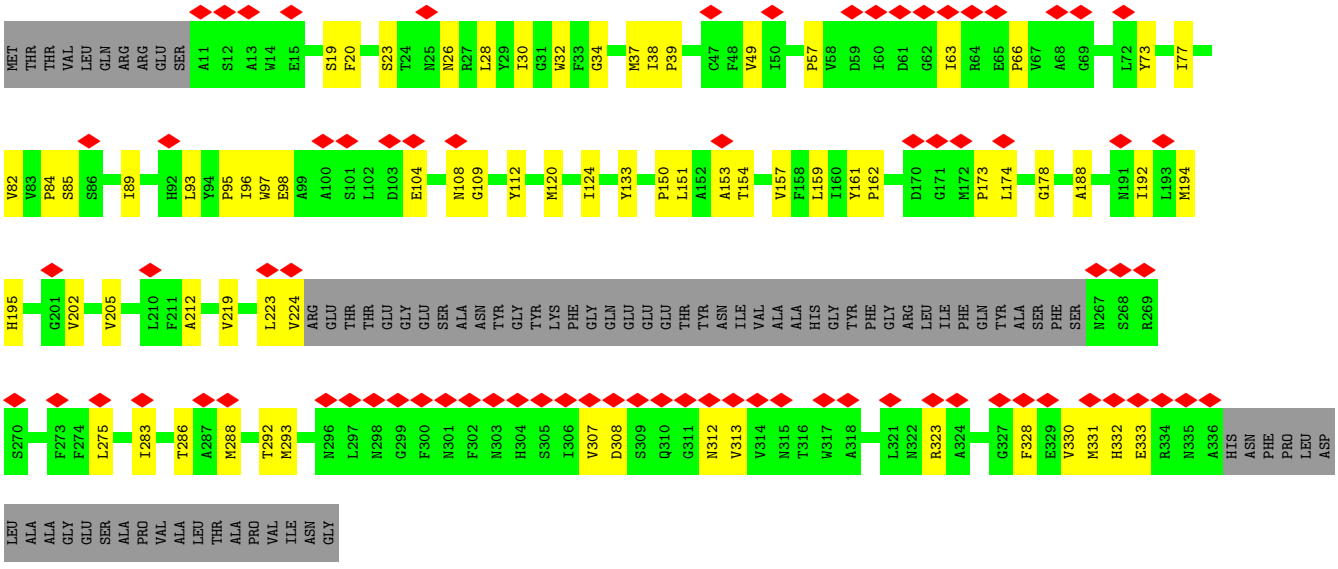




• Molecule 1: Photosystem II protein D1 2

Chain 4A:

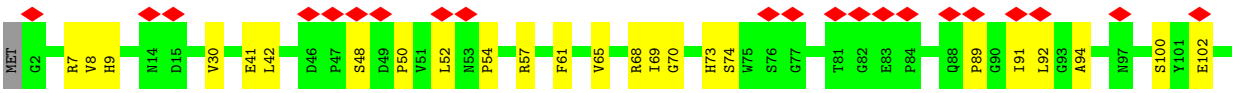


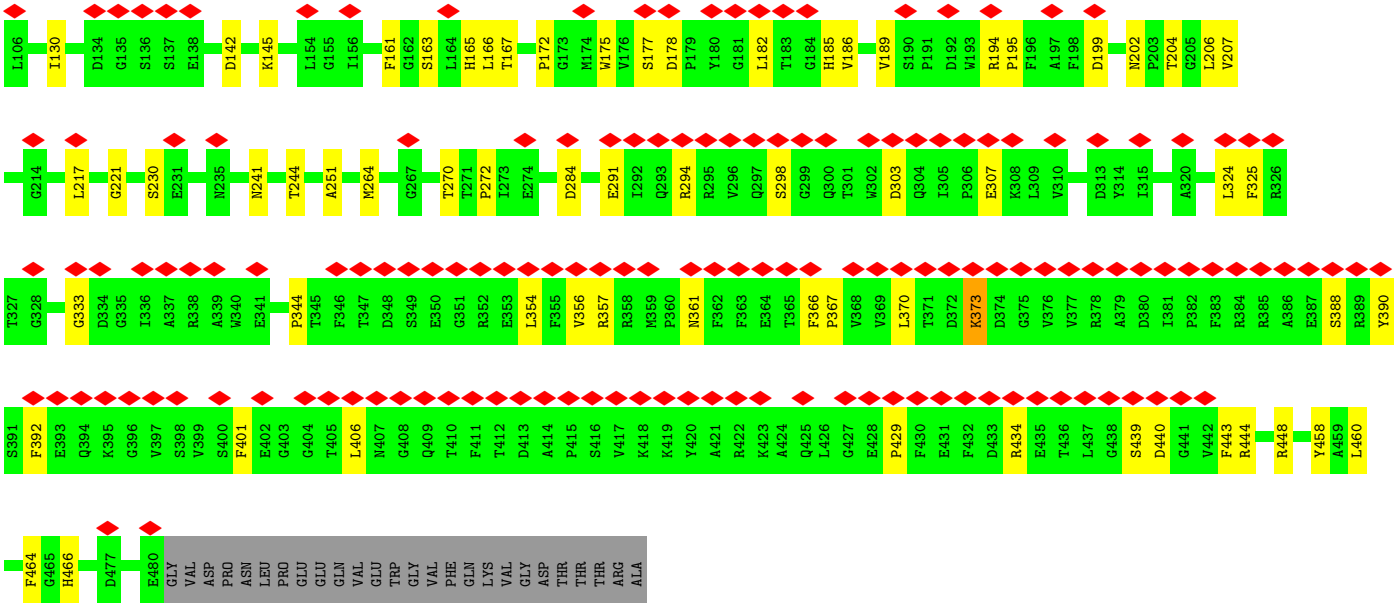


• Molecule 2: Photosystem II CP47 reaction center protein

Chain 1B:



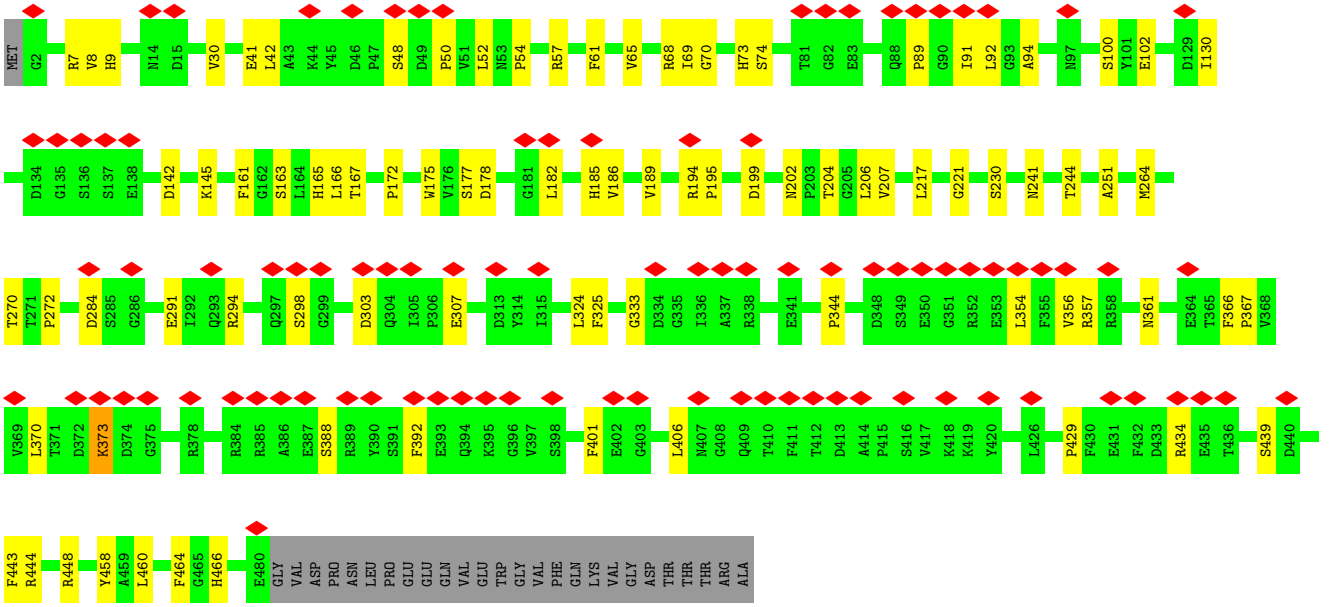




• Molecule 2: Photosystem II CP47 reaction center protein

Chain 2B:

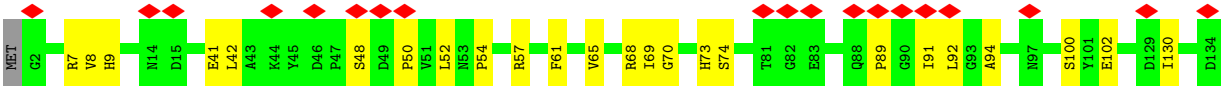


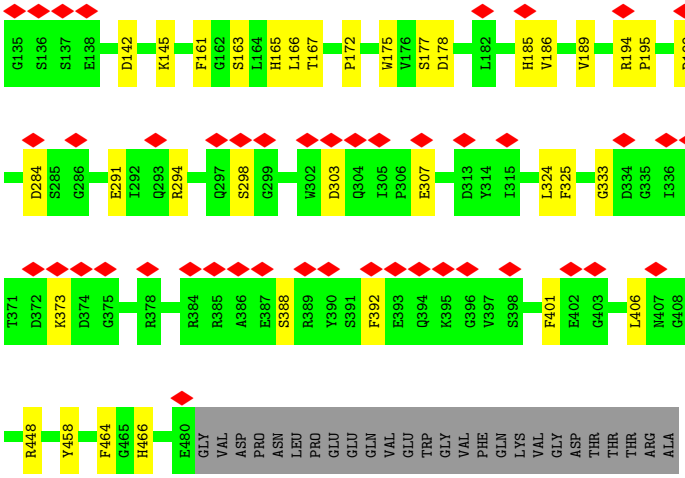


• Molecule 2: Photosystem II CP47 reaction center protein

Chain 3B:



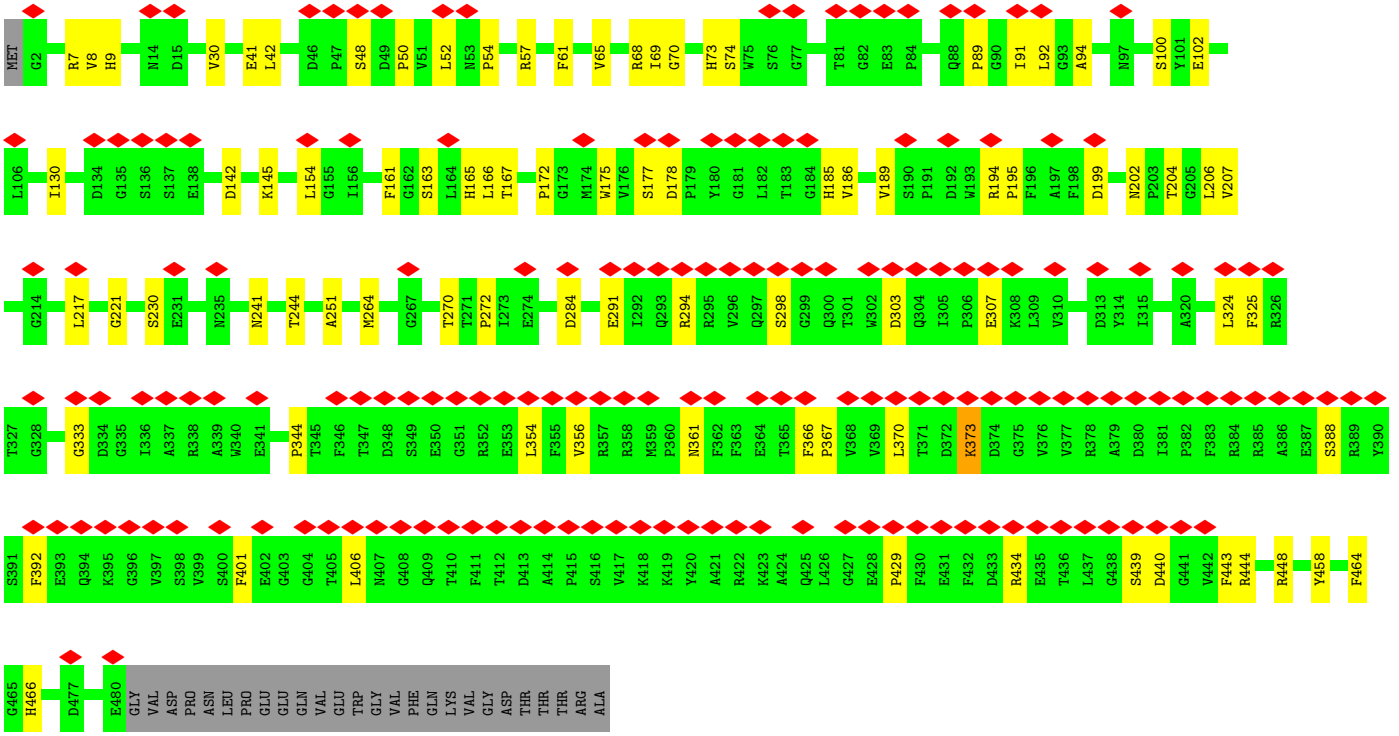




• Molecule 2: Photosystem II CP47 reaction center protein

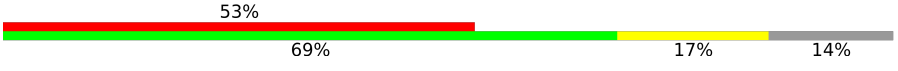
Chain 4B:

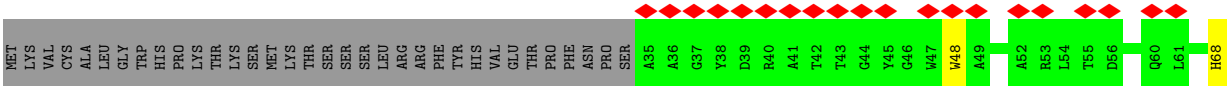


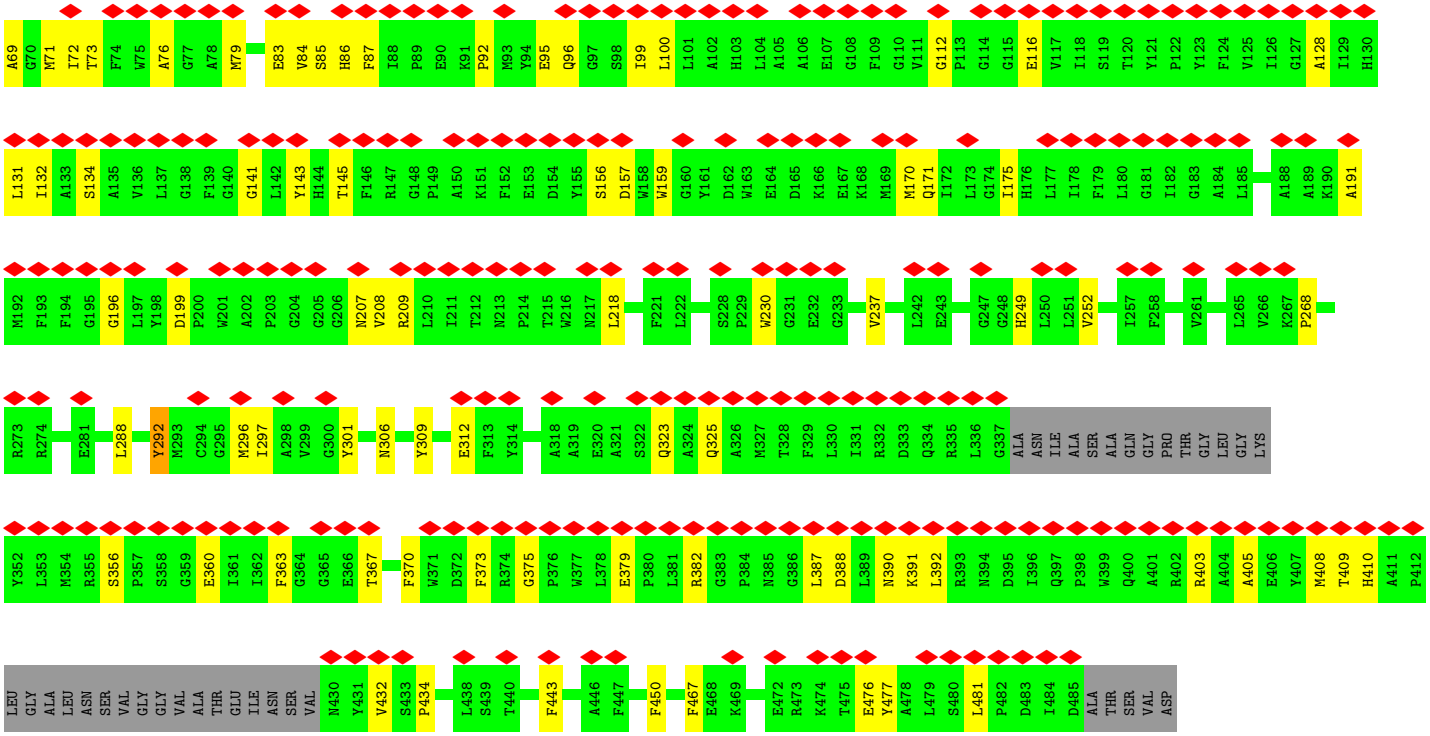


• Molecule 3: Photosystem II CP43 reaction center protein

Chain 1C:

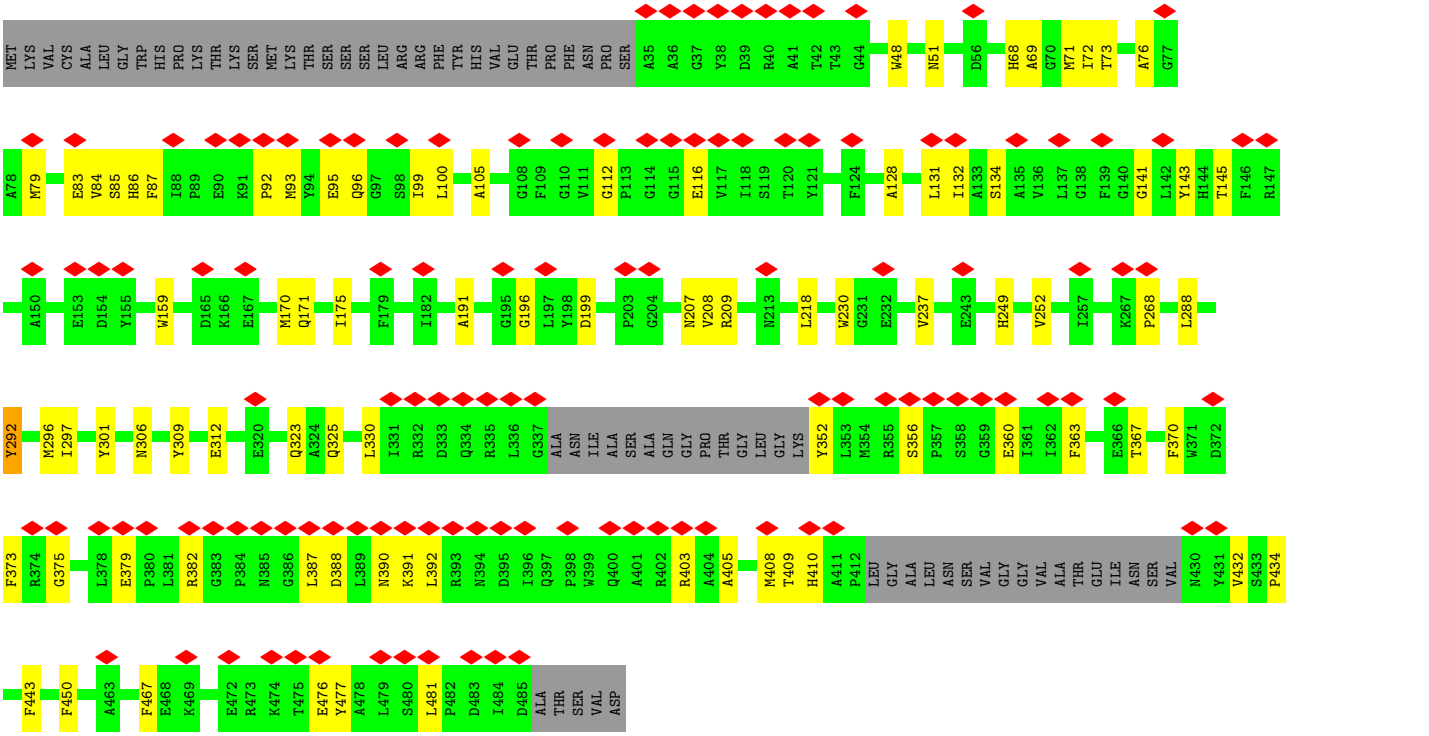






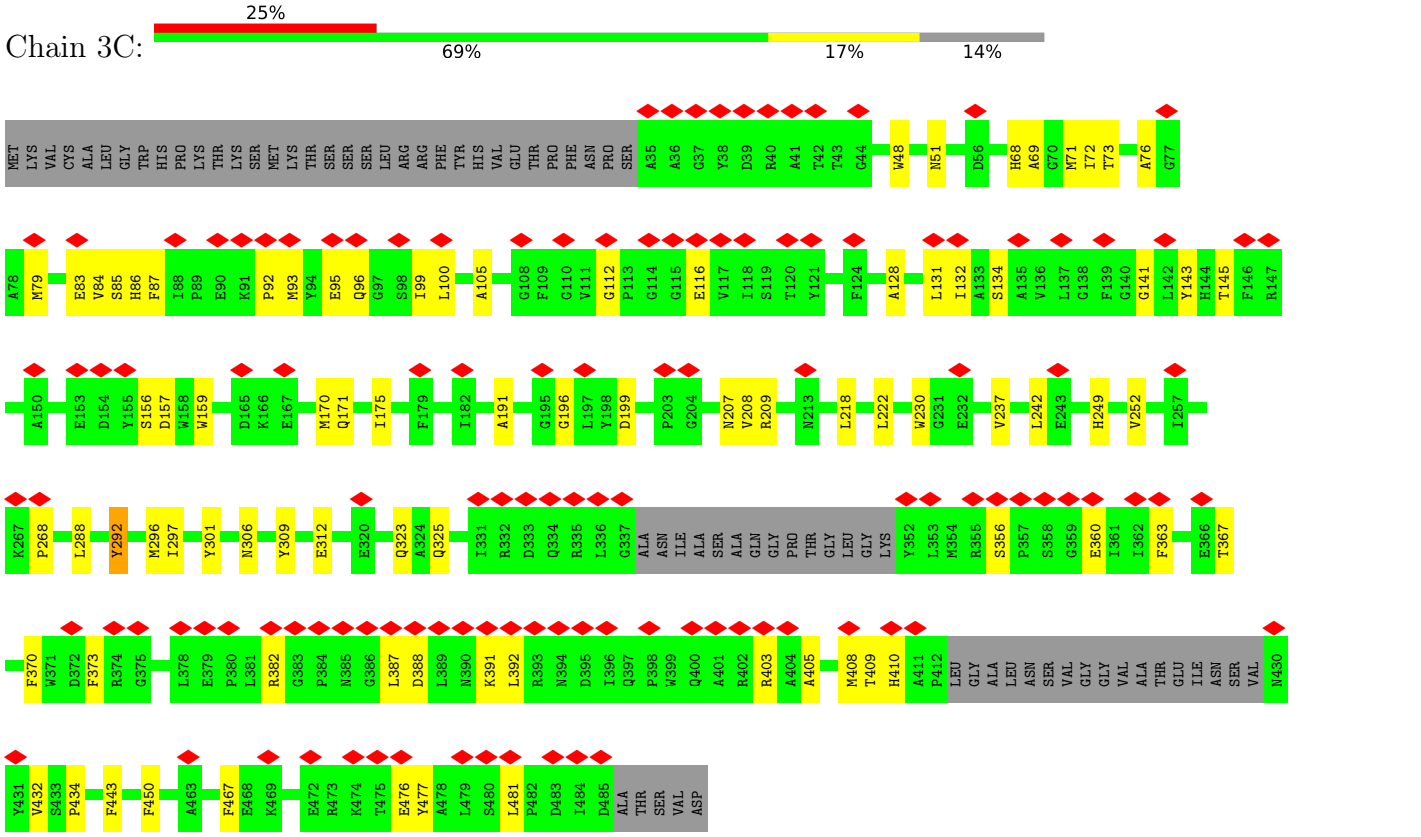
• Molecule 3: Photosystem II CP43 reaction center protein





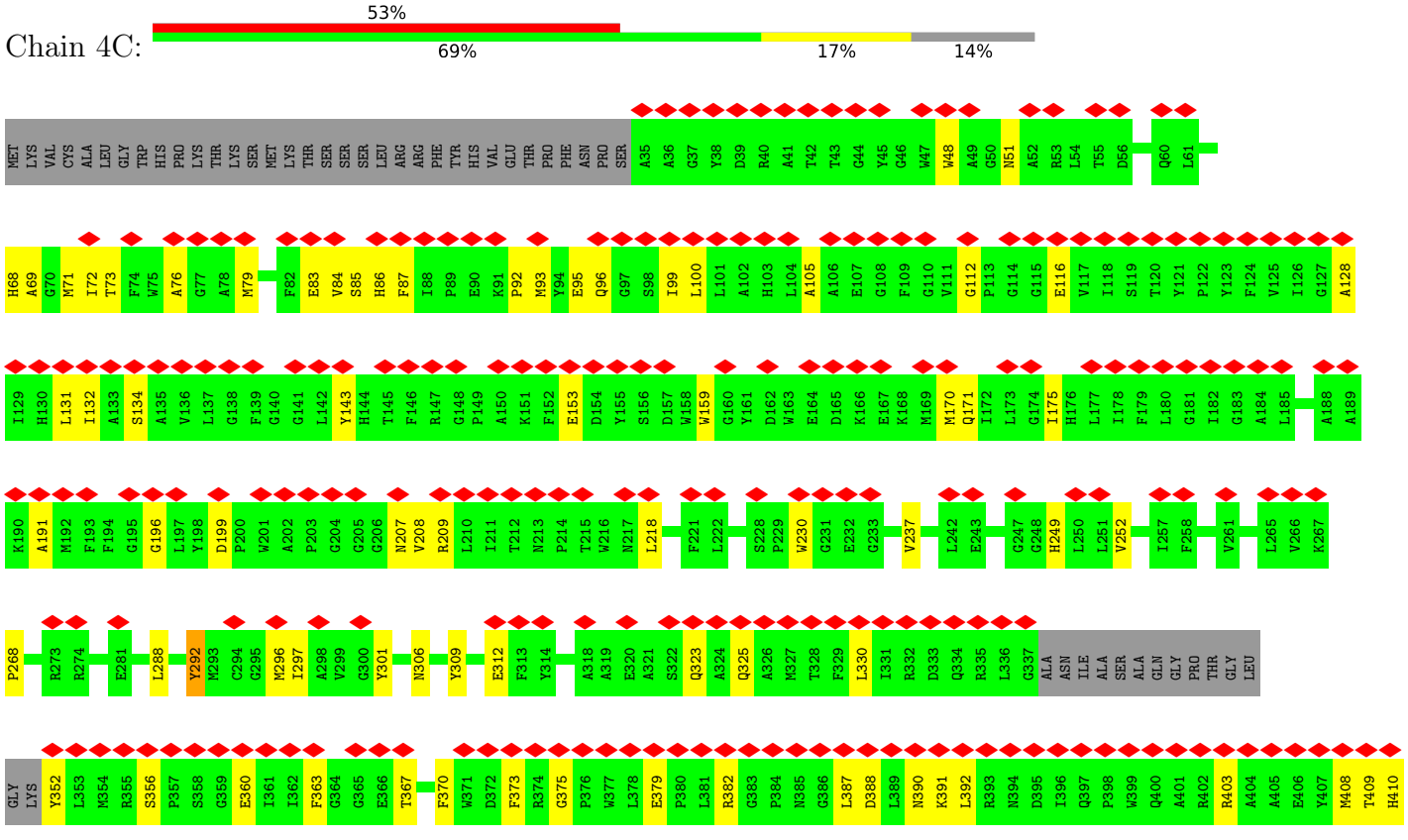
• Molecule 3: Photosystem II CP43 reaction center protein

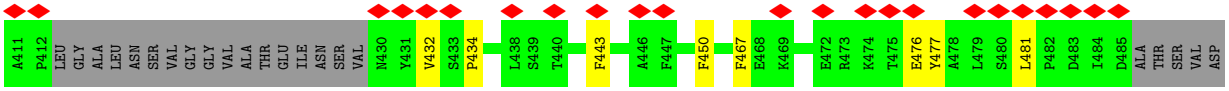
Chain 3C:



• Molecule 3: Photosystem II CP43 reaction center protein

Chain 4C:

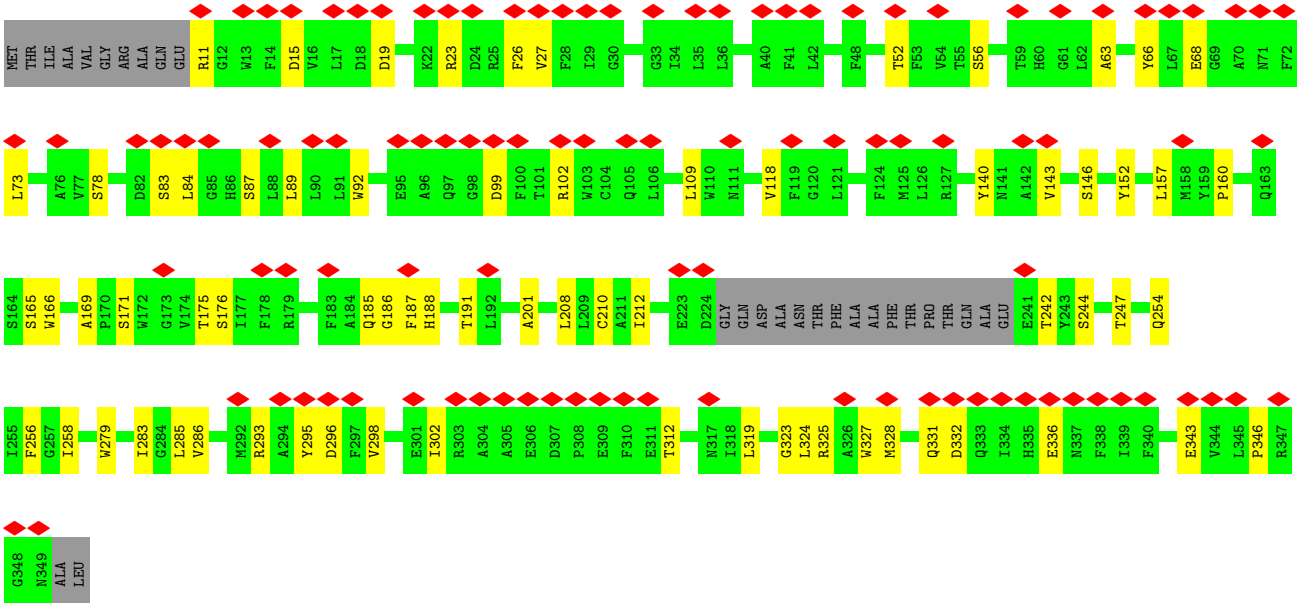




• Molecule 4: Photosystem II D2 protein 1

Chain 1D:

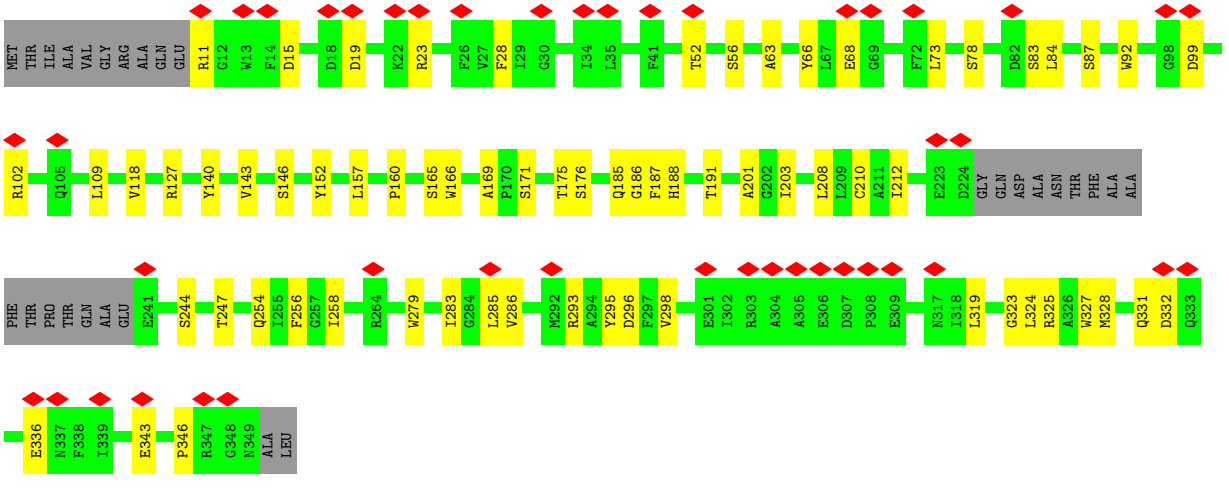




• Molecule 4: Photosystem II D2 protein 1

Chain 2D:

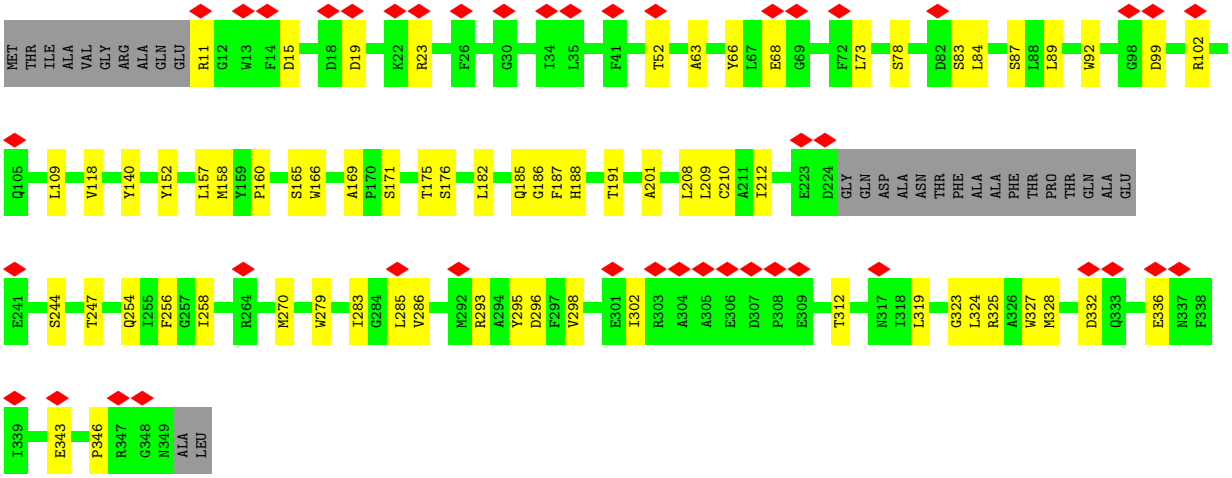




• Molecule 4: Photosystem II D2 protein 1

Chain 3D:





• Molecule 4: Photosystem II D2 protein 1

Chain 4D:

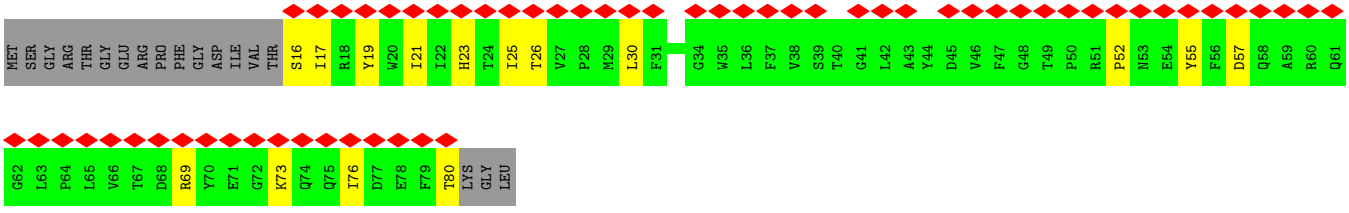




• Molecule 5: Cytochrome b559 subunit alpha

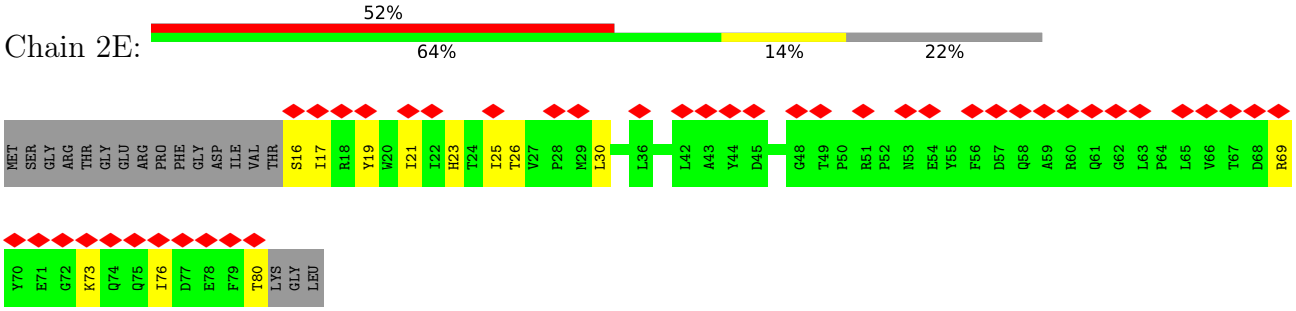
Chain 1E:





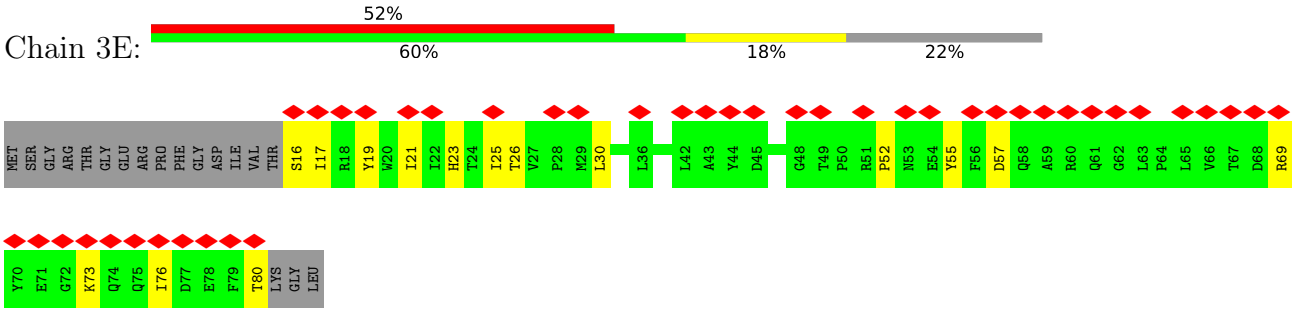
• Molecule 5: Cytochrome b559 subunit alpha

Chain 2E:



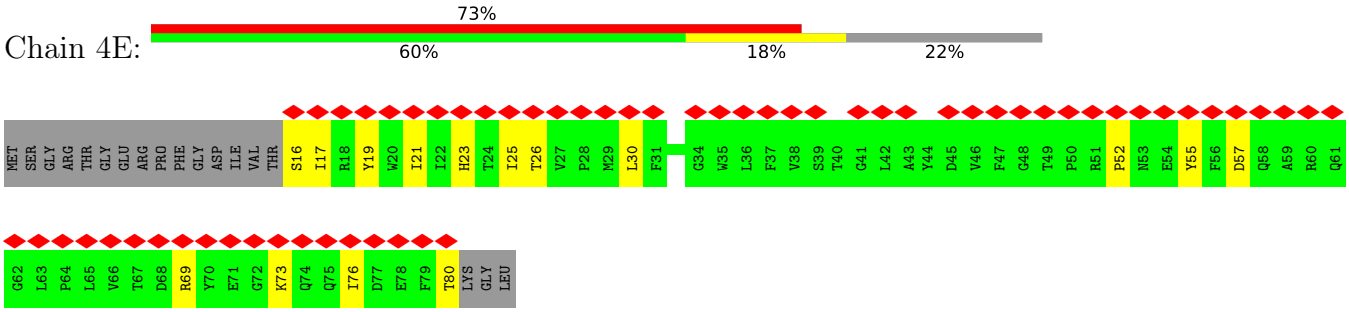
• Molecule 5: Cytochrome b559 subunit alpha

Chain 3E:



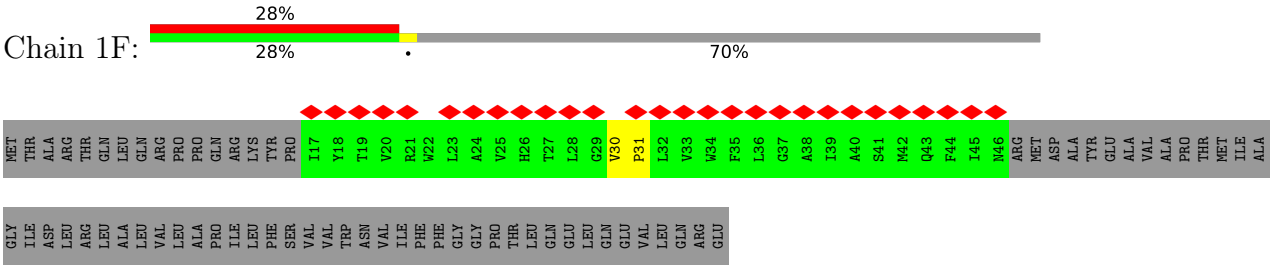
• Molecule 5: Cytochrome b559 subunit alpha

Chain 4E:



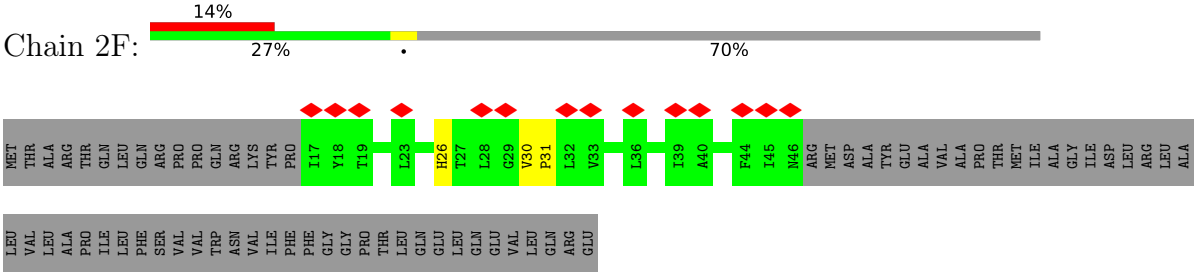
• Molecule 6: Photosystem II protein Y

Chain 1F:



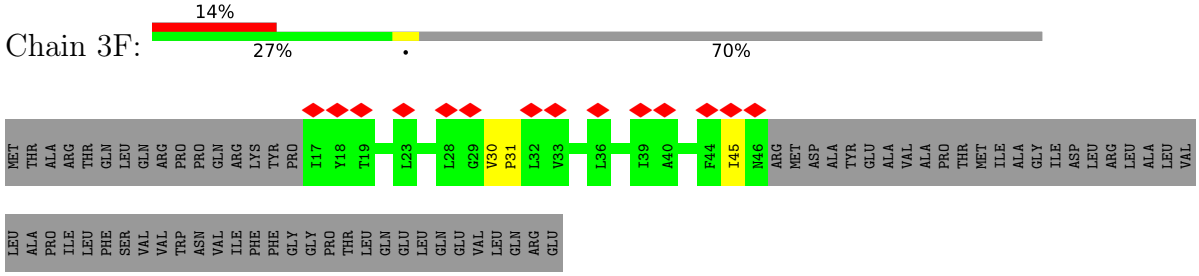
• Molecule 6: Photosystem II protein Y

Chain 2F:



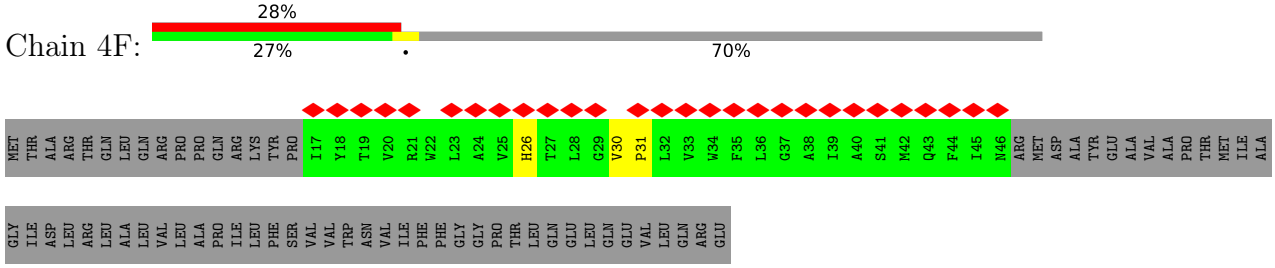
• Molecule 6: Photosystem II protein Y

Chain 3F:



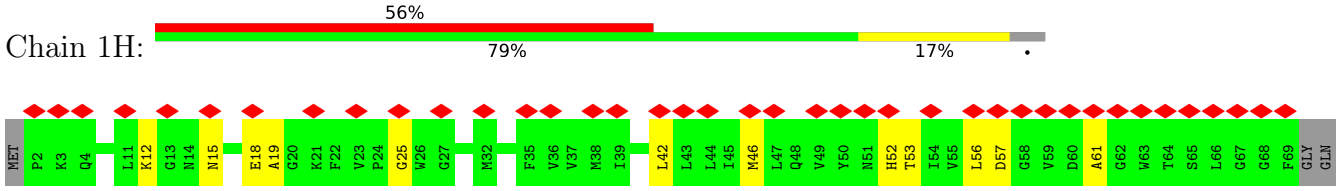
• Molecule 6: Photosystem II protein Y

Chain 4F:



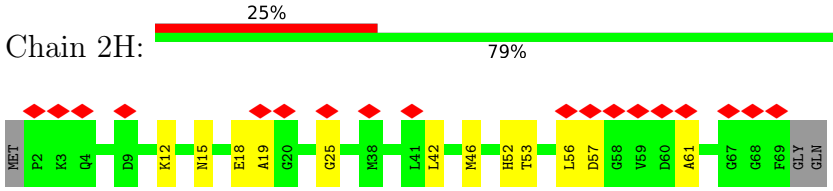
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 1H:



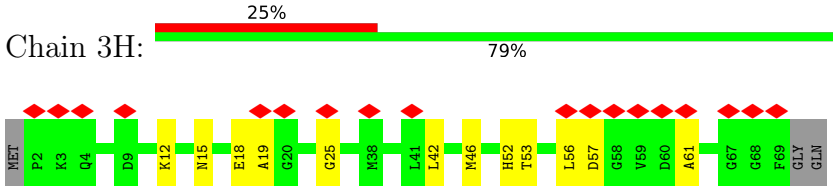
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 2H:



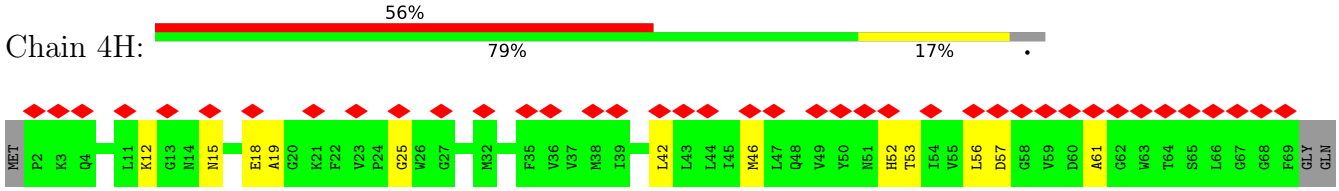
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 3H:



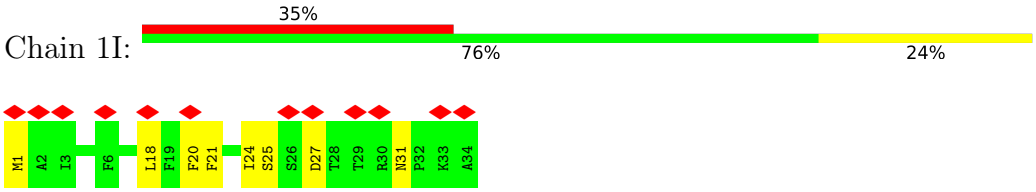
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH

Chain 4H:



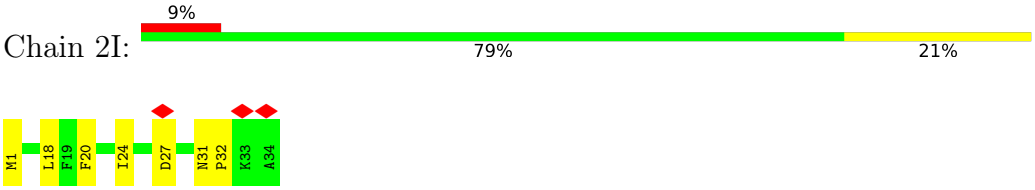
• Molecule 8: Photosystem II protein PsbI

Chain 1I:



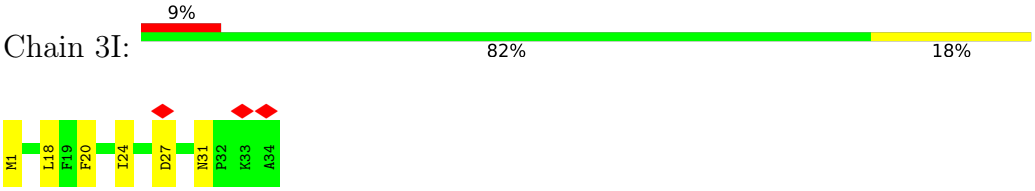
• Molecule 8: Photosystem II protein PsbI

Chain 2I:



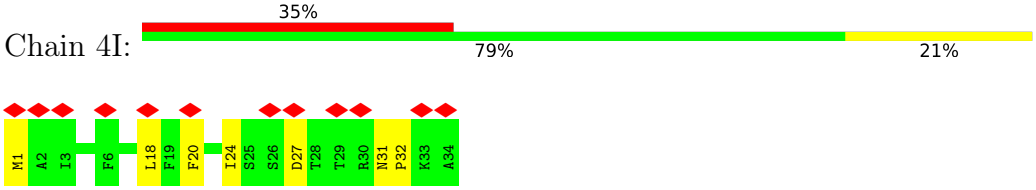
• Molecule 8: Photosystem II protein PsbI

Chain 3I:



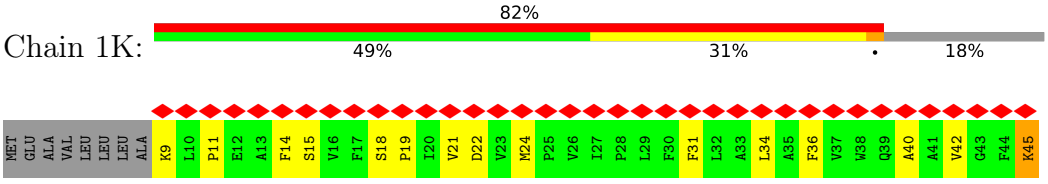
• Molecule 8: Photosystem II protein PsbI

Chain 4I:



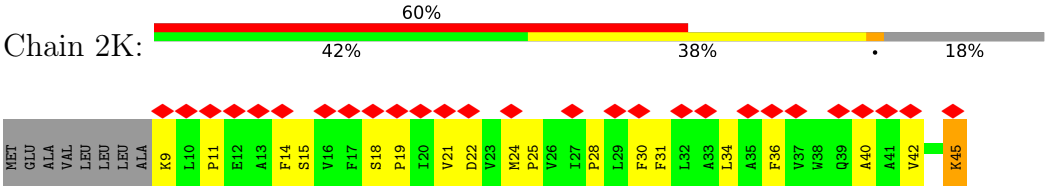
• Molecule 9: Photosystem II reaction center protein K

Chain 1K:



• Molecule 9: Photosystem II reaction center protein K

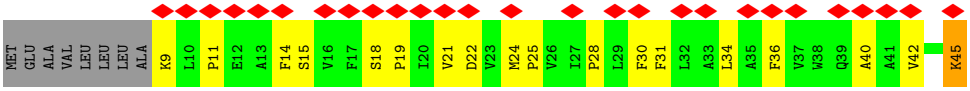
Chain 2K:



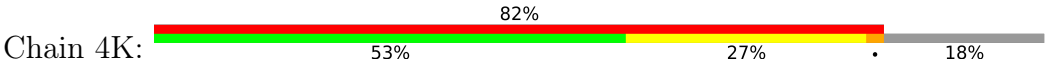
• Molecule 9: Photosystem II reaction center protein K

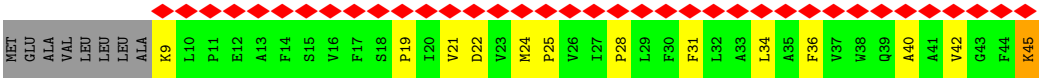
Chain 3K:



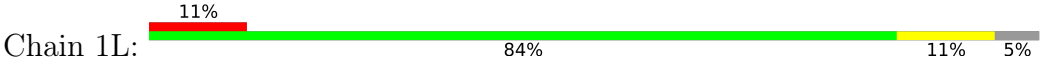


• Molecule 9: Photosystem II reaction center protein K



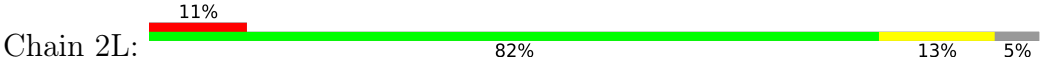


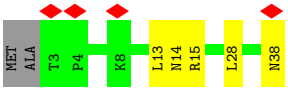
• Molecule 10: Photosystem II reaction center protein L



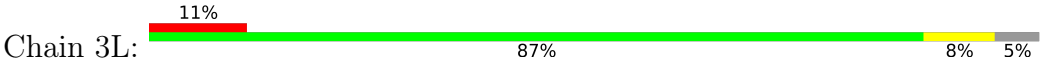


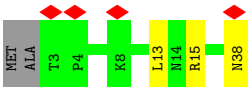
• Molecule 10: Photosystem II reaction center protein L



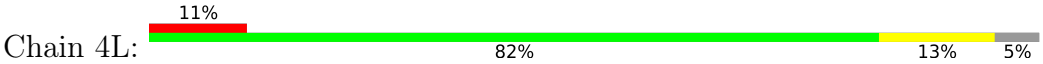


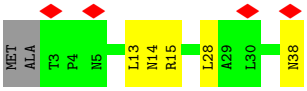
• Molecule 10: Photosystem II reaction center protein L



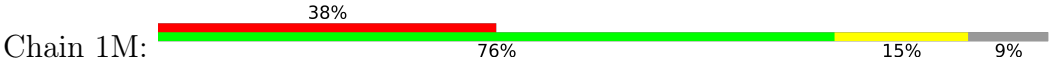


• Molecule 10: Photosystem II reaction center protein L





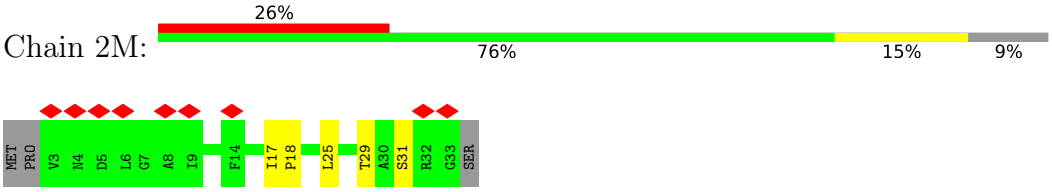
• Molecule 11: Photosystem II reaction center protein M





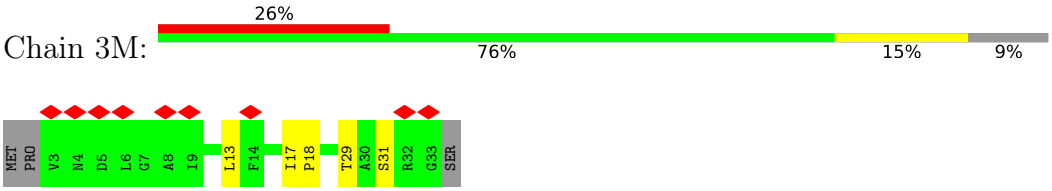
• Molecule 11: Photosystem II reaction center protein M

Chain 2M:



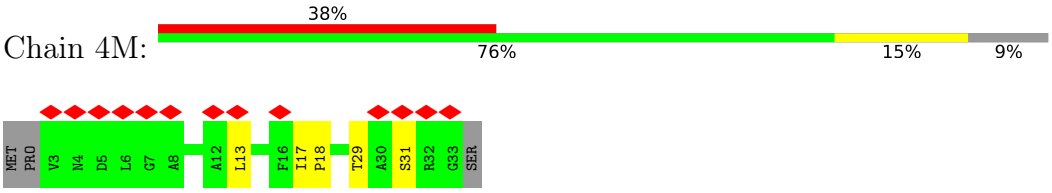
• Molecule 11: Photosystem II reaction center protein M

Chain 3M:



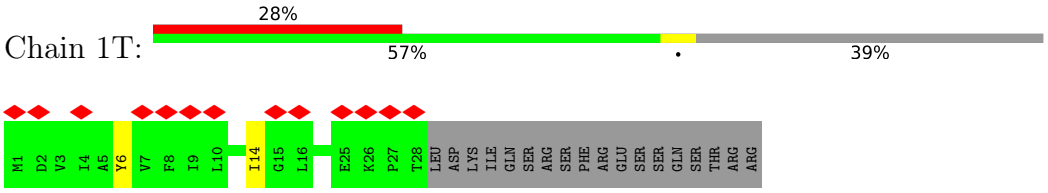
• Molecule 11: Photosystem II reaction center protein M

Chain 4M:



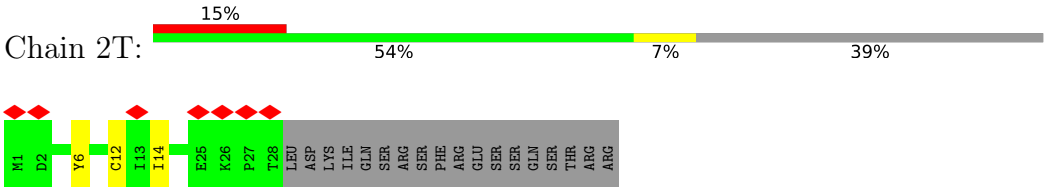
• Molecule 12: Photosystem II reaction center protein T

Chain 1T:



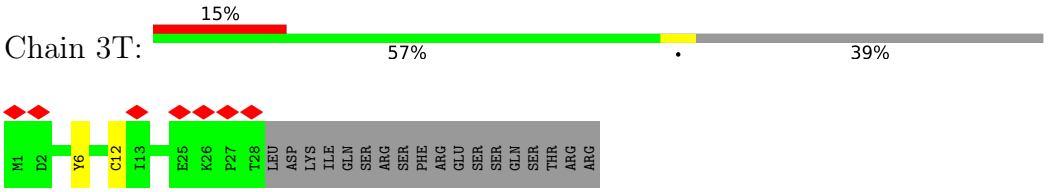
• Molecule 12: Photosystem II reaction center protein T

Chain 2T:



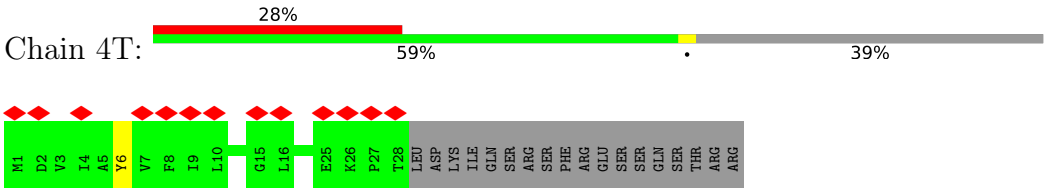
• Molecule 12: Photosystem II reaction center protein T

Chain 3T:



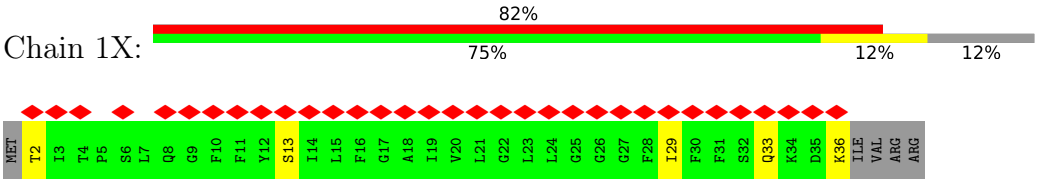
• Molecule 12: Photosystem II reaction center protein T

Chain 4T:



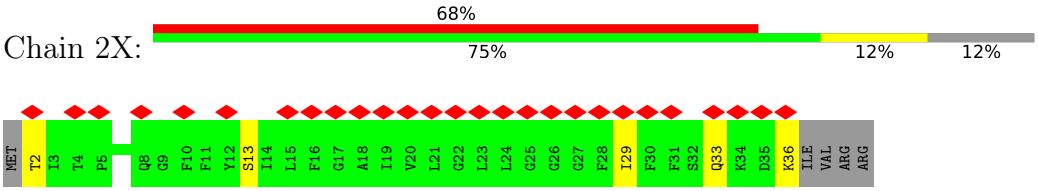
• Molecule 13: Photosystem II reaction center X protein

Chain 1X:



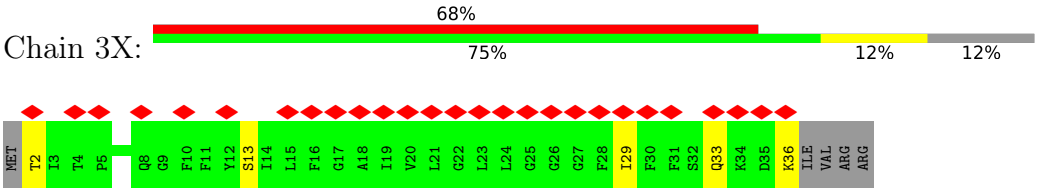
• Molecule 13: Photosystem II reaction center X protein

Chain 2X:



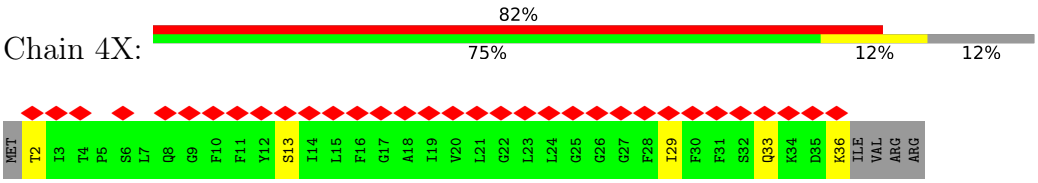
• Molecule 13: Photosystem II reaction center X protein

Chain 3X:



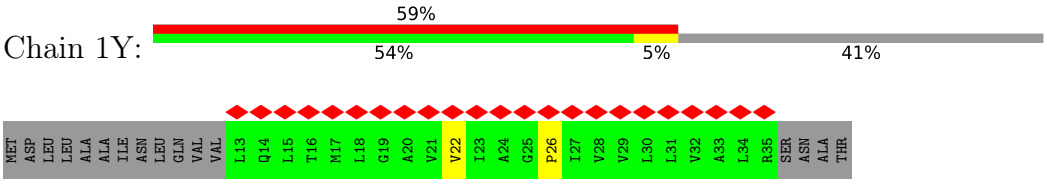
• Molecule 13: Photosystem II reaction center X protein

Chain 4X:



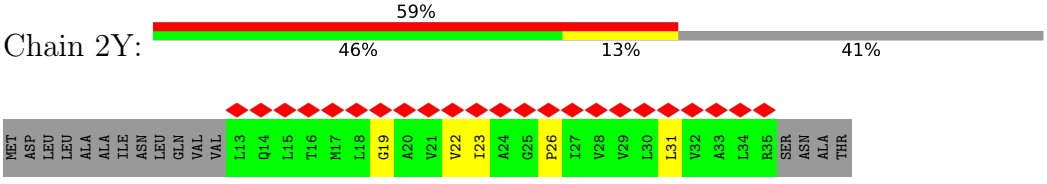
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain 1Y:



• Molecule 14: Photosystem II reaction center protein Ycf12

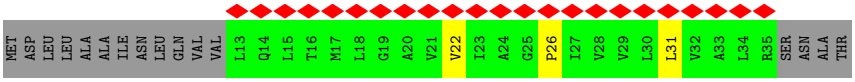
Chain 2Y:



• Molecule 14: Photosystem II reaction center protein Ycf12

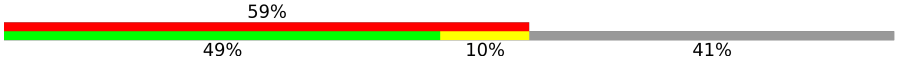
Chain 3Y:

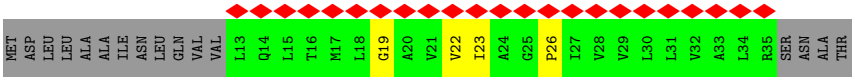




• Molecule 14: Photosystem II reaction center protein Ycf12

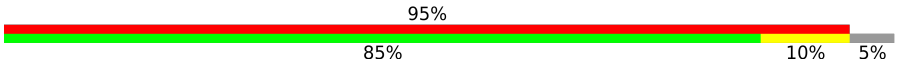
Chain 4Y:

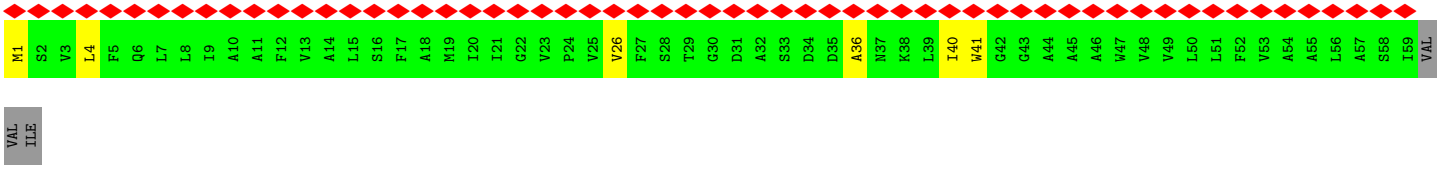




• Molecule 15: Photosystem II reaction center protein Z

Chain 1Z:

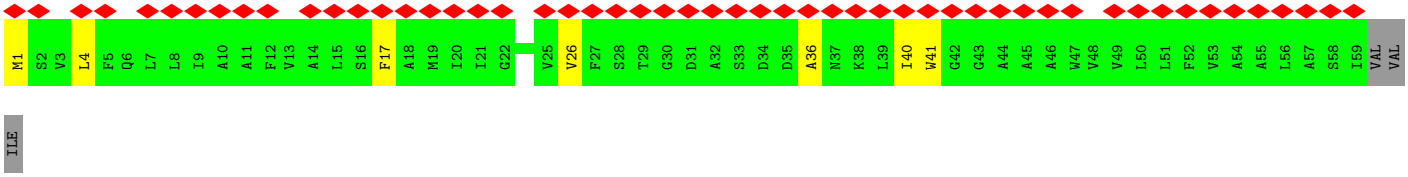




• Molecule 15: Photosystem II reaction center protein Z

Chain 2Z:

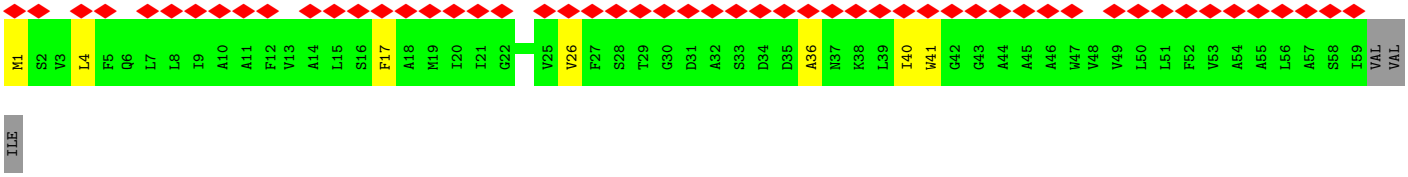




• Molecule 15: Photosystem II reaction center protein Z

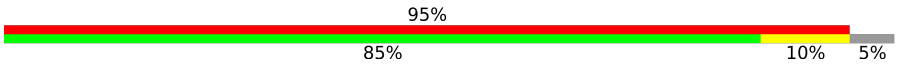
Chain 3Z:

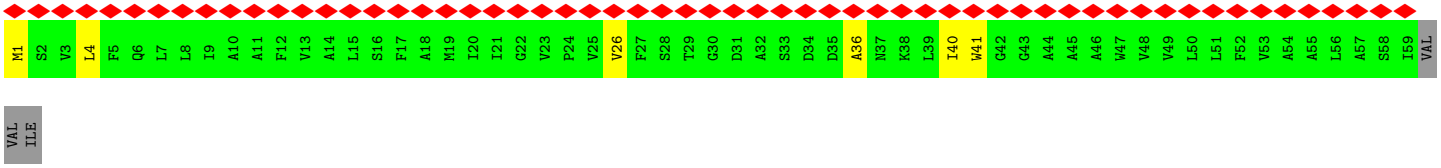




• Molecule 15: Photosystem II reaction center protein Z

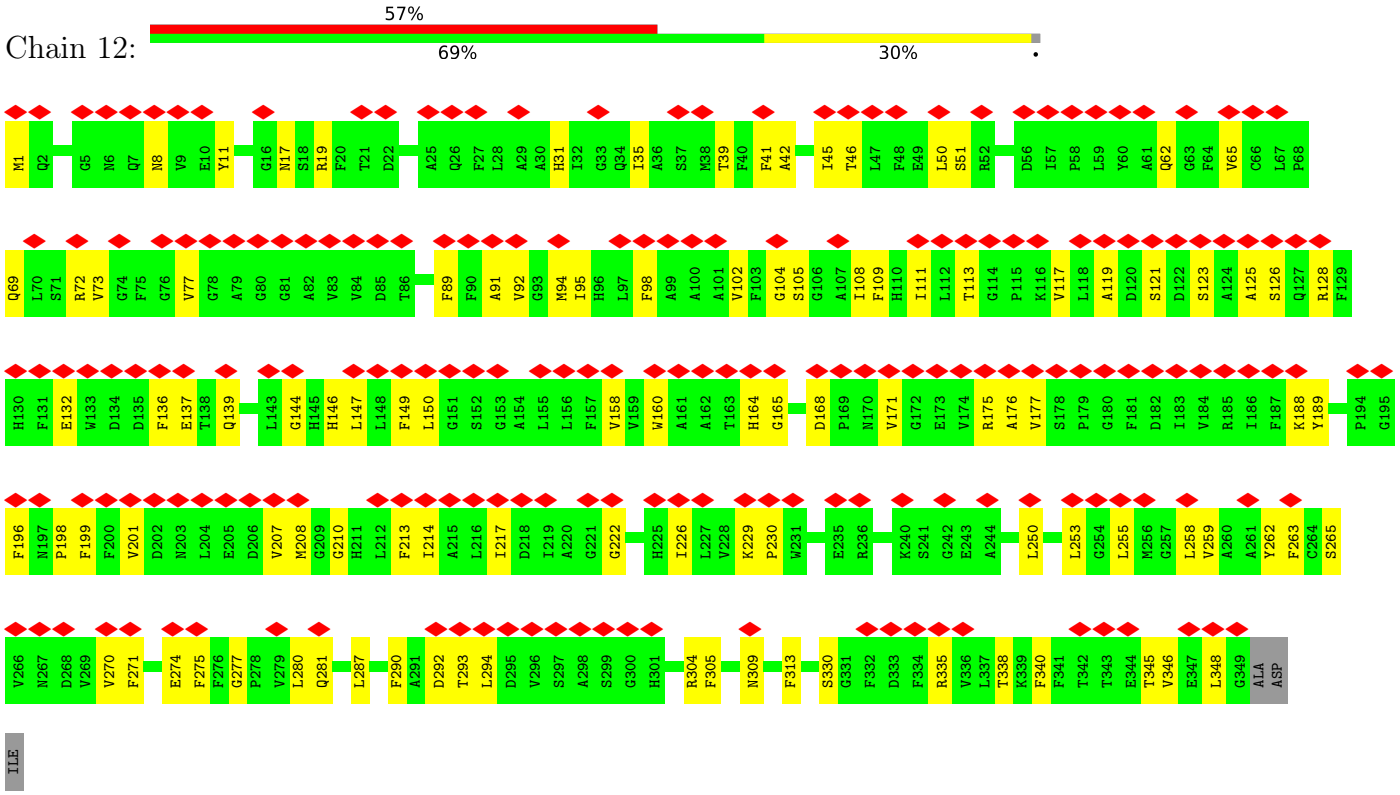
Chain 4Z:





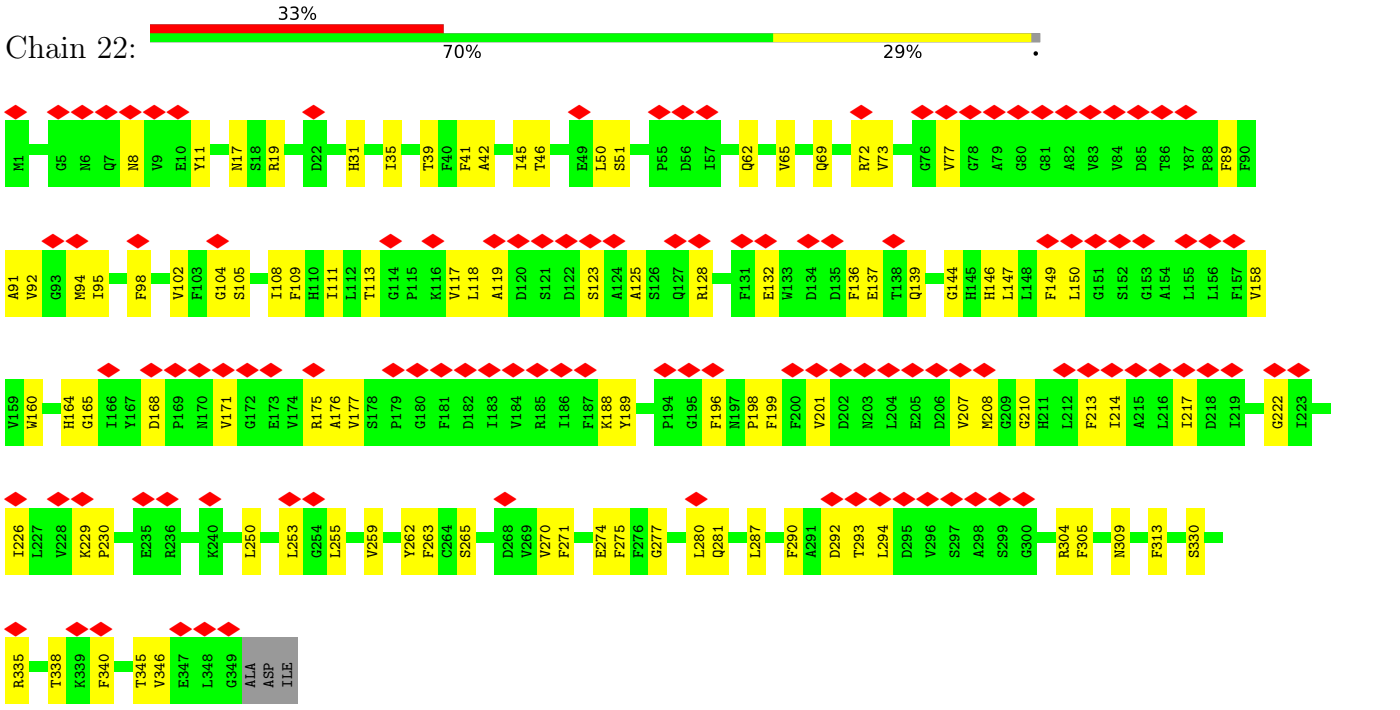
• Molecule 16: High light inducible protein

Chain 12:



• Molecule 16: High light inducible protein

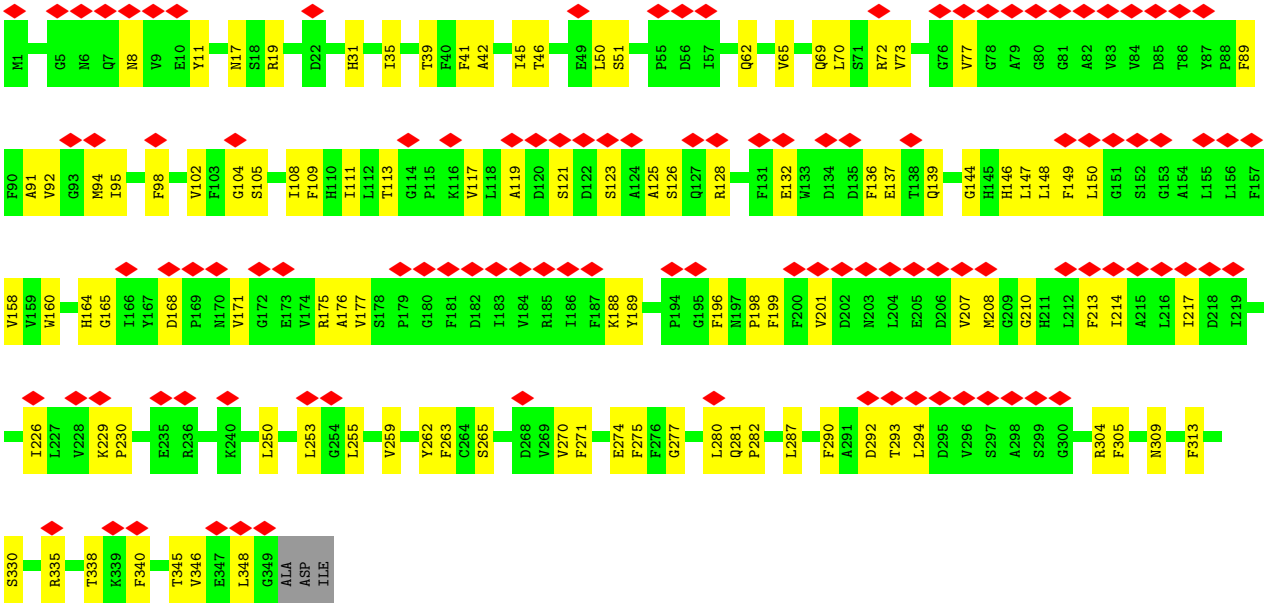
Chain 22:



• Molecule 16: High light inducible protein

Chain 32:

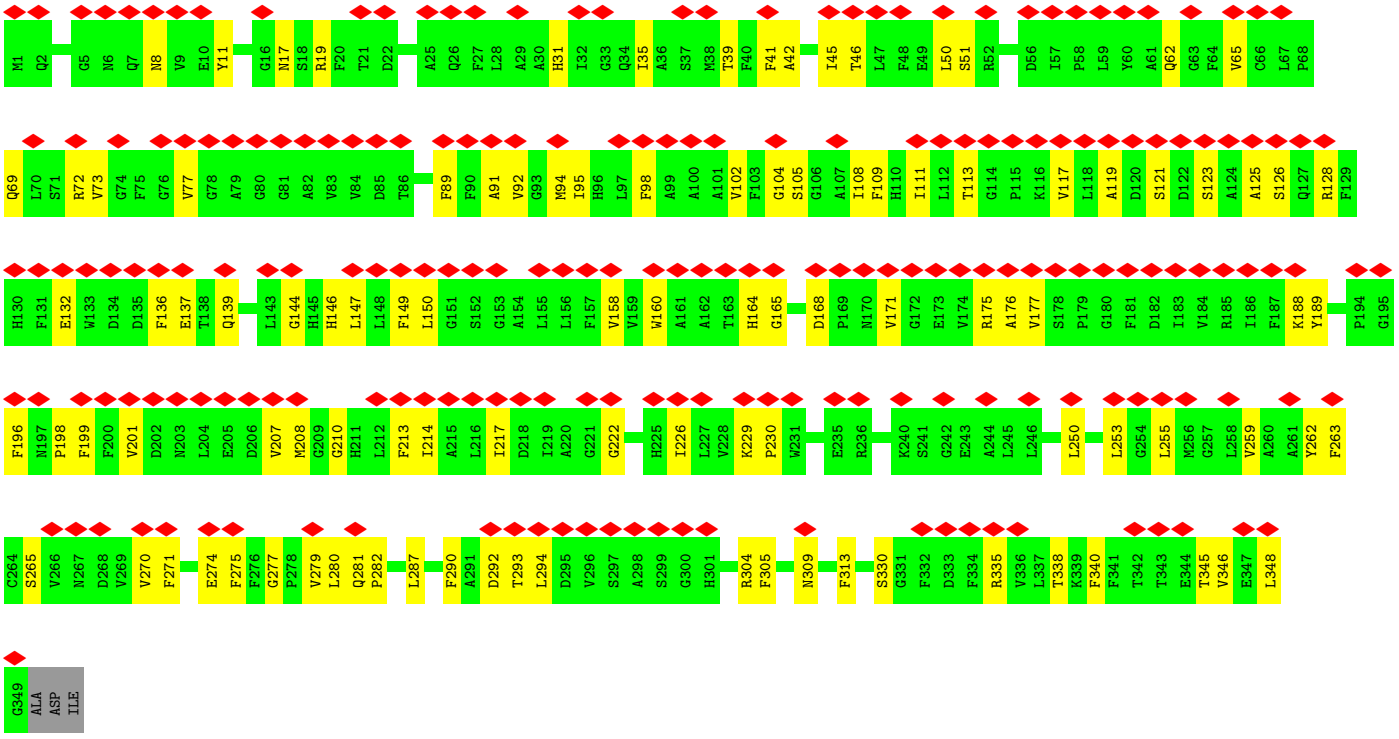




• Molecule 16: High light inducible protein

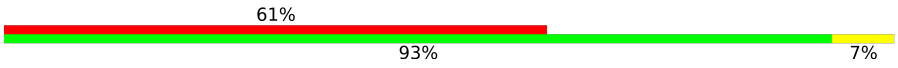
Chain 42:

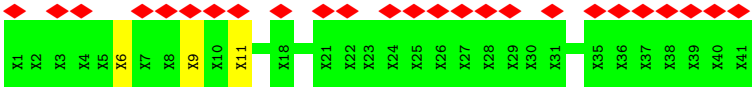




• Molecule 17: Unknown protein

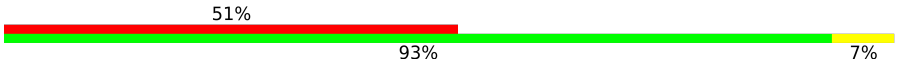
Chain 1G:

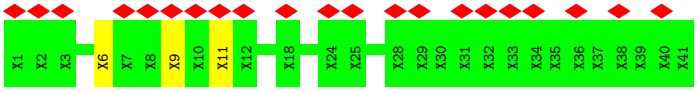




• Molecule 17: Unknown protein

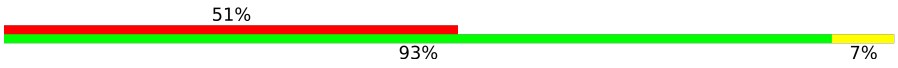
Chain 2G:

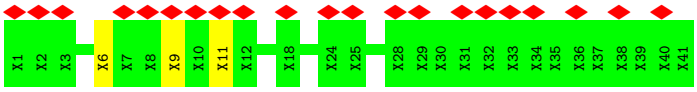




• Molecule 17: Unknown protein

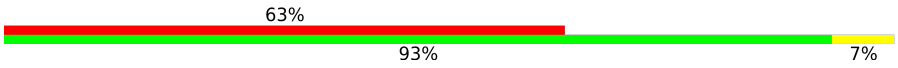
Chain 3G:

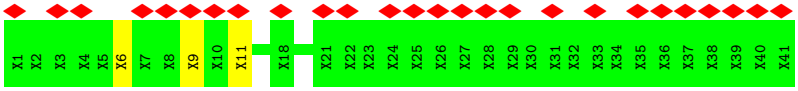




• Molecule 17: Unknown protein

Chain 4G:

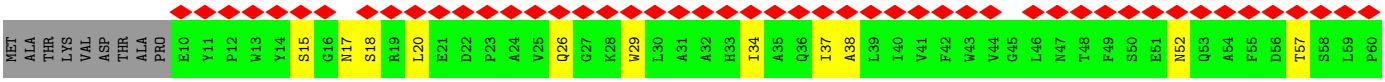


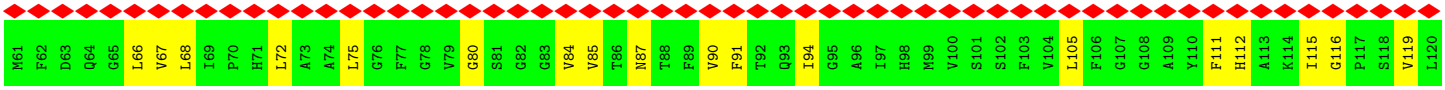


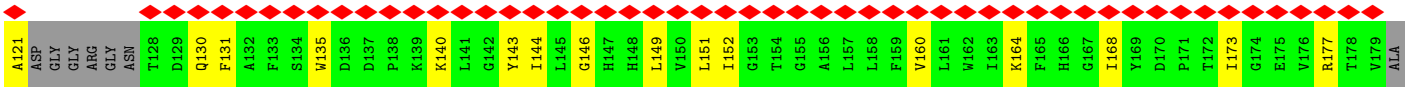
• Molecule 18: High light inducible protein

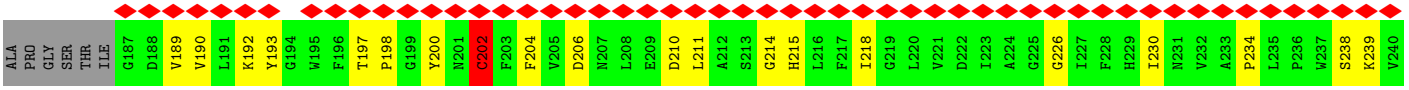
Chain 11:

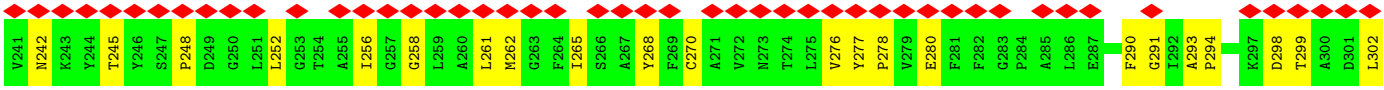


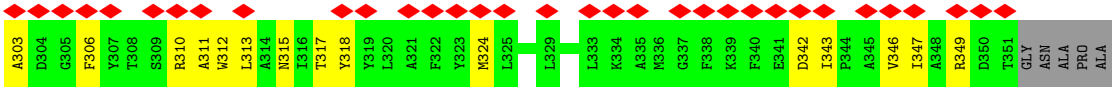








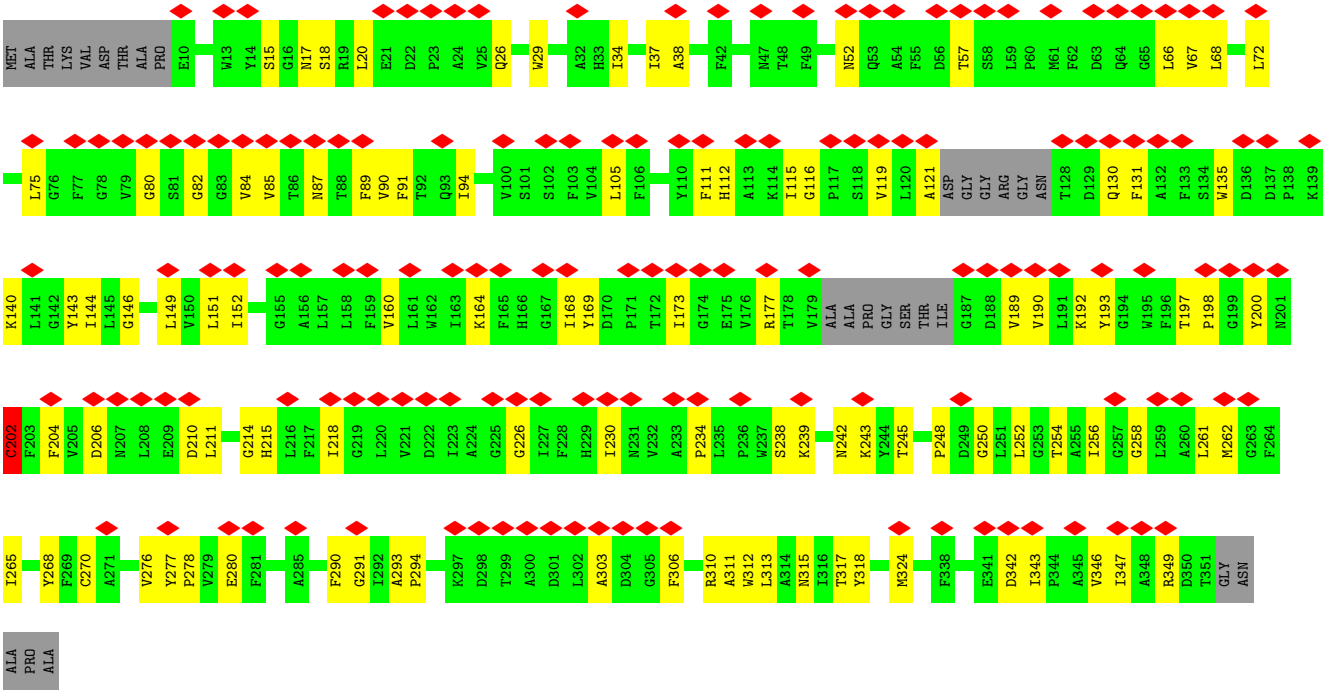




• Molecule 18: High light inducible protein

Chain 21:

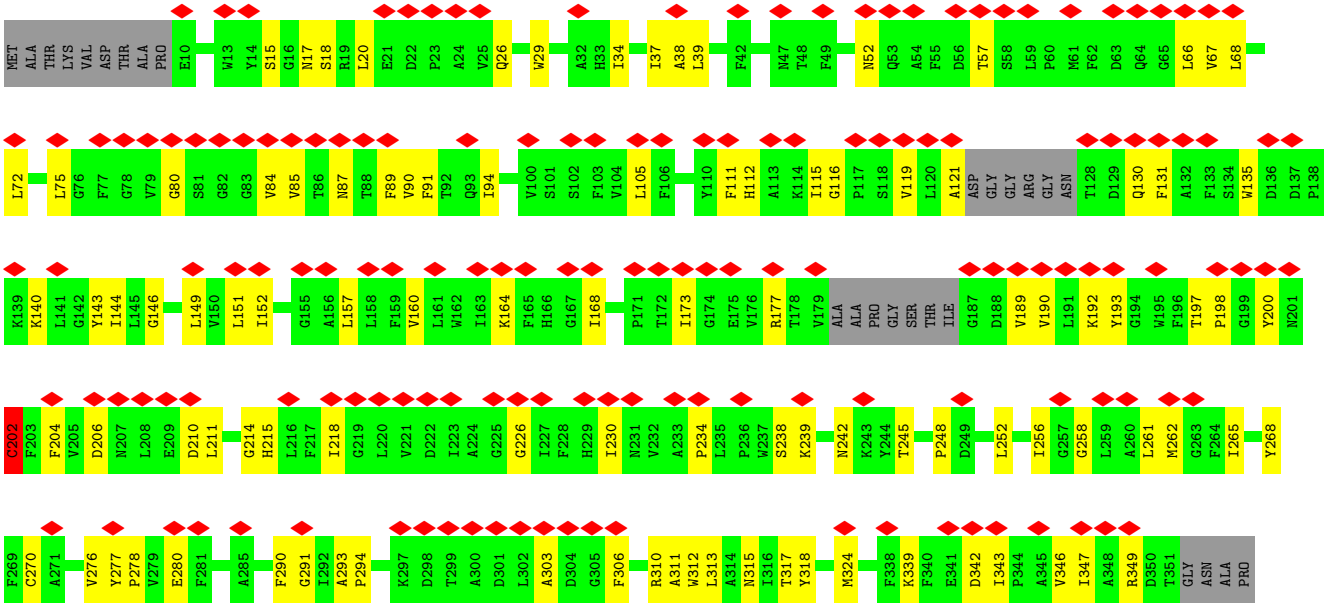




• Molecule 18: High light inducible protein

Chain 31:



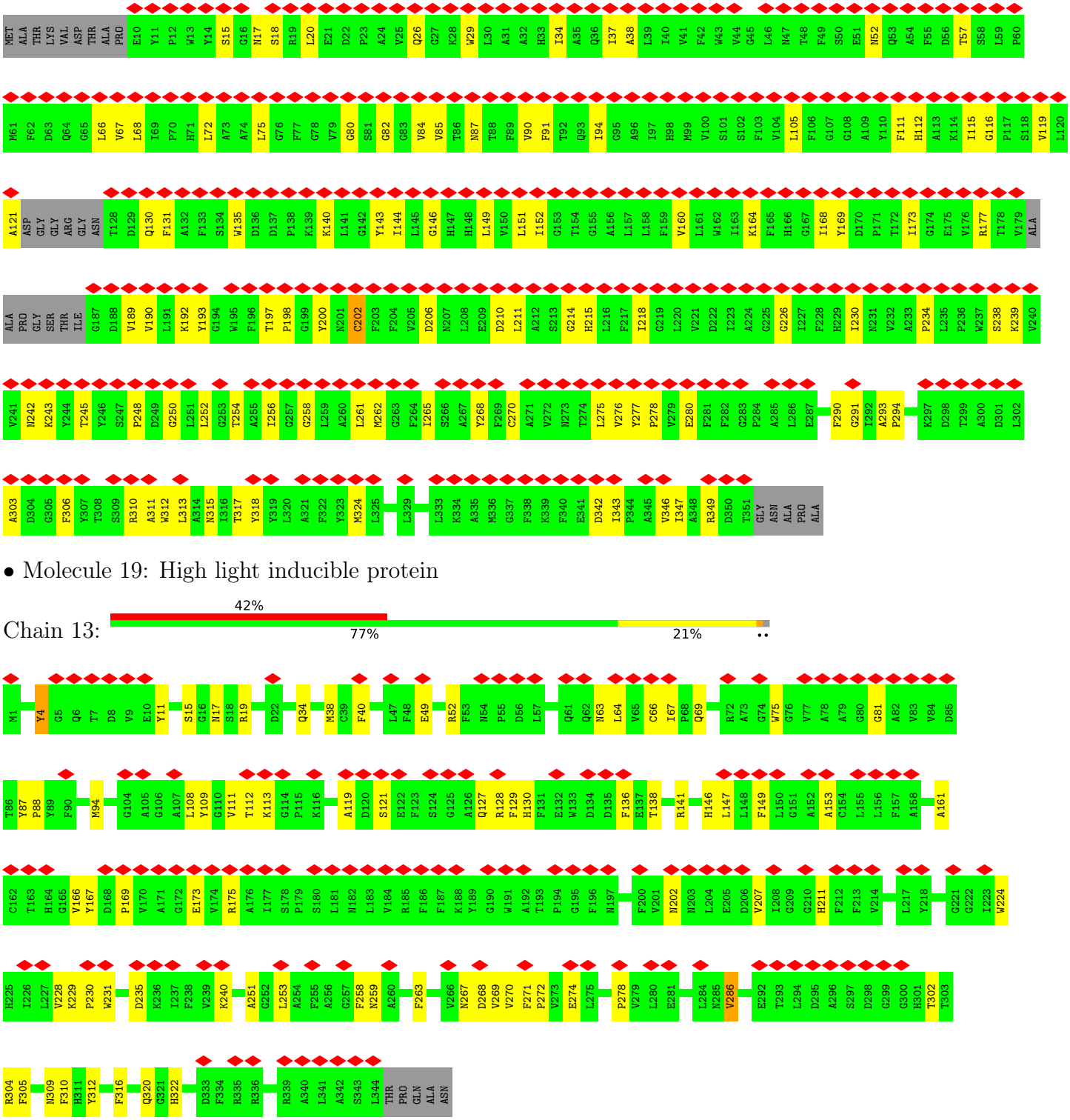




• Molecule 18: High light inducible protein

Chain 41:



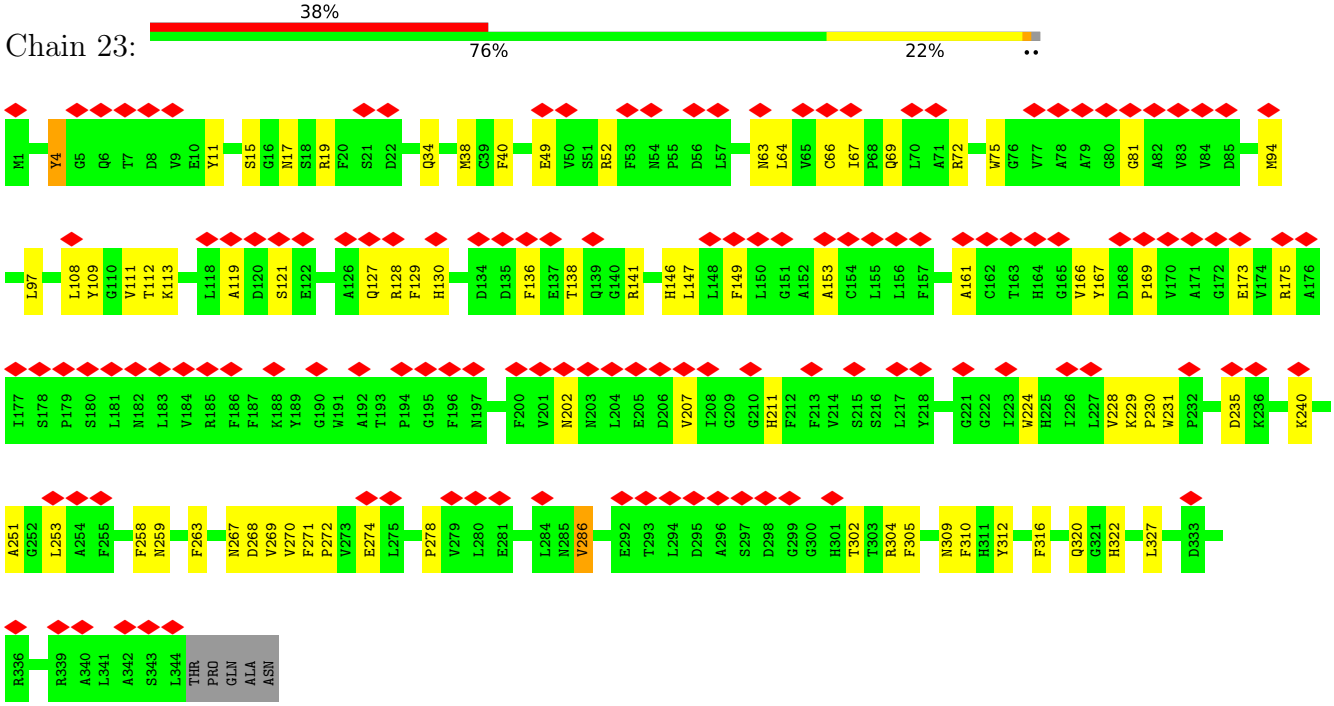


• Molecule 19: High light inducible protein

Chain 13:

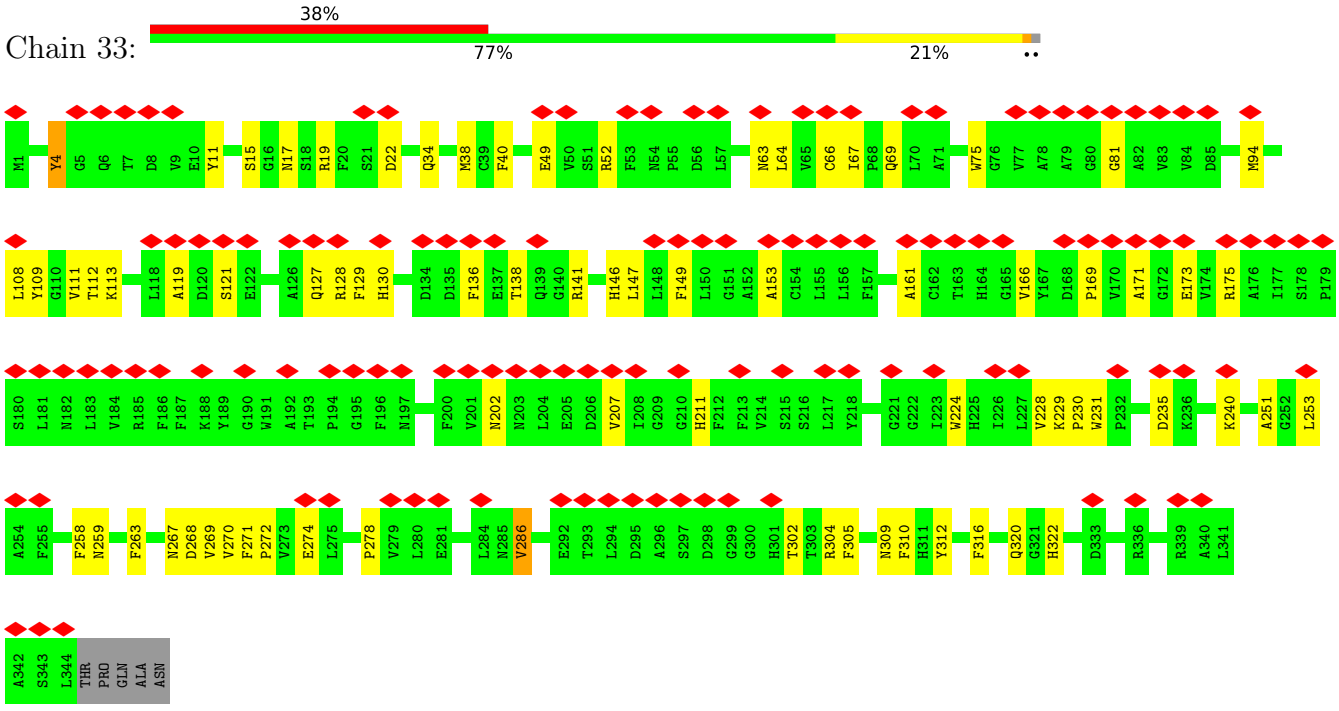
• Molecule 19: High light inducible protein

Chain 23:



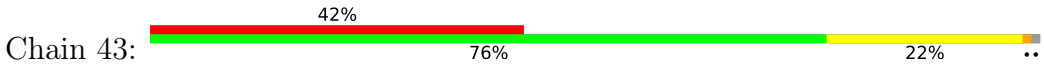
• Molecule 19: High light inducible protein

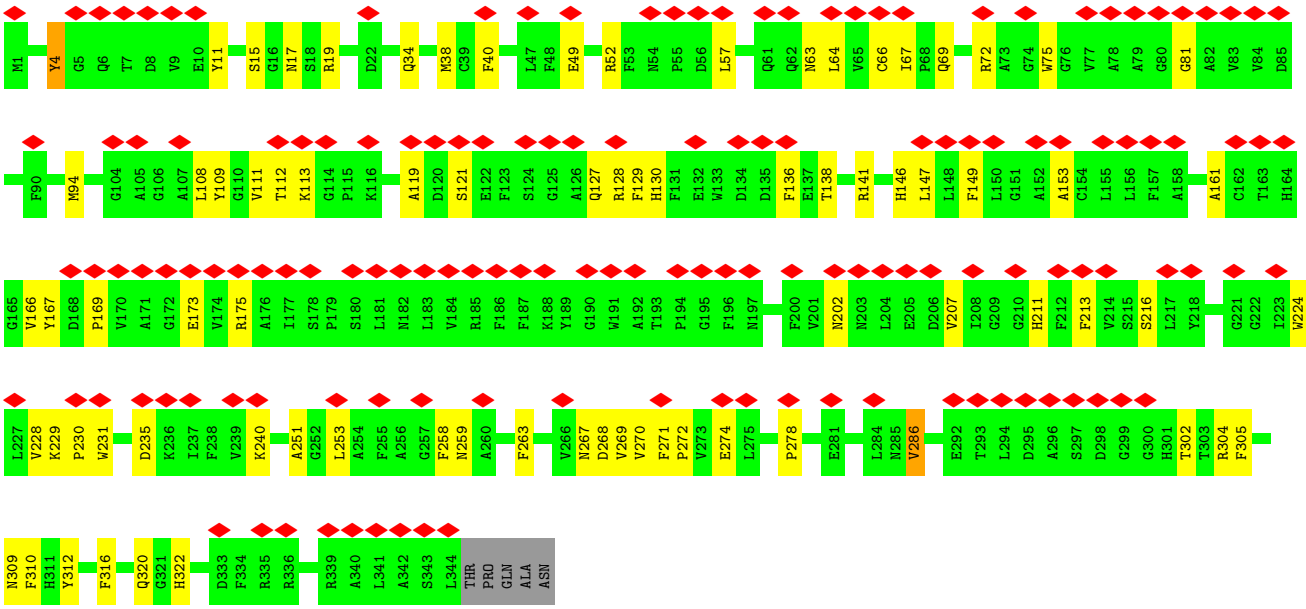
Chain 33:



• Molecule 19: High light inducible protein

Chain 43:

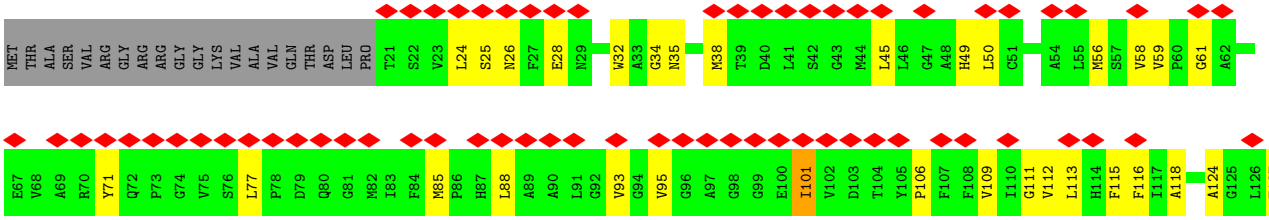




• Molecule 20: High light inducible protein

Chain 14:

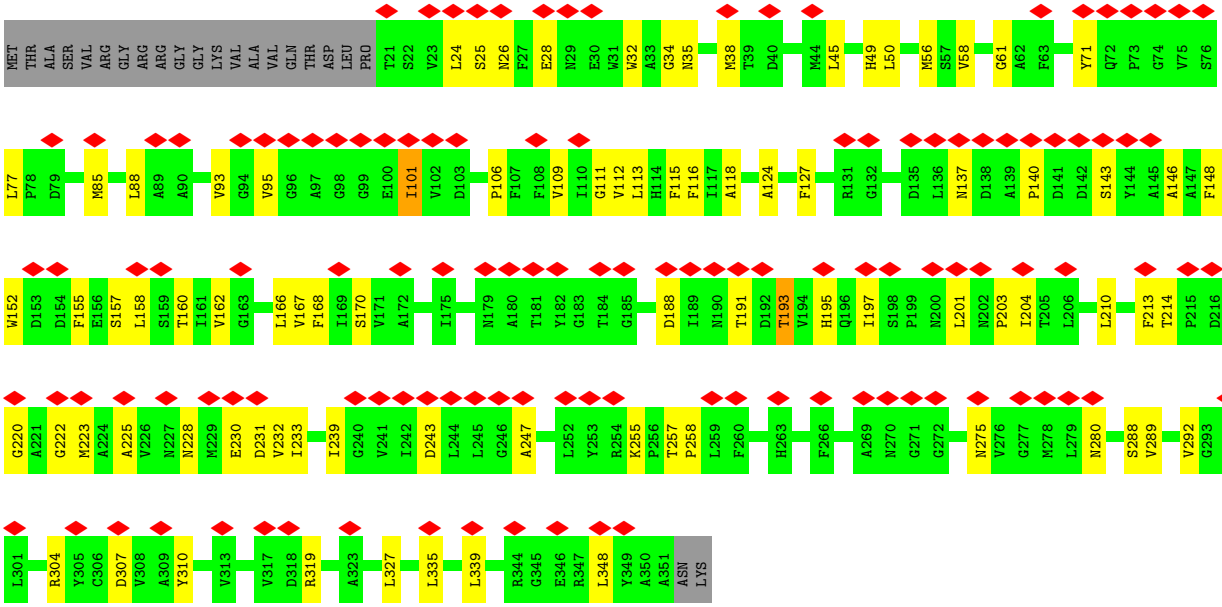




• Molecule 20: High light inducible protein

Chain 24:

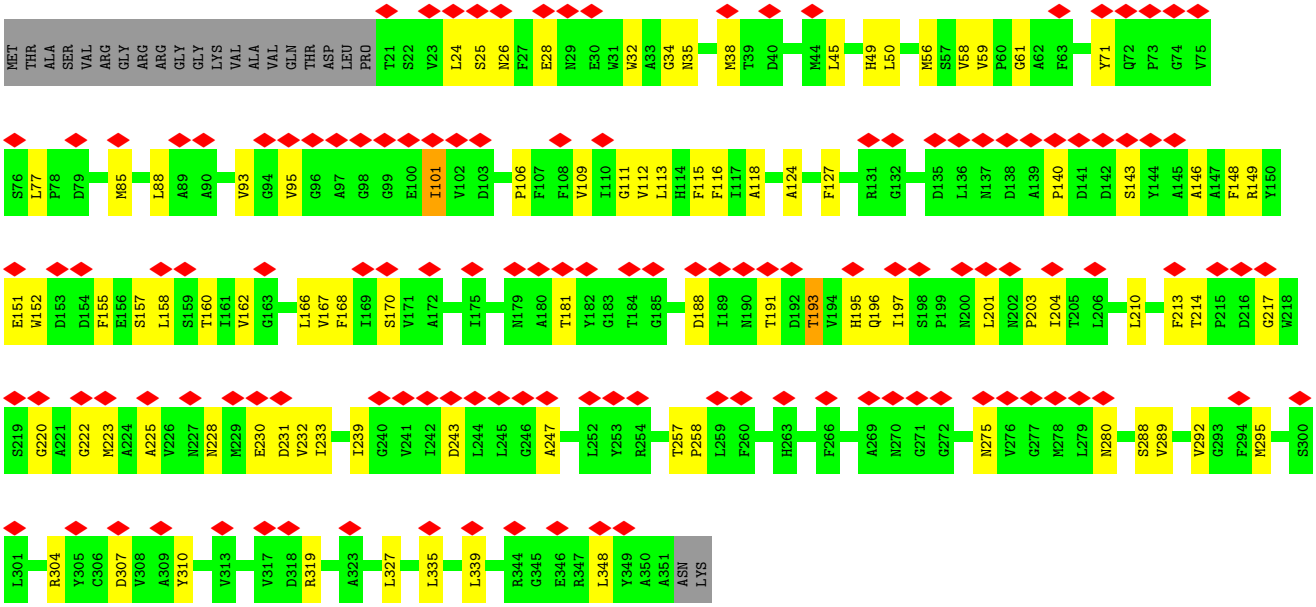




• Molecule 20: High light inducible protein

Chain 34:

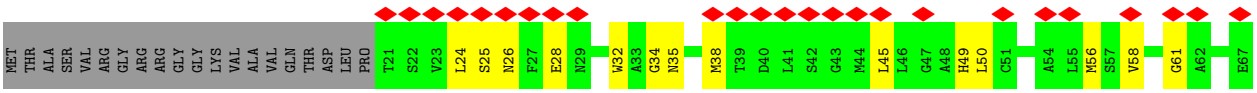


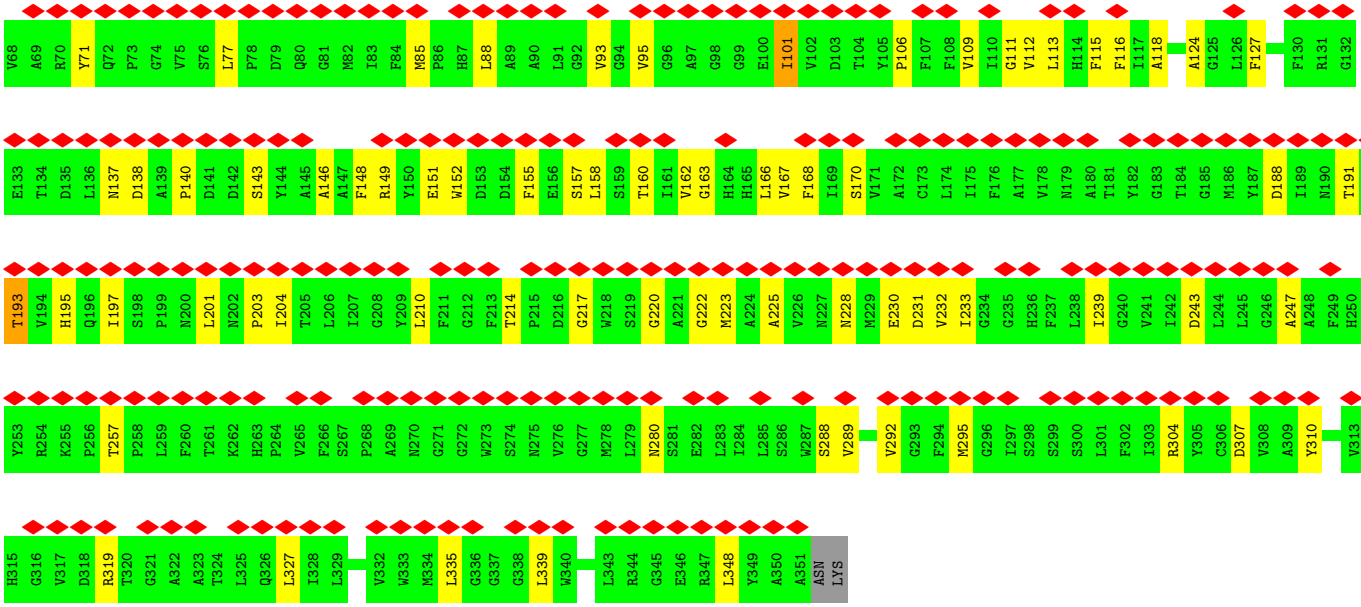


• Molecule 20: High light inducible protein

Chain 44:






V68 A69 R70 Y71 Q72 P73 G74 V75 S76 L77 P78 D79 Q80 G81 M82 I83 F84 M85 P86 H87 L88 A89 A90 L91 G92 V93 G94 V95 G96 A97 G98 G99 E100 I101 V102 D103 T104 Y105 P106 F107 F108 V109 I110 G111 V112 L113 H114 F115 F116 I117 A118 A124 G125 L126 F127 F130 R131 G132
E133 T134 D135 L136 N137 D138 A139 P140 D141 D142 S143 Y144 A145 A146 A147 F148 R149 Y150 E151 W152 D153 D154 F155 E156 S157 L158 S159 T160 I161 V162 G163 H164 H165 L166 V167 F168 I169 S170 V171 A172 C173 L174 I175 F176 A177 V178 N179 A180 T181 Y182 G183 T184 G185 M186 Y187 D188 I189 N190 T191 D192
T193 V194 H195 Q196 I197 S198 P199 N200 L201 N202 P203 I204 T205 L206 I207 G208 Y209 L210 F211 G212 F213 T214 P215 D216 G217 W218 S219 G220 A221 G222 M223 A224 A225 V226 N227 N228 M229 E230 D231 V232 I233 G234 G235 H236 F237 L238 I239 G240 V241 I242 D243 L244 L245 G246 A247 A248 F249 H250 I251 L252
Y253 R254 K255 P256 T257 P258 L259 F260 T261 K262 H263 P264 V265 P266 S267 P268 A269 N270 G271 G272 W273 S274 N275 V276 G277 M278 L279 N280 S281 E282 L283 I284 L285 S286 W287 S288 V289 V292 G293 P294 M295 G296 I297 S298 S299 S300 L301 F302 I303 R304 Y305 C306 D307 V308 A309 Y310 V313 F314
H315 G316 V317 D318 R319 T320 G321 A322 A323 T324 L325 Q326 L327 I328 L329 V332 W333 M334 L335 G336 G337 G338 L339 W340 L343 R344 G345 E346 R347 L348 Y349 A350 A351 ASN LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0171	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CL7, ZEX, LMG, SQD, PL9, 8CT, FE2, DGD, PHO, BCT, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1A	0.39	0/2280	0.41	0/3112
1	2A	0.39	0/2280	0.41	0/3112
1	3A	0.39	0/2280	0.41	0/3112
1	4A	0.39	0/2280	0.41	0/3112
2	1B	0.37	0/3929	0.43	1/5360 (0.0%)
2	2B	0.37	0/3929	0.42	0/5360
2	3B	0.37	0/3929	0.42	0/5360
2	4B	0.37	0/3929	0.42	0/5360
3	1C	0.34	0/3431	0.41	0/4669
3	2C	0.34	0/3431	0.41	0/4669
3	3C	0.34	0/3431	0.41	0/4669
3	4C	0.34	0/3431	0.41	0/4669
4	1D	0.38	0/2672	0.40	0/3641
4	2D	0.38	0/2672	0.40	0/3641
4	3D	0.38	0/2672	0.40	0/3641
4	4D	0.38	0/2672	0.40	0/3641
5	1E	0.25	0/555	0.38	0/757
5	2E	0.25	0/555	0.38	0/757
5	3E	0.25	0/555	0.38	0/757
5	4E	0.25	0/555	0.38	0/757
6	1F	0.33	0/250	0.39	0/343
6	2F	0.33	0/250	0.39	0/343
6	3F	0.33	0/250	0.39	0/343
6	4F	0.33	0/250	0.39	0/343
7	1H	0.32	0/534	0.49	1/729 (0.1%)
7	2H	0.32	0/534	0.49	1/729 (0.1%)
7	3H	0.32	0/534	0.49	1/729 (0.1%)
7	4H	0.32	0/534	0.49	1/729 (0.1%)
8	1I	0.39	0/290	0.37	0/391
8	2I	0.39	0/290	0.37	0/391
8	3I	0.39	0/290	0.37	0/391
8	4I	0.39	0/290	0.37	0/391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	1K	0.26	0/303	0.39	0/413
9	2K	0.26	0/303	0.39	0/413
9	3K	0.26	0/303	0.39	0/413
9	4K	0.26	0/303	0.39	0/413
10	1L	0.37	0/295	0.38	0/401
10	2L	0.37	0/295	0.38	0/401
10	3L	0.37	0/295	0.38	0/401
10	4L	0.37	0/295	0.38	0/401
11	1M	0.33	0/236	0.44	0/322
11	2M	0.33	0/236	0.44	0/322
11	3M	0.33	0/236	0.44	0/322
11	4M	0.33	0/236	0.44	0/322
12	1T	0.31	0/238	0.35	0/321
12	2T	0.31	0/238	0.35	0/321
12	3T	0.31	0/238	0.35	0/321
12	4T	0.31	0/238	0.35	0/321
13	1X	0.25	0/276	0.29	0/370
13	2X	0.25	0/276	0.29	0/370
13	3X	0.25	0/276	0.29	0/370
13	4X	0.25	0/276	0.29	0/370
14	1Y	0.17	0/164	0.33	0/224
14	2Y	0.17	0/164	0.33	0/224
14	3Y	0.18	0/164	0.33	0/224
14	4Y	0.18	0/164	0.33	0/224
15	1Z	0.20	0/438	0.29	0/599
15	2Z	0.20	0/438	0.29	0/599
15	3Z	0.20	0/438	0.29	0/599
15	4Z	0.19	0/438	0.29	0/599
16	12	0.36	0/2830	0.42	0/3855
16	22	0.36	0/2830	0.42	0/3855
16	32	0.36	0/2830	0.42	0/3855
16	42	0.35	0/2830	0.42	0/3855
18	11	0.28	0/2652	0.41	0/3618
18	21	0.28	0/2652	0.41	0/3618
18	31	0.29	0/2652	0.41	0/3618
18	41	0.28	0/2652	0.41	0/3618
19	13	0.38	0/2814	0.46	1/3841 (0.0%)
19	23	0.38	0/2814	0.46	1/3841 (0.0%)
19	33	0.38	0/2814	0.46	1/3841 (0.0%)
19	43	0.38	0/2814	0.46	1/3841 (0.0%)
20	14	0.33	0/2590	0.43	0/3537
20	24	0.33	0/2590	0.43	0/3537
20	34	0.33	0/2590	0.43	0/3537

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
20	44	0.33	0/2590	0.43	0/3537
All	All	0.35	0/107108	0.42	9/146012 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2H	53	THR	N-CA-C	-7.26	101.88	111.24
7	1H	53	THR	N-CA-C	-7.24	101.90	111.24
7	4H	53	THR	N-CA-C	-7.24	101.90	111.24
7	3H	53	THR	N-CA-C	-7.21	101.93	111.24
19	23	286	VAL	N-CA-C	-6.79	102.78	112.35
19	43	286	VAL	N-CA-C	-6.79	102.78	112.35
19	13	286	VAL	N-CA-C	-6.78	102.79	112.35
19	33	286	VAL	N-CA-C	-6.76	102.81	112.35
2	1B	390	TYR	N-CA-C	-5.91	97.69	108.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2209	0	2142	61	0
1	2A	2209	0	2142	61	0
1	3A	2209	0	2142	59	0
1	4A	2209	0	2142	64	0
2	1B	3794	0	3626	66	0
2	2B	3794	0	3626	67	0
2	3B	3794	0	3626	63	0
2	4B	3794	0	3626	64	0
3	1C	3313	0	3162	58	0
3	2C	3313	0	3162	61	0
3	3C	3313	0	3162	59	0
3	4C	3313	0	3162	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1D	2583	0	2493	61	0
4	2D	2583	0	2493	58	0
4	3D	2583	0	2493	61	0
4	4D	2583	0	2493	59	0
5	1E	538	0	520	14	0
5	2E	538	0	520	18	0
5	3E	538	0	520	20	0
5	4E	538	0	520	14	0
6	1F	242	0	249	1	0
6	2F	242	0	249	2	0
6	3F	242	0	249	2	0
6	4F	242	0	249	2	0
7	1H	519	0	518	10	0
7	2H	519	0	518	10	0
7	3H	519	0	518	10	0
7	4H	519	0	518	10	0
8	1I	281	0	289	8	0
8	2I	281	0	289	8	0
8	3I	281	0	289	7	0
8	4I	281	0	289	8	0
9	1K	292	0	302	8	0
9	2K	292	0	302	10	0
9	3K	292	0	302	10	0
9	4K	292	0	302	7	0
10	1L	288	0	301	7	0
10	2L	288	0	301	8	0
10	3L	288	0	301	6	0
10	4L	288	0	301	8	0
11	1M	232	0	243	4	0
11	2M	232	0	243	4	0
11	3M	232	0	243	4	0
11	4M	232	0	243	4	0
12	1T	231	0	240	2	0
12	2T	231	0	240	3	0
12	3T	231	0	240	2	0
12	4T	231	0	240	1	0
13	1X	269	0	275	4	0
13	2X	269	0	275	4	0
13	3X	269	0	275	4	0
13	4X	269	0	275	5	0
14	1Y	164	0	197	1	0
14	2Y	164	0	197	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	3Y	164	0	197	3	0
14	4Y	164	0	197	2	0
15	1Z	429	0	450	3	0
15	2Z	429	0	450	7	0
15	3Z	429	0	450	7	0
15	4Z	429	0	450	3	0
16	12	2734	0	2611	108	0
16	22	2734	0	2611	101	0
16	32	2734	0	2611	108	0
16	42	2734	0	2611	106	0
17	1G	205	0	46	2	0
17	2G	205	0	46	2	0
17	3G	205	0	46	2	0
17	4G	205	0	46	2	0
18	11	2567	0	2508	97	0
18	21	2567	0	2508	106	0
18	31	2567	0	2508	107	0
18	41	2567	0	2508	100	0
19	13	2715	0	2580	77	0
19	23	2715	0	2580	79	0
19	33	2715	0	2580	79	0
19	43	2715	0	2580	78	0
20	14	2514	0	2436	79	0
20	24	2514	0	2436	91	0
20	34	2514	0	2436	90	0
20	44	2514	0	2436	78	0
21	11	972	0	822	78	0
21	12	1065	0	1050	104	0
21	13	1024	0	962	117	0
21	14	757	0	681	59	0
21	1A	185	0	187	30	0
21	1B	991	0	947	59	0
21	1C	799	0	763	40	0
21	1D	153	0	121	8	0
21	21	972	0	822	90	0
21	22	1065	0	1050	104	0
21	23	1024	0	962	118	0
21	24	757	0	681	57	0
21	2A	185	0	187	27	0
21	2B	991	0	947	60	0
21	2C	799	0	763	40	0
21	2D	153	0	121	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	31	972	0	821	88	0
21	32	1065	0	1050	103	0
21	33	1024	0	962	117	0
21	34	757	0	681	59	0
21	3A	185	0	187	29	0
21	3B	991	0	946	55	0
21	3C	799	0	763	39	0
21	3D	153	0	121	8	0
21	41	972	0	822	85	0
21	42	1065	0	1050	101	0
21	43	1024	0	962	124	0
21	44	757	0	681	58	0
21	4A	185	0	187	28	0
21	4B	991	0	947	56	0
21	4C	799	0	763	39	0
21	4D	153	0	121	9	0
22	1A	64	0	74	3	0
22	1D	64	0	74	4	0
22	2A	64	0	74	3	0
22	2D	64	0	74	3	0
22	3A	64	0	74	3	0
22	3D	64	0	74	4	0
22	4A	64	0	74	3	0
22	4D	64	0	74	3	0
23	14	40	0	0	0	0
23	1A	40	0	0	0	0
23	1B	160	0	0	0	0
23	1C	120	0	0	2	0
23	1D	40	0	0	0	0
23	1K	40	0	0	0	0
23	24	40	0	0	0	0
23	2A	40	0	0	0	0
23	2B	160	0	0	0	0
23	2C	120	0	0	2	0
23	2D	40	0	0	0	0
23	2K	40	0	0	0	0
23	34	40	0	0	0	0
23	3A	40	0	0	0	0
23	3B	160	0	0	0	0
23	3C	120	0	0	2	0
23	3D	40	0	0	0	0
23	3K	40	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	44	40	0	0	0	0
23	4A	40	0	0	0	0
23	4B	160	0	0	0	0
23	4C	120	0	0	2	0
23	4D	40	0	0	0	0
23	4K	40	0	0	0	0
24	11	51	0	72	2	0
24	1A	50	0	70	2	0
24	1B	51	0	72	5	0
24	1D	33	0	36	1	0
24	21	51	0	72	2	0
24	2A	50	0	70	2	0
24	2B	51	0	72	5	0
24	2D	33	0	36	1	0
24	31	51	0	72	3	0
24	3A	50	0	70	2	0
24	3B	51	0	72	6	0
24	3D	33	0	36	1	0
24	41	51	0	72	2	0
24	4A	50	0	70	2	0
24	4B	51	0	72	6	0
24	4D	33	0	36	1	0
25	11	32	0	28	1	0
25	12	91	0	113	2	0
25	13	96	0	123	6	0
25	1A	34	0	32	3	0
25	1B	54	0	78	3	0
25	21	32	0	28	1	0
25	22	91	0	113	2	0
25	23	96	0	123	6	0
25	2A	34	0	32	2	0
25	2B	54	0	78	2	0
25	31	32	0	28	1	0
25	32	91	0	113	1	0
25	33	96	0	123	5	0
25	3A	34	0	32	1	0
25	3B	54	0	78	2	0
25	41	32	0	28	1	0
25	42	91	0	113	2	0
25	43	96	0	123	5	0
25	4A	34	0	32	2	0
25	4B	54	0	78	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	13	36	0	42	1	0
26	14	49	0	74	2	0
26	1A	46	0	65	0	0
26	1B	94	0	137	7	0
26	1D	49	0	74	3	0
26	23	36	0	42	1	0
26	24	49	0	74	2	0
26	2A	46	0	65	0	0
26	2B	94	0	137	8	0
26	2D	49	0	74	4	0
26	33	36	0	42	1	0
26	34	49	0	74	2	0
26	3A	46	0	65	0	0
26	3B	94	0	137	7	0
26	3D	49	0	74	3	0
26	43	36	0	42	1	0
26	44	49	0	74	2	0
26	4A	46	0	65	0	0
26	4B	94	0	137	8	0
26	4D	49	0	74	3	0
27	1B	62	0	82	2	0
27	1C	62	0	82	5	0
27	2B	62	0	82	2	0
27	2C	62	0	82	4	0
27	3B	62	0	82	2	0
27	3C	62	0	82	5	0
27	4B	62	0	82	2	0
27	4C	62	0	82	4	0
28	1D	1	0	0	0	0
28	2D	1	0	0	0	0
28	3D	1	0	0	0	0
28	4D	1	0	0	0	0
29	1D	4	0	0	0	0
29	2D	4	0	0	0	0
29	3D	4	0	0	0	0
29	4D	4	0	0	0	0
30	1D	55	0	80	7	0
30	2D	55	0	80	7	0
30	3D	55	0	80	7	0
30	4D	55	0	80	7	0
31	1F	43	0	30	3	0
31	2F	43	0	30	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3F	43	0	30	3	0
31	4F	43	0	30	4	0
32	11	84	0	112	34	0
32	12	168	0	224	70	0
32	13	168	0	224	77	0
32	14	168	0	224	49	0
32	21	84	0	112	36	0
32	22	168	0	224	66	0
32	23	168	0	224	77	0
32	24	168	0	224	51	0
32	31	84	0	112	37	0
32	32	168	0	224	67	0
32	33	168	0	224	77	0
32	34	168	0	224	48	0
32	41	84	0	112	38	0
32	42	168	0	224	70	0
32	43	168	0	224	79	0
32	44	168	0	224	51	0
All	All	136856	0	131770	4187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (4187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:315:ASN:HB3	32:41:421:ZEX:C36	1.32	1.58
18:11:315:ASN:CB	32:11:421:ZEX:C36	1.81	1.58
18:41:315:ASN:CB	32:41:421:ZEX:C36	1.81	1.57
18:21:315:ASN:CB	32:21:421:ZEX:C36	1.81	1.57
18:31:315:ASN:CB	32:31:421:ZEX:C36	1.81	1.57
18:21:315:ASN:HB3	32:21:421:ZEX:C36	1.32	1.56
18:31:315:ASN:HB3	32:31:421:ZEX:C36	1.32	1.55
18:11:315:ASN:HB3	32:11:421:ZEX:C36	1.32	1.54
21:43:409:CL7:H42C	32:43:420:ZEX:C17	1.38	1.51
21:23:409:CL7:H42C	32:23:420:ZEX:C17	1.38	1.50
21:13:508:CL7:H42C	32:13:519:ZEX:C17	1.38	1.49
21:33:508:CL7:H42C	32:33:519:ZEX:C17	1.38	1.47
18:31:315:ASN:CG	32:31:421:ZEX:C36	1.91	1.44
18:11:315:ASN:CG	32:11:421:ZEX:C36	1.91	1.43
18:21:315:ASN:CG	32:21:421:ZEX:C36	1.91	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:315:ASN:CG	32:41:421:ZEX:C36	1.91	1.41
18:31:315:ASN:CG	32:31:421:ZEX:H362	1.43	1.40
18:41:315:ASN:CG	32:41:421:ZEX:H362	1.43	1.40
21:23:406:CL7:C14	32:24:403:ZEX:C39	2.00	1.39
21:13:505:CL7:C14	32:14:403:ZEX:C39	2.00	1.39
21:43:406:CL7:C14	32:44:403:ZEX:C39	2.00	1.39
18:21:315:ASN:CG	32:21:421:ZEX:H362	1.43	1.38
16:42:94:MET:SD	32:42:524:ZEX:C36	2.13	1.37
18:11:315:ASN:CG	32:11:421:ZEX:H362	1.43	1.37
16:12:94:MET:SD	32:12:524:ZEX:C36	2.13	1.37
16:22:94:MET:SD	32:22:524:ZEX:C36	2.13	1.37
21:33:505:CL7:C14	32:34:403:ZEX:C39	2.00	1.36
16:32:94:MET:SD	32:32:524:ZEX:C36	2.12	1.36
21:23:409:CL7:C4	32:23:420:ZEX:H173	1.59	1.32
21:33:508:CL7:C4	32:33:519:ZEX:H173	1.59	1.32
21:13:508:CL7:C4	32:13:519:ZEX:H173	1.59	1.31
16:32:210:GLY:HA3	32:32:520:ZEX:C36	1.60	1.30
21:43:409:CL7:C4	32:43:420:ZEX:H173	1.59	1.30
16:12:210:GLY:HA3	32:12:520:ZEX:C36	1.60	1.29
21:43:409:CL7:C4	32:43:420:ZEX:C17	2.11	1.28
16:42:210:GLY:HA3	32:42:520:ZEX:C36	1.61	1.28
16:22:210:GLY:HA3	32:22:520:ZEX:C36	1.61	1.27
21:33:508:CL7:C4	32:33:519:ZEX:C17	2.11	1.27
21:13:505:CL7:H141	32:14:403:ZEX:C39	1.62	1.26
21:13:508:CL7:C4	32:13:519:ZEX:C17	2.11	1.26
21:33:505:CL7:H141	32:34:403:ZEX:C39	1.61	1.26
18:21:315:ASN:CB	32:21:421:ZEX:H362	1.52	1.26
21:23:409:CL7:C4	32:23:420:ZEX:C17	2.11	1.26
18:41:315:ASN:CB	32:41:421:ZEX:H362	1.52	1.23
21:43:406:CL7:H141	32:44:403:ZEX:C39	1.61	1.23
16:12:201:VAL:HG21	32:12:520:ZEX:O23	1.38	1.22
21:23:406:CL7:H141	32:24:403:ZEX:C39	1.61	1.21
18:31:315:ASN:CB	32:31:421:ZEX:H362	1.52	1.21
16:22:201:VAL:HG21	32:22:520:ZEX:O23	1.38	1.21
21:43:406:CL7:C14	32:44:403:ZEX:H393	1.65	1.21
19:43:111:VAL:HG21	32:43:401:ZEX:H42	1.24	1.20
16:42:201:VAL:HG21	32:42:520:ZEX:O23	1.38	1.20
16:32:201:VAL:HG21	32:32:520:ZEX:O23	1.38	1.19
16:42:210:GLY:CA	32:42:520:ZEX:H363	1.73	1.19
16:12:210:GLY:CA	32:12:520:ZEX:H363	1.72	1.18
18:11:315:ASN:CB	32:11:421:ZEX:H362	1.52	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:22:210:GLY:CA	32:22:520:ZEX:H363	1.72	1.18
16:32:210:GLY:CA	32:32:520:ZEX:H363	1.72	1.17
21:13:505:CL7:C14	32:14:403:ZEX:H393	1.65	1.17
21:33:505:CL7:C14	32:34:403:ZEX:H393	1.65	1.17
19:23:111:VAL:HG21	32:23:401:ZEX:H42	1.28	1.16
21:21:414:CL7:OBD	20:34:258:PRO:HG2	1.46	1.14
19:13:111:VAL:HG21	32:13:525:ZEX:H42	1.24	1.14
21:43:409:CL7:H42C	32:43:420:ZEX:H171	1.30	1.14
21:23:406:CL7:C14	32:24:403:ZEX:H393	1.65	1.13
16:32:94:MET:SD	32:32:524:ZEX:H363	1.84	1.12
16:42:94:MET:SD	32:42:524:ZEX:H363	1.84	1.12
21:23:409:CL7:H42C	32:23:420:ZEX:H171	1.30	1.12
20:24:258:PRO:HG2	21:31:414:CL7:OBD	1.47	1.12
16:12:94:MET:SD	32:12:524:ZEX:H363	1.84	1.11
18:41:315:ASN:CG	32:41:421:ZEX:H361	1.75	1.11
19:33:111:VAL:HG21	32:33:525:ZEX:H42	1.27	1.11
21:33:513:CL7:C4B	32:33:522:ZEX:C17	2.30	1.10
21:13:513:CL7:C4B	32:13:522:ZEX:C17	2.30	1.10
18:21:315:ASN:CG	32:21:421:ZEX:H361	1.75	1.10
21:43:414:CL7:C4B	32:43:423:ZEX:C17	2.30	1.10
21:33:513:CL7:NB	32:33:522:ZEX:C17	2.16	1.09
21:43:414:CL7:NB	32:43:423:ZEX:C17	2.16	1.09
21:23:414:CL7:NB	32:23:423:ZEX:C17	2.16	1.09
21:23:409:CL7:H43C	32:23:420:ZEX:H173	1.30	1.09
21:23:414:CL7:C4B	32:23:423:ZEX:C17	2.30	1.09
21:33:508:CL7:H42C	32:33:519:ZEX:H171	1.30	1.09
21:13:513:CL7:NB	32:13:522:ZEX:C17	2.16	1.08
21:13:513:CL7:NB	32:13:522:ZEX:H171	1.66	1.08
21:33:513:CL7:NB	32:33:522:ZEX:H171	1.66	1.08
21:43:414:CL7:NB	32:43:423:ZEX:H171	1.66	1.08
16:22:94:MET:SD	32:22:524:ZEX:H363	1.84	1.08
18:11:315:ASN:CG	32:11:421:ZEX:H361	1.75	1.08
21:43:409:CL7:H43C	32:43:420:ZEX:H173	1.30	1.08
21:23:414:CL7:NB	32:23:423:ZEX:H171	1.66	1.07
21:13:508:CL7:H43C	32:13:519:ZEX:H173	1.30	1.07
21:13:513:CL7:C4B	32:13:522:ZEX:H172	1.85	1.06
21:23:414:CL7:C4B	32:23:423:ZEX:H172	1.85	1.06
21:43:414:CL7:C4B	32:43:423:ZEX:H172	1.85	1.06
16:32:210:GLY:HA3	32:32:520:ZEX:H363	1.06	1.06
21:43:406:CL7:H142	32:44:403:ZEX:C39	1.75	1.05
21:33:513:CL7:C4B	32:33:522:ZEX:H172	1.85	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:31:315:ASN:CG	32:31:421:ZEX:H361	1.75	1.05
16:12:210:GLY:HA3	32:12:520:ZEX:H363	1.06	1.05
21:23:406:CL7:H142	32:24:403:ZEX:C39	1.75	1.05
16:12:94:MET:SD	32:12:524:ZEX:H362	1.95	1.04
21:13:508:CL7:H42C	32:13:519:ZEX:H171	1.30	1.04
16:22:210:GLY:HA3	32:22:520:ZEX:H363	1.06	1.04
21:33:508:CL7:H43C	32:33:519:ZEX:H173	1.30	1.04
15:2Z:17:PHE:CE2	5:3E:25:ILE:HD12	1.93	1.04
21:13:505:CL7:H142	32:14:403:ZEX:C39	1.75	1.04
16:22:94:MET:SD	32:22:524:ZEX:H362	1.95	1.03
16:32:94:MET:SD	32:32:524:ZEX:H362	1.95	1.02
16:42:210:GLY:HA3	32:42:520:ZEX:H363	1.06	1.02
5:2E:25:ILE:HD12	15:3Z:17:PHE:CE2	1.93	1.01
19:13:94:MET:CE	32:13:525:ZEX:C36	2.38	1.01
16:42:94:MET:SD	32:42:524:ZEX:H362	1.95	1.01
21:33:505:CL7:H142	32:34:403:ZEX:C39	1.75	1.01
18:11:315:ASN:CB	32:11:421:ZEX:H363	1.63	1.01
19:43:94:MET:CE	32:43:401:ZEX:C36	2.39	1.01
32:42:524:ZEX:H193	21:41:418:CL7:H8	1.41	1.00
32:32:524:ZEX:H193	21:31:418:CL7:H8	1.41	1.00
21:33:505:CL7:H141	32:34:403:ZEX:H391	1.00	1.00
21:13:505:CL7:H141	32:14:403:ZEX:H391	1.00	0.99
32:22:524:ZEX:H193	21:21:418:CL7:H8	1.41	0.99
19:43:94:MET:HE1	32:43:401:ZEX:H363	1.44	0.99
19:23:94:MET:CE	32:23:401:ZEX:C36	2.40	0.99
19:33:94:MET:CE	32:33:525:ZEX:C36	2.41	0.99
21:23:406:CL7:H142	32:24:403:ZEX:H393	0.99	0.99
19:13:94:MET:HE1	32:13:525:ZEX:H363	1.45	0.98
18:31:315:ASN:CB	32:31:421:ZEX:H363	1.63	0.98
21:43:406:CL7:H142	32:44:403:ZEX:H393	0.99	0.98
21:13:505:CL7:H142	32:14:403:ZEX:H393	0.99	0.98
21:23:406:CL7:H141	32:24:403:ZEX:H391	1.00	0.98
21:33:505:CL7:H142	32:34:403:ZEX:H393	0.99	0.97
32:12:524:ZEX:H193	21:11:418:CL7:H8	1.41	0.97
21:33:516:CL7:H3A	21:33:516:CL7:H11C	1.47	0.96
21:13:516:CL7:H11C	21:13:516:CL7:H3A	1.48	0.96
18:41:315:ASN:OD1	32:41:421:ZEX:H361	1.66	0.96
18:21:315:ASN:OD1	32:21:421:ZEX:H361	1.66	0.96
21:43:406:CL7:H141	32:44:403:ZEX:H391	1.00	0.96
19:33:94:MET:HE1	32:33:525:ZEX:H363	1.47	0.96
19:23:94:MET:HE1	32:23:401:ZEX:H363	1.48	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:23:417:CL7:H11C	21:23:417:CL7:H3A	1.47	0.96
21:33:505:CL7:C14	32:34:403:ZEX:H391	1.80	0.96
18:31:315:ASN:OD1	32:31:421:ZEX:H361	1.66	0.95
18:11:315:ASN:OD1	32:11:421:ZEX:H361	1.66	0.95
21:42:505:CL7:H11C	32:42:520:ZEX:H172	1.48	0.95
21:22:505:CL7:H11C	32:22:520:ZEX:H172	1.48	0.95
21:12:505:CL7:H11C	32:12:520:ZEX:H172	1.48	0.95
19:13:94:MET:HE1	32:13:525:ZEX:C36	1.96	0.95
19:23:309:ASN:OD1	32:23:420:ZEX:H363	1.66	0.95
18:41:315:ASN:CB	32:41:421:ZEX:H363	1.63	0.94
19:13:94:MET:CE	32:13:525:ZEX:H362	1.97	0.94
21:32:505:CL7:H11C	32:32:520:ZEX:H172	1.48	0.94
21:43:417:CL7:H11C	21:43:417:CL7:H3A	1.47	0.94
19:43:309:ASN:OD1	32:43:420:ZEX:H363	1.66	0.94
32:33:522:ZEX:H363	21:42:518:CL7:CMA	1.97	0.93
18:21:315:ASN:CB	32:21:421:ZEX:H363	1.63	0.93
19:13:309:ASN:OD1	32:13:519:ZEX:H363	1.66	0.93
19:43:94:MET:HE1	32:43:401:ZEX:C36	1.97	0.93
19:33:309:ASN:OD1	32:33:519:ZEX:H363	1.66	0.93
21:13:505:CL7:C14	32:14:403:ZEX:H391	1.80	0.92
19:43:94:MET:CE	32:43:401:ZEX:H362	1.99	0.92
21:12:518:CL7:CMA	32:23:423:ZEX:H363	2.00	0.92
19:13:111:VAL:HG21	32:13:525:ZEX:C4	2.00	0.92
19:23:94:MET:CE	32:23:401:ZEX:H362	1.99	0.92
16:22:214:ILE:HD11	32:22:520:ZEX:H392	1.52	0.91
16:12:214:ILE:HD11	32:12:520:ZEX:H392	1.52	0.91
21:22:512:CL7:H61C	32:22:522:ZEX:H202	1.53	0.91
18:11:315:ASN:ND2	32:11:421:ZEX:H362	1.85	0.91
19:23:94:MET:HE1	32:23:401:ZEX:C36	2.00	0.91
32:13:522:ZEX:H363	21:22:518:CL7:CMA	2.01	0.91
21:12:512:CL7:H61C	32:12:522:ZEX:H202	1.52	0.91
16:42:214:ILE:HD11	32:42:520:ZEX:H392	1.52	0.91
19:33:94:MET:HE1	32:33:525:ZEX:C36	2.01	0.91
21:32:518:CL7:CMA	32:43:423:ZEX:H363	1.99	0.91
19:43:111:VAL:HG21	32:43:401:ZEX:C4	2.00	0.91
4:1D:185:GLN:HB2	21:1D:404:CL7:HBC1	1.53	0.90
18:11:276:VAL:HG11	21:11:402:CL7:HAA2	1.53	0.90
19:33:94:MET:CE	32:33:525:ZEX:H362	2.00	0.90
4:2D:185:GLN:HB2	21:2D:404:CL7:HBC1	1.53	0.90
18:41:315:ASN:ND2	32:41:421:ZEX:H362	1.85	0.90
18:21:315:ASN:ND2	32:21:421:ZEX:H362	1.85	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:31:315:ASN:ND2	32:31:421:ZEX:H362	1.85	0.90
21:42:512:CL7:H61C	32:42:522:ZEX:H202	1.53	0.90
18:21:276:VAL:HG11	21:21:402:CL7:HAA2	1.53	0.90
21:43:414:CL7:C1B	32:43:423:ZEX:C17	2.50	0.90
20:44:304:ARG:HG3	32:44:418:ZEX:H373	1.52	0.90
20:24:213:PHE:HB3	18:31:89:PHE:HZ	1.37	0.90
4:4D:185:GLN:HB2	21:4D:404:CL7:HBC1	1.53	0.90
16:42:201:VAL:HG21	32:42:520:ZEX:H1	1.30	0.90
16:32:214:ILE:HD11	32:32:520:ZEX:H392	1.52	0.89
21:33:513:CL7:C1B	32:33:522:ZEX:C17	2.50	0.89
16:22:210:GLY:CA	32:22:520:ZEX:C36	2.42	0.89
21:23:414:CL7:C1B	32:23:423:ZEX:C17	2.50	0.89
18:31:276:VAL:HG11	21:31:402:CL7:HAA2	1.53	0.89
20:34:304:ARG:HG3	32:34:418:ZEX:H373	1.52	0.89
21:32:512:CL7:H61C	32:32:522:ZEX:H202	1.53	0.89
21:13:513:CL7:C1B	32:13:522:ZEX:C17	2.49	0.89
4:3D:185:GLN:HB2	21:3D:404:CL7:HBC1	1.53	0.89
20:24:115:PHE:CE2	32:24:403:ZEX:H363	2.08	0.89
20:44:115:PHE:CE2	32:44:403:ZEX:H363	2.08	0.89
18:41:276:VAL:HG11	21:41:402:CL7:HAA2	1.53	0.89
16:32:210:GLY:CA	32:32:520:ZEX:C36	2.42	0.88
20:14:115:PHE:CE2	32:14:403:ZEX:H363	2.08	0.88
18:21:89:PHE:HZ	20:34:213:PHE:HB3	1.38	0.88
20:14:304:ARG:HG3	32:14:418:ZEX:H373	1.52	0.88
20:34:115:PHE:CE2	32:34:403:ZEX:H363	2.08	0.88
16:12:210:GLY:HA3	32:12:520:ZEX:H362	1.56	0.87
20:24:304:ARG:HG3	32:24:418:ZEX:H373	1.52	0.87
19:33:111:VAL:HG21	32:33:525:ZEX:C4	2.04	0.87
16:12:207:VAL:HA	32:12:520:ZEX:H382	1.58	0.86
16:22:207:VAL:HA	32:22:520:ZEX:H382	1.58	0.86
16:22:210:GLY:HA3	32:22:520:ZEX:H362	1.56	0.86
16:22:201:VAL:HG21	32:22:520:ZEX:H1	1.37	0.86
16:42:210:GLY:CA	32:42:520:ZEX:C36	2.43	0.86
19:23:94:MET:SD	32:23:401:ZEX:C36	2.63	0.86
19:23:111:VAL:HG21	32:23:401:ZEX:C4	2.04	0.86
16:32:207:VAL:HA	32:32:520:ZEX:H382	1.57	0.86
16:42:207:VAL:HA	32:42:520:ZEX:H382	1.58	0.86
16:32:210:GLY:HA3	32:32:520:ZEX:H362	1.56	0.85
16:12:210:GLY:CA	32:12:520:ZEX:C36	2.42	0.85
15:2Z:17:PHE:HE2	5:3E:25:ILE:HD12	1.40	0.85
32:34:403:ZEX:O3	21:34:413:CL7:O2A	1.94	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:13:94:MET:SD	32:13:525:ZEX:C36	2.65	0.85
19:33:94:MET:SD	32:33:525:ZEX:C36	2.65	0.85
16:42:210:GLY:HA3	32:42:520:ZEX:H362	1.56	0.85
32:14:403:ZEX:O3	21:14:413:CL7:O2A	1.94	0.84
32:24:403:ZEX:O3	21:24:413:CL7:O2A	1.94	0.84
32:44:403:ZEX:O3	21:44:413:CL7:O2A	1.94	0.84
21:2A:401:CL7:H41C	21:2A:407:CL7:CAB	2.08	0.83
21:4A:401:CL7:H41C	21:4A:407:CL7:CAB	2.09	0.83
21:1A:401:CL7:H41C	21:1A:407:CL7:CAB	2.08	0.83
21:32:505:CL7:O1A	32:32:520:ZEX:H171	1.77	0.83
16:32:201:VAL:HG21	32:32:520:ZEX:H1	1.41	0.83
21:12:505:CL7:O1A	32:12:520:ZEX:H171	1.77	0.83
21:42:505:CL7:O1A	32:42:520:ZEX:H171	1.77	0.83
21:22:505:CL7:O1A	32:22:520:ZEX:H171	1.77	0.83
19:43:94:MET:SD	32:43:401:ZEX:C36	2.67	0.83
18:11:211:LEU:HD12	32:11:422:ZEX:C38	2.10	0.82
21:3A:401:CL7:H41C	21:3A:407:CL7:CAB	2.09	0.82
18:21:211:LEU:HD12	32:21:422:ZEX:C38	2.10	0.82
21:12:502:CL7:H2	21:12:503:CL7:H12C	1.62	0.82
21:23:406:CL7:HBA2	20:24:127:PHE:HB2	1.62	0.82
21:33:508:CL7:H42C	32:33:519:ZEX:H172	1.59	0.82
21:12:513:CL7:C1B	32:12:522:ZEX:H41	2.09	0.82
21:13:505:CL7:HBA2	20:14:127:PHE:HB2	1.62	0.82
16:32:290:PHE:CZ	32:43:401:ZEX:O23	2.33	0.82
18:31:211:LEU:HD12	32:31:422:ZEX:C38	2.10	0.82
5:2E:25:ILE:HD12	15:3Z:17:PHE:HE2	1.40	0.81
21:33:505:CL7:HBA2	20:34:127:PHE:HB2	1.62	0.81
16:12:290:PHE:CZ	32:23:401:ZEX:O23	2.33	0.81
21:22:502:CL7:H2	21:22:503:CL7:H12C	1.62	0.81
21:22:513:CL7:C1B	32:22:522:ZEX:H41	2.09	0.81
21:32:513:CL7:C1B	32:32:522:ZEX:H41	2.09	0.81
18:11:214:GLY:HA3	32:11:422:ZEX:H362	1.63	0.81
18:21:214:GLY:HA3	32:21:422:ZEX:H362	1.63	0.81
21:32:502:CL7:H2	21:32:503:CL7:H12C	1.62	0.81
18:41:315:ASN:HB2	32:41:421:ZEX:H362	1.63	0.81
21:43:406:CL7:HBA2	20:44:127:PHE:HB2	1.62	0.81
16:12:201:VAL:HG21	32:12:520:ZEX:H1	1.42	0.81
21:42:513:CL7:C1B	32:42:522:ZEX:H41	2.09	0.81
18:41:211:LEU:HD12	32:41:422:ZEX:C38	2.10	0.81
18:31:214:GLY:HA3	32:31:422:ZEX:H362	1.63	0.81
32:33:525:ZEX:O23	16:42:290:PHE:CZ	2.33	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:12:69:GLN:HE22	21:12:502:CL7:HAA1	1.47	0.80
16:32:94:MET:HB3	32:32:522:ZEX:H25	1.63	0.80
32:33:525:ZEX:H203	21:42:517:CL7:H42C	1.63	0.80
32:13:525:ZEX:H203	21:22:517:CL7:H42C	1.63	0.80
21:42:502:CL7:H2	21:42:503:CL7:H12C	1.62	0.80
18:41:214:GLY:HA3	32:41:422:ZEX:H362	1.63	0.80
16:22:94:MET:HB3	32:22:522:ZEX:H25	1.63	0.80
16:32:69:GLN:HE22	21:32:502:CL7:HAA1	1.47	0.80
16:12:94:MET:HB3	32:12:522:ZEX:H25	1.63	0.80
3:4C:296:MET:HE2	27:4C:516:DGD:HB81	1.64	0.80
18:41:315:ASN:ND2	32:41:421:ZEX:H382	1.97	0.80
16:22:69:GLN:HE22	21:22:502:CL7:HAA1	1.47	0.80
3:2C:296:MET:HE2	27:2C:516:DGD:HB81	1.64	0.79
21:4B:614:CL7:H43C	26:4B:624:LHG:H362	1.64	0.79
21:2B:614:CL7:H43C	26:2B:624:LHG:H362	1.65	0.79
21:23:409:CL7:H42C	32:23:420:ZEX:H172	1.59	0.79
20:24:258:PRO:CG	21:31:414:CL7:OBD	2.29	0.79
21:43:406:CL7:C14	32:44:403:ZEX:H391	1.80	0.79
21:12:517:CL7:H42C	32:23:401:ZEX:H203	1.63	0.79
16:42:94:MET:HB3	32:42:522:ZEX:H25	1.63	0.79
18:21:315:ASN:ND2	32:21:421:ZEX:H382	1.97	0.79
21:42:505:CL7:C1	32:42:520:ZEX:H172	2.13	0.79
21:1B:613:CL7:H43C	26:1B:623:LHG:H362	1.64	0.79
21:13:508:CL7:H42C	32:13:519:ZEX:H172	1.59	0.79
21:22:505:CL7:C1	32:22:520:ZEX:H172	2.13	0.79
21:21:414:CL7:OBD	20:34:258:PRO:CG	2.29	0.79
18:11:315:ASN:ND2	32:11:421:ZEX:H382	1.97	0.79
18:11:315:ASN:HB2	32:11:421:ZEX:H362	1.63	0.79
32:13:525:ZEX:O23	16:22:290:PHE:CZ	2.33	0.79
21:12:505:CL7:C1	32:12:520:ZEX:H172	2.13	0.79
21:32:517:CL7:H42C	32:43:401:ZEX:H203	1.63	0.79
21:33:513:CL7:C1B	32:33:522:ZEX:H173	2.13	0.79
3:1C:296:MET:HE2	27:1C:516:DGD:HB81	1.64	0.79
16:42:69:GLN:HE22	21:42:502:CL7:HAA1	1.47	0.78
21:32:505:CL7:C1	32:32:520:ZEX:H172	2.13	0.78
18:31:315:ASN:HB2	32:31:421:ZEX:H362	1.63	0.78
21:13:513:CL7:C1B	32:13:522:ZEX:H173	2.13	0.78
20:24:258:PRO:HB2	21:31:414:CL7:HMD1	1.64	0.78
21:3B:613:CL7:H43C	26:3B:623:LHG:H362	1.65	0.78
18:31:315:ASN:ND2	32:31:421:ZEX:H382	1.97	0.78
1:4A:133:TYR:OH	4:4D:254:GLN:OE1	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:149:LEU:HD21	21:41:407:CL7:HAB	1.66	0.78
15:2Z:17:PHE:HE2	5:3E:25:ILE:CD1	1.97	0.78
21:23:414:CL7:C1B	32:23:423:ZEX:H173	2.13	0.78
3:3C:296:MET:HE2	27:3C:516:DGD:HB81	1.64	0.78
21:43:414:CL7:C1B	32:43:423:ZEX:H173	2.13	0.78
21:21:414:CL7:HMD1	20:34:258:PRO:HB2	1.64	0.78
20:34:239:ILE:HD11	32:34:419:ZEX:C30	2.15	0.77
21:13:503:CL7:H143	21:13:509:CL7:H2	1.67	0.77
20:14:239:ILE:HD11	32:14:419:ZEX:C30	2.15	0.77
1:2A:133:TYR:OH	4:2D:254:GLN:OE1	2.01	0.77
21:23:404:CL7:H143	21:23:410:CL7:H2	1.66	0.77
20:24:239:ILE:HD11	32:24:419:ZEX:C30	2.15	0.77
21:43:404:CL7:H143	21:43:410:CL7:H2	1.66	0.77
1:1A:133:TYR:OH	4:1D:254:GLN:OE1	2.01	0.77
18:31:149:LEU:HD21	21:31:407:CL7:HAB	1.66	0.77
20:44:239:ILE:HD11	32:44:419:ZEX:C30	2.15	0.77
18:21:149:LEU:HD21	21:21:407:CL7:HAB	1.66	0.77
21:33:503:CL7:H143	21:33:509:CL7:H2	1.66	0.77
18:11:149:LEU:HD21	21:11:407:CL7:HAB	1.66	0.76
21:13:513:CL7:C1B	32:13:522:ZEX:H171	2.15	0.76
5:2E:25:ILE:CD1	15:3Z:17:PHE:HE2	1.97	0.76
21:43:414:CL7:C1B	32:43:423:ZEX:H171	2.15	0.76
19:43:94:MET:CE	32:43:401:ZEX:H363	2.11	0.76
21:43:409:CL7:H42C	32:43:420:ZEX:H172	1.59	0.76
21:33:513:CL7:C1B	32:33:522:ZEX:H171	2.15	0.76
21:23:406:CL7:C14	32:24:403:ZEX:H391	1.80	0.76
1:3A:133:TYR:OH	4:3D:254:GLN:OE1	2.01	0.76
21:23:414:CL7:C1B	32:23:423:ZEX:H171	2.15	0.75
21:33:505:CL7:H2	21:34:415:CL7:HBC1	1.68	0.75
21:1C:501:CL7:H142	21:1C:507:CL7:H71C	1.68	0.75
21:3C:501:CL7:H142	21:3C:507:CL7:H71C	1.68	0.75
16:22:109:PHE:HB2	21:21:406:CL7:HBA2	1.69	0.75
16:12:109:PHE:HB2	21:11:406:CL7:HBA2	1.69	0.75
21:2C:501:CL7:H142	21:2C:507:CL7:H71C	1.68	0.75
21:3A:401:CL7:H42C	21:3A:407:CL7:CHC	2.16	0.75
16:42:109:PHE:HB2	21:41:406:CL7:HBA2	1.69	0.75
21:13:512:CL7:H91C	32:13:522:ZEX:H182	1.69	0.75
21:1A:401:CL7:H42C	21:1A:407:CL7:CHC	2.16	0.75
21:1B:602:CL7:H42C	27:1B:624:DGD:HB51	1.68	0.75
19:23:94:MET:CE	32:23:401:ZEX:H363	2.11	0.75
21:3B:602:CL7:H42C	27:3B:624:DGD:HB51	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:33:94:MET:CE	32:33:525:ZEX:H363	2.11	0.75
21:13:505:CL7:H2	21:14:415:CL7:HBC1	1.69	0.75
21:2A:401:CL7:H42C	21:2A:407:CL7:CHC	2.16	0.75
21:23:413:CL7:H91C	32:23:423:ZEX:H182	1.69	0.75
21:33:512:CL7:H91C	32:33:522:ZEX:H182	1.69	0.74
2:1B:130:ILE:O	7:1H:15:ASN:ND2	2.20	0.74
21:4A:401:CL7:H42C	21:4A:407:CL7:CHC	2.16	0.74
2:4B:130:ILE:O	7:4H:15:ASN:ND2	2.20	0.74
21:43:406:CL7:H2	21:44:415:CL7:HBC1	1.69	0.74
16:32:109:PHE:HB2	21:31:406:CL7:HBA2	1.69	0.74
21:4B:603:CL7:H42C	27:4B:625:DGD:HB51	1.68	0.74
21:44:404:CL7:H41C	21:44:404:CL7:H92C	1.70	0.74
2:2B:130:ILE:O	7:2H:15:ASN:ND2	2.20	0.74
21:14:404:CL7:H92C	21:14:404:CL7:H41C	1.70	0.74
21:2B:603:CL7:H42C	27:2B:625:DGD:HB51	1.68	0.74
21:23:406:CL7:H2	21:24:415:CL7:HBC1	1.69	0.74
16:22:201:VAL:CG2	32:22:520:ZEX:O23	2.30	0.74
2:3B:130:ILE:O	7:3H:15:ASN:ND2	2.20	0.74
21:34:404:CL7:H41C	21:34:404:CL7:H92C	1.70	0.74
18:41:315:ASN:HB3	32:41:421:ZEX:H363	0.74	0.74
18:21:315:ASN:HB3	32:21:421:ZEX:H363	0.74	0.74
21:24:404:CL7:H41C	21:24:404:CL7:H92C	1.70	0.74
21:4C:501:CL7:H142	21:4C:507:CL7:H71C	1.68	0.74
21:43:413:CL7:H91C	32:43:423:ZEX:H182	1.69	0.74
1:1A:153:ALA:CB	21:1A:401:CL7:HED1	2.19	0.73
21:1C:503:CL7:HBD	21:1C:503:CL7:HBA2	1.70	0.73
21:1C:505:CL7:H41C	21:1C:505:CL7:H92C	1.70	0.73
19:43:129:PHE:CZ	32:43:423:ZEX:O3	2.41	0.73
21:2C:503:CL7:HBA2	21:2C:503:CL7:HBD	1.70	0.73
16:32:201:VAL:CG2	32:32:520:ZEX:O23	2.30	0.73
4:4D:191:THR:HG23	21:4D:404:CL7:HBC2	1.71	0.73
1:2A:153:ALA:CB	21:2A:401:CL7:HED1	2.19	0.73
21:13:513:CL7:C2B	32:13:522:ZEX:H173	2.18	0.73
18:31:315:ASN:HB3	32:31:421:ZEX:H363	0.74	0.73
18:11:315:ASN:HB3	32:11:421:ZEX:H363	0.74	0.73
19:13:94:MET:HE2	32:13:525:ZEX:H362	1.69	0.73
19:13:129:PHE:CZ	32:13:522:ZEX:O3	2.40	0.73
21:2C:505:CL7:H41C	21:2C:505:CL7:H92C	1.70	0.73
32:23:401:ZEX:H172	21:23:412:CL7:C1B	2.18	0.73
1:3A:153:ALA:CB	21:3A:401:CL7:HED1	2.19	0.73
19:23:129:PHE:CZ	32:23:423:ZEX:O3	2.41	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3C:503:CL7:HBA2	21:3C:503:CL7:HBD	1.70	0.73
21:3C:505:CL7:H41C	21:3C:505:CL7:H92C	1.70	0.73
19:33:129:PHE:CZ	32:33:522:ZEX:O3	2.40	0.73
1:4A:153:ALA:CB	21:4A:401:CL7:HED1	2.19	0.73
21:4C:505:CL7:H41C	21:4C:505:CL7:H92C	1.70	0.73
21:33:505:CL7:HMD2	21:33:507:CL7:HAB	1.71	0.73
21:33:513:CL7:C2B	32:33:522:ZEX:H173	2.19	0.73
21:4C:503:CL7:HBD	21:4C:503:CL7:HBA2	1.70	0.73
19:43:94:MET:HE2	32:43:401:ZEX:H362	1.69	0.72
21:13:505:CL7:HMD2	21:13:507:CL7:HAB	1.71	0.72
4:3D:191:THR:HG23	21:3D:404:CL7:HBC2	1.71	0.72
20:24:258:PRO:HB2	21:31:414:CL7:CMD	2.19	0.72
21:43:414:CL7:C2B	32:43:423:ZEX:H173	2.19	0.72
2:1B:163:SER:O	2:1B:167:THR:OG1	2.08	0.72
4:2D:191:THR:HG23	21:2D:404:CL7:HBC2	1.71	0.72
3:3C:476:GLU:OE2	4:3D:244:SER:OG	2.08	0.72
2:2B:163:SER:O	2:2B:167:THR:OG1	2.08	0.72
21:23:414:CL7:C2B	32:23:423:ZEX:H173	2.19	0.72
18:21:115:ILE:HG12	20:34:275:ASN:ND2	2.05	0.72
19:23:94:MET:HE2	32:23:401:ZEX:H362	1.71	0.72
2:3B:163:SER:O	2:3B:167:THR:OG1	2.08	0.72
3:1C:476:GLU:OE2	4:1D:244:SER:OG	2.08	0.72
18:41:130:GLN:O	18:41:140:LYS:NZ	2.23	0.72
21:11:402:CL7:HMA2	32:11:422:ZEX:H383	1.72	0.72
21:23:406:CL7:HMD2	21:23:408:CL7:HAB	1.71	0.72
16:42:94:MET:SD	32:42:524:ZEX:H361	2.29	0.72
20:24:275:ASN:ND2	18:31:115:ILE:HG12	2.05	0.71
21:31:402:CL7:HMA2	32:31:422:ZEX:H383	1.72	0.71
21:21:402:CL7:HMA2	32:21:422:ZEX:H383	1.72	0.71
21:13:511:CL7:C1B	32:13:525:ZEX:H172	2.19	0.71
18:21:130:GLN:O	18:21:140:LYS:NZ	2.23	0.71
21:43:406:CL7:HMD2	21:43:408:CL7:HAB	1.71	0.71
4:1D:191:THR:HG23	21:1D:404:CL7:HBC2	1.71	0.71
21:21:414:CL7:CMD	20:34:258:PRO:HB2	2.19	0.71
16:42:201:VAL:CG2	32:42:520:ZEX:O23	2.30	0.71
21:43:419:CL7:HMA1	32:44:420:ZEX:H372	1.73	0.71
3:2C:476:GLU:OE2	4:2D:244:SER:OG	2.08	0.71
21:41:402:CL7:HMA2	32:41:422:ZEX:H383	1.72	0.71
24:1A:405:LMG:H411	8:1I:20:PHE:HB2	1.73	0.71
2:1B:284:ASP:OD1	2:1B:361:ASN:ND2	2.24	0.71
19:33:94:MET:HE2	32:33:525:ZEX:H362	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:33:511:CL7:C1B	32:33:525:ZEX:H172	2.20	0.71
2:4B:163:SER:O	2:4B:167:THR:OG1	2.08	0.71
2:3B:284:ASP:OD1	2:3B:361:ASN:ND2	2.24	0.70
24:2A:405:LMG:H411	8:2I:20:PHE:HB2	1.74	0.70
21:23:419:CL7:HMA1	32:24:420:ZEX:H372	1.73	0.70
32:33:522:ZEX:H363	21:42:518:CL7:HMA2	1.73	0.70
21:1A:401:CL7:C4	21:1A:407:CL7:CAB	2.70	0.70
16:12:201:VAL:CG2	32:12:520:ZEX:O23	2.30	0.70
16:42:17:ASN:ND2	21:42:509:CL7:OBB	2.24	0.70
16:12:17:ASN:ND2	21:12:509:CL7:OBB	2.24	0.70
16:32:147:LEU:HD21	21:32:506:CL7:HAB	1.74	0.70
2:4B:284:ASP:OD1	2:4B:361:ASN:ND2	2.24	0.70
2:2B:284:ASP:OD1	2:2B:361:ASN:ND2	2.24	0.70
18:21:315:ASN:HB2	32:21:421:ZEX:H362	1.63	0.70
21:32:518:CL7:HMA2	32:43:423:ZEX:H363	1.74	0.70
16:22:17:ASN:ND2	21:22:509:CL7:OBB	2.25	0.70
18:31:130:GLN:O	18:31:140:LYS:NZ	2.23	0.70
19:33:312:TYR:OH	21:33:517:CL7:OBB	2.10	0.70
16:12:158:VAL:HA	16:12:208:MET:HE1	1.74	0.70
19:13:312:TYR:OH	21:13:517:CL7:OBB	2.10	0.70
24:3A:405:LMG:H411	8:3I:20:PHE:HB2	1.73	0.70
16:32:17:ASN:ND2	21:32:509:CL7:OBB	2.24	0.70
24:4A:405:LMG:H411	8:4I:20:PHE:HB2	1.73	0.70
16:22:147:LEU:HD21	21:22:506:CL7:HAB	1.74	0.69
16:32:158:VAL:HA	16:32:208:MET:HE1	1.74	0.69
21:33:508:CL7:C4	32:33:519:ZEX:H171	2.03	0.69
3:4C:288:LEU:HD21	21:4C:508:CL7:HAB	1.74	0.69
16:12:147:LEU:HD21	21:12:506:CL7:HAB	1.74	0.69
21:13:518:CL7:HMA1	32:14:420:ZEX:H372	1.73	0.69
21:3A:401:CL7:C4	21:3A:407:CL7:CAB	2.70	0.69
21:33:518:CL7:HMA1	32:34:420:ZEX:H372	1.73	0.69
3:4C:476:GLU:OE2	4:4D:244:SER:OG	2.08	0.69
21:13:513:CL7:CHC	32:13:522:ZEX:H172	2.23	0.69
21:2A:401:CL7:C4	21:2A:407:CL7:CAB	2.70	0.69
3:2C:288:LEU:HD21	21:2C:508:CL7:HAB	1.74	0.69
16:22:335:ARG:NH2	25:22:521:SQD:O7	2.26	0.69
19:23:312:TYR:OH	21:23:418:CL7:OBB	2.10	0.69
18:11:130:GLN:O	18:11:140:LYS:NZ	2.23	0.69
21:4A:401:CL7:C4	21:4A:407:CL7:CAB	2.70	0.69
20:14:220:GLY:O	21:14:417:CL7:OBD	2.11	0.69
16:22:158:VAL:HA	16:22:208:MET:HE1	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:22:522:ZEX:C36	21:21:420:CL7:HMA1	2.23	0.69
21:33:513:CL7:CHC	32:33:522:ZEX:H172	2.23	0.69
20:34:220:GLY:O	21:34:417:CL7:OBD	2.11	0.69
16:42:147:LEU:HD21	21:42:506:CL7:HAB	1.74	0.69
32:43:401:ZEX:H172	21:43:412:CL7:C1B	2.22	0.69
16:22:98:PHE:CD1	32:22:522:ZEX:H31	2.28	0.69
32:42:522:ZEX:C36	21:41:420:CL7:HMA1	2.23	0.69
5:2E:21:ILE:HG12	14:3Y:31:LEU:HD11	1.75	0.69
19:43:312:TYR:OH	21:43:418:CL7:OBB	2.10	0.69
3:1C:288:LEU:HD21	21:1C:508:CL7:HAB	1.74	0.68
1:4A:153:ALA:HB1	21:4A:401:CL7:HED1	1.75	0.68
16:42:335:ARG:NH2	25:42:521:SQD:O7	2.26	0.68
32:12:522:ZEX:C36	21:11:420:CL7:HMA1	2.23	0.68
19:13:94:MET:CE	32:13:525:ZEX:H363	2.11	0.68
16:32:335:ARG:NH2	25:32:521:SQD:O7	2.26	0.68
16:42:98:PHE:CD1	32:42:522:ZEX:H31	2.28	0.68
20:24:304:ARG:HG3	32:24:418:ZEX:C37	2.24	0.68
3:3C:288:LEU:HD21	21:3C:508:CL7:HAB	1.74	0.68
21:32:505:CL7:H11C	32:32:520:ZEX:C17	2.22	0.68
21:12:518:CL7:HMA2	32:23:423:ZEX:H363	1.74	0.68
20:24:220:GLY:O	21:24:417:CL7:OBD	2.11	0.68
20:14:304:ARG:HG3	32:14:418:ZEX:C37	2.24	0.68
19:33:81:GLY:HA3	19:33:274:GLU:HG3	1.75	0.68
16:12:335:ARG:NH2	25:12:521:SQD:O7	2.26	0.68
21:12:505:CL7:H11C	32:12:520:ZEX:C17	2.22	0.68
16:32:94:MET:SD	32:32:524:ZEX:H361	2.29	0.68
16:42:214:ILE:CD1	32:42:520:ZEX:H392	2.24	0.68
21:13:508:CL7:C4	32:13:519:ZEX:H171	2.03	0.68
16:22:214:ILE:CD1	32:22:520:ZEX:H392	2.24	0.68
1:3A:153:ALA:HB1	21:3A:401:CL7:HED1	1.75	0.68
32:32:522:ZEX:C36	21:31:420:CL7:HMA1	2.23	0.68
16:32:150:LEU:HD13	21:32:507:CL7:H43C	1.76	0.68
18:31:131:PHE:CD2	21:31:414:CL7:H3A	2.29	0.68
16:12:98:PHE:CD1	32:12:522:ZEX:H31	2.28	0.68
18:11:131:PHE:CD2	21:11:414:CL7:H3A	2.29	0.68
32:13:522:ZEX:H363	21:22:518:CL7:HMA2	1.75	0.68
20:34:304:ARG:HG3	32:34:418:ZEX:C37	2.24	0.68
16:12:290:PHE:HZ	32:23:401:ZEX:O23	1.78	0.67
19:13:81:GLY:HA3	19:13:274:GLU:HG3	1.75	0.67
1:2A:153:ALA:HB1	21:2A:401:CL7:HED1	1.75	0.67
20:44:220:GLY:O	21:44:417:CL7:OBD	2.11	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:12:505:CL7:H41C	21:12:505:CL7:H101	1.76	0.67
21:23:414:CL7:CHC	32:23:423:ZEX:H172	2.23	0.67
16:32:137:GLU:HG2	16:32:229:LYS:HG3	1.76	0.67
32:33:522:ZEX:H363	21:42:518:CL7:HMA3	1.76	0.67
2:3B:70:GLY:HA2	2:3B:186:VAL:HG11	1.76	0.67
16:32:98:PHE:CD1	32:32:522:ZEX:H31	2.28	0.67
21:42:501:CL7:H121	21:42:507:CL7:H61C	1.77	0.67
21:42:505:CL7:H11C	32:42:520:ZEX:C17	2.22	0.67
19:23:81:GLY:HA3	19:23:274:GLU:HG3	1.75	0.67
16:32:98:PHE:CD1	32:32:522:ZEX:C31	2.78	0.67
19:33:66:CYS:HA	21:33:503:CL7:HED1	1.75	0.67
16:42:158:VAL:HA	16:42:208:MET:HE1	1.74	0.67
21:12:501:CL7:H121	21:12:507:CL7:H61C	1.77	0.67
21:22:501:CL7:H121	21:22:507:CL7:H61C	1.77	0.67
18:21:89:PHE:CZ	20:34:213:PHE:HB3	2.27	0.67
16:32:290:PHE:HZ	32:43:401:ZEX:O23	1.78	0.67
17:3G:6:UNK:O	19:43:52:ARG:NH1	2.28	0.67
21:43:414:CL7:CHC	32:43:423:ZEX:H172	2.23	0.67
16:12:150:LEU:HD13	21:12:507:CL7:H43C	1.76	0.67
14:2Y:31:LEU:HD11	5:3E:21:ILE:HG12	1.74	0.67
21:22:505:CL7:H101	21:22:505:CL7:H41C	1.76	0.67
19:43:81:GLY:HA3	19:43:274:GLU:HG3	1.75	0.67
2:1B:70:GLY:HA2	2:1B:186:VAL:HG11	1.76	0.67
16:12:132:GLU:O	16:12:139:GLN:NE2	2.28	0.67
21:22:505:CL7:H11C	32:22:520:ZEX:C17	2.22	0.67
16:12:137:GLU:HG2	16:12:229:LYS:HG3	1.76	0.67
19:13:66:CYS:HA	21:13:503:CL7:HED1	1.75	0.67
21:32:501:CL7:H121	21:32:507:CL7:H61C	1.77	0.67
19:33:153:ALA:HB2	21:33:502:CL7:H101	1.77	0.67
19:43:66:CYS:HA	21:43:404:CL7:HED1	1.75	0.67
1:1A:153:ALA:HB1	21:1A:401:CL7:HED1	1.75	0.67
20:14:166:LEU:HD21	21:14:408:CL7:HAB	1.76	0.67
18:21:131:PHE:CD2	21:21:414:CL7:H3A	2.29	0.67
20:24:166:LEU:HD21	21:24:408:CL7:HAB	1.75	0.67
20:24:280:ASN:HD21	20:24:348:LEU:HD23	1.61	0.67
21:32:505:CL7:H41C	21:32:505:CL7:H101	1.76	0.67
2:4B:70:GLY:HA2	2:4B:186:VAL:HG11	1.77	0.67
19:43:153:ALA:HB2	21:43:403:CL7:H101	1.77	0.67
20:44:166:LEU:HD21	21:44:408:CL7:HAB	1.76	0.67
16:12:98:PHE:CD1	32:12:522:ZEX:C31	2.78	0.66
16:22:132:GLU:O	16:22:139:GLN:NE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:23:413:CL7:OBB	21:23:415:CL7:O1D	2.13	0.66
20:24:232:VAL:HA	32:24:419:ZEX:O23	1.96	0.66
20:34:166:LEU:HD21	21:34:408:CL7:HAB	1.76	0.66
16:42:98:PHE:CD1	32:42:522:ZEX:C31	2.78	0.66
16:42:132:GLU:O	16:42:139:GLN:NE2	2.28	0.66
20:44:232:VAL:HA	32:44:419:ZEX:O23	1.95	0.66
16:22:98:PHE:CD1	32:22:522:ZEX:C31	2.78	0.66
19:23:66:CYS:HA	21:23:404:CL7:HED1	1.75	0.66
3:4C:476:GLU:OE2	4:4D:247:THR:OG1	2.13	0.66
21:12:505:CL7:C1	32:12:520:ZEX:C17	2.73	0.66
16:22:150:LEU:HD13	21:22:507:CL7:H43C	1.76	0.66
19:23:94:MET:HG3	32:23:423:ZEX:H24	1.77	0.66
16:32:132:GLU:O	16:32:139:GLN:NE2	2.28	0.66
21:42:505:CL7:H101	21:42:505:CL7:H41C	1.76	0.66
18:41:131:PHE:CD2	21:41:414:CL7:H3A	2.29	0.66
3:3C:476:GLU:OE2	4:3D:247:THR:OG1	2.13	0.66
21:32:505:CL7:C1	32:32:520:ZEX:C17	2.73	0.66
19:43:94:MET:HG3	32:43:423:ZEX:H24	1.77	0.66
16:12:175:ARG:HH11	16:12:177:VAL:HG22	1.61	0.66
16:22:175:ARG:HH11	16:22:177:VAL:HG22	1.61	0.66
20:34:232:VAL:HA	32:34:419:ZEX:O23	1.96	0.66
20:34:280:ASN:HD21	20:34:348:LEU:HD23	1.60	0.66
20:44:280:ASN:HD21	20:44:348:LEU:HD23	1.60	0.66
16:32:175:ARG:HH11	16:32:177:VAL:HG22	1.61	0.66
21:33:512:CL7:OBB	21:33:514:CL7:O1D	2.13	0.66
32:33:525:ZEX:H392	21:42:517:CL7:OBB	1.96	0.66
21:13:512:CL7:OBB	21:13:514:CL7:O1D	2.13	0.66
20:14:232:VAL:HA	32:14:419:ZEX:O23	1.96	0.66
16:42:175:ARG:HH11	16:42:177:VAL:HG22	1.61	0.66
21:43:413:CL7:OBB	21:43:415:CL7:O1D	2.12	0.66
19:13:94:MET:HG3	32:13:522:ZEX:H24	1.77	0.66
3:2C:476:GLU:OE2	4:2D:247:THR:OG1	2.13	0.66
16:22:137:GLU:HG2	16:22:229:LYS:HG3	1.77	0.66
21:11:402:CL7:HMA2	32:11:422:ZEX:C38	2.26	0.66
32:13:525:ZEX:H392	21:22:517:CL7:OBB	1.96	0.66
1:3A:89:ILE:HD11	1:3A:108:ASN:HB3	1.78	0.66
19:33:94:MET:HG3	32:33:522:ZEX:H24	1.77	0.66
1:1A:89:ILE:HD11	1:1A:108:ASN:HB3	1.78	0.66
19:13:153:ALA:HB2	21:13:502:CL7:H101	1.77	0.66
21:22:505:CL7:C1	32:22:520:ZEX:C17	2.73	0.66
21:21:402:CL7:HMA2	32:21:422:ZEX:C38	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:70:GLY:HA2	2:2B:186:VAL:HG11	1.77	0.65
19:23:207:VAL:HA	32:23:421:ZEX:O23	1.96	0.65
16:42:150:LEU:HD13	21:42:507:CL7:H43C	1.76	0.65
3:1C:476:GLU:OE2	4:1D:247:THR:OG1	2.13	0.65
18:11:218:ILE:HG22	32:11:422:ZEX:H392	1.78	0.65
19:13:52:ARG:NH1	17:2G:6:UNK:O	2.29	0.65
20:14:280:ASN:HD21	20:14:348:LEU:HD23	1.60	0.65
21:32:518:CL7:HMA3	32:43:423:ZEX:H363	1.77	0.65
21:41:402:CL7:HMA2	32:41:422:ZEX:C38	2.26	0.65
19:43:207:VAL:HA	32:43:421:ZEX:O23	1.97	0.65
16:12:94:MET:SD	32:12:524:ZEX:H361	2.29	0.65
21:44:404:CL7:HMB2	32:44:419:ZEX:H24	1.79	0.65
16:22:207:VAL:HG13	32:22:520:ZEX:C38	2.27	0.65
18:21:218:ILE:HG22	32:21:422:ZEX:H392	1.78	0.65
19:23:153:ALA:HB2	21:23:403:CL7:H101	1.77	0.65
1:3A:57:PRO:HB2	1:3A:66:PRO:HB2	1.78	0.65
21:31:402:CL7:HMA2	32:31:422:ZEX:C38	2.26	0.65
1:4A:57:PRO:HB2	1:4A:66:PRO:HB2	1.78	0.65
16:42:137:GLU:HG2	16:42:229:LYS:HG3	1.76	0.65
1:2A:89:ILE:HD11	1:2A:108:ASN:HB3	1.78	0.65
19:33:207:VAL:HA	32:33:520:ZEX:O23	1.97	0.65
21:24:404:CL7:HMB2	32:24:419:ZEX:H24	1.79	0.65
3:3C:306:ASN:N	27:3C:516:DGD:O5E	2.28	0.65
21:42:505:CL7:C1	32:42:520:ZEX:C17	2.73	0.65
19:13:207:VAL:HA	32:13:520:ZEX:O23	1.96	0.65
18:31:218:ILE:HG22	32:31:422:ZEX:H392	1.78	0.65
21:12:517:CL7:OBB	32:23:401:ZEX:H392	1.96	0.65
32:13:522:ZEX:H363	21:22:518:CL7:HMA3	1.79	0.65
16:42:207:VAL:HG13	32:42:520:ZEX:C38	2.27	0.65
21:12:518:CL7:HMA3	32:23:423:ZEX:H363	1.79	0.65
16:22:210:GLY:HA2	32:22:520:ZEX:H363	1.78	0.65
18:31:15:SER:O	18:31:18:SER:OG	2.15	0.65
16:42:207:VAL:HG13	32:42:520:ZEX:H381	1.79	0.65
16:12:214:ILE:CD1	32:12:520:ZEX:H392	2.24	0.64
16:22:94:MET:SD	32:22:524:ZEX:H361	2.29	0.64
20:24:213:PHE:CB	18:31:89:PHE:HZ	2.10	0.64
16:32:207:VAL:HG13	32:32:520:ZEX:C38	2.27	0.64
21:14:404:CL7:HMB2	32:14:419:ZEX:H24	1.79	0.64
18:41:190:VAL:HG22	32:41:422:ZEX:C36	2.27	0.64
20:14:115:PHE:CE2	32:14:403:ZEX:C36	2.80	0.64
20:44:115:PHE:CE2	32:44:403:ZEX:C36	2.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:44:304:ARG:HG3	32:44:418:ZEX:C37	2.24	0.64
10:1L:15:ARG:HD2	25:2B:621:SQD:H241	1.80	0.64
2:3B:68:ARG:HH12	21:3B:604:CL7:HED1	1.62	0.64
21:32:517:CL7:OBB	32:43:401:ZEX:H392	1.96	0.64
19:33:52:ARG:NH1	17:4G:6:UNK:O	2.31	0.64
4:4D:102:ARG:HG3	5:4E:73:LYS:HB2	1.79	0.64
18:41:218:ILE:HG22	32:41:422:ZEX:H392	1.78	0.64
2:1B:68:ARG:HH12	21:1B:604:CL7:HED1	1.62	0.64
3:1C:323:GLN:OE1	3:1C:367:THR:OG1	2.15	0.64
2:2B:68:ARG:HH12	21:2B:605:CL7:HED1	1.62	0.64
13:2X:33:GLN:OE1	13:2X:36:LYS:NZ	2.26	0.64
15:2Z:17:PHE:CE2	5:3E:25:ILE:CD1	2.72	0.64
16:22:207:VAL:HG13	32:22:520:ZEX:H381	1.79	0.64
3:3C:323:GLN:OE1	3:3C:367:THR:OG1	2.15	0.64
2:1B:264:MET:O	2:1B:448:ARG:NH1	2.30	0.64
32:13:525:ZEX:H193	21:22:517:CL7:H92C	1.80	0.64
1:3A:153:ALA:HB1	21:3A:401:CL7:CED	2.28	0.64
2:3B:356:VAL:HG22	2:3B:370:LEU:HG	1.79	0.64
1:1A:153:ALA:HB1	21:1A:401:CL7:CED	2.28	0.64
18:11:15:SER:O	18:11:18:SER:OG	2.15	0.64
32:13:525:ZEX:H383	16:22:262:TYR:HB2	1.80	0.64
1:2A:57:PRO:HB2	1:2A:66:PRO:HB2	1.78	0.64
2:2B:356:VAL:HG22	2:2B:370:LEU:HG	1.79	0.64
18:21:190:VAL:HG22	32:21:422:ZEX:C36	2.28	0.64
16:32:262:TYR:HB2	32:43:401:ZEX:H383	1.80	0.64
21:21:403:CL7:HMB2	21:21:405:CL7:HHC	1.80	0.64
19:23:94:MET:SD	32:23:401:ZEX:H361	2.37	0.64
21:33:518:CL7:HMA2	32:34:420:ZEX:H27	1.80	0.64
32:33:525:ZEX:H383	16:42:262:TYR:HB2	1.80	0.64
13:1X:33:GLN:OE1	13:1X:36:LYS:NZ	2.26	0.64
16:12:262:TYR:HB2	32:23:401:ZEX:H383	1.80	0.64
21:11:403:CL7:HMB2	21:11:405:CL7:HHC	1.80	0.64
21:13:512:CL7:H91C	32:13:522:ZEX:C18	2.28	0.64
32:13:525:ZEX:O23	16:22:290:PHE:HZ	1.77	0.64
1:2A:308:ASP:N	1:2A:312:ASN:O	2.30	0.64
21:31:403:CL7:HMB2	21:31:405:CL7:HHC	1.80	0.64
21:34:404:CL7:HMB2	32:34:419:ZEX:H24	1.79	0.64
1:4A:89:ILE:HD11	1:4A:108:ASN:HB3	1.78	0.64
2:4B:356:VAL:HG22	2:4B:370:LEU:HG	1.79	0.64
2:1B:356:VAL:HG22	2:1B:370:LEU:HG	1.79	0.64
16:12:207:VAL:HG13	32:12:520:ZEX:C38	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:21:119:VAL:HG22	18:21:121:ALA:H	1.62	0.64
32:33:525:ZEX:H193	21:42:517:CL7:H92C	1.80	0.64
2:4B:68:ARG:HH12	21:4B:605:CL7:HED1	1.62	0.64
3:4C:306:ASN:N	27:4C:516:DGD:O5E	2.28	0.64
16:12:207:VAL:HG13	32:12:520:ZEX:H381	1.79	0.63
21:12:517:CL7:H92C	32:23:401:ZEX:H193	1.80	0.63
3:2C:323:GLN:OE1	3:2C:367:THR:OG1	2.15	0.63
21:23:413:CL7:H91C	32:23:423:ZEX:C18	2.28	0.63
21:33:512:CL7:C9	32:33:522:ZEX:H182	2.28	0.63
1:4A:308:ASP:N	1:4A:312:ASN:O	2.30	0.63
18:41:119:VAL:HG22	18:41:121:ALA:H	1.62	0.63
21:41:403:CL7:HMB2	21:41:405:CL7:HHC	1.80	0.63
1:1A:57:PRO:HB2	1:1A:66:PRO:HB2	1.78	0.63
16:32:207:VAL:HG13	32:32:520:ZEX:H381	1.79	0.63
21:13:518:CL7:HMA2	32:14:420:ZEX:H27	1.80	0.63
20:24:115:PHE:CE2	32:24:403:ZEX:C36	2.80	0.63
16:32:214:ILE:CD1	32:32:520:ZEX:H392	2.24	0.63
32:33:525:ZEX:O23	16:42:290:PHE:HZ	1.78	0.63
3:4C:323:GLN:OE1	3:4C:367:THR:OG1	2.15	0.63
19:13:94:MET:SD	32:13:525:ZEX:H361	2.37	0.63
1:2A:153:ALA:HB1	21:2A:401:CL7:CED	2.28	0.63
16:22:265:SER:HB2	16:22:280:LEU:HB2	1.80	0.63
2:4B:264:MET:O	2:4B:448:ARG:NH1	2.30	0.63
21:43:414:CL7:C3B	32:43:423:ZEX:C17	2.77	0.63
21:12:501:CL7:HMA1	32:12:520:ZEX:H24	1.81	0.63
21:2B:615:CL7:HBA2	21:2B:615:CL7:CBD	2.29	0.63
21:23:414:CL7:C3B	32:23:423:ZEX:C17	2.77	0.63
20:24:213:PHE:HB3	18:31:89:PHE:CZ	2.27	0.63
20:24:307:ASP:HB3	20:24:319:ARG:HH22	1.64	0.63
20:34:115:PHE:CE2	32:34:403:ZEX:C36	2.80	0.63
21:4B:615:CL7:HBA2	21:4B:615:CL7:CBD	2.29	0.63
16:42:265:SER:HB2	16:42:280:LEU:HB2	1.81	0.63
19:43:94:MET:SD	32:43:401:ZEX:H361	2.38	0.63
21:43:413:CL7:H91C	32:43:423:ZEX:C18	2.28	0.63
18:11:119:VAL:HG22	18:11:121:ALA:H	1.62	0.63
4:2D:102:ARG:HG3	5:2E:73:LYS:HB2	1.79	0.63
21:32:501:CL7:HMA1	32:32:520:ZEX:H24	1.81	0.63
32:32:524:ZEX:H35	21:31:417:CL7:HBA2	1.81	0.63
21:31:402:CL7:HMB2	21:31:402:CL7:H43C	1.80	0.63
19:33:173:GLU:OE1	19:33:175:ARG:NH2	2.32	0.63
21:33:512:CL7:H91C	32:33:522:ZEX:C18	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:153:ALA:HB1	21:4A:401:CL7:CED	2.28	0.63
20:14:307:ASP:HB3	20:14:319:ARG:HH22	1.64	0.63
21:22:501:CL7:HMA1	32:22:520:ZEX:H24	1.80	0.63
1:3A:95:PRO:HD2	1:3A:98:GLU:HB2	1.80	0.63
16:32:165:GLY:HA2	16:32:176:ALA:HA	1.81	0.63
21:32:517:CL7:H92C	32:43:401:ZEX:H193	1.80	0.63
18:31:119:VAL:HG22	18:31:121:ALA:H	1.62	0.63
18:31:190:VAL:HG22	32:31:422:ZEX:C36	2.27	0.63
18:41:15:SER:O	18:41:18:SER:OG	2.15	0.63
21:13:512:CL7:C9	32:13:522:ZEX:H182	2.28	0.63
21:23:406:CL7:HMD3	32:23:421:ZEX:C17	2.29	0.63
2:3B:264:MET:O	2:3B:448:ARG:NH1	2.30	0.63
21:33:518:CL7:CMA	32:34:420:ZEX:H372	2.28	0.63
16:42:146:HIS:ND1	21:42:507:CL7:OBD	2.31	0.63
32:12:524:ZEX:H35	21:11:417:CL7:HBA2	1.81	0.63
18:11:190:VAL:HG22	32:11:422:ZEX:C36	2.27	0.63
21:13:513:CL7:C3B	32:13:522:ZEX:C17	2.77	0.63
21:13:513:CL7:C3B	32:13:522:ZEX:H173	2.29	0.63
21:23:419:CL7:HMA2	32:24:420:ZEX:H27	1.80	0.63
16:32:146:HIS:ND1	21:32:507:CL7:OBD	2.31	0.63
21:33:513:CL7:C3B	32:33:522:ZEX:C17	2.77	0.63
19:43:173:GLU:OE1	19:43:175:ARG:NH2	2.32	0.63
21:43:413:CL7:C9	32:43:423:ZEX:H182	2.28	0.63
3:1C:356:SER:OG	3:1C:360:GLU:N	2.31	0.62
21:13:505:CL7:CMD	21:13:507:CL7:HAB	2.29	0.62
21:23:413:CL7:C9	32:23:423:ZEX:H182	2.28	0.62
21:33:513:CL7:C3B	32:33:522:ZEX:H173	2.29	0.62
20:34:307:ASP:HB3	20:34:319:ARG:HH22	1.64	0.62
15:4Z:26:VAL:HG13	15:4Z:36:ALA:HB1	1.81	0.62
21:43:406:CL7:HMD3	32:43:421:ZEX:C17	2.29	0.62
20:44:34:GLY:HA3	21:44:413:CL7:HMD2	1.81	0.62
3:1C:312:GLU:HG3	3:1C:403:ARG:HH12	1.64	0.62
16:12:265:SER:HB2	16:12:280:LEU:HB2	1.81	0.62
17:1G:6:UNK:O	19:23:52:ARG:NH1	2.33	0.62
19:13:173:GLU:OE1	19:13:175:ARG:NH2	2.32	0.62
19:23:121:SER:O	19:23:127:GLN:NE2	2.33	0.62
19:33:94:MET:SD	32:33:525:ZEX:H361	2.39	0.62
4:1D:102:ARG:HG3	5:1E:73:LYS:HB2	1.79	0.62
21:11:402:CL7:HMB2	21:11:402:CL7:H43C	1.81	0.62
15:2Z:26:VAL:HG13	15:2Z:36:ALA:HB1	1.82	0.62
3:3C:312:GLU:OE1	3:3C:312:GLU:N	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:33:505:CL7:CMD	21:33:507:CL7:HAB	2.29	0.62
3:4C:312:GLU:N	3:4C:312:GLU:OE1	2.31	0.62
21:41:402:CL7:HMB2	21:41:402:CL7:H43C	1.80	0.62
1:1A:124:ILE:HD12	1:1A:151:LEU:HD21	1.82	0.62
21:11:406:CL7:C4	32:11:422:ZEX:H192	2.29	0.62
1:2A:124:ILE:HD12	1:2A:151:LEU:HD21	1.82	0.62
32:22:524:ZEX:H35	21:21:417:CL7:HBA2	1.81	0.62
18:21:15:SER:O	18:21:18:SER:OG	2.15	0.62
19:23:17:ASN:ND2	21:23:410:CL7:OBB	2.32	0.62
4:3D:102:ARG:HG3	5:3E:73:LYS:HB2	1.79	0.62
1:4A:95:PRO:HD2	1:4A:98:GLU:HB2	1.80	0.62
3:4C:312:GLU:HG3	3:4C:403:ARG:HH12	1.64	0.62
19:43:121:SER:O	19:43:127:GLN:NE2	2.33	0.62
3:3C:312:GLU:HG3	3:3C:403:ARG:HH12	1.64	0.62
4:3D:66:TYR:O	24:3D:410:LMG:O5	2.15	0.62
21:41:406:CL7:C4	32:41:422:ZEX:H192	2.29	0.62
21:43:419:CL7:HMA2	32:44:420:ZEX:H27	1.80	0.62
21:43:419:CL7:CMA	32:44:420:ZEX:H372	2.28	0.62
21:13:518:CL7:CMA	32:14:420:ZEX:H372	2.28	0.62
21:21:406:CL7:C4	32:21:422:ZEX:H192	2.29	0.62
21:23:406:CL7:CMD	21:23:408:CL7:HAB	2.29	0.62
19:33:17:ASN:ND2	21:33:509:CL7:OBB	2.33	0.62
1:4A:124:ILE:HD12	1:4A:151:LEU:HD21	1.82	0.62
4:4D:118:VAL:HG21	4:4D:157:LEU:HD11	1.82	0.62
21:43:406:CL7:CMD	21:43:408:CL7:HAB	2.29	0.62
16:12:146:HIS:ND1	21:12:507:CL7:OBD	2.31	0.62
16:12:165:GLY:HA2	16:12:176:ALA:HA	1.81	0.62
21:13:505:CL7:HMD3	32:13:520:ZEX:C17	2.29	0.62
21:23:414:CL7:C3B	32:23:423:ZEX:H173	2.29	0.62
4:3D:187:PHE:O	4:3D:293:ARG:NH2	2.33	0.62
21:32:507:CL7:HMD2	21:32:509:CL7:H203	1.82	0.62
20:44:307:ASP:HB3	20:44:319:ARG:HH22	1.64	0.62
15:1Z:26:VAL:HG13	15:1Z:36:ALA:HB1	1.81	0.62
21:23:419:CL7:CMA	32:24:420:ZEX:H372	2.28	0.62
1:3A:124:ILE:HD12	1:3A:151:LEU:HD21	1.82	0.62
16:42:165:GLY:HA2	16:42:176:ALA:HA	1.81	0.62
21:43:414:CL7:C3B	32:43:423:ZEX:H173	2.29	0.62
21:1B:614:CL7:HBA2	21:1B:614:CL7:CBD	2.29	0.62
4:1D:187:PHE:O	4:1D:293:ARG:NH2	2.33	0.62
3:2C:312:GLU:OE1	3:2C:312:GLU:N	2.31	0.62
4:2D:118:VAL:HG21	4:2D:157:LEU:HD11	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:43:17:ASN:ND2	21:43:410:CL7:OBB	2.33	0.62
4:1D:66:TYR:O	24:1D:410:LMG:O5	2.15	0.62
1:2A:95:PRO:HD2	1:2A:98:GLU:HB2	1.80	0.62
2:2B:264:MET:O	2:2B:448:ARG:NH1	2.30	0.62
21:21:402:CL7:HMB2	21:21:402:CL7:H43C	1.80	0.62
19:23:173:GLU:OE1	19:23:175:ARG:NH2	2.32	0.62
20:44:77:LEU:HD11	20:44:101:ILE:HD11	1.82	0.62
21:44:412:CL7:HBD	21:44:412:CL7:HBA1	1.82	0.62
3:1C:84:VAL:O	9:1K:9:LYS:N	2.33	0.61
3:1C:312:GLU:OE1	3:1C:312:GLU:N	2.31	0.61
20:24:77:LEU:HD11	20:24:101:ILE:HD11	1.82	0.61
21:31:406:CL7:C4	32:31:422:ZEX:H192	2.29	0.61
4:1D:118:VAL:HG21	4:1D:157:LEU:HD11	1.82	0.61
16:22:146:HIS:ND1	21:22:507:CL7:OBD	2.31	0.61
16:32:265:SER:HB2	16:32:280:LEU:HB2	1.80	0.61
4:4D:66:TYR:O	24:4D:410:LMG:O5	2.15	0.61
21:42:501:CL7:HMA1	32:42:520:ZEX:H24	1.81	0.61
16:12:72:ARG:NH2	21:12:501:CL7:OBD	2.34	0.61
1:2A:26:ASN:O	4:2D:254:GLN:NE2	2.33	0.61
4:2D:187:PHE:O	4:2D:293:ARG:NH2	2.33	0.61
20:24:34:GLY:HA3	21:24:413:CL7:HMD2	1.81	0.61
21:3B:614:CL7:CBD	21:3B:614:CL7:HBA2	2.29	0.61
19:33:121:SER:O	19:33:127:GLN:NE2	2.33	0.61
25:33:521:SQD:H172	21:34:413:CL7:H143	1.82	0.61
20:34:34:GLY:HA3	21:34:413:CL7:HMD2	1.81	0.61
21:12:518:CL7:HMA3	32:23:423:ZEX:H372	1.83	0.61
19:13:17:ASN:ND2	21:13:509:CL7:OBB	2.33	0.61
3:2C:312:GLU:HG3	3:2C:403:ARG:HH12	1.64	0.61
16:32:72:ARG:NH2	21:32:501:CL7:OBD	2.33	0.61
21:34:411:CL7:HBD	21:34:411:CL7:HBA1	1.83	0.61
21:4C:502:CL7:HBD	21:4C:503:CL7:H43C	1.83	0.61
4:4D:187:PHE:O	4:4D:293:ARG:NH2	2.33	0.61
16:32:136:PHE:HB3	16:32:230:PRO:HG2	1.83	0.61
3:4C:84:VAL:O	9:4K:9:LYS:N	2.33	0.61
32:42:524:ZEX:H35	21:41:417:CL7:HBA2	1.81	0.61
19:43:267:ASN:O	19:43:304:ARG:NH1	2.34	0.61
1:1A:95:PRO:HD2	1:1A:98:GLU:HB2	1.80	0.61
16:12:136:PHE:HB3	16:12:230:PRO:HG2	1.83	0.61
16:22:165:GLY:HA2	16:22:176:ALA:HA	1.81	0.61
3:3C:356:SER:OG	3:3C:360:GLU:N	2.31	0.61
21:41:406:CL7:H43C	32:41:422:ZEX:H7	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:521:SQD:H172	21:14:413:CL7:H143	1.82	0.61
20:14:214:THR:OG1	20:14:217:GLY:O	2.16	0.61
3:2C:306:ASN:N	27:2C:516:DGD:O5E	2.28	0.61
21:21:406:CL7:H43C	32:21:422:ZEX:H7	1.82	0.61
3:3C:84:VAL:O	9:3K:9:LYS:N	2.33	0.61
13:3X:33:GLN:OE1	13:3X:36:LYS:NZ	2.26	0.61
15:3Z:26:VAL:HG13	15:3Z:36:ALA:HB1	1.81	0.61
21:34:412:CL7:HBD	21:34:412:CL7:HBA1	1.82	0.61
1:1A:26:ASN:O	4:1D:254:GLN:NE2	2.33	0.61
18:41:318:TYR:OH	21:41:418:CL7:OBB	2.19	0.61
20:44:214:THR:OG1	20:44:217:GLY:O	2.16	0.61
20:14:77:LEU:HD11	20:14:101:ILE:HD11	1.82	0.61
21:2C:502:CL7:HBD	21:2C:503:CL7:H43C	1.83	0.61
18:21:318:TYR:OH	21:21:418:CL7:OBB	2.19	0.61
21:33:505:CL7:HMD3	32:33:520:ZEX:C17	2.29	0.61
1:4A:26:ASN:O	4:4D:254:GLN:NE2	2.33	0.61
3:2C:84:VAL:O	9:2K:9:LYS:N	2.33	0.61
3:2C:143:TYR:OH	21:2C:513:CL7:O1D	2.19	0.61
19:23:267:ASN:O	19:23:304:ARG:NH1	2.34	0.61
19:23:305:PHE:CZ	32:23:420:ZEX:H362	2.36	0.61
21:24:412:CL7:HBD	21:24:412:CL7:HBA1	1.82	0.61
25:3B:620:SQD:H241	10:4L:15:ARG:HD2	1.81	0.61
21:43:402:CL7:H191	21:43:408:CL7:H172	1.83	0.61
21:43:409:CL7:C4	32:43:420:ZEX:H171	2.03	0.61
19:13:64:LEU:HD23	19:13:67:ILE:HB	1.83	0.60
19:13:121:SER:O	19:13:127:GLN:NE2	2.33	0.60
2:2B:161:PHE:HB2	21:2B:607:CL7:HAB	1.83	0.60
21:24:411:CL7:HBD	21:24:411:CL7:HBA1	1.83	0.60
17:4G:9:UNK:O	17:4G:11:UNK:N	2.35	0.60
21:14:411:CL7:HBD	21:14:411:CL7:HBA1	1.83	0.60
16:22:72:ARG:NH2	21:22:501:CL7:OBD	2.34	0.60
16:22:136:PHE:HB3	16:22:230:PRO:HG2	1.83	0.60
21:31:406:CL7:H43C	32:31:422:ZEX:H7	1.82	0.60
32:33:522:ZEX:H372	21:42:518:CL7:HMA3	1.83	0.60
21:11:406:CL7:H43C	32:11:422:ZEX:H7	1.82	0.60
18:21:26:GLN:O	18:21:29:TRP:HB3	2.02	0.60
19:23:64:LEU:HD23	19:23:67:ILE:HB	1.83	0.60
19:33:64:LEU:HD23	19:33:67:ILE:HB	1.83	0.60
3:4C:79:MET:HB3	3:4C:100:LEU:HD12	1.82	0.60
18:41:242:ASN:HB3	18:41:245:THR:HG22	1.83	0.60
19:43:305:PHE:CZ	32:43:420:ZEX:H362	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:161:PHE:HB2	21:1B:606:CL7:HAB	1.83	0.60
18:11:318:TYR:OH	21:11:418:CL7:OBB	2.19	0.60
20:14:34:GLY:HA3	21:14:413:CL7:HMD2	1.81	0.60
17:2G:9:UNK:O	17:2G:11:UNK:N	2.35	0.60
26:3B:623:LHG:O4	4:3D:140:TYR:OH	2.19	0.60
19:33:267:ASN:O	19:33:304:ARG:NH1	2.34	0.60
18:41:26:GLN:O	18:41:29:TRP:HB3	2.02	0.60
21:14:412:CL7:HBD	21:14:412:CL7:HBA1	1.82	0.60
5:2E:25:ILE:CD1	15:3Z:17:PHE:CE2	2.72	0.60
25:23:422:SQD:H172	21:24:413:CL7:H143	1.82	0.60
20:34:214:THR:OG1	20:34:217:GLY:O	2.16	0.60
16:42:117:VAL:HG12	16:42:119:ALA:H	1.66	0.60
18:41:189:VAL:HG22	18:41:192:LYS:HB2	1.83	0.60
25:43:422:SQD:H172	21:44:413:CL7:H143	1.82	0.60
2:1B:73:HIS:CE1	2:1B:100:SER:HB3	2.37	0.60
21:1C:502:CL7:HBD	21:1C:503:CL7:H43C	1.83	0.60
17:1G:9:UNK:O	17:1G:11:UNK:N	2.35	0.60
16:22:117:VAL:HG12	16:22:119:ALA:H	1.66	0.60
21:23:409:CL7:C4	32:23:420:ZEX:H171	2.03	0.60
4:3D:118:VAL:HG21	4:3D:157:LEU:HD11	1.82	0.60
18:31:242:ASN:HB3	18:31:245:THR:HG22	1.83	0.60
20:34:77:LEU:HD11	20:34:101:ILE:HD11	1.82	0.60
2:4B:161:PHE:HB2	21:4B:607:CL7:HAB	1.83	0.60
3:4C:143:TYR:OH	21:4C:513:CL7:O1D	2.19	0.60
21:4C:513:CL7:H2A	21:4C:513:CL7:HED3	1.83	0.60
3:1C:79:MET:HB3	3:1C:100:LEU:HD12	1.82	0.60
19:13:267:ASN:O	19:13:304:ARG:NH1	2.34	0.60
19:13:305:PHE:CZ	32:13:519:ZEX:H362	2.36	0.60
20:24:35:ASN:ND2	21:24:410:CL7:O1A	2.33	0.60
1:3A:26:ASN:O	4:3D:254:GLN:NE2	2.33	0.60
3:3C:79:MET:HB3	3:3C:100:LEU:HD12	1.82	0.60
18:31:189:VAL:HG22	18:31:192:LYS:HB2	1.83	0.60
18:31:311:ALA:O	18:31:315:ASN:ND2	2.35	0.60
21:33:501:CL7:H191	21:33:507:CL7:H172	1.83	0.60
2:4B:73:HIS:CE1	2:4B:100:SER:HB3	2.37	0.60
16:42:72:ARG:NH2	21:42:501:CL7:OBD	2.33	0.60
21:42:505:CL7:HBC2	32:42:520:ZEX:H191	1.84	0.60
19:43:64:LEU:HD23	19:43:67:ILE:HB	1.84	0.60
2:2B:73:HIS:CE1	2:2B:100:SER:HB3	2.37	0.60
21:2C:513:CL7:H2A	21:2C:513:CL7:HED3	1.84	0.60
20:24:214:THR:OG1	20:24:217:GLY:O	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:42:98:PHE:CG	32:42:522:ZEX:C31	2.85	0.60
20:44:35:ASN:ND2	21:44:410:CL7:O1A	2.33	0.60
25:1B:620:SQD:H241	10:2L:15:ARG:HD2	1.83	0.60
16:22:98:PHE:CG	32:22:522:ZEX:C31	2.85	0.60
21:23:402:CL7:H191	21:23:408:CL7:H172	1.83	0.60
21:3C:502:CL7:HBD	21:3C:503:CL7:H43C	1.83	0.60
16:32:117:VAL:HG12	16:32:119:ALA:H	1.66	0.60
19:33:305:PHE:CZ	32:33:519:ZEX:H362	2.36	0.60
18:21:242:ASN:HB3	18:21:245:THR:HG22	1.83	0.60
18:31:211:LEU:CD1	32:31:422:ZEX:C38	2.80	0.60
20:34:35:ASN:ND2	21:34:410:CL7:O1A	2.33	0.60
9:1K:36:PHE:O	9:1K:40:ALA:N	2.35	0.59
20:14:35:ASN:ND2	21:14:410:CL7:O1A	2.33	0.59
17:3G:9:UNK:O	17:3G:11:UNK:N	2.35	0.59
18:41:211:LEU:CD1	32:41:422:ZEX:C38	2.80	0.59
21:44:411:CL7:HBD	21:44:411:CL7:HBA1	1.83	0.59
21:1C:513:CL7:H2A	21:1C:513:CL7:HED3	1.83	0.59
16:12:117:VAL:HG12	16:12:119:ALA:H	1.66	0.59
18:11:311:ALA:O	18:11:315:ASN:ND2	2.35	0.59
1:3A:308:ASP:N	1:3A:312:ASN:O	2.30	0.59
2:3B:73:HIS:CE1	2:3B:100:SER:HB3	2.37	0.59
21:32:505:CL7:HBC2	32:32:520:ZEX:H191	1.84	0.59
21:14:406:CL7:HAA2	21:14:406:CL7:HBD	1.85	0.59
9:2K:36:PHE:O	9:2K:40:ALA:N	2.35	0.59
3:1C:143:TYR:OH	21:1C:513:CL7:O1D	2.19	0.59
4:1D:11:ARG:NH2	4:1D:19:ASP:OD2	2.36	0.59
16:12:98:PHE:CG	32:12:522:ZEX:C31	2.85	0.59
21:22:505:CL7:HBC2	32:22:520:ZEX:H191	1.84	0.59
2:3B:161:PHE:HB2	21:3B:606:CL7:HAB	1.83	0.59
10:3L:15:ARG:HD2	25:4B:621:SQD:H241	1.85	0.59
16:32:98:PHE:CG	32:32:522:ZEX:C31	2.85	0.59
18:31:318:TYR:OH	21:31:418:CL7:OBB	2.19	0.59
16:42:136:PHE:HB3	16:42:230:PRO:HG2	1.83	0.59
18:21:189:VAL:HG22	18:21:192:LYS:HB2	1.83	0.59
21:3C:513:CL7:HED3	21:3C:513:CL7:H2A	1.83	0.59
4:3D:11:ARG:NH2	4:3D:19:ASP:OD2	2.36	0.59
21:34:406:CL7:HBD	21:34:406:CL7:HAA2	1.85	0.59
3:2C:79:MET:HB3	3:2C:100:LEU:HD12	1.82	0.59
18:21:89:PHE:HZ	20:34:213:PHE:CB	2.10	0.59
32:23:401:ZEX:H172	21:23:412:CL7:CHB	2.33	0.59
18:31:26:GLN:O	18:31:29:TRP:HB3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:42:508:CL7:HAC2	21:42:516:CL7:HBC3	1.85	0.59
19:43:267:ASN:OD1	19:43:268:ASP:N	2.36	0.59
18:11:189:VAL:HG22	18:11:192:LYS:HB2	1.83	0.59
18:11:211:LEU:CD1	32:11:422:ZEX:C38	2.80	0.59
18:11:242:ASN:HB3	18:11:245:THR:HG22	1.83	0.59
20:14:327:LEU:HD22	32:14:418:ZEX:C36	2.33	0.59
20:24:327:LEU:HD22	32:24:418:ZEX:C36	2.33	0.59
18:31:280:GLU:OE1	18:31:280:GLU:N	2.30	0.59
3:4C:356:SER:OG	3:4C:360:GLU:N	2.31	0.59
21:13:511:CL7:CHB	32:13:525:ZEX:H172	2.31	0.59
19:23:267:ASN:OD1	19:23:268:ASP:N	2.36	0.59
3:3C:143:TYR:OH	21:3C:513:CL7:O1D	2.19	0.59
9:3K:36:PHE:O	9:3K:40:ALA:N	2.36	0.59
19:33:267:ASN:OD1	19:33:268:ASP:N	2.36	0.59
21:13:501:CL7:H191	21:13:507:CL7:H172	1.83	0.59
20:14:168:PHE:CE1	21:14:414:CL7:HHB	2.38	0.59
2:2B:291:GLU:OE2	2:2B:294:ARG:NH2	2.36	0.59
21:22:508:CL7:HAC2	21:22:516:CL7:HBC3	1.85	0.59
18:21:211:LEU:CD1	32:21:422:ZEX:C38	2.80	0.59
32:43:401:ZEX:H172	21:43:412:CL7:CHB	2.33	0.59
18:11:26:GLN:O	18:11:29:TRP:HB3	2.02	0.59
3:2C:356:SER:OG	3:2C:360:GLU:N	2.31	0.59
18:21:311:ALA:O	18:21:315:ASN:ND2	2.35	0.59
18:41:311:ALA:O	18:41:315:ASN:ND2	2.35	0.59
19:13:267:ASN:OD1	19:13:268:ASP:N	2.36	0.58
20:24:228:ASN:ND2	20:24:231:ASP:OD2	2.36	0.58
21:24:406:CL7:HAA2	21:24:406:CL7:HBD	1.85	0.58
21:24:407:CL7:CAD	32:24:419:ZEX:H163	2.33	0.58
20:34:228:ASN:ND2	20:34:231:ASP:OD2	2.36	0.58
20:34:327:LEU:HD22	32:34:418:ZEX:C36	2.33	0.58
14:4Y:22:VAL:O	14:4Y:26:PRO:HD2	2.03	0.58
20:44:228:ASN:ND2	20:44:231:ASP:OD2	2.36	0.58
21:44:407:CL7:CAD	32:44:419:ZEX:H163	2.33	0.58
1:1A:308:ASP:N	1:1A:312:ASN:O	2.30	0.58
16:12:11:TYR:O	16:12:19:ARG:NH2	2.36	0.58
32:12:520:ZEX:C10	25:23:424:SQD:H221	2.32	0.58
20:14:193:THR:HG23	20:14:195:HIS:CE1	2.38	0.58
16:22:11:TYR:O	16:22:19:ARG:NH2	2.36	0.58
16:32:11:TYR:O	16:32:19:ARG:NH2	2.36	0.58
2:4B:291:GLU:OE2	2:4B:294:ARG:NH2	2.36	0.58
9:4K:36:PHE:O	9:4K:40:ALA:N	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:291:GLU:OE2	2:1B:294:ARG:NH2	2.36	0.58
14:1Y:22:VAL:O	14:1Y:26:PRO:HD2	2.03	0.58
21:12:505:CL7:HBC2	32:12:520:ZEX:H191	1.84	0.58
21:12:508:CL7:HAC2	21:12:516:CL7:HBC3	1.85	0.58
32:13:522:ZEX:H372	21:22:518:CL7:HMA3	1.86	0.58
21:2C:510:CL7:HBD	21:2C:510:CL7:HBA1	1.85	0.58
14:3Y:22:VAL:O	14:3Y:26:PRO:HD2	2.03	0.58
20:34:168:PHE:CE1	21:34:414:CL7:HHB	2.38	0.58
20:34:193:THR:HG23	20:34:195:HIS:CE1	2.38	0.58
4:4D:11:ARG:NH2	4:4D:19:ASP:OD2	2.36	0.58
20:44:327:LEU:HD22	32:44:418:ZEX:C36	2.33	0.58
21:12:505:CL7:O1A	32:12:520:ZEX:C17	2.51	0.58
18:11:280:GLU:OE1	18:11:280:GLU:N	2.30	0.58
1:4A:188:ALA:HB2	1:4A:328:PHE:HB3	1.85	0.58
20:24:193:THR:HG23	20:24:195:HIS:CE1	2.38	0.58
1:3A:188:ALA:HB2	1:3A:328:PHE:HB3	1.85	0.58
21:32:505:CL7:O1A	32:32:520:ZEX:C17	2.51	0.58
1:1A:188:ALA:HB2	1:1A:328:PHE:HB3	1.85	0.58
2:1B:91:ILE:HG23	2:1B:92:LEU:O	2.04	0.58
18:11:17:ASN:HB2	21:11:409:CL7:HBA2	1.86	0.58
20:14:222:GLY:N	21:14:417:CL7:OBD	2.36	0.58
21:14:407:CL7:CAD	32:14:419:ZEX:H163	2.33	0.58
2:2B:91:ILE:HG23	2:2B:92:LEU:O	2.04	0.58
21:4C:510:CL7:HBA1	21:4C:510:CL7:HBD	1.85	0.58
1:2A:188:ALA:HB2	1:2A:328:PHE:HB3	1.85	0.58
4:2D:11:ARG:NH2	4:2D:19:ASP:OD2	2.36	0.58
14:2Y:22:VAL:O	14:2Y:26:PRO:HD2	2.03	0.58
1:3A:192:ILE:HG13	1:3A:293:MET:HE1	1.85	0.58
18:31:17:ASN:HB2	21:31:409:CL7:HBA2	1.86	0.58
20:34:222:GLY:N	21:34:417:CL7:OBD	2.36	0.58
18:21:17:ASN:HB2	21:21:409:CL7:HBA2	1.86	0.58
19:33:310:PHE:HA	32:33:519:ZEX:H393	1.86	0.58
20:44:168:PHE:CE1	21:44:414:CL7:HHB	2.38	0.58
1:1A:192:ILE:HG13	1:1A:293:MET:HE1	1.85	0.58
21:1C:510:CL7:HBA1	21:1C:510:CL7:HBD	1.85	0.58
20:14:228:ASN:ND2	20:14:231:ASP:OD2	2.36	0.58
20:24:168:PHE:CE1	21:24:414:CL7:HHB	2.38	0.58
21:3C:504:CL7:HBA2	21:3C:504:CL7:HBD	1.86	0.58
21:34:407:CL7:CAD	32:34:419:ZEX:H163	2.33	0.58
16:12:41:PHE:CE2	16:12:45:ILE:HG13	2.39	0.58
1:2A:192:ILE:HG13	1:2A:293:MET:HE1	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:22:41:PHE:CE2	16:22:45:ILE:HG13	2.39	0.58
21:32:508:CL7:HAC2	21:32:516:CL7:HBC3	1.85	0.58
19:33:211:HIS:CE1	32:33:520:ZEX:H383	2.39	0.58
2:4B:91:ILE:HG23	2:4B:92:LEU:O	2.04	0.58
16:42:11:TYR:O	16:42:19:ARG:NH2	2.36	0.58
4:1D:73:LEU:O	4:1D:175:THR:OG1	2.16	0.57
16:12:210:GLY:HA2	32:12:520:ZEX:H363	1.78	0.57
14:2Y:31:LEU:HD21	5:3E:21:ILE:HD11	1.86	0.57
2:3B:291:GLU:OE2	2:3B:294:ARG:NH2	2.36	0.57
21:1D:404:CL7:H111	22:1D:408:PHO:H11	1.87	0.57
16:32:41:PHE:CE2	16:32:45:ILE:HG13	2.39	0.57
25:33:523:SQD:H221	32:42:520:ZEX:C10	2.34	0.57
16:42:41:PHE:CE2	16:42:45:ILE:HG13	2.39	0.57
16:12:345:THR:HG22	19:23:19:ARG:HD3	1.85	0.57
19:13:211:HIS:CE1	32:13:520:ZEX:H383	2.39	0.57
19:13:310:PHE:HA	32:13:519:ZEX:H393	1.86	0.57
21:13:515:CL7:CAB	32:14:420:ZEX:H401	2.35	0.57
21:23:416:CL7:CAB	32:24:420:ZEX:H401	2.35	0.57
2:3B:91:ILE:HG23	2:3B:92:LEU:O	2.04	0.57
21:32:518:CL7:HMA3	32:43:423:ZEX:H372	1.86	0.57
19:33:309:ASN:OD1	32:33:519:ZEX:C36	2.49	0.57
32:42:522:ZEX:H363	21:41:420:CL7:HMA1	1.85	0.57
20:44:193:THR:HG23	20:44:195:HIS:CE1	2.38	0.57
21:44:406:CL7:HAA2	21:44:406:CL7:HBD	1.85	0.57
21:1C:504:CL7:HBD	21:1C:504:CL7:HBA2	1.86	0.57
19:23:211:HIS:CE1	32:23:421:ZEX:H383	2.39	0.57
21:33:515:CL7:CAB	32:34:420:ZEX:H401	2.35	0.57
26:4B:624:LHG:O4	4:4D:140:TYR:OH	2.19	0.57
21:41:406:CL7:HAA2	21:41:406:CL7:HBD	1.86	0.57
20:44:112:VAL:HG11	32:44:420:ZEX:H24	1.86	0.57
20:44:222:GLY:N	21:44:417:CL7:OBD	2.36	0.57
20:14:115:PHE:HE2	32:14:403:ZEX:C36	2.17	0.57
32:22:522:ZEX:H363	21:21:420:CL7:HMA1	1.85	0.57
21:3D:404:CL7:H111	22:3D:408:PHO:H11	1.87	0.57
1:4A:192:ILE:HG13	1:4A:293:MET:HE1	1.85	0.57
3:1C:306:ASN:N	27:1C:516:DGD:O5E	2.28	0.57
21:2C:504:CL7:HBD	21:2C:504:CL7:HBA2	1.86	0.57
21:2D:404:CL7:H111	22:2D:408:PHO:H11	1.87	0.57
21:3C:510:CL7:HBD	21:3C:510:CL7:HBA1	1.85	0.57
21:33:508:CL7:HAA2	21:33:508:CL7:HBD	1.86	0.57
21:43:416:CL7:CAB	32:44:420:ZEX:H401	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:12:522:ZEX:H363	21:11:420:CL7:HMA1	1.85	0.57
21:23:409:CL7:HBD	21:23:409:CL7:HAA2	1.86	0.57
20:24:112:VAL:HG11	32:24:420:ZEX:H24	1.86	0.57
32:32:522:ZEX:H363	21:31:420:CL7:HMA1	1.86	0.57
19:33:211:HIS:CE1	32:33:520:ZEX:C38	2.88	0.57
18:41:17:ASN:HB2	21:41:409:CL7:HBA2	1.86	0.57
7:2H:57:ASP:OD2	13:2X:2:THR:OG1	2.23	0.57
18:21:215:HIS:HA	18:21:218:ILE:HG12	1.87	0.57
18:21:280:GLU:OE1	18:21:280:GLU:N	2.30	0.57
21:21:406:CL7:HAA2	21:21:406:CL7:HBD	1.86	0.57
1:3A:307:VAL:HG12	1:3A:313:VAL:HG22	1.86	0.57
21:4B:603:CL7:HBD	21:4B:603:CL7:HAA1	1.87	0.57
21:4D:404:CL7:H111	22:4D:408:PHO:H11	1.87	0.57
20:44:335:LEU:O	20:44:339:LEU:HB2	2.05	0.57
20:24:115:PHE:HE2	32:24:403:ZEX:C36	2.17	0.57
20:24:335:LEU:O	20:24:339:LEU:HB2	2.05	0.57
4:3D:73:LEU:O	4:3D:175:THR:OG1	2.16	0.57
16:32:105:SER:HB2	21:31:406:CL7:H2	1.86	0.57
20:34:115:PHE:HE2	32:34:403:ZEX:C36	2.17	0.57
20:44:115:PHE:HE2	32:44:403:ZEX:C36	2.17	0.57
21:11:406:CL7:HAA2	21:11:406:CL7:HBD	1.86	0.57
21:13:508:CL7:HAA2	21:13:508:CL7:HBD	1.86	0.57
21:22:502:CL7:HAA2	21:22:502:CL7:HBD	1.87	0.57
20:24:222:GLY:N	21:24:417:CL7:OBD	2.37	0.57
1:2A:153:ALA:CB	21:2A:401:CL7:CED	2.83	0.56
19:23:310:PHE:HA	32:23:420:ZEX:H393	1.86	0.56
18:31:315:ASN:HD22	32:31:421:ZEX:H382	1.68	0.56
19:33:149:PHE:CE2	21:33:512:CL7:HHB	2.40	0.56
1:4A:307:VAL:HG12	1:4A:313:VAL:HG22	1.86	0.56
21:42:502:CL7:HBD	21:42:502:CL7:HAA2	1.87	0.56
18:41:215:HIS:HA	18:41:218:ILE:HG12	1.87	0.56
19:43:310:PHE:HA	32:43:420:ZEX:H393	1.86	0.56
20:44:25:SER:OG	20:44:26:ASN:N	2.38	0.56
21:12:502:CL7:HBD	21:12:502:CL7:HAA2	1.87	0.56
20:14:112:VAL:HG11	32:14:420:ZEX:H24	1.87	0.56
32:33:525:ZEX:H392	21:42:517:CL7:CAB	2.35	0.56
21:34:404:CL7:H2	21:34:406:CL7:H41C	1.87	0.56
18:41:280:GLU:OE1	18:41:280:GLU:N	2.30	0.56
16:12:105:SER:HB2	21:11:406:CL7:H2	1.86	0.56
18:11:160:VAL:HG12	18:11:164:LYS:HE3	1.87	0.56
18:11:215:HIS:HA	18:11:218:ILE:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2B:603:CL7:HBD	21:2B:603:CL7:HAA1	1.87	0.56
5:2E:21:ILE:HD11	14:3Y:31:LEU:HD21	1.86	0.56
16:22:105:SER:HB2	21:21:406:CL7:H2	1.86	0.56
19:33:19:ARG:HD3	16:42:345:THR:HG22	1.87	0.56
21:33:502:CL7:C2B	21:33:504:CL7:HAB	2.35	0.56
21:42:507:CL7:H111	32:42:520:ZEX:H402	1.88	0.56
18:41:160:VAL:HG12	18:41:164:LYS:HE3	1.87	0.56
19:43:149:PHE:CE2	21:43:413:CL7:HHB	2.40	0.56
19:43:211:HIS:CE1	32:43:421:ZEX:C38	2.88	0.56
19:43:211:HIS:CE1	32:43:421:ZEX:H383	2.39	0.56
21:43:403:CL7:C2B	21:43:405:CL7:HAB	2.35	0.56
21:43:409:CL7:HAA2	21:43:409:CL7:HBD	1.86	0.56
19:13:211:HIS:CE1	32:13:520:ZEX:C38	2.88	0.56
20:14:335:LEU:O	20:14:339:LEU:HB2	2.05	0.56
18:21:160:VAL:HG12	18:21:164:LYS:HE3	1.87	0.56
19:23:94:MET:SD	32:23:401:ZEX:H363	2.43	0.56
32:23:401:ZEX:C17	21:23:412:CL7:CHB	2.84	0.56
20:34:112:VAL:HG11	32:34:420:ZEX:H24	1.86	0.56
21:4C:504:CL7:HBD	21:4C:504:CL7:HBA2	1.86	0.56
18:41:20:LEU:HD11	21:41:412:CL7:HMA2	1.88	0.56
16:12:98:PHE:CE1	32:12:522:ZEX:H31	2.41	0.56
21:13:502:CL7:C2B	21:13:504:CL7:HAB	2.35	0.56
20:14:45:LEU:HG	20:14:49:HIS:CE1	2.41	0.56
21:2B:608:CL7:H11C	24:2B:622:LMG:H152	1.88	0.56
2:4B:89:PRO:HB3	2:4B:94:ALA:HB1	1.87	0.56
1:1A:153:ALA:CB	21:1A:401:CL7:CED	2.83	0.56
18:11:315:ASN:HD22	32:11:421:ZEX:H382	1.68	0.56
32:13:525:ZEX:H392	21:22:517:CL7:CAB	2.35	0.56
19:23:149:PHE:CE2	21:23:413:CL7:HHB	2.40	0.56
20:24:45:LEU:HG	20:24:49:HIS:CE1	2.41	0.56
21:24:404:CL7:H2	21:24:406:CL7:H41C	1.87	0.56
21:33:510:CL7:H42C	32:33:519:ZEX:H172	1.87	0.56
20:34:115:PHE:HE2	32:34:403:ZEX:H363	1.69	0.56
19:13:235:ASP:OD1	19:13:240:LYS:NZ	2.28	0.56
21:14:404:CL7:H2	21:14:406:CL7:H41C	1.87	0.56
21:2A:407:CL7:HED1	30:2D:407:PL9:H362	1.88	0.56
20:24:25:SER:OG	20:24:26:ASN:N	2.38	0.56
3:3C:141:GLY:O	3:3C:145:THR:OG1	2.20	0.56
18:31:20:LEU:HD11	21:31:412:CL7:HMA2	1.87	0.56
20:34:45:LEU:HG	20:34:49:HIS:CE1	2.41	0.56
21:1B:602:CL7:HBD	21:1B:602:CL7:HAA1	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:12:513:CL7:C1B	32:12:522:ZEX:C4	2.84	0.56
25:13:523:SQD:H221	32:22:520:ZEX:C10	2.36	0.56
16:22:98:PHE:CE1	32:22:522:ZEX:H31	2.41	0.56
21:22:507:CL7:H111	32:22:520:ZEX:H402	1.88	0.56
2:3B:89:PRO:HB3	2:3B:94:ALA:HB1	1.87	0.56
18:31:160:VAL:HG12	18:31:164:LYS:HE3	1.87	0.56
21:31:406:CL7:HBD	21:31:406:CL7:HAA2	1.86	0.56
21:33:511:CL7:CHB	32:33:525:ZEX:H172	2.35	0.56
21:4A:407:CL7:HED1	30:4D:407:PL9:H362	1.88	0.56
16:42:105:SER:HB2	21:41:406:CL7:H2	1.86	0.56
16:42:168:ASP:OD2	16:42:171:VAL:N	2.30	0.56
21:1A:407:CL7:HED1	30:1D:407:PL9:H362	1.88	0.56
7:1H:57:ASP:OD2	13:1X:2:THR:OG1	2.23	0.56
19:13:149:PHE:CE2	21:13:512:CL7:HHB	2.40	0.56
18:21:197:THR:HB	18:21:200:TYR:HD2	1.71	0.56
19:23:211:HIS:CE1	32:23:421:ZEX:C38	2.88	0.56
20:24:257:THR:HG23	21:24:408:CL7:HED2	1.88	0.56
16:32:210:GLY:HA2	32:32:520:ZEX:H363	1.78	0.56
21:32:517:CL7:CAB	32:43:401:ZEX:H392	2.35	0.56
21:1B:607:CL7:H11C	24:1B:621:LMG:H152	1.88	0.56
16:12:1:MET:HE1	21:12:508:CL7:HMA3	1.88	0.56
21:12:517:CL7:CAB	32:23:401:ZEX:H392	2.35	0.56
20:14:257:THR:HG23	21:14:408:CL7:HED2	1.88	0.56
3:2C:409:THR:OG1	3:2C:410:HIS:ND1	2.35	0.56
18:21:211:LEU:CD1	32:21:422:ZEX:H383	2.36	0.56
21:31:402:CL7:HBA2	21:31:402:CL7:CHA	2.35	0.56
19:33:63:ASN:HB3	21:33:504:CL7:HAA2	1.88	0.56
16:42:305:PHE:O	16:42:309:ASN:ND2	2.39	0.56
32:42:522:ZEX:H363	21:41:420:CL7:CMA	2.36	0.56
19:13:63:ASN:HB3	21:13:504:CL7:HAA2	1.88	0.55
20:14:288:SER:O	20:14:292:VAL:HG23	2.06	0.55
21:23:403:CL7:C2B	21:23:405:CL7:HAB	2.35	0.55
20:34:239:ILE:HD11	32:34:419:ZEX:C29	2.36	0.55
16:42:98:PHE:CE1	32:42:522:ZEX:H31	2.41	0.55
18:41:197:THR:HB	18:41:200:TYR:HD2	1.72	0.55
1:1A:307:VAL:HG12	1:1A:313:VAL:HG22	1.86	0.55
16:12:305:PHE:O	16:12:309:ASN:ND2	2.39	0.55
21:11:402:CL7:HBA2	21:11:402:CL7:CHA	2.35	0.55
21:13:511:CL7:CHB	32:13:525:ZEX:C17	2.84	0.55
21:22:505:CL7:O1A	32:22:520:ZEX:C17	2.51	0.55
21:21:410:CL7:H143	21:21:410:CL7:HAA1	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:34:407:CL7:HHB	32:34:418:ZEX:H172	1.88	0.55
26:4B:624:LHG:H172	30:4D:407:PL9:H303	1.88	0.55
18:11:197:THR:HB	18:11:200:TYR:HD2	1.71	0.55
21:11:410:CL7:H143	21:11:410:CL7:HAA1	1.89	0.55
26:2B:624:LHG:H172	30:2D:407:PL9:H303	1.88	0.55
16:22:305:PHE:O	16:22:309:ASN:ND2	2.39	0.55
32:22:522:ZEX:H363	21:21:420:CL7:CMA	2.36	0.55
18:21:20:LEU:HD11	21:21:412:CL7:HMA2	1.88	0.55
1:3A:124:ILE:HG21	21:3C:505:CL7:H122	1.89	0.55
3:3C:99:ILE:HG22	3:3C:434:PRO:HB3	1.89	0.55
16:32:77:VAL:HG21	16:32:275:PHE:HZ	1.71	0.55
16:32:98:PHE:CE1	32:32:522:ZEX:H31	2.41	0.55
16:32:168:ASP:OD2	16:32:171:VAL:N	2.30	0.55
21:32:502:CL7:HAA2	21:32:502:CL7:HBD	1.87	0.55
21:32:507:CL7:H111	32:32:520:ZEX:H402	1.88	0.55
21:4B:608:CL7:H11C	24:4B:622:LMG:H152	1.88	0.55
18:41:211:LEU:CD1	32:41:422:ZEX:H383	2.36	0.55
1:1A:124:ILE:HG21	21:1C:505:CL7:H122	1.89	0.55
2:1B:89:PRO:HB3	2:1B:94:ALA:HB1	1.87	0.55
32:12:522:ZEX:H363	21:11:420:CL7:CMA	2.36	0.55
32:12:522:ZEX:O23	18:11:268:TYR:CE2	2.60	0.55
20:14:239:ILE:HD11	32:14:419:ZEX:C29	2.36	0.55
20:24:239:ILE:HD11	32:24:419:ZEX:C29	2.36	0.55
21:32:513:CL7:C1B	32:32:522:ZEX:C4	2.84	0.55
3:4C:323:GLN:NE2	3:4C:370:PHE:O	2.40	0.55
21:41:410:CL7:H143	21:41:410:CL7:HAA1	1.89	0.55
21:44:404:CL7:H2	21:44:406:CL7:H41C	1.87	0.55
21:1B:613:CL7:H12C	21:1B:613:CL7:HED3	1.89	0.55
1:2A:307:VAL:HG12	1:2A:313:VAL:HG22	1.86	0.55
26:2B:624:LHG:O4	4:2D:140:TYR:OH	2.19	0.55
32:22:522:ZEX:O23	18:21:268:TYR:CE2	2.60	0.55
3:3C:323:GLN:NE2	3:3C:370:PHE:O	2.40	0.55
16:32:305:PHE:O	16:32:309:ASN:ND2	2.39	0.55
20:34:288:SER:O	20:34:292:VAL:HG23	2.06	0.55
20:34:335:LEU:O	20:34:339:LEU:HB2	2.05	0.55
21:34:405:CL7:H111	21:34:414:CL7:H12C	1.88	0.55
21:41:408:CL7:HMD2	21:41:410:CL7:H193	1.89	0.55
20:44:45:LEU:HG	20:44:49:HIS:CE1	2.41	0.55
21:44:407:CL7:HHB	32:44:418:ZEX:H172	1.88	0.55
21:12:507:CL7:H111	32:12:520:ZEX:H402	1.88	0.55
21:2B:614:CL7:H12C	21:2B:614:CL7:HED3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:31:215:HIS:HA	18:31:218:ILE:HG12	1.87	0.55
18:31:346:VAL:HG13	18:31:349:ARG:HH11	1.72	0.55
20:34:257:THR:HG23	21:34:408:CL7:HED2	1.88	0.55
21:42:511:CL7:CHB	32:42:524:ZEX:C17	2.85	0.55
21:41:402:CL7:HBA2	21:41:402:CL7:CHA	2.35	0.55
21:43:411:CL7:H42C	32:43:420:ZEX:H172	1.87	0.55
20:44:257:THR:HG23	21:44:408:CL7:HED2	1.88	0.55
21:44:405:CL7:H111	21:44:414:CL7:H12C	1.88	0.55
3:1C:323:GLN:NE2	3:1C:370:PHE:O	2.40	0.55
21:13:510:CL7:H42C	32:13:519:ZEX:H172	1.87	0.55
20:14:115:PHE:HE2	32:14:403:ZEX:H363	1.69	0.55
21:14:407:CL7:HHB	32:14:418:ZEX:H172	1.88	0.55
21:22:511:CL7:CHB	32:22:524:ZEX:C17	2.85	0.55
18:21:315:ASN:HD22	32:21:421:ZEX:H382	1.68	0.55
21:21:402:CL7:HBA2	21:21:402:CL7:CHA	2.35	0.55
21:21:408:CL7:HMD2	21:21:410:CL7:H193	1.89	0.55
21:3B:607:CL7:H11C	24:3B:621:LMG:H152	1.88	0.55
21:31:406:CL7:H41C	32:31:422:ZEX:H192	1.89	0.55
21:31:410:CL7:H143	21:31:410:CL7:HAA1	1.89	0.55
21:34:411:CL7:HBA1	21:34:411:CL7:HED3	1.89	0.55
16:42:77:VAL:HG21	16:42:275:PHE:HZ	1.71	0.55
16:42:210:GLY:HA2	32:42:520:ZEX:H363	1.78	0.55
18:41:151:LEU:HD12	21:41:413:CL7:H3A	1.89	0.55
18:11:20:LEU:HD11	21:11:412:CL7:HMA2	1.87	0.55
18:11:211:LEU:CD1	32:11:422:ZEX:H383	2.36	0.55
2:2B:89:PRO:HB3	2:2B:94:ALA:HB1	1.87	0.55
20:24:288:SER:O	20:24:292:VAL:HG23	2.06	0.55
1:3A:77:ILE:HD11	12:3T:6:TYR:HB3	1.88	0.55
21:3A:407:CL7:HED1	30:3D:407:PL9:H362	1.88	0.55
19:33:94:MET:SD	32:33:525:ZEX:H363	2.45	0.55
1:1A:219:VAL:O	1:1A:223:LEU:HB2	2.07	0.55
26:1B:623:LHG:H172	30:1D:407:PL9:H303	1.88	0.55
3:1C:99:ILE:HG22	3:1C:434:PRO:HB3	1.88	0.55
16:12:109:PHE:O	16:12:113:THR:OG1	2.22	0.55
21:14:405:CL7:H111	21:14:414:CL7:H12C	1.88	0.55
1:2A:124:ILE:HG21	21:2C:505:CL7:H122	1.89	0.55
3:2C:196:GLY:HA3	3:2C:209:ARG:O	2.07	0.55
19:23:63:ASN:HB3	21:23:405:CL7:HAA2	1.88	0.55
20:24:223:MET:HE3	21:24:417:CL7:H3A	1.89	0.55
21:3A:407:CL7:HMD2	21:3D:404:CL7:HAB	1.89	0.55
7:3H:57:ASP:OD2	13:3X:2:THR:OG1	2.23	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:32:522:ZEX:O23	18:31:268:TYR:CE2	2.60	0.55
3:4C:196:GLY:HA3	3:4C:209:ARG:O	2.07	0.55
21:2B:616:CL7:HAA2	21:2B:616:CL7:HBD	1.89	0.55
3:2C:99:ILE:HG22	3:2C:434:PRO:HB3	1.89	0.55
21:21:406:CL7:H41C	32:21:422:ZEX:H192	1.89	0.55
21:24:405:CL7:H111	21:24:414:CL7:H12C	1.88	0.55
21:24:407:CL7:HHB	32:24:418:ZEX:H172	1.88	0.55
1:3A:153:ALA:CB	21:3A:401:CL7:CED	2.83	0.55
21:3B:613:CL7:H12C	21:3B:613:CL7:HED3	1.89	0.55
18:31:238:SER:O	18:31:242:ASN:ND2	2.37	0.55
1:4A:77:ILE:HD11	12:4T:6:TYR:HB3	1.88	0.55
27:4B:625:DGD:O5D	27:4B:625:DGD:O4D	2.18	0.55
21:43:405:CL7:H161	21:43:411:CL7:H41C	1.89	0.55
20:44:223:MET:HE3	21:44:417:CL7:H3A	1.89	0.55
20:44:239:ILE:HD11	32:44:419:ZEX:C29	2.36	0.55
20:44:288:SER:O	20:44:292:VAL:HG23	2.06	0.55
21:44:405:CL7:H42C	21:44:406:CL7:H72C	1.90	0.55
21:12:511:CL7:CHB	32:12:524:ZEX:C17	2.85	0.54
21:11:406:CL7:H41C	32:11:422:ZEX:H192	1.89	0.54
21:14:405:CL7:H42C	21:14:406:CL7:H72C	1.89	0.54
21:23:417:CL7:HED1	32:24:403:ZEX:H10	1.89	0.54
20:24:115:PHE:HE2	32:24:403:ZEX:H363	1.69	0.54
32:32:522:ZEX:H363	21:31:420:CL7:CMA	2.36	0.54
20:34:295:MET:HG2	21:34:404:CL7:H93C	1.89	0.54
21:4B:616:CL7:HAA2	21:4B:616:CL7:HBD	1.89	0.54
32:42:522:ZEX:O23	18:41:268:TYR:CE2	2.60	0.54
21:1B:615:CL7:HAA2	21:1B:615:CL7:HBD	1.89	0.54
3:1C:196:GLY:HA3	3:1C:209:ARG:O	2.07	0.54
21:14:411:CL7:HBA1	21:14:411:CL7:HED3	1.89	0.54
21:23:411:CL7:H42C	32:23:420:ZEX:H172	1.87	0.54
21:24:405:CL7:H42C	21:24:406:CL7:H72C	1.89	0.54
21:3B:602:CL7:HAA1	21:3B:602:CL7:HBD	1.87	0.54
18:31:197:THR:HB	18:31:200:TYR:HD2	1.71	0.54
21:33:504:CL7:H161	21:33:510:CL7:H41C	1.89	0.54
21:34:407:CL7:CAD	32:34:419:ZEX:C16	2.86	0.54
21:34:407:CL7:CMD	21:34:409:CL7:HAB	2.38	0.54
21:42:505:CL7:O1A	32:42:520:ZEX:C17	2.52	0.54
21:11:408:CL7:HMD2	21:11:410:CL7:H193	1.89	0.54
21:14:407:CL7:CMD	21:14:409:CL7:HAB	2.38	0.54
2:2B:217:LEU:O	2:2B:221:GLY:N	2.38	0.54
21:42:513:CL7:C1B	32:42:522:ZEX:C4	2.84	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:312:TRP:CZ2	21:41:405:CL7:HBA2	2.43	0.54
2:1B:74:SER:OG	2:1B:102:GLU:OE2	2.19	0.54
3:1C:159:TRP:NE1	21:1C:513:CL7:O2A	2.41	0.54
16:12:77:VAL:HG21	16:12:275:PHE:HZ	1.71	0.54
18:11:346:VAL:HG13	18:11:349:ARG:HH11	1.72	0.54
21:13:516:CL7:HED1	32:14:403:ZEX:H10	1.89	0.54
3:2C:323:GLN:NE2	3:2C:370:PHE:O	2.40	0.54
18:21:151:LEU:HD12	21:21:413:CL7:H3A	1.89	0.54
20:24:115:PHE:CD2	32:24:403:ZEX:H363	2.43	0.54
26:24:401:LHG:HC81	21:24:405:CL7:HMA1	1.90	0.54
1:3A:219:VAL:O	1:3A:223:LEU:HB2	2.07	0.54
26:3B:623:LHG:H172	30:3D:407:PL9:H303	1.88	0.54
1:4A:124:ILE:HG21	21:4C:505:CL7:H122	1.89	0.54
19:43:63:ASN:HB3	21:43:405:CL7:HAA2	1.88	0.54
21:43:417:CL7:HED1	32:44:403:ZEX:H10	1.89	0.54
20:44:45:LEU:HG	20:44:49:HIS:HE1	1.73	0.54
20:44:115:PHE:CD2	32:44:403:ZEX:H363	2.43	0.54
21:2B:605:CL7:H2	21:2B:606:CL7:H12C	1.90	0.54
16:22:77:VAL:HG21	16:22:275:PHE:HZ	1.71	0.54
16:22:277:GLY:O	16:22:304:ARG:NH1	2.41	0.54
21:3A:403:CL7:H52C	24:3A:405:LMG:O10	2.08	0.54
7:3H:42:LEU:HD11	7:3H:46:MET:HE3	1.89	0.54
21:33:516:CL7:HED1	32:34:403:ZEX:H10	1.90	0.54
2:4B:217:LEU:O	2:4B:221:GLY:N	2.38	0.54
21:4B:614:CL7:H12C	21:4B:614:CL7:HED3	1.89	0.54
18:41:315:ASN:HD22	32:41:421:ZEX:H382	1.68	0.54
21:41:406:CL7:H41C	32:41:422:ZEX:H192	1.89	0.54
26:44:401:LHG:HC81	21:44:405:CL7:HMA1	1.90	0.54
21:44:407:CL7:CAD	32:44:419:ZEX:C16	2.86	0.54
1:1A:77:ILE:HD11	12:1T:6:TYR:HB3	1.88	0.54
20:14:223:MET:HE3	21:14:417:CL7:H3A	1.89	0.54
20:24:275:ASN:HD22	18:31:115:ILE:HG12	1.72	0.54
20:24:310:TYR:CE2	21:24:404:CL7:HBA2	2.43	0.54
16:32:277:GLY:O	16:32:304:ARG:NH1	2.41	0.54
18:31:211:LEU:CD1	32:31:422:ZEX:H383	2.36	0.54
3:4C:99:ILE:HG22	3:4C:434:PRO:HB3	1.89	0.54
19:43:34:GLN:HE21	21:43:410:CL7:HMB3	1.73	0.54
21:1B:604:CL7:H2	21:1B:605:CL7:H12C	1.90	0.54
26:1B:623:LHG:H101	26:1B:623:LHG:H352	1.90	0.54
21:11:406:CL7:HBC2	32:11:422:ZEX:H191	1.90	0.54
19:13:309:ASN:OD1	32:13:519:ZEX:C36	2.49	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:14:58:VAL:HG23	20:14:118:ALA:HB1	1.90	0.54
26:3B:623:LHG:H352	26:3B:623:LHG:H101	1.90	0.54
21:4A:403:CL7:H52C	24:4A:405:LMG:O10	2.08	0.54
16:42:277:GLY:O	16:42:304:ARG:NH1	2.41	0.54
16:12:277:GLY:O	16:12:304:ARG:NH1	2.41	0.54
20:14:310:TYR:CE2	21:14:404:CL7:HBA2	2.43	0.54
26:14:401:LHG:HC81	21:14:405:CL7:HMA1	1.90	0.54
3:3C:159:TRP:NE1	21:3C:513:CL7:O2A	2.41	0.54
21:32:511:CL7:CHB	32:32:524:ZEX:C17	2.85	0.54
21:31:406:CL7:HBC2	32:31:422:ZEX:H191	1.90	0.54
21:31:408:CL7:HMD2	21:31:410:CL7:H193	1.89	0.54
20:34:310:TYR:CE2	21:34:404:CL7:HBA2	2.43	0.54
21:34:405:CL7:H42C	21:34:406:CL7:H72C	1.89	0.54
7:4H:57:ASP:OD2	13:4X:2:THR:OG1	2.23	0.54
20:44:310:TYR:CE2	21:44:404:CL7:HBA2	2.43	0.54
1:1A:205:VAL:HG21	21:1A:401:CL7:HHB	1.89	0.54
7:1H:42:LEU:HD11	7:1H:46:MET:HE3	1.89	0.54
21:13:504:CL7:H161	21:13:510:CL7:H41C	1.89	0.54
21:14:407:CL7:CAD	32:14:419:ZEX:C16	2.86	0.54
21:21:414:CL7:HMD1	20:34:258:PRO:CB	2.35	0.54
21:23:405:CL7:H161	21:23:411:CL7:H41C	1.89	0.54
20:24:58:VAL:HG23	20:24:118:ALA:HB1	1.90	0.54
21:24:411:CL7:HBA1	21:24:411:CL7:HED3	1.89	0.54
2:3B:344:PRO:HG3	2:3B:429:PRO:HG3	1.90	0.54
16:32:105:SER:CB	21:31:406:CL7:H2	2.38	0.54
18:31:312:TRP:CZ2	21:31:405:CL7:HBA2	2.43	0.54
20:34:58:VAL:HG23	20:34:118:ALA:HB1	1.90	0.54
1:4A:153:ALA:CB	21:4A:401:CL7:CED	2.83	0.54
32:43:401:ZEX:C17	21:43:412:CL7:CHB	2.86	0.54
18:21:206:ASP:N	18:21:206:ASP:OD1	2.41	0.54
20:24:45:LEU:HG	20:24:49:HIS:HE1	1.73	0.54
1:3A:205:VAL:HG21	21:3A:401:CL7:HHB	1.89	0.54
32:32:522:ZEX:C36	21:31:420:CL7:CMA	2.86	0.54
18:31:111:PHE:O	18:31:116:GLY:N	2.37	0.54
21:4A:407:CL7:HMD2	21:4D:404:CL7:HAB	1.89	0.54
2:4B:166:LEU:HB3	2:4B:207:VAL:HG22	1.90	0.54
16:42:213:PHE:O	16:42:217:ILE:HG12	2.08	0.54
18:41:206:ASP:OD1	18:41:206:ASP:N	2.41	0.54
21:1A:403:CL7:H52C	24:1A:405:LMG:O10	2.08	0.53
16:12:105:SER:CB	21:11:406:CL7:H2	2.38	0.53
1:2A:77:ILE:HD11	12:2T:6:TYR:HB3	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2C:159:TRP:NE1	21:2C:513:CL7:O2A	2.41	0.53
4:2D:73:LEU:O	4:2D:175:THR:OG1	2.16	0.53
18:21:312:TRP:CZ2	21:21:405:CL7:HBA2	2.43	0.53
21:23:402:CL7:H41C	21:23:402:CL7:H92C	1.90	0.53
20:24:275:ASN:ND2	18:31:115:ILE:CD1	2.71	0.53
2:3B:74:SER:OG	2:3B:102:GLU:OE2	2.19	0.53
21:3B:604:CL7:H2	21:3B:605:CL7:H12C	1.90	0.53
21:32:512:CL7:C6	32:32:522:ZEX:H202	2.34	0.53
1:4A:205:VAL:HG21	21:4A:401:CL7:HHB	1.89	0.53
1:4A:219:VAL:O	1:4A:223:LEU:HB2	2.07	0.53
20:44:295:MET:HG2	21:44:404:CL7:H93C	1.89	0.53
1:1A:283:ILE:HG13	22:1A:402:PHO:HBC3	1.90	0.53
18:11:206:ASP:OD1	18:11:206:ASP:N	2.41	0.53
21:13:501:CL7:H41C	21:13:501:CL7:H92C	1.90	0.53
20:14:25:SER:OG	20:14:26:ASN:N	2.38	0.53
2:2B:166:LEU:HB3	2:2B:207:VAL:HG22	1.90	0.53
26:2B:624:LHG:H101	26:2B:624:LHG:H352	1.90	0.53
27:2B:625:DGD:O5D	27:2B:625:DGD:O4D	2.18	0.53
21:22:513:CL7:C1B	32:22:522:ZEX:C4	2.84	0.53
21:3B:615:CL7:HAA2	21:3B:615:CL7:HBD	1.89	0.53
3:3C:196:GLY:HA3	3:3C:209:ARG:O	2.07	0.53
4:3D:160:PRO:HB3	4:3D:169:ALA:HB2	1.90	0.53
21:44:411:CL7:HBA1	21:44:411:CL7:HED3	1.89	0.53
21:1B:607:CL7:H121	24:1B:621:LMG:H362	1.91	0.53
18:11:312:TRP:CZ2	21:11:405:CL7:HBA2	2.43	0.53
20:14:295:MET:HG2	21:14:404:CL7:H93C	1.89	0.53
1:2A:219:VAL:O	1:2A:223:LEU:HB2	2.08	0.53
21:2A:407:CL7:HMD2	21:2D:404:CL7:HAB	1.89	0.53
4:2D:52:THR:HA	4:2D:66:TYR:HD2	1.74	0.53
21:2D:404:CL7:HAA2	21:2D:404:CL7:HBD	1.90	0.53
21:24:407:CL7:CAD	32:24:419:ZEX:C16	2.86	0.53
1:3A:283:ILE:HG13	22:3A:402:PHO:HBC3	1.90	0.53
21:3B:607:CL7:H121	24:3B:621:LMG:H362	1.91	0.53
19:33:235:ASP:OD1	19:33:240:LYS:NZ	2.28	0.53
2:1B:344:PRO:HG3	2:1B:429:PRO:HG3	1.90	0.53
4:1D:84:LEU:HA	5:1E:69:ARG:HB2	1.91	0.53
16:12:35:ILE:O	16:12:39:THR:HG22	2.09	0.53
32:12:522:ZEX:C36	21:11:420:CL7:CMA	2.86	0.53
18:11:151:LEU:HD12	21:11:413:CL7:H3A	1.89	0.53
1:2A:283:ILE:HG13	22:2A:402:PHO:HBC3	1.90	0.53
2:2B:7:ARG:NH2	26:2B:624:LHG:O5	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:22:51:SER:OG	18:21:290:PHE:N	2.41	0.53
32:22:522:ZEX:C36	21:21:420:CL7:CMA	2.86	0.53
18:21:115:ILE:CD1	20:34:275:ASN:ND2	2.72	0.53
1:3A:57:PRO:HD3	1:3A:73:TYR:CE1	2.44	0.53
4:3D:298:VAL:HG22	10:3L:38:ASN:OXT	2.09	0.53
19:33:34:GLN:HE21	21:33:509:CL7:HMB3	1.73	0.53
26:34:401:LHG:HC81	21:34:405:CL7:HMA1	1.90	0.53
4:4D:52:THR:HA	4:4D:66:TYR:HD2	1.74	0.53
32:42:522:ZEX:C36	21:41:420:CL7:CMA	2.86	0.53
18:41:146:GLY:HA3	18:41:230:ILE:HG13	1.91	0.53
18:41:234:PRO:HA	21:41:407:CL7:HED3	1.91	0.53
21:43:405:CL7:HBD	21:43:405:CL7:HBA2	1.90	0.53
21:44:407:CL7:CMD	21:44:409:CL7:HAB	2.38	0.53
19:13:109:TYR:HB2	21:22:505:CL7:HBA2	1.89	0.53
21:2B:608:CL7:H121	24:2B:622:LMG:H362	1.91	0.53
3:2C:69:ALA:O	3:2C:73:THR:HG22	2.08	0.53
16:22:213:PHE:O	16:22:217:ILE:HG12	2.08	0.53
18:21:346:VAL:HG13	18:21:349:ARG:HH11	1.72	0.53
21:21:406:CL7:HBC2	32:21:422:ZEX:H191	1.90	0.53
19:23:34:GLN:HE21	21:23:410:CL7:HMB3	1.73	0.53
16:32:213:PHE:O	16:32:217:ILE:HG12	2.08	0.53
20:34:56:MET:HE1	21:34:411:CL7:H12C	1.91	0.53
3:4C:159:TRP:NE1	21:4C:513:CL7:O2A	2.41	0.53
19:43:278:PRO:HD2	19:43:302:THR:HG21	1.91	0.53
19:43:309:ASN:OD1	32:43:420:ZEX:C36	2.49	0.53
2:1B:166:LEU:HB3	2:1B:207:VAL:HG22	1.91	0.53
26:1B:623:LHG:O4	4:1D:140:TYR:OH	2.19	0.53
27:1B:624:DGD:O5D	27:1B:624:DGD:O4D	2.18	0.53
18:11:238:SER:O	18:11:242:ASN:ND2	2.37	0.53
4:2D:298:VAL:HG22	10:2L:38:ASN:OXT	2.09	0.53
18:21:146:GLY:HA3	18:21:230:ILE:HG13	1.91	0.53
19:23:278:PRO:HD2	19:23:302:THR:HG21	1.91	0.53
21:3B:607:CL7:H101	24:3B:621:LMG:H351	1.90	0.53
4:3D:84:LEU:HA	5:3E:69:ARG:HB2	1.91	0.53
16:32:35:ILE:O	16:32:39:THR:HG22	2.09	0.53
16:32:51:SER:OG	18:31:290:PHE:N	2.41	0.53
16:32:92:VAL:HG22	21:32:512:CL7:H201	1.91	0.53
18:31:151:LEU:HD12	21:31:413:CL7:H3A	1.89	0.53
21:4B:605:CL7:H2	21:4B:606:CL7:H12C	1.90	0.53
16:42:51:SER:OG	18:41:290:PHE:N	2.41	0.53
21:42:511:CL7:C1B	32:42:524:ZEX:H172	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:346:VAL:HG13	18:41:349:ARG:HH11	1.72	0.53
20:44:56:MET:HE1	21:44:411:CL7:H12C	1.91	0.53
20:44:58:VAL:HG23	20:44:118:ALA:HB1	1.90	0.53
1:1A:57:PRO:HD3	1:1A:73:TYR:CE1	2.44	0.53
16:12:51:SER:OG	18:11:290:PHE:N	2.41	0.53
19:13:19:ARG:HD3	16:22:345:THR:HG22	1.90	0.53
19:13:94:MET:SD	32:13:525:ZEX:H363	2.47	0.53
21:2A:403:CL7:H52C	24:2A:405:LMG:O10	2.08	0.53
4:2D:84:LEU:HA	5:2E:69:ARG:HB2	1.91	0.53
16:22:35:ILE:O	16:22:39:THR:HG22	2.09	0.53
16:22:105:SER:CB	21:21:406:CL7:H2	2.38	0.53
21:32:511:CL7:C1B	32:32:524:ZEX:H172	2.39	0.53
21:4D:404:CL7:HAA2	21:4D:404:CL7:HBD	1.90	0.53
2:1B:217:LEU:O	2:1B:221:GLY:N	2.38	0.53
4:1D:298:VAL:HG22	10:1L:38:ASN:OXT	2.09	0.53
16:12:213:PHE:O	16:12:217:ILE:HG12	2.08	0.53
21:12:511:CL7:C1B	32:12:524:ZEX:H172	2.39	0.53
18:11:146:GLY:HA3	18:11:230:ILE:HG13	1.91	0.53
1:2A:205:VAL:HG21	21:2A:401:CL7:HHB	1.89	0.53
18:21:262:MET:HG2	21:21:402:CL7:H102	1.91	0.53
20:24:295:MET:HG2	21:24:404:CL7:H93C	1.89	0.53
2:3B:294:ARG:O	2:3B:298:SER:OG	2.23	0.53
20:34:223:MET:HE3	21:34:417:CL7:H3A	1.89	0.53
26:4B:624:LHG:H101	26:4B:624:LHG:H352	1.90	0.53
16:42:35:ILE:O	16:42:39:THR:HG22	2.09	0.53
3:1C:69:ALA:O	3:1C:73:THR:HG22	2.08	0.53
21:13:501:CL7:H101	21:13:507:CL7:H41C	1.91	0.53
3:2C:141:GLY:O	3:2C:145:THR:OG1	2.20	0.53
7:2H:42:LEU:HD11	7:2H:46:MET:HE3	1.89	0.53
21:22:513:CL7:HBA2	21:22:513:CL7:CHA	2.38	0.53
18:21:234:PRO:HA	21:21:407:CL7:HED3	1.91	0.53
19:23:235:ASP:OD1	19:23:240:LYS:NZ	2.28	0.53
21:33:511:CL7:CHB	32:33:525:ZEX:C17	2.86	0.53
4:4D:298:VAL:HG22	10:4L:38:ASN:OXT	2.09	0.53
18:41:262:MET:HG2	21:41:402:CL7:H102	1.91	0.53
21:43:402:CL7:H92C	21:43:402:CL7:H41C	1.90	0.53
20:44:151:GLU:OE2	20:44:152:TRP:N	2.42	0.53
2:1B:294:ARG:O	2:1B:298:SER:OG	2.23	0.53
4:1D:160:PRO:HB3	4:1D:169:ALA:HB2	1.90	0.53
21:13:508:CL7:H51C	21:13:511:CL7:HAC1	1.90	0.53
20:14:45:LEU:HG	20:14:49:HIS:HE1	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:22:512:CL7:C6	32:22:522:ZEX:H202	2.34	0.53
21:23:405:CL7:HBA2	21:23:405:CL7:HBD	1.90	0.53
21:24:407:CL7:CMD	21:24:409:CL7:HAB	2.37	0.53
3:3C:83:GLU:HG2	21:3C:504:CL7:HED1	1.91	0.53
21:32:513:CL7:HBA2	21:32:513:CL7:CHA	2.38	0.53
21:31:412:CL7:HBA2	21:31:412:CL7:HBD	1.91	0.53
21:33:501:CL7:H41C	21:33:501:CL7:H92C	1.90	0.53
20:34:45:LEU:HG	20:34:49:HIS:HE1	1.73	0.53
3:4C:230:TRP:CE3	27:4C:516:DGD:HA21	2.44	0.53
3:4C:409:THR:OG1	3:4C:410:HIS:ND1	2.35	0.53
21:41:412:CL7:HBA2	21:41:412:CL7:HBD	1.91	0.53
21:1B:607:CL7:H101	24:1B:621:LMG:H351	1.90	0.52
3:1C:83:GLU:HG2	21:1C:504:CL7:HED1	1.91	0.52
16:12:92:VAL:HG22	21:12:512:CL7:H201	1.91	0.52
21:12:511:CL7:CHB	32:12:524:ZEX:H173	2.39	0.52
21:12:513:CL7:HBA2	21:12:513:CL7:CHA	2.38	0.52
18:11:270:CYS:O	18:11:310:ARG:NH1	2.40	0.52
21:11:412:CL7:HBA2	21:11:412:CL7:HBD	1.91	0.52
19:13:278:PRO:HD2	19:13:302:THR:HG21	1.91	0.52
2:2B:344:PRO:HG3	2:2B:429:PRO:HG3	1.90	0.52
21:2B:608:CL7:H101	24:2B:622:LMG:H351	1.90	0.52
3:2C:230:TRP:CE3	27:2C:516:DGD:HA21	2.44	0.52
21:23:402:CL7:H101	21:23:408:CL7:H41C	1.91	0.52
18:31:234:PRO:HA	21:31:407:CL7:HED3	1.91	0.52
21:31:408:CL7:H13	32:31:422:ZEX:H402	1.91	0.52
20:34:58:VAL:HG21	32:34:403:ZEX:H15	1.91	0.52
21:4B:608:CL7:H101	24:4B:622:LMG:H351	1.90	0.52
21:42:513:CL7:HBA2	21:42:513:CL7:CHA	2.38	0.52
21:1D:404:CL7:HAA2	21:1D:404:CL7:HBD	1.90	0.52
18:11:262:MET:HG2	21:11:402:CL7:H102	1.91	0.52
18:11:303:ALA:HB3	18:11:306:PHE:HD2	1.74	0.52
21:13:504:CL7:HBD	21:13:504:CL7:HBA2	1.90	0.52
1:2A:32:TRP:NE1	8:2I:27:ASP:OD1	2.43	0.52
21:22:511:CL7:C1B	32:22:524:ZEX:H172	2.39	0.52
18:21:146:GLY:HA2	18:21:226:GLY:HA2	1.91	0.52
32:32:520:ZEX:C10	25:43:424:SQD:H221	2.38	0.52
18:31:303:ALA:HB3	18:31:306:PHE:HD2	1.74	0.52
21:4C:510:CL7:OBD	21:4C:511:CL7:OBB	2.27	0.52
7:4H:42:LEU:HD11	7:4H:46:MET:HE3	1.89	0.52
21:41:406:CL7:HBC2	32:41:422:ZEX:H191	1.90	0.52
21:43:409:CL7:H51C	21:43:412:CL7:HAC1	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1C:510:CL7:OBD	21:1C:511:CL7:OBB	2.27	0.52
21:2C:510:CL7:OBD	21:2C:511:CL7:OBB	2.27	0.52
21:21:412:CL7:HBD	21:21:412:CL7:HBA2	1.91	0.52
21:23:409:CL7:H51C	21:23:412:CL7:HAC1	1.90	0.52
3:3C:69:ALA:O	3:3C:73:THR:HG22	2.08	0.52
3:3C:230:TRP:CE3	27:3C:516:DGD:HA21	2.44	0.52
21:3C:510:CL7:OBD	21:3C:511:CL7:OBB	2.27	0.52
21:32:511:CL7:CHB	32:32:524:ZEX:H173	2.39	0.52
21:33:501:CL7:H101	21:33:507:CL7:H41C	1.91	0.52
21:4B:604:CL7:O1A	21:4B:604:CL7:H3A	2.09	0.52
16:42:105:SER:CB	21:41:406:CL7:H2	2.38	0.52
21:42:507:CL7:HMD3	21:42:509:CL7:H171	1.91	0.52
18:41:146:GLY:HA2	18:41:226:GLY:HA2	1.92	0.52
2:1B:458:TYR:HB3	21:1B:604:CL7:HBC2	1.91	0.52
16:12:201:VAL:CG2	32:12:520:ZEX:H1	2.18	0.52
19:13:34:GLN:HE21	21:13:509:CL7:HMB3	1.73	0.52
20:14:292:VAL:HG13	21:14:406:CL7:H141	1.92	0.52
1:2A:57:PRO:HD3	1:2A:73:TYR:CE1	2.44	0.52
3:2C:363:PHE:CE2	3:2C:387:LEU:HD11	2.45	0.52
21:23:408:CL7:H2A	21:23:408:CL7:O2D	2.09	0.52
20:24:258:PRO:CB	21:31:414:CL7:HMD1	2.35	0.52
1:3A:32:TRP:NE1	8:3I:27:ASP:OD1	2.43	0.52
21:33:508:CL7:H51C	21:33:511:CL7:HAC1	1.90	0.52
26:33:524:LHG:H242	21:34:413:CL7:C3D	2.40	0.52
20:34:25:SER:OG	20:34:26:ASN:N	2.38	0.52
21:34:414:CL7:HMA1	32:34:420:ZEX:H162	1.91	0.52
1:4A:32:TRP:NE1	8:4I:27:ASP:OD1	2.43	0.52
1:4A:57:PRO:HD3	1:4A:73:TYR:CE1	2.44	0.52
3:4C:363:PHE:CE2	3:4C:387:LEU:HD11	2.45	0.52
16:42:109:PHE:O	16:42:113:THR:OG1	2.22	0.52
16:42:250:LEU:HD21	21:42:508:CL7:HAB	1.92	0.52
20:44:58:VAL:HG21	32:44:403:ZEX:H15	1.91	0.52
21:44:414:CL7:HMA1	32:44:420:ZEX:H162	1.91	0.52
21:1A:407:CL7:H41C	30:1D:407:PL9:H211	1.91	0.52
3:1C:230:TRP:CE3	27:1C:516:DGD:HA21	2.44	0.52
6:1F:30:VAL:HB	6:1F:31:PRO:HD3	1.91	0.52
18:11:146:GLY:HA2	18:11:226:GLY:HA2	1.92	0.52
20:14:115:PHE:CD2	32:14:403:ZEX:H363	2.43	0.52
2:2B:458:TYR:HB3	21:2B:605:CL7:HBC2	1.91	0.52
4:2D:160:PRO:HB3	4:2D:169:ALA:HB2	1.90	0.52
21:24:414:CL7:HMA1	32:24:420:ZEX:H162	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3F:30:VAL:HB	6:3F:31:PRO:HD3	1.91	0.52
18:31:146:GLY:HA3	18:31:230:ILE:HG13	1.91	0.52
18:31:270:CYS:O	18:31:310:ARG:NH1	2.40	0.52
21:4B:608:CL7:H121	24:4B:622:LMG:H362	1.91	0.52
3:4C:69:ALA:O	3:4C:73:THR:HG22	2.08	0.52
4:4D:84:LEU:HA	5:4E:69:ARG:HB2	1.91	0.52
4:4D:160:PRO:HB3	4:4D:169:ALA:HB2	1.90	0.52
16:42:92:VAL:HG22	21:42:512:CL7:H201	1.91	0.52
21:42:511:CL7:CHB	32:42:524:ZEX:H173	2.39	0.52
21:42:512:CL7:C6	32:42:522:ZEX:H202	2.34	0.52
16:12:207:VAL:HA	32:12:520:ZEX:C38	2.37	0.52
18:11:234:PRO:HA	21:11:407:CL7:HED3	1.91	0.52
21:22:511:CL7:CHB	32:22:524:ZEX:H173	2.39	0.52
18:21:37:ILE:HG22	18:21:105:LEU:HD13	1.92	0.52
20:24:58:VAL:HG21	32:24:403:ZEX:H15	1.91	0.52
21:3A:407:CL7:H41C	30:3D:407:PL9:H211	1.91	0.52
2:3B:458:TYR:HB3	21:3B:604:CL7:HBC2	1.91	0.52
21:32:505:CL7:HMD3	32:32:520:ZEX:C16	2.40	0.52
18:31:206:ASP:N	18:31:206:ASP:OD1	2.41	0.52
21:43:408:CL7:H2A	21:43:408:CL7:O2D	2.09	0.52
1:1A:32:TRP:NE1	8:1I:27:ASP:OD1	2.43	0.52
1:1A:283:ILE:HA	1:1A:286:THR:HG22	1.91	0.52
1:1A:286:THR:OG1	21:1A:401:CL7:O1D	2.23	0.52
32:12:524:ZEX:C19	21:11:418:CL7:H8	2.28	0.52
21:14:414:CL7:HMA1	32:14:420:ZEX:H162	1.91	0.52
3:2C:83:GLU:HG2	21:2C:504:CL7:HED1	1.91	0.52
6:2F:30:VAL:HB	6:2F:31:PRO:HD3	1.91	0.52
18:21:111:PHE:O	18:21:116:GLY:N	2.37	0.52
18:21:276:VAL:O	18:21:278:PRO:HD3	2.09	0.52
20:24:56:MET:HE1	21:24:411:CL7:H12C	1.91	0.52
20:24:151:GLU:OE2	20:24:152:TRP:N	2.42	0.52
3:3C:363:PHE:CE2	3:3C:387:LEU:HD11	2.45	0.52
18:31:276:VAL:O	18:31:278:PRO:HD3	2.09	0.52
21:33:504:CL7:HBD	21:33:504:CL7:HBA2	1.90	0.52
21:33:507:CL7:O2D	21:33:507:CL7:H2A	2.09	0.52
1:4A:283:ILE:HG13	22:4A:402:PHO:HBC3	1.90	0.52
18:41:37:ILE:HG22	18:41:105:LEU:HD13	1.92	0.52
18:41:80:GLY:H	18:41:84:VAL:HB	1.75	0.52
21:44:408:CL7:O1A	21:44:409:CL7:OBB	2.28	0.52
3:1C:363:PHE:CE2	3:1C:387:LEU:HD11	2.45	0.52
4:1D:258:ILE:HG21	26:1D:409:LHG:H262	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:14:56:MET:HE1	21:14:411:CL7:H12C	1.91	0.52
20:14:58:VAL:HG21	32:14:403:ZEX:H15	1.91	0.52
2:2B:74:SER:OG	2:2B:102:GLU:OE2	2.19	0.52
21:2B:604:CL7:O1A	21:2B:604:CL7:H3A	2.09	0.52
16:22:250:LEU:HD21	21:22:508:CL7:HAB	1.92	0.52
18:21:80:GLY:H	18:21:84:VAL:HB	1.75	0.52
20:24:292:VAL:HG13	21:24:406:CL7:H141	1.92	0.52
21:24:408:CL7:O1A	21:24:409:CL7:OBB	2.28	0.52
2:3B:166:LEU:HB3	2:3B:207:VAL:HG22	1.91	0.52
4:3D:258:ILE:HD13	26:3D:409:LHG:HC82	1.92	0.52
21:32:505:CL7:HBA2	19:43:109:TYR:HB2	1.91	0.52
18:31:80:GLY:H	18:31:84:VAL:HB	1.75	0.52
18:31:214:GLY:CA	32:31:422:ZEX:H362	2.37	0.52
18:31:262:MET:HG2	21:31:402:CL7:H102	1.91	0.52
21:31:417:CL7:H3A	21:31:417:CL7:CGA	2.39	0.52
20:34:292:VAL:HG13	21:34:406:CL7:H141	1.92	0.52
21:4A:407:CL7:H41C	30:4D:407:PL9:H211	1.91	0.52
3:4C:83:GLU:HG2	21:4C:504:CL7:HED1	1.91	0.52
25:43:422:SQD:H141	25:43:422:SQD:H271	1.92	0.52
21:2A:407:CL7:H41C	30:2D:407:PL9:H211	1.91	0.52
21:24:415:CL7:HAA2	21:24:415:CL7:HBD	1.92	0.52
3:3C:409:THR:OG1	3:3C:410:HIS:ND1	2.35	0.52
19:33:108:LEU:O	19:33:112:THR:HG22	2.10	0.52
20:34:115:PHE:CD2	32:34:403:ZEX:H363	2.43	0.52
1:4A:283:ILE:HA	1:4A:286:THR:HG22	1.91	0.52
19:43:235:ASP:OD1	19:43:240:LYS:NZ	2.28	0.52
21:43:402:CL7:H101	21:43:408:CL7:H41C	1.91	0.52
21:44:407:CL7:C3D	32:44:419:ZEX:H163	2.40	0.52
2:1B:100:SER:OG	2:1B:102:GLU:OE1	2.20	0.52
4:1D:52:THR:HA	4:1D:66:TYR:HD2	1.74	0.52
21:12:512:CL7:C6	32:12:522:ZEX:H202	2.34	0.52
21:11:408:CL7:H13	32:11:422:ZEX:H402	1.91	0.52
21:13:507:CL7:H2A	21:13:507:CL7:O2D	2.09	0.52
26:13:524:LHG:H242	21:14:413:CL7:C3D	2.40	0.52
4:2D:258:ILE:HG21	26:2D:409:LHG:H262	1.92	0.52
16:22:92:VAL:HG22	21:22:512:CL7:H201	1.91	0.52
21:22:507:CL7:HMD3	21:22:509:CL7:H171	1.91	0.52
18:21:115:ILE:HG12	20:34:275:ASN:HD22	1.72	0.52
18:21:303:ALA:HB3	18:21:306:PHE:HD2	1.74	0.52
1:3A:283:ILE:HA	1:3A:286:THR:HG22	1.91	0.52
21:3B:603:CL7:O1A	21:3B:603:CL7:H3A	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3D:404:CL7:HBD	21:3D:404:CL7:HAA2	1.90	0.52
16:32:280:LEU:HD13	16:32:290:PHE:HB3	1.92	0.52
18:31:146:GLY:HA2	18:31:226:GLY:HA2	1.91	0.52
21:41:408:CL7:H13	32:41:422:ZEX:H402	1.91	0.52
21:43:416:CL7:HMC2	32:44:420:ZEX:H391	1.92	0.52
18:11:37:ILE:HG22	18:11:105:LEU:HD13	1.92	0.51
4:2D:66:TYR:O	24:2D:410:LMG:O5	2.15	0.51
18:21:270:CYS:O	18:21:310:ARG:NH1	2.40	0.51
19:23:108:LEU:O	19:23:112:THR:HG22	2.10	0.51
26:23:425:LHG:H242	21:24:413:CL7:C3D	2.40	0.51
21:24:407:CL7:C3D	32:24:419:ZEX:H163	2.40	0.51
2:3B:217:LEU:O	2:3B:221:GLY:N	2.38	0.51
27:3B:624:DGD:O5D	27:3B:624:DGD:O4D	2.18	0.51
18:31:258:GLY:O	18:31:262:MET:HG3	2.10	0.51
21:33:510:CL7:HBA1	21:33:510:CL7:HBD	1.92	0.51
20:34:93:VAL:HG13	20:34:106:PRO:HB2	1.92	0.51
4:4D:258:ILE:HG21	26:4D:409:LHG:H262	1.92	0.51
4:4D:258:ILE:HD13	26:4D:409:LHG:HC82	1.92	0.51
18:41:258:GLY:O	18:41:262:MET:HG3	2.11	0.51
26:43:425:LHG:H242	21:44:413:CL7:C3D	2.40	0.51
3:1C:388:ASP:HB3	3:1C:391:LYS:HG2	1.91	0.51
4:1D:258:ILE:HD13	26:1D:409:LHG:HC82	1.92	0.51
16:12:280:LEU:HD13	16:12:290:PHE:HB3	1.93	0.51
18:11:80:GLY:H	18:11:84:VAL:HB	1.75	0.51
21:14:408:CL7:O1A	21:14:409:CL7:OBB	2.28	0.51
21:14:415:CL7:HAA2	21:14:415:CL7:HBD	1.93	0.51
2:2B:100:SER:OG	2:2B:102:GLU:OE1	2.20	0.51
18:21:258:GLY:O	18:21:262:MET:HG3	2.11	0.51
2:4B:458:TYR:HB3	21:4B:605:CL7:HBC2	1.91	0.51
21:4B:604:CL7:H3A	21:4B:604:CL7:CGA	2.40	0.51
20:44:292:VAL:HG13	21:44:406:CL7:H141	1.92	0.51
21:1B:603:CL7:H3A	21:1B:603:CL7:CGA	2.40	0.51
16:12:250:LEU:HD21	21:12:508:CL7:HAB	1.92	0.51
18:11:111:PHE:O	18:11:116:GLY:N	2.37	0.51
18:11:214:GLY:CA	32:11:422:ZEX:H362	2.37	0.51
18:11:276:VAL:O	18:11:278:PRO:HD3	2.09	0.51
2:2B:65:VAL:HG11	21:2B:605:CL7:HAA1	1.91	0.51
16:22:280:LEU:HD13	16:22:290:PHE:HB3	1.92	0.51
20:24:109:VAL:O	20:24:113:LEU:HG	2.11	0.51
4:3D:52:THR:HA	4:3D:66:TYR:HD2	1.74	0.51
4:3D:258:ILE:HG21	26:3D:409:LHG:H262	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:34:109:VAL:O	20:34:113:LEU:HG	2.11	0.51
6:4F:30:VAL:HB	6:4F:31:PRO:HD3	1.91	0.51
32:42:524:ZEX:C19	21:41:418:CL7:H8	2.28	0.51
2:1B:65:VAL:HG11	21:1B:604:CL7:HAA1	1.91	0.51
16:12:168:ASP:OD2	16:12:171:VAL:N	2.30	0.51
21:12:505:CL7:HBA2	19:23:109:TYR:HB2	1.92	0.51
18:11:258:GLY:O	18:11:262:MET:HG3	2.11	0.51
20:14:93:VAL:HG13	20:14:106:PRO:HB2	1.92	0.51
21:3B:603:CL7:H3A	21:3B:603:CL7:CGA	2.40	0.51
19:33:147:LEU:HD21	21:33:506:CL7:HAB	1.93	0.51
2:4B:344:PRO:HG3	2:4B:429:PRO:HG3	1.90	0.51
21:4B:608:CL7:H12C	24:4B:622:LMG:H132	1.92	0.51
20:14:109:VAL:O	20:14:113:LEU:HG	2.11	0.51
21:14:407:CL7:C3D	32:14:419:ZEX:H163	2.40	0.51
1:2A:283:ILE:HA	1:2A:286:THR:HG22	1.91	0.51
25:23:422:SQD:H141	25:23:422:SQD:H271	1.92	0.51
3:3C:388:ASP:HB3	3:3C:391:LYS:HG2	1.91	0.51
19:33:278:PRO:HD2	19:33:302:THR:HG21	1.91	0.51
21:34:407:CL7:C3D	32:34:419:ZEX:H163	2.40	0.51
21:34:415:CL7:HAA2	21:34:415:CL7:HBD	1.93	0.51
4:4D:63:ALA:HB1	4:4D:68:GLU:HB3	1.93	0.51
18:41:276:VAL:O	18:41:278:PRO:HD3	2.09	0.51
18:41:303:ALA:HB3	18:41:306:PHE:HD2	1.74	0.51
21:41:417:CL7:H3A	21:41:417:CL7:CGA	2.39	0.51
21:12:505:CL7:HMD3	32:12:520:ZEX:C16	2.40	0.51
21:11:417:CL7:CGA	21:11:417:CL7:H3A	2.39	0.51
19:13:108:LEU:O	19:13:112:THR:HG22	2.10	0.51
3:2C:388:ASP:HB3	3:2C:391:LYS:HG2	1.91	0.51
21:21:417:CL7:H3A	21:21:417:CL7:CGA	2.39	0.51
20:24:93:VAL:HG13	20:24:106:PRO:HB2	1.93	0.51
20:24:148:PHE:HZ	32:24:420:ZEX:HO3	1.58	0.51
2:3B:65:VAL:HG11	21:3B:604:CL7:HAA1	1.91	0.51
21:32:501:CL7:HMD2	21:32:503:CL7:O2A	2.10	0.51
3:4C:199:ASP:OD2	3:4C:209:ARG:NH2	2.36	0.51
7:4H:52:HIS:NE2	7:4H:61:ALA:O	2.40	0.51
13:4X:33:GLN:OE1	13:4X:36:LYS:NZ	2.26	0.51
16:42:102:VAL:O	16:42:105:SER:OG	2.29	0.51
21:42:505:CL7:HMD3	32:42:520:ZEX:C16	2.40	0.51
18:41:111:PHE:O	18:41:116:GLY:N	2.37	0.51
18:41:211:LEU:HD12	32:41:422:ZEX:H382	1.93	0.51
21:1B:603:CL7:H3A	21:1B:603:CL7:O1A	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:13:147:LEU:HD21	21:13:506:CL7:HAB	1.93	0.51
21:13:510:CL7:HBD	21:13:510:CL7:HBA1	1.92	0.51
19:23:147:LEU:HD21	21:23:407:CL7:HAB	1.93	0.51
4:3D:186:GLY:HA3	4:3D:324:LEU:HD22	1.93	0.51
3:4C:388:ASP:HB3	3:4C:391:LYS:HG2	1.91	0.51
21:42:501:CL7:HMD2	21:42:503:CL7:O2A	2.10	0.51
21:44:415:CL7:HAA2	21:44:415:CL7:HBD	1.93	0.51
16:12:199:PHE:CE2	32:23:423:ZEX:H382	2.46	0.51
21:12:501:CL7:HMD2	21:12:503:CL7:O2A	2.10	0.51
21:12:507:CL7:HMD3	21:12:509:CL7:H171	1.91	0.51
20:14:304:ARG:HG3	32:14:418:ZEX:H23	1.93	0.51
8:2I:20:PHE:O	8:2I:24:ILE:HG23	2.11	0.51
21:22:513:CL7:NB	32:22:522:ZEX:H41	2.26	0.51
21:42:513:CL7:NB	32:42:522:ZEX:H41	2.26	0.51
18:41:315:ASN:CB	32:41:421:ZEX:H361	2.10	0.51
20:44:109:VAL:O	20:44:113:LEU:HG	2.11	0.51
1:1A:19:SER:O	1:1A:23:SER:HB3	2.11	0.51
21:1B:607:CL7:H12C	24:1B:621:LMG:H132	1.92	0.51
21:2B:604:CL7:H3A	21:2B:604:CL7:CGA	2.40	0.51
18:21:197:THR:HB	18:21:200:TYR:CD2	2.46	0.51
1:3A:28:LEU:HD12	25:3A:406:SQD:H112	1.93	0.51
21:3A:401:CL7:H41C	21:3A:407:CL7:OBB	2.11	0.51
16:32:345:THR:HG22	19:43:19:ARG:HD3	1.92	0.51
19:33:271:PHE:O	19:33:304:ARG:NH2	2.43	0.51
20:34:304:ARG:HG3	32:34:418:ZEX:H23	1.93	0.51
2:4B:65:VAL:HG11	21:4B:605:CL7:HAA1	1.91	0.51
16:42:280:LEU:HD13	16:42:290:PHE:HB3	1.92	0.51
18:41:270:CYS:O	18:41:310:ARG:NH1	2.40	0.51
1:1A:28:LEU:HD12	25:1A:406:SQD:H112	1.93	0.51
1:1A:195:HIS:CD2	1:1A:293:MET:HE2	2.46	0.51
4:1D:186:GLY:HA3	4:1D:324:LEU:HD22	1.93	0.51
20:14:151:GLU:OE2	20:14:152:TRP:N	2.42	0.51
2:2B:91:ILE:HG12	2:2B:92:LEU:H	1.76	0.51
21:2B:608:CL7:H12C	24:2B:622:LMG:H132	1.92	0.51
4:2D:186:GLY:HA3	4:2D:324:LEU:HD22	1.93	0.51
4:2D:258:ILE:HD13	26:2D:409:LHG:HC82	1.92	0.51
21:21:408:CL7:H13	32:21:422:ZEX:H402	1.91	0.51
19:23:309:ASN:OD1	32:23:420:ZEX:C36	2.49	0.51
21:23:411:CL7:HBD	21:23:411:CL7:HBA1	1.92	0.51
21:23:416:CL7:HMC2	32:24:420:ZEX:H391	1.92	0.51
1:3A:19:SER:O	1:3A:23:SER:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:195:HIS:CD2	1:3A:293:MET:HE2	2.46	0.51
16:32:250:LEU:HD21	21:32:508:CL7:HAB	1.92	0.51
21:32:518:CL7:HAA2	21:32:518:CL7:HBD	1.93	0.51
21:33:515:CL7:HMC2	32:34:420:ZEX:H391	1.92	0.51
25:33:521:SQD:H271	25:33:521:SQD:H141	1.92	0.51
1:4A:84:PRO:HA	1:4A:112:TYR:CG	2.47	0.51
8:4I:20:PHE:O	8:4I:24:ILE:HG23	2.11	0.51
18:41:197:THR:HB	18:41:200:TYR:CD2	2.46	0.51
19:43:108:LEU:O	19:43:112:THR:HG22	2.10	0.51
21:1A:401:CL7:H41C	21:1A:407:CL7:OBB	2.11	0.50
4:2D:63:ALA:HB1	4:2D:68:GLU:HB3	1.93	0.50
18:21:211:LEU:HD12	32:21:422:ZEX:H382	1.93	0.50
20:24:304:ARG:HG3	32:24:418:ZEX:H23	1.93	0.50
26:3B:625:LHG:HC11	10:3L:13:LEU:HA	1.93	0.50
21:43:411:CL7:HBD	21:43:411:CL7:HBA1	1.92	0.50
20:44:304:ARG:HG3	32:44:418:ZEX:H23	1.93	0.50
16:12:69:GLN:NE2	21:12:502:CL7:HAA1	2.23	0.50
21:12:513:CL7:NB	32:12:522:ZEX:H41	2.26	0.50
21:12:518:CL7:HAA2	21:12:518:CL7:HBD	1.93	0.50
25:13:521:SQD:H141	25:13:521:SQD:H271	1.92	0.50
20:14:116:PHE:CD2	32:14:420:ZEX:H32	2.46	0.50
1:2A:19:SER:O	1:2A:23:SER:HB3	2.11	0.50
4:2D:171:SER:HB2	4:2D:176:SER:HB2	1.94	0.50
21:22:501:CL7:HMD2	21:22:503:CL7:O2A	2.10	0.50
21:21:408:CL7:C14	32:21:422:ZEX:H402	2.41	0.50
3:3C:87:PHE:HA	3:3C:96:GLN:NE2	2.27	0.50
3:3C:268:PRO:HA	21:3C:506:CL7:HED2	1.93	0.50
16:32:340:PHE:HA	16:32:346:VAL:HG21	1.94	0.50
21:34:408:CL7:O1A	21:34:409:CL7:OBB	2.28	0.50
2:4B:142:ASP:HB2	7:4H:19:ALA:HA	1.92	0.50
3:4C:268:PRO:HA	21:4C:506:CL7:HED2	1.93	0.50
4:4D:171:SER:HB2	4:4D:176:SER:HB2	1.94	0.50
16:12:340:PHE:HA	16:12:346:VAL:HG21	1.94	0.50
18:11:197:THR:HB	18:11:200:TYR:CD2	2.46	0.50
3:2C:477:TYR:CZ	3:2C:481:LEU:HD21	2.46	0.50
21:3A:401:CL7:H141	21:3A:407:CL7:H152	1.94	0.50
2:3B:91:ILE:HG12	2:3B:92:LEU:H	1.76	0.50
18:31:37:ILE:HG22	18:31:105:LEU:HD13	1.92	0.50
1:4A:19:SER:O	1:4A:23:SER:HB3	2.11	0.50
2:4B:251:ALA:HB2	2:4B:466:HIS:CG	2.46	0.50
4:4D:11:ARG:HG3	4:4D:15:ASP:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:87:PHE:HA	3:1C:96:GLN:NE2	2.27	0.50
21:13:515:CL7:HMC2	32:14:420:ZEX:H391	1.92	0.50
4:2D:143:VAL:O	4:2D:146:SER:OG	2.21	0.50
21:22:505:CL7:HMD3	32:22:520:ZEX:C16	2.40	0.50
18:21:68:LEU:HB3	21:21:404:CL7:HED1	1.94	0.50
3:3C:477:TYR:CZ	3:3C:481:LEU:HD21	2.46	0.50
18:41:68:LEU:HB3	21:41:404:CL7:HED1	1.94	0.50
19:43:147:LEU:HD21	21:43:407:CL7:HAB	1.93	0.50
20:44:93:VAL:HG13	20:44:106:PRO:HB2	1.93	0.50
21:1A:401:CL7:H141	21:1A:407:CL7:H152	1.94	0.50
2:1B:251:ALA:HB2	2:1B:466:HIS:CG	2.46	0.50
1:2A:195:HIS:CD2	1:2A:293:MET:HE2	2.46	0.50
32:33:525:ZEX:C38	16:42:262:TYR:HB2	2.41	0.50
21:4B:604:CL7:H101	21:4B:606:CL7:H193	1.94	0.50
26:4B:626:LHG:HC11	10:4L:13:LEU:HA	1.93	0.50
4:4D:186:GLY:HA3	4:4D:324:LEU:HD22	1.93	0.50
18:41:190:VAL:HG22	32:41:422:ZEX:H361	1.94	0.50
18:11:68:LEU:HB3	21:11:404:CL7:HED1	1.94	0.50
21:13:502:CL7:H51C	21:22:518:CL7:H201	1.93	0.50
1:2A:28:LEU:HD12	25:2A:406:SQD:H112	1.93	0.50
1:2A:84:PRO:HA	1:2A:112:TYR:CG	2.46	0.50
2:2B:54:PRO:HD2	2:2B:57:ARG:HG3	1.94	0.50
21:2B:604:CL7:H101	21:2B:606:CL7:H193	1.94	0.50
1:4A:195:HIS:CD2	1:4A:293:MET:HE2	2.46	0.50
3:4C:477:TYR:CZ	3:4C:481:LEU:HD21	2.46	0.50
21:1B:603:CL7:H101	21:1B:605:CL7:H193	1.94	0.50
3:1C:268:PRO:HA	21:1C:506:CL7:HED2	1.93	0.50
4:1D:171:SER:HB2	4:1D:176:SER:HB2	1.94	0.50
25:11:423:SQD:O7	25:11:423:SQD:O4	2.28	0.50
32:13:522:ZEX:H382	16:22:199:PHE:CE2	2.46	0.50
2:2B:251:ALA:HB2	2:2B:466:HIS:CG	2.46	0.50
2:2B:344:PRO:HB3	2:2B:401:PHE:CE1	2.47	0.50
7:2H:52:HIS:NE2	7:2H:61:ALA:O	2.40	0.50
20:24:210:LEU:HD21	21:24:417:CL7:C1B	2.42	0.50
21:3B:603:CL7:H101	21:3B:605:CL7:H193	1.94	0.50
18:31:315:ASN:HB2	32:31:421:ZEX:C36	2.20	0.50
2:4B:54:PRO:HD2	2:4B:57:ARG:HG3	1.94	0.50
21:41:408:CL7:C14	32:41:422:ZEX:H402	2.41	0.50
4:1D:63:ALA:HB1	4:1D:68:GLU:HB3	1.93	0.50
7:1H:52:HIS:NE2	7:1H:61:ALA:O	2.40	0.50
21:2A:401:CL7:H141	21:2A:407:CL7:H152	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2C:87:PHE:HA	3:2C:96:GLN:NE2	2.27	0.50
32:22:524:ZEX:C19	21:21:418:CL7:H8	2.28	0.50
21:32:513:CL7:NB	32:32:522:ZEX:H41	2.26	0.50
32:32:524:ZEX:C19	21:31:418:CL7:H8	2.28	0.50
21:31:408:CL7:C14	32:31:422:ZEX:H402	2.41	0.50
2:4B:91:ILE:HG12	2:4B:92:LEU:H	1.76	0.50
2:4B:344:PRO:HB3	2:4B:401:PHE:CE1	2.47	0.50
19:43:94:MET:SD	32:43:401:ZEX:H363	2.48	0.50
20:44:61:GLY:HA2	20:44:111:GLY:HA2	1.94	0.50
2:1B:54:PRO:HD2	2:1B:57:ARG:HG3	1.94	0.50
3:1C:477:TYR:CZ	3:1C:481:LEU:HD21	2.46	0.50
5:1E:16:SER:OG	5:1E:17:ILE:N	2.45	0.50
3:2C:199:ASP:OD2	3:2C:209:ARG:NH2	2.36	0.50
8:3I:20:PHE:O	8:3I:24:ILE:HG23	2.11	0.50
2:4B:7:ARG:NH2	26:4B:624:LHG:O5	2.35	0.50
19:43:34:GLN:HG3	19:43:38:MET:HE3	1.94	0.50
19:13:305:PHE:HZ	32:13:519:ZEX:H362	1.77	0.49
4:2D:11:ARG:HG3	4:2D:15:ASP:HB2	1.94	0.49
16:22:340:PHE:HA	16:22:346:VAL:HG21	1.94	0.49
21:22:518:CL7:HBD	21:22:518:CL7:HAA2	1.93	0.49
20:24:116:PHE:CD2	32:24:420:ZEX:H32	2.47	0.49
20:24:275:ASN:ND2	18:31:115:ILE:CG1	2.75	0.49
1:3A:84:PRO:HA	1:3A:112:TYR:CG	2.46	0.49
2:3B:54:PRO:HD2	2:3B:57:ARG:HG3	1.94	0.49
2:3B:251:ALA:HB2	2:3B:466:HIS:CG	2.46	0.49
4:3D:63:ALA:HB1	4:3D:68:GLU:HB3	1.93	0.49
11:3M:31:SER:OG	11:4M:31:SER:OG	2.30	0.49
21:32:502:CL7:C2B	21:32:504:CL7:HAB	2.42	0.49
20:34:116:PHE:CD2	32:34:420:ZEX:H32	2.46	0.49
4:4D:73:LEU:O	4:4D:175:THR:OG1	2.16	0.49
2:1B:344:PRO:HB3	2:1B:401:PHE:CE1	2.47	0.49
26:1B:625:LHG:HC11	10:1L:13:LEU:HA	1.93	0.49
18:11:211:LEU:HD12	32:11:422:ZEX:H382	1.93	0.49
21:11:408:CL7:C14	32:11:422:ZEX:H402	2.41	0.49
21:2A:401:CL7:H41C	21:2A:407:CL7:OBB	2.11	0.49
3:2C:268:PRO:HA	21:2C:506:CL7:HED2	1.93	0.49
18:21:190:VAL:HG22	32:21:422:ZEX:H361	1.94	0.49
20:24:61:GLY:HA2	20:24:111:GLY:HA2	1.94	0.49
2:3B:142:ASP:HB2	7:3H:19:ALA:HA	1.92	0.49
21:3B:607:CL7:H12C	24:3B:621:LMG:H132	1.92	0.49
4:3D:171:SER:HB2	4:3D:176:SER:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:32:502:CL7:HMD2	21:32:503:CL7:H141	1.94	0.49
20:44:210:LEU:HD21	21:44:417:CL7:C1B	2.42	0.49
2:1B:91:ILE:HG12	2:1B:92:LEU:H	1.76	0.49
8:1I:20:PHE:O	8:1I:24:ILE:HG23	2.11	0.49
32:13:525:ZEX:C38	16:22:262:TYR:HB2	2.41	0.49
20:14:210:LEU:HD21	21:14:417:CL7:C1B	2.42	0.49
21:22:510:CL7:O2A	21:22:510:CL7:H2A	2.12	0.49
18:21:238:SER:O	18:21:242:ASN:ND2	2.37	0.49
1:3A:49:VAL:HG22	30:3D:407:PL9:H503	1.94	0.49
1:3A:174:LEU:HD22	22:3A:402:PHO:H143	1.95	0.49
18:31:68:LEU:HB3	21:31:404:CL7:HED1	1.94	0.49
18:31:197:THR:HB	18:31:200:TYR:CD2	2.46	0.49
2:4B:333:GLY:O	2:4B:439:SER:HB3	2.13	0.49
16:42:42:ALA:O	16:42:46:THR:OG1	2.30	0.49
16:42:69:GLN:NE2	21:42:502:CL7:HAA1	2.23	0.49
21:42:518:CL7:HAA2	21:42:518:CL7:HBD	1.93	0.49
2:1B:142:ASP:HB2	7:1H:19:ALA:HA	1.92	0.49
2:2B:333:GLY:O	2:2B:439:SER:HB3	2.13	0.49
19:23:34:GLN:HG3	19:23:38:MET:HE3	1.94	0.49
19:33:305:PHE:HZ	32:33:519:ZEX:H362	1.77	0.49
1:4A:28:LEU:HD12	25:4A:406:SQD:H112	1.93	0.49
3:4C:87:PHE:HA	3:4C:96:GLN:NE2	2.27	0.49
21:41:402:CL7:C2D	21:41:404:CL7:H42C	2.43	0.49
1:1A:174:LEU:HD22	22:1A:402:PHO:H143	1.95	0.49
2:1B:7:ARG:NH2	26:1B:623:LHG:O5	2.35	0.49
16:12:262:TYR:HB2	32:23:401:ZEX:C38	2.41	0.49
26:2B:626:LHG:HC11	10:2L:13:LEU:HA	1.93	0.49
21:21:418:CL7:H2A	21:21:418:CL7:CED	2.43	0.49
19:23:129:PHE:HZ	32:23:423:ZEX:O3	1.95	0.49
2:3B:344:PRO:HB3	2:3B:401:PHE:CE1	2.47	0.49
20:34:95:VAL:HG12	20:34:101:ILE:HA	1.95	0.49
1:1A:84:PRO:HA	1:1A:112:TYR:CG	2.46	0.49
21:12:502:CL7:C2B	21:12:504:CL7:HAB	2.42	0.49
21:21:402:CL7:C2D	21:21:404:CL7:H42C	2.43	0.49
21:4A:401:CL7:H141	21:4A:407:CL7:H152	1.94	0.49
2:4B:270:THR:O	2:4B:272:PRO:HD3	2.13	0.49
21:41:418:CL7:H2A	21:41:418:CL7:CED	2.43	0.49
20:44:116:PHE:CD2	32:44:420:ZEX:H32	2.46	0.49
20:44:327:LEU:HD22	32:44:418:ZEX:H362	1.94	0.49
21:1B:612:CL7:H62C	21:1B:615:CL7:HMB3	1.95	0.49
19:13:34:GLN:HG3	19:13:38:MET:HE3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2B:613:CL7:H62C	21:2B:616:CL7:HMB3	1.95	0.49
18:21:115:ILE:CG1	20:34:275:ASN:ND2	2.75	0.49
20:34:210:LEU:HD21	21:34:417:CL7:C1B	2.42	0.49
16:42:340:PHE:HA	16:42:346:VAL:HG21	1.94	0.49
3:1C:409:THR:OG1	3:1C:410:HIS:ND1	2.35	0.49
21:11:418:CL7:H2A	21:11:418:CL7:CED	2.43	0.49
21:13:508:CL7:H41C	21:13:508:CL7:H61C	1.53	0.49
4:3D:283:ILE:HA	4:3D:286:VAL:HG12	1.94	0.49
18:31:152:ILE:HG21	21:31:408:CL7:H43C	1.94	0.49
21:33:508:CL7:H61C	21:33:508:CL7:H41C	1.53	0.49
1:4A:288:MET:O	1:4A:292:THR:HG23	2.13	0.49
4:4D:295:TYR:OH	4:4D:325:ARG:NH1	2.32	0.49
19:43:167:TYR:OH	19:43:274:GLU:OE2	2.29	0.49
1:1A:49:VAL:HG22	30:1D:407:PL9:H503	1.94	0.49
4:1D:295:TYR:OH	4:1D:325:ARG:NH1	2.32	0.49
18:11:190:VAL:HG22	32:11:422:ZEX:H361	1.93	0.49
1:2A:288:MET:O	1:2A:292:THR:HG23	2.13	0.49
1:2A:331:MET:CG	4:2D:323:GLY:HA3	2.43	0.49
2:2B:142:ASP:HB2	7:2H:19:ALA:HA	1.92	0.49
2:4B:206:LEU:HD13	21:4B:604:CL7:HED3	1.95	0.49
21:1A:401:CL7:H41C	21:1A:401:CL7:H62C	1.48	0.49
19:23:167:TYR:OH	19:23:274:GLU:OE2	2.29	0.49
2:3B:7:ARG:NH2	26:3B:623:LHG:O5	2.35	0.49
25:31:423:SQD:O7	25:31:423:SQD:O4	2.28	0.49
20:34:61:GLY:HA2	20:34:111:GLY:HA2	1.94	0.49
19:43:259:ASN:HB3	21:43:402:CL7:H42C	1.94	0.49
20:44:188:ASP:HB3	20:44:191:THR:OG1	2.13	0.49
3:1C:323:GLN:HG3	3:1C:373:PHE:CD2	2.48	0.48
4:1D:11:ARG:HG3	4:1D:15:ASP:HB2	1.94	0.48
21:12:502:CL7:HMD2	21:12:503:CL7:H141	1.94	0.48
20:14:61:GLY:HA2	20:14:111:GLY:HA2	1.94	0.48
16:22:8:ASN:O	16:22:8:ASN:ND2	2.46	0.48
21:23:406:CL7:H71C	32:23:421:ZEX:C19	2.43	0.48
1:3A:288:MET:O	1:3A:292:THR:HG23	2.13	0.48
1:3A:331:MET:CG	4:3D:323:GLY:HA3	2.43	0.48
21:31:418:CL7:H2A	21:31:418:CL7:CED	2.43	0.48
19:33:109:TYR:HB2	21:42:505:CL7:HBA2	1.93	0.48
1:4A:331:MET:CG	4:4D:323:GLY:HA3	2.43	0.48
2:4B:241:ASN:O	2:4B:244:THR:HG22	2.13	0.48
4:4D:283:ILE:HA	4:4D:286:VAL:HG12	1.95	0.48
21:42:510:CL7:O2A	21:42:510:CL7:H2A	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:333:GLY:O	2:1B:439:SER:HB3	2.13	0.48
16:12:77:VAL:HG21	16:12:275:PHE:CZ	2.49	0.48
16:12:330:SER:HB2	19:23:113:LYS:HG3	1.96	0.48
21:11:402:CL7:C2D	21:11:404:CL7:H42C	2.43	0.48
20:14:95:VAL:HG12	20:14:101:ILE:HA	1.95	0.48
2:2B:270:THR:O	2:2B:272:PRO:HD3	2.13	0.48
3:2C:71:MET:HE3	23:2C:518:8CT:C40	2.43	0.48
16:22:77:VAL:HG21	16:22:275:PHE:CZ	2.49	0.48
21:22:502:CL7:HMD2	21:22:503:CL7:H141	1.94	0.48
2:3B:145:LYS:NZ	7:3H:18:GLU:OE1	2.40	0.48
2:3B:270:THR:O	2:3B:272:PRO:HD3	2.12	0.48
16:32:262:TYR:HB2	32:43:401:ZEX:C38	2.41	0.48
19:33:149:PHE:HE2	21:33:512:CL7:HHB	1.78	0.48
20:34:230:GLU:OE1	20:34:230:GLU:N	2.37	0.48
21:34:406:CL7:H61C	21:34:406:CL7:H101	1.53	0.48
21:4A:401:CL7:H41C	21:4A:407:CL7:OBB	2.11	0.48
3:4C:325:GLN:HB2	3:4C:408:MET:HG3	1.95	0.48
1:1A:331:MET:CG	4:1D:323:GLY:HA3	2.43	0.48
21:1B:612:CL7:H62C	21:1B:612:CL7:H102	1.71	0.48
11:1M:31:SER:OG	11:2M:31:SER:OG	2.30	0.48
1:2A:174:LEU:HD22	22:2A:402:PHO:H143	1.95	0.48
21:22:502:CL7:C2B	21:22:504:CL7:HAB	2.42	0.48
21:3B:612:CL7:H62C	21:3B:615:CL7:HMB3	1.95	0.48
3:3C:323:GLN:HG3	3:3C:373:PHE:CD2	2.48	0.48
16:32:270:VAL:HG23	16:32:271:PHE:CD2	2.48	0.48
21:32:518:CL7:H201	21:43:403:CL7:H51C	1.93	0.48
2:4B:74:SER:OG	2:4B:102:GLU:OE2	2.19	0.48
3:4C:71:MET:HE3	23:4C:518:8CT:C40	2.43	0.48
16:42:113:THR:HG21	21:42:513:CL7:HED1	1.96	0.48
21:43:406:CL7:H71C	32:43:421:ZEX:C19	2.43	0.48
16:12:8:ASN:O	16:12:8:ASN:ND2	2.46	0.48
21:11:406:CL7:H12C	32:11:422:ZEX:H3	1.96	0.48
16:22:168:ASP:OD2	16:22:171:VAL:N	2.30	0.48
16:22:270:VAL:HG23	16:22:271:PHE:CD2	2.48	0.48
21:21:406:CL7:H12C	32:21:422:ZEX:H3	1.96	0.48
4:3D:11:ARG:HG3	4:3D:15:ASP:HB2	1.94	0.48
4:3D:118:VAL:HG23	4:3D:152:TYR:HE1	1.78	0.48
32:33:522:ZEX:H382	16:42:199:PHE:CE2	2.48	0.48
20:34:151:GLU:OE2	20:34:152:TRP:N	2.42	0.48
21:4B:605:CL7:HBA2	21:4B:606:CL7:CAD	2.44	0.48
16:42:270:VAL:HG23	16:42:271:PHE:CD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:42:502:CL7:C2B	21:42:504:CL7:HAB	2.42	0.48
21:42:505:CL7:H41C	21:42:505:CL7:H62C	1.49	0.48
18:41:214:GLY:CA	32:41:422:ZEX:H362	2.37	0.48
18:41:256:ILE:HG23	18:41:324:MET:HE3	1.96	0.48
4:1D:118:VAL:HG23	4:1D:152:TYR:HE1	1.78	0.48
16:12:270:VAL:HG23	16:12:271:PHE:CD2	2.48	0.48
21:13:504:CL7:H93C	21:13:504:CL7:H111	1.73	0.48
21:14:406:CL7:H41C	21:14:406:CL7:H62C	1.51	0.48
2:2B:241:ASN:O	2:2B:244:THR:HG22	2.13	0.48
4:2D:118:VAL:HG23	4:2D:152:TYR:HE1	1.78	0.48
19:23:259:ASN:HB3	21:23:402:CL7:H42C	1.95	0.48
1:3A:202:VAL:HG22	21:3A:401:CL7:C1B	2.44	0.48
16:32:77:VAL:HG21	16:32:275:PHE:CZ	2.49	0.48
18:31:291:GLY:HA3	24:31:401:LMG:HC72	1.96	0.48
21:31:406:CL7:H12C	32:31:422:ZEX:H3	1.96	0.48
19:33:259:ASN:HB3	21:33:501:CL7:H42C	1.95	0.48
32:34:418:ZEX:H201	32:34:418:ZEX:H15	1.61	0.48
16:42:77:VAL:HG21	16:42:275:PHE:CZ	2.49	0.48
21:42:510:CL7:H61C	21:42:510:CL7:H41C	1.54	0.48
21:42:516:CL7:H3A	21:42:516:CL7:HBA1	1.55	0.48
20:44:95:VAL:HG12	20:44:101:ILE:HA	1.95	0.48
1:1A:212:ALA:HB2	4:1D:210:CYS:HB2	1.95	0.48
2:1B:241:ASN:O	2:1B:244:THR:HG22	2.13	0.48
21:13:505:CL7:H71C	32:13:520:ZEX:C19	2.43	0.48
3:2C:323:GLN:HG3	3:2C:373:PHE:CD2	2.48	0.48
21:22:510:CL7:H141	21:22:510:CL7:H162	1.62	0.48
1:3A:212:ALA:HB2	4:3D:210:CYS:HB2	1.95	0.48
2:3B:100:SER:OG	2:3B:102:GLU:OE1	2.20	0.48
2:3B:206:LEU:HD13	21:3B:603:CL7:HED3	1.95	0.48
21:3B:608:CL7:HBA1	21:3B:608:CL7:H3A	1.54	0.48
3:3C:71:MET:HE3	23:3C:518:8CT:C40	2.44	0.48
19:33:34:GLN:HG3	19:33:38:MET:HE3	1.94	0.48
21:33:505:CL7:H71C	32:33:520:ZEX:C19	2.43	0.48
21:4B:613:CL7:H62C	21:4B:616:CL7:HMB3	1.95	0.48
21:42:509:CL7:H161	21:42:509:CL7:H141	1.49	0.48
18:41:152:ILE:HG21	21:41:408:CL7:H43C	1.94	0.48
21:41:406:CL7:H12C	32:41:422:ZEX:H3	1.96	0.48
20:44:214:THR:HG21	20:44:225:ALA:HB3	1.96	0.48
18:11:152:ILE:HG21	21:11:408:CL7:H43C	1.94	0.48
19:13:259:ASN:HB3	21:13:501:CL7:H42C	1.94	0.48
1:2A:223:LEU:O	1:2A:224:VAL:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:206:LEU:HD13	21:2B:604:CL7:HED3	1.95	0.48
21:2D:404:CL7:H61C	21:2D:404:CL7:H41C	1.67	0.48
18:21:152:ILE:HG21	21:21:408:CL7:H43C	1.94	0.48
2:3B:241:ASN:O	2:3B:244:THR:HG22	2.13	0.48
16:32:69:GLN:NE2	21:32:502:CL7:HAA1	2.23	0.48
19:33:129:PHE:HZ	32:33:522:ZEX:O3	1.95	0.48
16:42:8:ASN:O	16:42:8:ASN:ND2	2.46	0.48
1:1A:202:VAL:HG22	21:1A:401:CL7:C1B	2.44	0.48
2:1B:270:THR:O	2:1B:272:PRO:HD3	2.12	0.48
21:1B:607:CL7:HED3	21:1B:607:CL7:HBD	1.66	0.48
16:12:271:PHE:O	16:12:304:ARG:NH2	2.47	0.48
19:13:69:GLN:HB2	21:13:503:CL7:HED2	1.96	0.48
19:13:129:PHE:HZ	32:13:522:ZEX:O3	1.94	0.48
2:2B:195:PRO:HB2	7:2H:56:LEU:HD13	1.95	0.48
3:2C:131:LEU:O	3:2C:134:SER:OG	2.27	0.48
3:2C:325:GLN:HB2	3:2C:408:MET:HG3	1.95	0.48
19:23:69:GLN:HB2	21:23:404:CL7:HED2	1.96	0.48
20:24:95:VAL:HG12	20:24:101:ILE:HA	1.95	0.48
20:24:327:LEU:HD22	32:24:418:ZEX:H362	1.94	0.48
1:3A:223:LEU:O	1:3A:224:VAL:C	2.56	0.48
21:3B:604:CL7:HBA2	21:3B:605:CL7:CAD	2.44	0.48
7:3H:52:HIS:NE2	7:3H:61:ALA:O	2.40	0.48
16:32:271:PHE:O	16:32:304:ARG:NH2	2.47	0.48
21:31:416:CL7:HED3	21:31:416:CL7:HBD	1.71	0.48
19:33:40:PHE:CD1	21:42:517:CL7:H2	2.49	0.48
21:33:507:CL7:H41C	21:33:507:CL7:H61C	1.62	0.48
2:4B:195:PRO:HB2	7:4H:56:LEU:HD13	1.95	0.48
16:42:65:VAL:HG13	21:42:504:CL7:HMA2	1.96	0.48
1:1A:223:LEU:O	1:1A:224:VAL:C	2.56	0.48
1:1A:288:MET:O	1:1A:292:THR:HG23	2.13	0.48
3:1C:71:MET:HE3	23:1C:518:8CT:C40	2.43	0.48
21:12:510:CL7:H2A	21:12:510:CL7:O2A	2.12	0.48
18:11:291:GLY:HA3	24:11:401:LMG:HC72	1.96	0.48
19:13:149:PHE:HE2	21:13:512:CL7:HHB	1.78	0.48
19:13:253:LEU:HD12	21:13:509:CL7:HED3	1.96	0.48
16:22:65:VAL:HG13	21:22:504:CL7:HMA2	1.96	0.48
16:22:113:THR:HG21	21:22:513:CL7:HED1	1.96	0.48
21:3A:401:CL7:H91C	21:3A:401:CL7:H111	1.69	0.48
3:3C:325:GLN:HB2	3:3C:408:MET:HG3	1.95	0.48
16:32:102:VAL:O	16:32:105:SER:OG	2.29	0.48
16:32:113:THR:HG21	21:32:513:CL7:HED1	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:31:190:VAL:HG22	32:31:422:ZEX:H361	1.93	0.48
20:34:214:THR:HG21	20:34:225:ALA:HB3	1.96	0.48
1:4A:223:LEU:O	1:4A:224:VAL:C	2.56	0.48
5:4E:26:THR:HG21	31:4F:101:HEM:HMB2	1.96	0.48
21:42:502:CL7:HMD2	21:42:503:CL7:H141	1.94	0.48
5:1E:26:THR:HG21	31:1F:101:HEM:HMB2	1.96	0.48
19:13:49:GLU:CD	19:13:66:CYS:H	2.22	0.48
21:2B:605:CL7:HBA2	21:2B:606:CL7:CAD	2.43	0.48
21:2B:609:CL7:H41C	21:2B:609:CL7:H62C	1.50	0.48
4:2D:256:PHE:O	26:2D:409:LHG:H321	2.14	0.48
4:2D:283:ILE:HA	4:2D:286:VAL:HG12	1.95	0.48
5:2E:26:THR:HG21	31:2F:101:HEM:HMB2	1.96	0.48
20:24:188:ASP:HB3	20:24:191:THR:OG1	2.13	0.48
2:3B:189:VAL:HB	2:3B:207:VAL:HG21	1.96	0.48
5:3E:26:THR:HG21	31:3F:101:HEM:HMB2	1.96	0.48
21:31:402:CL7:C2D	21:31:404:CL7:H42C	2.43	0.48
19:33:69:GLN:HB2	21:33:503:CL7:HED2	1.96	0.48
1:4A:49:VAL:HG22	30:4D:407:PL9:H503	1.94	0.48
2:4B:189:VAL:HB	2:4B:207:VAL:HG21	1.96	0.48
16:42:271:PHE:O	16:42:304:ARG:NH2	2.47	0.48
4:1D:283:ILE:HA	4:1D:286:VAL:HG12	1.95	0.47
19:13:271:PHE:O	19:13:304:ARG:NH2	2.43	0.47
1:2A:49:VAL:HG22	30:2D:407:PL9:H503	1.95	0.47
16:22:69:GLN:NE2	21:22:502:CL7:HAA1	2.23	0.47
16:22:271:PHE:O	16:22:304:ARG:NH2	2.47	0.47
21:21:404:CL7:H41C	21:21:404:CL7:H62C	1.62	0.47
19:23:149:PHE:HE2	21:23:413:CL7:HHB	1.78	0.47
16:32:42:ALA:O	16:32:46:THR:OG1	2.30	0.47
21:4B:609:CL7:HBA1	21:4B:609:CL7:H3A	1.54	0.47
3:4C:323:GLN:HG3	3:4C:373:PHE:CD2	2.48	0.47
4:4D:143:VAL:O	4:4D:146:SER:OG	2.21	0.47
4:4D:256:PHE:O	26:4D:409:LHG:H321	2.14	0.47
3:1C:199:ASP:OD2	3:1C:209:ARG:NH2	2.36	0.47
3:1C:325:GLN:HB2	3:1C:408:MET:HG3	1.95	0.47
21:1D:405:CL7:HBA1	21:1D:405:CL7:H3A	1.59	0.47
21:12:512:CL7:H2	21:12:512:CL7:HMA2	1.96	0.47
19:13:229:LYS:HG2	19:13:230:PRO:HD2	1.97	0.47
21:13:506:CL7:HBA2	21:13:506:CL7:CHA	2.45	0.47
21:13:508:CL7:H8	21:22:516:CL7:H201	1.96	0.47
21:14:405:CL7:CGA	21:14:406:CL7:H12C	2.44	0.47
21:23:407:CL7:HBA2	21:23:407:CL7:CHA	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:24:404:CL7:H3A	21:24:404:CL7:HBA1	1.27	0.47
21:24:406:CL7:H3A	21:24:406:CL7:HBA1	1.62	0.47
2:3B:195:PRO:HB2	7:3H:56:LEU:HD13	1.95	0.47
2:3B:333:GLY:O	2:3B:439:SER:HB3	2.13	0.47
3:3C:301:TYR:HB3	3:3C:309:TYR:HE2	1.79	0.47
16:32:8:ASN:O	16:32:8:ASN:ND2	2.47	0.47
18:31:211:LEU:HD12	32:31:422:ZEX:H382	1.93	0.47
1:4A:174:LEU:HD22	22:4A:402:PHO:H143	1.95	0.47
1:4A:212:ALA:HB2	4:4D:210:CYS:HB2	1.95	0.47
22:4D:408:PHO:HBB1	22:4D:408:PHO:HMB1	1.97	0.47
19:43:136:PHE:HB3	19:43:230:PRO:HG3	1.96	0.47
20:14:327:LEU:HD22	32:14:418:ZEX:H362	1.94	0.47
2:2B:189:VAL:HB	2:2B:207:VAL:HG21	1.96	0.47
4:2D:201:ALA:HB2	30:2D:407:PL9:H353	1.97	0.47
22:2D:408:PHO:HMB1	22:2D:408:PHO:HBB1	1.96	0.47
21:3C:505:CL7:H42C	21:3C:505:CL7:C1C	2.45	0.47
22:3D:408:PHO:H62	22:3D:408:PHO:H41	1.73	0.47
16:32:199:PHE:CE2	32:43:423:ZEX:H382	2.49	0.47
19:33:253:LEU:HD12	21:33:509:CL7:HED3	1.96	0.47
21:33:506:CL7:HBA2	21:33:506:CL7:CHA	2.45	0.47
20:34:327:LEU:HD22	32:34:418:ZEX:H362	1.94	0.47
21:4C:505:CL7:H42C	21:4C:505:CL7:C1C	2.44	0.47
18:41:238:SER:O	18:41:242:ASN:ND2	2.37	0.47
19:43:271:PHE:CZ	21:43:402:CL7:HBA2	2.49	0.47
21:43:407:CL7:HBA2	21:43:407:CL7:CHA	2.45	0.47
2:1B:195:PRO:HB2	7:1H:56:LEU:HD13	1.95	0.47
4:1D:201:ALA:HB2	30:1D:407:PL9:H353	1.97	0.47
20:14:188:ASP:HB3	20:14:191:THR:OG1	2.13	0.47
1:2A:212:ALA:HB2	4:2D:210:CYS:HB2	1.95	0.47
18:21:256:ILE:HG23	18:21:324:MET:HE3	1.96	0.47
18:21:291:GLY:HA3	24:21:401:LMG:HC72	1.96	0.47
21:21:404:CL7:H102	21:21:404:CL7:H13	1.51	0.47
19:23:229:LYS:HG2	19:23:230:PRO:HD2	1.97	0.47
19:23:253:LEU:HD12	21:23:410:CL7:HED3	1.96	0.47
2:3B:42:LEU:HA	2:3B:42:LEU:HD23	1.73	0.47
21:32:510:CL7:H2A	21:32:510:CL7:O2A	2.12	0.47
21:32:512:CL7:HMA2	21:32:512:CL7:H2	1.96	0.47
19:33:49:GLU:CD	19:33:66:CYS:H	2.22	0.47
21:4B:604:CL7:H203	21:4B:604:CL7:H161	1.75	0.47
3:4C:301:TYR:HB3	3:4C:309:TYR:HE2	1.79	0.47
4:4D:118:VAL:HG23	4:4D:152:TYR:HE1	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:42:348:LEU:HD23	16:42:348:LEU:HA	1.64	0.47
2:1B:206:LEU:HD13	21:1B:603:CL7:HED3	1.95	0.47
21:1B:603:CL7:H62C	21:1B:603:CL7:H41C	1.73	0.47
21:1B:604:CL7:H121	21:1B:604:CL7:H162	1.77	0.47
3:1C:301:TYR:HB3	3:1C:309:TYR:HE2	1.79	0.47
21:2B:610:CL7:H3A	21:2B:610:CL7:HBA1	1.50	0.47
21:21:420:CL7:H2A	21:21:420:CL7:O2D	2.14	0.47
19:23:136:PHE:HB3	19:23:230:PRO:HG3	1.96	0.47
21:24:406:CL7:H121	21:24:406:CL7:H162	1.73	0.47
4:3D:201:ALA:HB2	30:3D:407:PL9:H353	1.97	0.47
21:33:504:CL7:H93C	21:33:504:CL7:H111	1.73	0.47
21:34:406:CL7:H41C	21:34:406:CL7:H62C	1.51	0.47
1:4A:202:VAL:HG22	21:4A:401:CL7:C1B	2.44	0.47
3:4C:131:LEU:O	3:4C:134:SER:OG	2.27	0.47
21:43:405:CL7:H93C	21:43:405:CL7:H111	1.74	0.47
4:1D:256:PHE:O	26:1D:409:LHG:H321	2.14	0.47
9:1K:19:PRO:O	9:1K:22:ASP:HB2	2.15	0.47
16:12:102:VAL:O	16:12:105:SER:OG	2.29	0.47
21:11:420:CL7:H2A	21:11:420:CL7:O2D	2.14	0.47
21:13:506:CL7:O1D	21:13:506:CL7:H2A	2.15	0.47
1:2A:202:VAL:HG22	21:2A:401:CL7:C1B	2.44	0.47
3:2C:112:GLY:N	3:2C:116:GLU:O	2.48	0.47
3:2C:301:TYR:HB3	3:2C:309:TYR:HE2	1.79	0.47
18:21:214:GLY:CA	32:21:422:ZEX:H362	2.37	0.47
21:23:404:CL7:H112	21:23:404:CL7:H72C	1.52	0.47
21:3C:503:CL7:H162	21:3C:503:CL7:H141	1.62	0.47
19:33:119:ALA:HB2	19:33:130:HIS:CG	2.50	0.47
20:34:188:ASP:HB3	20:34:191:THR:OG1	2.13	0.47
3:4C:76:ALA:HB2	21:4C:503:CL7:HMD2	1.97	0.47
4:4D:84:LEU:HD23	5:4E:69:ARG:HA	1.96	0.47
21:41:404:CL7:H13	21:41:404:CL7:H102	1.51	0.47
19:43:129:PHE:HZ	32:43:423:ZEX:O3	1.94	0.47
21:43:406:CL7:H43C	32:43:421:ZEX:H8	1.96	0.47
21:43:407:CL7:O1D	21:43:407:CL7:H2A	2.15	0.47
20:44:38:MET:HE3	20:44:38:MET:HB2	1.71	0.47
32:44:403:ZEX:H11	32:44:403:ZEX:H191	1.76	0.47
2:1B:8:VAL:HG23	2:1B:9:HIS:CD2	2.50	0.47
2:1B:189:VAL:HB	2:1B:207:VAL:HG21	1.96	0.47
21:1C:505:CL7:H42C	21:1C:505:CL7:C1C	2.44	0.47
4:1D:84:LEU:HD23	5:1E:69:ARG:HA	1.96	0.47
22:1D:408:PHO:HBB1	22:1D:408:PHO:HMB1	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:12:65:VAL:HG13	21:12:504:CL7:HMA2	1.96	0.47
21:12:517:CL7:H3A	21:12:517:CL7:HBA1	1.48	0.47
18:11:256:ILE:HG23	18:11:324:MET:HE3	1.96	0.47
2:2B:8:VAL:HG23	2:2B:9:HIS:CD2	2.50	0.47
3:2C:476:GLU:CD	4:2D:244:SER:HG	2.18	0.47
21:2C:505:CL7:H3A	21:2C:505:CL7:HBA1	1.63	0.47
4:2D:84:LEU:HD23	5:2E:69:ARG:HA	1.96	0.47
21:22:512:CL7:HMA2	21:22:512:CL7:H2	1.96	0.47
19:23:271:PHE:CZ	21:23:402:CL7:HBA2	2.50	0.47
21:23:407:CL7:H2A	21:23:407:CL7:O1D	2.15	0.47
20:24:214:THR:HG21	20:24:225:ALA:HB3	1.96	0.47
21:24:405:CL7:CGA	21:24:406:CL7:H12C	2.45	0.47
1:3A:154:THR:HG22	21:3A:401:CL7:H43C	1.97	0.47
21:3C:506:CL7:H121	21:3C:507:CL7:H192	1.97	0.47
4:3D:256:PHE:O	26:3D:409:LHG:H321	2.14	0.47
21:3D:405:CL7:HBA1	21:3D:405:CL7:H3A	1.59	0.47
9:3K:31:PHE:O	9:3K:34:LEU:HB3	2.15	0.47
18:31:57:THR:HG23	18:31:85:VAL:HB	1.97	0.47
19:33:229:LYS:HG2	19:33:230:PRO:HD2	1.97	0.47
21:33:502:CL7:CGA	21:33:503:CL7:H12C	2.45	0.47
21:34:405:CL7:CGA	21:34:406:CL7:H12C	2.45	0.47
21:34:415:CL7:HBA1	21:34:415:CL7:H3A	1.40	0.47
21:4B:616:CL7:HBA2	21:4B:616:CL7:H11C	1.71	0.47
9:4K:19:PRO:O	9:4K:22:ASP:HB2	2.15	0.47
16:42:335:ARG:O	16:42:338:THR:OG1	2.30	0.47
25:41:423:SQD:O7	25:41:423:SQD:O4	2.28	0.47
32:44:403:ZEX:H15	32:44:403:ZEX:H201	1.65	0.47
21:44:406:CL7:H143	21:44:406:CL7:H111	1.80	0.47
21:1B:609:CL7:HBA1	21:1B:609:CL7:H3A	1.50	0.47
16:12:113:THR:HG21	21:12:513:CL7:HED1	1.96	0.47
21:12:516:CL7:H201	21:23:409:CL7:H8	1.96	0.47
19:13:119:ALA:HB2	19:13:130:HIS:CG	2.50	0.47
21:2C:505:CL7:H42C	21:2C:505:CL7:C1C	2.45	0.47
8:2I:18:LEU:HD23	8:2I:18:LEU:HA	1.73	0.47
19:23:146:HIS:ND1	21:23:408:CL7:OBD	2.48	0.47
21:23:406:CL7:H43C	32:23:421:ZEX:H8	1.97	0.47
2:3B:8:VAL:HG23	2:3B:9:HIS:CD2	2.50	0.47
3:3C:76:ALA:HB2	21:3C:503:CL7:HMD2	1.97	0.47
4:3D:84:LEU:HD23	5:3E:69:ARG:HA	1.96	0.47
16:32:330:SER:HB2	19:43:113:LYS:HG3	1.97	0.47
19:33:146:HIS:ND1	21:33:507:CL7:OBD	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:34:197:ILE:HD11	20:34:233:ILE:HG13	1.97	0.47
21:4C:509:CL7:H202	21:4C:512:CL7:HAC1	1.97	0.47
19:43:69:GLN:HB2	21:43:404:CL7:HED2	1.96	0.47
21:1B:604:CL7:HBA2	21:1B:605:CL7:CAD	2.44	0.47
21:1C:501:CL7:H202	21:1C:501:CL7:H162	1.69	0.47
9:1K:31:PHE:O	9:1K:34:LEU:HB3	2.15	0.47
4:2D:208:LEU:O	4:2D:212:ILE:HG23	2.15	0.47
21:22:516:CL7:HBA1	21:22:516:CL7:H12C	1.71	0.47
21:23:405:CL7:H93C	21:23:405:CL7:H111	1.74	0.47
25:23:422:SQD:H81	25:23:422:SQD:H45	1.53	0.47
21:3C:509:CL7:HBA2	21:3C:509:CL7:H3A	1.63	0.47
9:3K:19:PRO:O	9:3K:22:ASP:HB2	2.15	0.47
2:4B:8:VAL:HG23	2:4B:9:HIS:CD2	2.50	0.47
4:4D:201:ALA:HB2	30:4D:407:PL9:H353	1.97	0.47
21:41:417:CL7:HBA1	21:41:417:CL7:H12C	1.59	0.47
21:41:420:CL7:H2A	21:41:420:CL7:O2D	2.14	0.47
19:43:146:HIS:ND1	21:43:408:CL7:OBD	2.48	0.47
1:1A:154:THR:HG22	21:1A:401:CL7:H43C	1.97	0.47
4:1D:208:LEU:O	4:1D:212:ILE:HG23	2.15	0.47
21:12:517:CL7:H2	19:23:40:PHE:CD1	2.50	0.47
19:13:146:HIS:ND1	21:13:507:CL7:OBD	2.48	0.47
21:13:502:CL7:CGA	21:13:503:CL7:H12C	2.44	0.47
20:14:214:THR:HG21	20:14:225:ALA:HB3	1.96	0.47
1:2A:157:VAL:HG11	21:2A:407:CL7:HMC2	1.97	0.47
21:2B:613:CL7:H3A	21:2B:613:CL7:HBA1	1.60	0.47
21:22:505:CL7:H41C	21:22:505:CL7:H62C	1.49	0.47
19:23:305:PHE:HZ	32:23:420:ZEX:H362	1.77	0.47
21:23:417:CL7:CED	32:24:403:ZEX:H172	2.45	0.47
21:24:412:CL7:H61C	21:24:412:CL7:H41C	1.76	0.47
9:3K:15:SER:O	9:3K:18:SER:OG	2.20	0.47
21:33:504:CL7:H41C	21:33:504:CL7:H62C	1.36	0.47
21:33:516:CL7:CED	32:34:403:ZEX:H172	2.45	0.47
21:34:406:CL7:H202	21:34:406:CL7:H162	1.73	0.47
4:4D:208:LEU:O	4:4D:212:ILE:HG23	2.15	0.47
18:41:291:GLY:HA3	24:41:401:LMG:HC72	1.96	0.47
21:43:403:CL7:CGA	21:43:404:CL7:H12C	2.45	0.47
21:1C:506:CL7:H121	21:1C:507:CL7:H192	1.97	0.46
21:12:510:CL7:H162	21:12:510:CL7:H141	1.61	0.46
18:11:57:THR:HG23	18:11:85:VAL:HB	1.97	0.46
19:13:113:LYS:HG3	16:22:330:SER:HB2	1.96	0.46
19:13:136:PHE:HB3	19:13:230:PRO:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2B:604:CL7:H62C	21:2B:604:CL7:H41C	1.73	0.46
21:2B:612:CL7:H203	21:2B:612:CL7:H141	1.97	0.46
19:23:119:ALA:HB2	19:23:130:HIS:CG	2.50	0.46
2:3B:230:SER:OG	7:3H:25:GLY:O	2.33	0.46
4:3D:208:LEU:O	4:3D:212:ILE:HG23	2.15	0.46
16:32:65:VAL:HG13	21:32:504:CL7:HMA2	1.96	0.46
19:33:271:PHE:CZ	21:33:501:CL7:HBA2	2.49	0.46
21:33:506:CL7:O1D	21:33:506:CL7:H2A	2.15	0.46
32:33:522:ZEX:H11	32:33:522:ZEX:H191	1.48	0.46
16:42:253:LEU:HD12	21:42:509:CL7:HED3	1.97	0.46
19:43:229:LYS:HG2	19:43:230:PRO:HD2	1.97	0.46
19:43:253:LEU:HD12	21:43:410:CL7:HED3	1.96	0.46
20:44:170:SER:HB3	20:44:243:ASP:HB3	1.96	0.46
20:44:197:ILE:HD11	20:44:233:ILE:HG13	1.97	0.46
21:44:411:CL7:H162	21:44:411:CL7:H141	1.70	0.46
21:1B:611:CL7:H203	21:1B:611:CL7:H141	1.97	0.46
18:11:277:TYR:CE1	21:11:403:CL7:HED1	2.51	0.46
21:13:510:CL7:H143	21:13:510:CL7:H112	1.79	0.46
20:14:230:GLU:OE1	20:14:230:GLU:N	2.38	0.46
32:14:418:ZEX:H201	32:14:418:ZEX:H15	1.61	0.46
9:2K:19:PRO:O	9:2K:22:ASP:HB2	2.15	0.46
19:23:49:GLU:CD	19:23:66:CYS:H	2.22	0.46
1:3A:157:VAL:HG11	21:3A:407:CL7:HMC2	1.97	0.46
18:31:256:ILE:HG23	18:31:324:MET:HE3	1.96	0.46
21:31:410:CL7:H203	21:31:410:CL7:H161	1.73	0.46
21:4D:405:CL7:HBA1	21:4D:405:CL7:H3A	1.59	0.46
9:4K:31:PHE:O	9:4K:34:LEU:HB3	2.15	0.46
21:43:418:CL7:HBA2	21:43:418:CL7:H3A	1.69	0.46
21:44:405:CL7:CGA	21:44:406:CL7:H12C	2.45	0.46
1:1A:157:VAL:HG11	21:1A:407:CL7:HMC2	1.97	0.46
21:1B:615:CL7:H3A	21:1B:615:CL7:HBA1	1.45	0.46
21:1C:508:CL7:H61C	21:1C:508:CL7:H41C	1.41	0.46
8:1I:18:LEU:HD23	8:1I:18:LEU:HA	1.73	0.46
21:12:506:CL7:H143	21:12:518:CL7:HED1	1.98	0.46
18:11:313:LEU:O	18:11:317:THR:OG1	2.23	0.46
21:11:409:CL7:HBD	21:11:409:CL7:HAA2	1.97	0.46
21:13:505:CL7:H43C	32:13:520:ZEX:H8	1.97	0.46
1:2A:323:ARG:NH2	4:2D:327:TRP:O	2.40	0.46
2:2B:294:ARG:O	2:2B:298:SER:OG	2.23	0.46
21:2C:503:CL7:H141	21:2C:503:CL7:H162	1.62	0.46
21:2C:506:CL7:H121	21:2C:507:CL7:H192	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:21:409:CL7:HAA2	21:21:409:CL7:HBD	1.97	0.46
21:24:407:CL7:HHB	32:24:418:ZEX:C17	2.46	0.46
2:3B:202:ASN:OD1	2:3B:204:THR:OG1	2.27	0.46
21:3B:607:CL7:HED3	21:3B:607:CL7:HBD	1.66	0.46
18:31:277:TYR:CE1	21:31:403:CL7:HED1	2.51	0.46
20:34:170:SER:HB3	20:34:243:ASP:HB3	1.96	0.46
21:4B:612:CL7:H203	21:4B:612:CL7:H141	1.97	0.46
3:4C:112:GLY:N	3:4C:116:GLU:O	2.48	0.46
21:42:511:CL7:H41C	21:42:511:CL7:H61C	1.58	0.46
18:41:277:TYR:CE1	21:41:403:CL7:HED1	2.51	0.46
2:1B:145:LYS:NZ	7:1H:18:GLU:OE1	2.40	0.46
5:1E:21:ILE:O	5:1E:25:ILE:HG12	2.16	0.46
21:2B:616:CL7:H3A	21:2B:616:CL7:HBA1	1.45	0.46
21:2C:509:CL7:H202	21:2C:512:CL7:HAC1	1.97	0.46
18:21:57:THR:HG23	18:21:85:VAL:HB	1.97	0.46
18:21:277:TYR:CE1	21:21:403:CL7:HED1	2.51	0.46
20:24:170:SER:HB3	20:24:243:ASP:HB3	1.96	0.46
26:24:401:LHG:HC92	21:24:405:CL7:C1B	2.46	0.46
1:3A:331:MET:HG3	4:3D:323:GLY:HA3	1.98	0.46
21:3A:407:CL7:H3A	21:3A:407:CL7:HBA1	1.55	0.46
5:3E:16:SER:OG	5:3E:17:ILE:N	2.45	0.46
21:31:420:CL7:O2D	21:31:420:CL7:H2A	2.14	0.46
21:33:509:CL7:H111	21:33:509:CL7:H142	1.63	0.46
21:4C:506:CL7:H121	21:4C:507:CL7:H192	1.97	0.46
21:41:409:CL7:HAA2	21:41:409:CL7:HBD	1.97	0.46
19:43:63:ASN:O	19:43:64:LEU:HD12	2.15	0.46
19:43:271:PHE:O	19:43:304:ARG:NH2	2.43	0.46
1:1A:20:PHE:O	1:1A:23:SER:OG	2.29	0.46
21:1B:605:CL7:HAA2	21:1B:605:CL7:HBD	1.98	0.46
21:1C:509:CL7:H202	21:1C:512:CL7:HAC1	1.97	0.46
21:12:505:CL7:H41C	21:12:505:CL7:H62C	1.49	0.46
18:11:151:LEU:HD23	18:11:151:LEU:HA	1.71	0.46
21:11:416:CL7:HED3	21:11:416:CL7:HBD	1.71	0.46
19:13:271:PHE:CZ	21:13:501:CL7:HBA2	2.49	0.46
21:13:516:CL7:CED	32:14:403:ZEX:H172	2.45	0.46
20:14:170:SER:HB3	20:14:243:ASP:HB3	1.96	0.46
1:2A:154:THR:HG22	21:2A:401:CL7:H43C	1.97	0.46
21:2B:605:CL7:H41C	21:2B:605:CL7:H93C	1.98	0.46
3:2C:76:ALA:HB2	21:2C:503:CL7:HMD2	1.97	0.46
9:2K:31:PHE:O	9:2K:34:LEU:HB3	2.15	0.46
16:22:335:ARG:O	16:22:338:THR:OG1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:23:410:CL7:H111	21:23:410:CL7:H142	1.63	0.46
21:32:516:CL7:H61C	21:32:516:CL7:H41C	1.33	0.46
32:34:403:ZEX:H28	32:34:403:ZEX:H25	1.64	0.46
21:4A:401:CL7:H91C	21:4A:401:CL7:H111	1.69	0.46
21:41:418:CL7:HBA1	21:41:418:CL7:H3A	1.59	0.46
19:43:149:PHE:HE2	21:43:413:CL7:HHB	1.78	0.46
21:44:407:CL7:HHB	32:44:418:ZEX:C17	2.46	0.46
22:1D:408:PHO:H62	22:1D:408:PHO:H41	1.73	0.46
19:13:63:ASN:O	19:13:64:LEU:HD12	2.15	0.46
25:13:521:SQD:H45	25:13:521:SQD:H81	1.52	0.46
20:14:158:LEU:O	20:14:162:VAL:HG23	2.16	0.46
21:14:407:CL7:HHB	32:14:418:ZEX:C17	2.46	0.46
2:2B:145:LYS:NZ	7:2H:18:GLU:OE1	2.40	0.46
21:2B:606:CL7:HAA2	21:2B:606:CL7:HBD	1.98	0.46
16:22:287:LEU:HD23	21:22:517:CL7:HBC2	1.97	0.46
25:21:423:SQD:O7	25:21:423:SQD:O4	2.28	0.46
21:23:403:CL7:CGA	21:23:404:CL7:H12C	2.45	0.46
21:24:406:CL7:H41C	21:24:406:CL7:H62C	1.51	0.46
2:3B:366:PHE:CD1	2:3B:367:PRO:HD2	2.51	0.46
16:32:207:VAL:HA	32:32:520:ZEX:C38	2.37	0.46
16:32:253:LEU:HD12	21:32:509:CL7:HED3	1.97	0.46
16:32:287:LEU:HD23	21:32:517:CL7:HBC2	1.97	0.46
21:32:516:CL7:H201	21:43:409:CL7:H8	1.98	0.46
21:33:510:CL7:H143	21:33:510:CL7:H112	1.79	0.46
20:34:38:MET:HE3	20:34:38:MET:HB2	1.71	0.46
21:4A:401:CL7:C14	21:4A:407:CL7:H152	2.46	0.46
2:4B:324:LEU:O	21:4B:608:CL7:H43C	2.16	0.46
21:42:506:CL7:H143	21:42:518:CL7:HED1	1.98	0.46
21:42:516:CL7:H193	21:42:516:CL7:H162	1.75	0.46
18:41:303:ALA:HB3	18:41:306:PHE:CD2	2.50	0.46
19:43:49:GLU:CD	19:43:66:CYS:H	2.22	0.46
19:43:119:ALA:HB2	19:43:130:HIS:CG	2.50	0.46
1:1A:331:MET:HG3	4:1D:323:GLY:HA3	1.98	0.46
26:14:401:LHG:HC92	21:14:405:CL7:C1B	2.46	0.46
21:14:406:CL7:H3A	21:14:406:CL7:HBA1	1.62	0.46
16:22:102:VAL:O	16:22:105:SER:OG	2.29	0.46
21:22:506:CL7:H143	21:22:518:CL7:HED1	1.98	0.46
21:22:511:CL7:H61C	21:22:511:CL7:H41C	1.58	0.46
19:23:63:ASN:O	19:23:64:LEU:HD12	2.15	0.46
32:23:423:ZEX:H27	32:23:423:ZEX:H391	1.82	0.46
20:24:158:LEU:O	20:24:162:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:32:506:CL7:H143	21:32:518:CL7:HED1	1.98	0.46
21:32:516:CL7:H193	21:32:516:CL7:H162	1.75	0.46
21:32:517:CL7:H62C	21:32:517:CL7:H41C	1.42	0.46
21:33:502:CL7:H51C	21:42:518:CL7:H201	1.98	0.46
1:4A:157:VAL:HG11	21:4A:407:CL7:HMC2	1.97	0.46
2:4B:230:SER:OG	7:4H:25:GLY:O	2.33	0.46
21:4B:605:CL7:H41C	21:4B:605:CL7:H93C	1.98	0.46
21:4C:509:CL7:H62C	21:4C:509:CL7:H41C	1.60	0.46
21:42:512:CL7:H2	21:42:512:CL7:HMA2	1.96	0.46
2:1B:366:PHE:CD1	2:1B:367:PRO:HD2	2.51	0.46
3:1C:76:ALA:HB2	21:1C:503:CL7:HMD2	1.97	0.46
16:12:149:PHE:CE2	21:12:512:CL7:HHB	2.51	0.46
21:12:503:CL7:HAA2	21:12:503:CL7:HBD	1.98	0.46
20:14:197:ILE:HD11	20:14:233:ILE:HG13	1.97	0.46
2:2B:324:LEU:O	21:2B:608:CL7:H43C	2.16	0.46
3:2C:92:PRO:HD2	3:2C:95:GLU:HB3	1.97	0.46
21:22:513:CL7:NB	32:22:522:ZEX:C4	2.79	0.46
19:23:316:PHE:O	19:23:320:GLN:HG2	2.16	0.46
32:24:403:ZEX:H15	32:24:403:ZEX:H201	1.65	0.46
32:24:403:ZEX:H11	32:24:403:ZEX:H191	1.76	0.46
4:3D:295:TYR:OH	4:3D:325:ARG:NH1	2.32	0.46
19:33:136:PHE:HB3	19:33:230:PRO:HG3	1.96	0.46
1:4A:104:GLU:O	1:4A:108:ASN:ND2	2.48	0.46
2:4B:294:ARG:O	2:4B:298:SER:OG	2.23	0.46
15:4Z:1:MET:HE3	15:4Z:4:LEU:HD23	1.98	0.46
21:44:406:CL7:H41C	21:44:406:CL7:H62C	1.51	0.46
21:1A:401:CL7:H91C	21:1A:401:CL7:H111	1.69	0.46
21:1B:604:CL7:H41C	21:1B:604:CL7:H93C	1.98	0.46
4:1D:99:ASP:OD2	4:1D:102:ARG:HG2	2.16	0.46
21:11:409:CL7:OBB	21:11:411:CL7:HHB	2.16	0.46
21:13:501:CL7:H142	32:13:520:ZEX:C31	2.46	0.46
16:22:109:PHE:O	16:22:113:THR:OG1	2.22	0.46
19:23:271:PHE:O	19:23:304:ARG:NH2	2.43	0.46
21:23:402:CL7:H142	32:23:421:ZEX:C31	2.46	0.46
21:23:405:CL7:H62C	21:23:405:CL7:H41C	1.36	0.46
1:3A:323:ARG:NH2	4:3D:327:TRP:O	2.40	0.46
3:3C:199:ASP:OD2	3:3C:209:ARG:NH2	2.36	0.46
16:32:149:PHE:CE2	21:32:512:CL7:HHB	2.51	0.46
19:33:113:LYS:HG3	16:42:330:SER:HB2	1.97	0.46
21:4B:603:CL7:HBD	21:4B:603:CL7:H12C	1.98	0.46
3:4C:92:PRO:HD2	3:4C:95:GLU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:42:287:LEU:HD23	21:42:517:CL7:HBC2	1.97	0.46
19:43:258:PHE:HB3	21:43:406:CL7:H203	1.98	0.46
21:43:404:CL7:H112	21:43:404:CL7:H72C	1.53	0.46
26:44:401:LHG:HC92	21:44:405:CL7:C1B	2.46	0.46
2:1B:230:SER:OG	7:1H:25:GLY:O	2.33	0.46
21:1B:602:CL7:HBD	21:1B:602:CL7:H12C	1.98	0.46
21:12:503:CL7:H13	21:12:503:CL7:H102	1.67	0.46
21:12:513:CL7:NB	32:12:522:ZEX:C4	2.79	0.46
21:13:511:CL7:H62C	21:13:511:CL7:H41C	1.63	0.46
21:2B:603:CL7:HBD	21:2B:603:CL7:H12C	1.98	0.46
3:2C:85:SER:OG	3:2C:86:HIS:ND1	2.46	0.46
16:22:253:LEU:HD12	21:22:509:CL7:HED3	1.97	0.46
21:22:503:CL7:HAA2	21:22:503:CL7:HBD	1.98	0.46
18:21:135:TRP:CD1	18:21:248:PRO:HG3	2.51	0.46
18:21:303:ALA:HB3	18:21:306:PHE:CD2	2.50	0.46
32:23:423:ZEX:H191	32:23:423:ZEX:H11	1.48	0.46
2:3B:130:ILE:HG13	7:3H:12:LYS:HA	1.98	0.46
22:3D:408:PHO:HMB1	22:3D:408:PHO:HBB1	1.96	0.46
21:31:409:CL7:HAA2	21:31:409:CL7:HBD	1.97	0.46
20:34:158:LEU:O	20:34:162:VAL:HG23	2.16	0.46
21:42:503:CL7:HBD	21:42:503:CL7:HAA2	1.98	0.46
21:42:513:CL7:NB	32:42:522:ZEX:C4	2.79	0.46
32:42:524:ZEX:H15	32:42:524:ZEX:H201	1.81	0.46
21:43:413:CL7:H41C	21:43:413:CL7:H62C	1.78	0.46
21:44:406:CL7:H152	21:44:411:CL7:H43C	1.98	0.46
16:12:42:ALA:O	16:12:46:THR:OG1	2.30	0.45
21:12:518:CL7:H8	21:12:518:CL7:H52C	1.84	0.45
18:11:234:PRO:O	18:11:239:LYS:NZ	2.49	0.45
21:2A:401:CL7:C14	21:2A:407:CL7:H152	2.46	0.45
15:2Z:1:MET:HE3	15:2Z:4:LEU:HD23	1.98	0.45
18:21:234:PRO:O	18:21:239:LYS:NZ	2.49	0.45
21:3B:605:CL7:HAA2	21:3B:605:CL7:HBD	1.98	0.45
3:3C:249:HIS:HA	3:3C:252:VAL:HG22	1.98	0.45
21:3C:509:CL7:H202	21:3C:512:CL7:HAC1	1.97	0.45
21:32:510:CL7:HMA3	21:32:510:CL7:H51C	1.99	0.45
21:34:407:CL7:HHB	32:34:418:ZEX:C17	2.46	0.45
1:4A:323:ARG:NH2	4:4D:327:TRP:O	2.40	0.45
21:4B:606:CL7:HAA2	21:4B:606:CL7:HBD	1.98	0.45
18:41:135:TRP:CD1	18:41:248:PRO:HG3	2.52	0.45
21:43:408:CL7:H41C	21:43:408:CL7:H61C	1.62	0.45
21:43:412:CL7:H62C	21:43:412:CL7:H41C	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:43:417:CL7:CED	32:44:403:ZEX:H172	2.45	0.45
21:44:406:CL7:H61C	21:44:406:CL7:H101	1.53	0.45
3:1C:249:HIS:HA	3:1C:252:VAL:HG22	1.98	0.45
21:12:516:CL7:HBA1	21:12:516:CL7:H12C	1.71	0.45
21:11:404:CL7:H102	21:11:404:CL7:H13	1.51	0.45
3:2C:249:HIS:HA	3:2C:252:VAL:HG22	1.98	0.45
16:22:91:ALA:O	16:22:95:ILE:HG13	2.16	0.45
16:22:207:VAL:HA	32:22:520:ZEX:C38	2.37	0.45
21:22:510:CL7:HMA3	21:22:510:CL7:H51C	1.99	0.45
21:21:409:CL7:OBB	21:21:411:CL7:HHB	2.16	0.45
19:23:138:THR:HG22	19:23:141:ARG:HH21	1.81	0.45
21:24:406:CL7:H152	21:24:411:CL7:H43C	1.98	0.45
21:3A:401:CL7:H41C	21:3A:401:CL7:H62C	1.48	0.45
21:3B:611:CL7:H141	21:3B:611:CL7:H203	1.97	0.45
4:3D:99:ASP:OD2	4:3D:102:ARG:HG2	2.17	0.45
16:32:189:TYR:O	16:32:198:PRO:HG3	2.16	0.45
21:32:511:CL7:H41C	21:32:511:CL7:H61C	1.58	0.45
18:31:193:TYR:OH	18:31:210:ASP:OD2	2.35	0.45
19:33:75:TRP:HH2	21:42:518:CL7:H121	1.80	0.45
21:33:501:CL7:H142	32:33:520:ZEX:C31	2.46	0.45
21:33:505:CL7:H43C	32:33:520:ZEX:H8	1.97	0.45
21:33:513:CL7:CHA	21:33:513:CL7:HBA2	2.46	0.45
1:4A:194:MET:HE2	1:4A:194:MET:HB3	1.85	0.45
2:4B:366:PHE:CD1	2:4B:367:PRO:HD2	2.51	0.45
21:1A:401:CL7:C14	21:1A:407:CL7:H152	2.46	0.45
2:1B:130:ILE:HG13	7:1H:12:LYS:HA	1.99	0.45
21:1B:608:CL7:HBA1	21:1B:608:CL7:H3A	1.54	0.45
4:1D:143:VAL:O	4:1D:146:SER:OG	2.21	0.45
16:12:287:LEU:HD23	21:12:517:CL7:HBC2	1.97	0.45
16:12:335:ARG:O	16:12:338:THR:OG1	2.30	0.45
18:11:298:ASP:O	18:11:299:THR:OG1	2.32	0.45
21:11:410:CL7:H51C	21:11:410:CL7:H8	1.63	0.45
19:13:138:THR:HG22	19:13:141:ARG:HH21	1.81	0.45
21:13:508:CL7:H62C	21:13:508:CL7:H102	1.52	0.45
21:14:415:CL7:H3A	21:14:415:CL7:HBA1	1.40	0.45
21:2D:405:CL7:HBA1	21:2D:405:CL7:H3A	1.59	0.45
5:2E:21:ILE:O	5:2E:25:ILE:HG12	2.15	0.45
21:21:416:CL7:HED3	21:21:416:CL7:HBD	1.71	0.45
21:23:410:CL7:H12C	21:23:410:CL7:HBA1	1.68	0.45
20:24:197:ILE:HD11	20:24:233:ILE:HG13	1.97	0.45
5:3E:21:ILE:O	5:3E:25:ILE:HG12	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3Z:1:MET:HE3	15:3Z:4:LEU:HD23	1.98	0.45
21:32:513:CL7:NB	32:32:522:ZEX:C4	2.79	0.45
18:31:215:HIS:HE1	21:31:402:CL7:NC	2.15	0.45
21:31:409:CL7:OBB	21:31:411:CL7:HHB	2.16	0.45
19:33:63:ASN:O	19:33:64:LEU:HD12	2.15	0.45
19:33:138:THR:HG22	19:33:141:ARG:HH21	1.81	0.45
26:34:401:LHG:HC92	21:34:405:CL7:C1B	2.46	0.45
3:4C:85:SER:OG	3:4C:86:HIS:ND1	2.46	0.45
21:4C:502:CL7:CBD	21:4C:503:CL7:H43C	2.47	0.45
16:42:149:PHE:CE2	21:42:512:CL7:HHB	2.51	0.45
21:42:508:CL7:HAA2	21:42:508:CL7:HBD	1.98	0.45
21:42:510:CL7:H51C	21:42:510:CL7:HMA3	1.99	0.45
18:41:57:THR:HG23	18:41:85:VAL:HB	1.97	0.45
18:41:151:LEU:HA	18:41:151:LEU:HD23	1.71	0.45
18:41:215:HIS:HE1	21:41:402:CL7:NC	2.15	0.45
19:43:316:PHE:O	19:43:320:GLN:HG2	2.16	0.45
20:44:124:ALA:HB2	21:44:415:CL7:C2C	2.47	0.45
2:1B:324:LEU:O	21:1B:607:CL7:H43C	2.16	0.45
32:11:422:ZEX:H27	32:11:422:ZEX:H391	1.76	0.45
1:2A:331:MET:HG3	4:2D:323:GLY:HA3	1.98	0.45
2:2B:230:SER:OG	7:2H:25:GLY:O	2.33	0.45
2:2B:366:PHE:CD1	2:2B:367:PRO:HD2	2.51	0.45
21:2C:502:CL7:CBD	21:2C:503:CL7:H43C	2.47	0.45
4:2D:295:TYR:OH	4:2D:325:ARG:NH1	2.32	0.45
21:22:505:CL7:H101	21:22:505:CL7:H62C	1.69	0.45
21:23:412:CL7:H41C	21:23:412:CL7:H62C	1.63	0.45
21:3A:401:CL7:C14	21:3A:407:CL7:H152	2.46	0.45
21:3B:602:CL7:HBD	21:3B:602:CL7:H12C	1.98	0.45
21:3B:611:CL7:H143	24:3B:621:LMG:H411	1.99	0.45
3:3C:92:PRO:HD2	3:3C:95:GLU:HB3	1.97	0.45
4:3D:87:SER:HB3	5:3E:69:ARG:CZ	2.46	0.45
5:3E:30:LEU:HD21	31:3F:101:HEM:HBB1	1.98	0.45
25:33:521:SQD:H291	25:33:521:SQD:H161	1.99	0.45
21:34:406:CL7:H3A	21:34:406:CL7:HBA1	1.62	0.45
1:4A:331:MET:HG3	4:4D:323:GLY:HA3	1.98	0.45
21:4B:612:CL7:H143	24:4B:622:LMG:H411	1.99	0.45
4:4D:87:SER:HB3	5:4E:69:ARG:CZ	2.46	0.45
4:4D:99:ASP:OD2	4:4D:102:ARG:HG2	2.16	0.45
18:41:234:PRO:O	18:41:239:LYS:NZ	2.49	0.45
21:43:402:CL7:H142	32:43:421:ZEX:C31	2.46	0.45
2:1B:69:ILE:HD11	21:1B:605:CL7:HBA1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:19:TYR:HD1	5:1E:23:HIS:CD2	2.35	0.45
5:1E:30:LEU:HD21	31:1F:101:HEM:HBB1	1.98	0.45
16:12:91:ALA:O	16:12:95:ILE:HG13	2.16	0.45
16:12:189:TYR:O	16:12:198:PRO:HG3	2.16	0.45
16:12:253:LEU:HD12	21:12:509:CL7:HED3	1.97	0.45
16:12:348:LEU:HA	16:12:348:LEU:HD23	1.64	0.45
18:11:193:TYR:OH	18:11:210:ASP:OD2	2.35	0.45
18:11:215:HIS:HE1	21:11:402:CL7:NC	2.15	0.45
18:21:215:HIS:HE1	21:21:402:CL7:NC	2.15	0.45
19:23:258:PHE:HB3	21:23:406:CL7:H203	1.98	0.45
21:23:409:CL7:H62C	21:23:409:CL7:H102	1.52	0.45
32:23:423:ZEX:H173	32:23:423:ZEX:H3	1.69	0.45
21:3B:604:CL7:H93C	21:3B:604:CL7:H41C	1.98	0.45
3:3C:85:SER:OG	3:3C:86:HIS:ND1	2.46	0.45
3:3C:112:GLY:N	3:3C:116:GLU:O	2.48	0.45
5:3E:19:TYR:HD1	5:3E:23:HIS:CD2	2.35	0.45
21:32:510:CL7:H41C	21:32:510:CL7:H61C	1.54	0.45
19:33:258:PHE:HB3	21:33:505:CL7:H203	1.98	0.45
2:4B:291:GLU:CD	2:4B:294:ARG:HH21	2.24	0.45
21:4B:612:CL7:H141	21:4B:612:CL7:H161	1.65	0.45
3:4C:249:HIS:HA	3:4C:252:VAL:HG22	1.98	0.45
21:41:409:CL7:OBB	21:41:411:CL7:HHB	2.16	0.45
19:43:231:TRP:NE1	21:43:407:CL7:OBD	2.47	0.45
32:43:420:ZEX:H11	32:43:420:ZEX:H191	1.61	0.45
20:44:158:LEU:O	20:44:162:VAL:HG23	2.16	0.45
21:1C:502:CL7:CBD	21:1C:503:CL7:H43C	2.47	0.45
18:11:135:TRP:CD1	18:11:248:PRO:HG3	2.52	0.45
21:11:404:CL7:H202	21:11:411:CL7:HAB	1.99	0.45
19:13:128:ARG:HB3	21:13:514:CL7:HED1	1.99	0.45
21:13:513:CL7:CHA	21:13:513:CL7:HBA2	2.46	0.45
2:2B:69:ILE:HD11	21:2B:606:CL7:HBA1	1.99	0.45
21:2B:607:CL7:H3A	21:2B:607:CL7:HBA2	1.70	0.45
4:2D:87:SER:HB3	5:2E:69:ARG:CZ	2.46	0.45
4:2D:99:ASP:OD2	4:2D:102:ARG:HG2	2.17	0.45
5:2E:19:TYR:HD1	5:2E:23:HIS:CD2	2.35	0.45
5:2E:30:LEU:HD21	31:2F:101:HEM:HBB1	1.98	0.45
21:22:516:CL7:HBA1	21:22:516:CL7:H3A	1.55	0.45
19:23:128:ARG:HB3	21:23:415:CL7:HED1	1.99	0.45
32:24:403:ZEX:H401	32:24:403:ZEX:H31	1.75	0.45
21:24:406:CL7:H101	21:24:406:CL7:H61C	1.53	0.45
2:3B:291:GLU:CD	2:3B:294:ARG:HH21	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3C:510:CL7:H72C	21:3C:510:CL7:H111	1.48	0.45
16:32:335:ARG:O	16:32:338:THR:OG1	2.30	0.45
18:31:234:PRO:O	18:31:239:LYS:NZ	2.49	0.45
18:31:303:ALA:HB3	18:31:306:PHE:CD2	2.50	0.45
21:31:410:CL7:H51C	21:31:410:CL7:H8	1.63	0.45
21:34:406:CL7:H162	21:34:406:CL7:H121	1.73	0.45
2:4B:145:LYS:NZ	7:4H:18:GLU:OE1	2.40	0.45
21:4C:501:CL7:H162	21:4C:501:CL7:H202	1.70	0.45
5:4E:21:ILE:O	5:4E:25:ILE:HG12	2.16	0.45
2:1B:178:ASP:OD1	2:1B:182:LEU:N	2.38	0.45
21:1B:611:CL7:H143	24:1B:621:LMG:H411	1.99	0.45
3:1C:92:PRO:HD2	3:1C:95:GLU:HB3	1.97	0.45
3:1C:112:GLY:N	3:1C:116:GLU:O	2.48	0.45
3:1C:387:LEU:HD12	3:1C:392:LEU:HD21	1.98	0.45
21:1C:503:CL7:H162	21:1C:503:CL7:H141	1.62	0.45
4:1D:87:SER:HB3	5:1E:69:ARG:CZ	2.46	0.45
21:2B:612:CL7:H143	24:2B:622:LMG:H411	1.99	0.45
18:21:75:LEU:HA	18:21:168:ILE:HG22	1.99	0.45
20:24:157:SER:O	20:24:160:THR:HG22	2.17	0.45
21:3B:607:CL7:HBA1	21:3B:607:CL7:H3A	1.26	0.45
21:32:503:CL7:HAA2	21:32:503:CL7:HBD	1.98	0.45
19:33:316:PHE:O	19:33:320:GLN:HG2	2.16	0.45
3:4C:476:GLU:CD	4:4D:244:SER:HG	2.19	0.45
21:42:505:CL7:CMD	32:42:520:ZEX:H163	2.47	0.45
21:42:517:CL7:H193	21:42:517:CL7:H162	1.69	0.45
19:43:138:THR:HG22	19:43:141:ARG:HH21	1.81	0.45
21:43:408:CL7:H101	21:43:408:CL7:H62C	1.64	0.45
15:1Z:1:MET:HE3	15:1Z:4:LEU:HD23	1.98	0.45
21:12:518:CL7:H201	21:23:403:CL7:H51C	1.98	0.45
18:11:75:LEU:HA	18:11:168:ILE:HG22	1.99	0.45
18:11:140:LYS:O	18:11:144:ILE:HG13	2.17	0.45
21:13:503:CL7:H112	21:13:503:CL7:H72C	1.52	0.45
25:13:521:SQD:H161	25:13:521:SQD:H291	1.99	0.45
32:14:403:ZEX:H28	32:14:403:ZEX:H25	1.65	0.45
2:2B:130:ILE:HG13	7:2H:12:LYS:HA	1.98	0.45
2:2B:291:GLU:CD	2:2B:294:ARG:HH21	2.24	0.45
5:2E:16:SER:OG	5:2E:17:ILE:N	2.45	0.45
16:22:108:ILE:O	16:22:111:ILE:HG22	2.17	0.45
21:3B:604:CL7:HAA2	21:3B:604:CL7:HBD	1.99	0.45
3:3C:387:LEU:HD12	3:3C:392:LEU:HD21	1.98	0.45
21:32:508:CL7:HAA2	21:32:508:CL7:HBD	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:31:75:LEU:HA	18:31:168:ILE:HG22	1.99	0.45
18:31:140:LYS:O	18:31:144:ILE:HG13	2.17	0.45
21:33:508:CL7:H8	21:42:516:CL7:H201	1.98	0.45
21:33:509:CL7:H2A	21:33:509:CL7:O1A	2.16	0.45
21:34:406:CL7:H152	21:34:411:CL7:H43C	1.98	0.45
1:4A:154:THR:HG22	21:4A:401:CL7:H43C	1.97	0.45
16:42:94:MET:CE	32:42:524:ZEX:C36	2.94	0.45
21:42:505:CL7:H101	21:42:505:CL7:H62C	1.69	0.45
20:44:71:TYR:OH	20:44:101:ILE:HB	2.17	0.45
2:1B:41:GLU:OE2	2:1B:61:PHE:N	2.35	0.45
16:12:108:ILE:O	16:12:111:ILE:HG22	2.17	0.45
21:12:512:CL7:H161	21:12:512:CL7:H141	1.75	0.45
21:2A:401:CL7:H91C	21:2A:401:CL7:H111	1.69	0.45
21:2B:607:CL7:HBA2	21:2B:607:CL7:C4A	2.46	0.45
16:22:149:PHE:CE2	21:22:512:CL7:HHB	2.51	0.45
21:22:508:CL7:HAA2	21:22:508:CL7:HBD	1.98	0.45
21:22:514:CL7:HBA1	21:22:514:CL7:H3A	1.69	0.45
20:24:88:LEU:HG	21:24:406:CL7:HED3	1.99	0.45
20:24:124:ALA:HB2	21:24:415:CL7:C2C	2.47	0.45
2:3B:324:LEU:O	21:3B:607:CL7:H43C	2.16	0.45
21:3B:615:CL7:H11C	21:3B:615:CL7:HBA2	1.71	0.45
3:3C:191:ALA:HA	3:3C:196:GLY:HA2	1.99	0.45
16:32:208:MET:HE3	16:32:208:MET:HB3	1.85	0.45
18:31:135:TRP:CD1	18:31:248:PRO:HG3	2.51	0.45
20:34:148:PHE:CZ	32:34:420:ZEX:O3	2.70	0.45
3:4C:387:LEU:HD12	3:4C:392:LEU:HD21	1.98	0.45
21:4C:506:CL7:HBA1	21:4C:506:CL7:H3A	1.76	0.45
16:42:108:ILE:O	16:42:111:ILE:HG22	2.17	0.45
16:42:189:TYR:O	16:42:198:PRO:HG3	2.16	0.45
18:41:75:LEU:HA	18:41:168:ILE:HG22	1.99	0.45
20:44:88:LEU:HG	21:44:406:CL7:HED3	1.99	0.45
18:11:303:ALA:HB3	18:11:306:PHE:CD2	2.50	0.45
21:13:507:CL7:H101	21:13:507:CL7:H62C	1.64	0.45
32:14:403:ZEX:H11	32:14:403:ZEX:H191	1.76	0.45
21:14:406:CL7:H61C	21:14:406:CL7:H101	1.53	0.45
21:2B:609:CL7:HBA1	21:2B:609:CL7:H3A	1.54	0.45
16:22:31:HIS:ND1	21:22:509:CL7:H142	2.32	0.45
21:22:503:CL7:HBD	21:22:503:CL7:O1A	2.17	0.45
21:22:505:CL7:CMD	32:22:520:ZEX:H163	2.47	0.45
18:21:151:LEU:HA	18:21:151:LEU:HD23	1.71	0.45
2:3B:69:ILE:HD11	21:3B:605:CL7:HBA1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:32:91:ALA:O	16:32:95:ILE:HG13	2.16	0.45
32:32:520:ZEX:H27	32:32:520:ZEX:H391	1.75	0.45
21:31:404:CL7:H202	21:31:411:CL7:HAB	1.99	0.45
20:34:124:ALA:HB2	21:34:415:CL7:C2C	2.47	0.45
20:34:289:VAL:HG22	21:34:410:CL7:HAB	2.00	0.45
2:4B:69:ILE:HD11	21:4B:606:CL7:HBA1	1.99	0.45
8:4I:18:LEU:HA	8:4I:18:LEU:HD23	1.73	0.45
21:42:510:CL7:H141	21:42:510:CL7:H162	1.61	0.45
21:41:406:CL7:H121	21:41:406:CL7:H162	1.83	0.45
21:43:414:CL7:HBA2	21:43:414:CL7:CHA	2.46	0.45
1:1A:323:ARG:NH2	4:1D:327:TRP:O	2.40	0.44
3:1C:85:SER:OG	3:1C:86:HIS:ND1	2.46	0.44
21:1C:502:CL7:O1A	21:1C:503:CL7:H2	2.17	0.44
21:12:503:CL7:HBD	21:12:503:CL7:O1A	2.18	0.44
21:12:516:CL7:H61C	21:12:516:CL7:H41C	1.33	0.44
21:11:403:CL7:HAA2	21:11:403:CL7:HBD	1.99	0.44
21:11:408:CL7:C13	32:11:422:ZEX:H402	2.47	0.44
19:13:112:THR:HG23	19:13:113:LYS:H	1.82	0.44
21:13:517:CL7:H3A	21:13:517:CL7:HBA2	1.69	0.44
32:14:403:ZEX:H15	32:14:403:ZEX:H201	1.65	0.44
21:14:406:CL7:H152	21:14:411:CL7:H43C	1.98	0.44
21:2B:604:CL7:H203	21:2B:604:CL7:H161	1.75	0.44
21:21:404:CL7:H202	21:21:411:CL7:HAB	1.99	0.44
21:21:410:CL7:H8	21:21:410:CL7:H51C	1.63	0.44
32:24:418:ZEX:H15	32:24:418:ZEX:H201	1.61	0.44
21:3C:502:CL7:CBD	21:3C:503:CL7:H43C	2.47	0.44
30:3D:407:PL9:H321	30:3D:407:PL9:H28	1.78	0.44
16:32:108:ILE:O	16:32:111:ILE:HG22	2.17	0.44
19:33:251:ALA:HB2	19:33:322:HIS:CD2	2.52	0.44
19:33:270:VAL:O	19:33:272:PRO:HD3	2.17	0.44
16:42:31:HIS:ND1	21:42:509:CL7:H142	2.32	0.44
19:43:128:ARG:HB3	21:43:415:CL7:HED1	1.99	0.44
19:43:251:ALA:HB2	19:43:322:HIS:CD2	2.52	0.44
19:43:305:PHE:HZ	32:43:420:ZEX:H362	1.77	0.44
25:43:422:SQD:H161	25:43:422:SQD:H291	1.99	0.44
22:1A:402:PHO:NC	22:1A:402:PHO:ND	2.66	0.44
21:1A:407:CL7:HMD1	21:1D:404:CL7:HAB	1.97	0.44
2:1B:291:GLU:CD	2:1B:294:ARG:HH21	2.24	0.44
21:1C:503:CL7:H151	21:1C:503:CL7:H112	1.75	0.44
19:13:258:PHE:HB3	21:13:505:CL7:H203	1.98	0.44
19:13:270:VAL:O	19:13:272:PRO:HD3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:13:316:PHE:O	19:13:320:GLN:HG2	2.16	0.44
21:2B:608:CL7:HBA1	21:2B:608:CL7:H3A	1.26	0.44
21:22:511:CL7:H91C	21:22:511:CL7:H111	1.81	0.44
21:22:516:CL7:H41C	21:22:516:CL7:H61C	1.33	0.44
21:21:403:CL7:HAA2	21:21:403:CL7:HBD	1.99	0.44
21:21:417:CL7:H3A	21:21:417:CL7:HBA1	1.70	0.44
21:21:418:CL7:H3A	21:21:418:CL7:HBA1	1.59	0.44
19:23:224:TRP:CZ3	19:23:228:VAL:HG21	2.53	0.44
20:24:155:PHE:CZ	21:24:408:CL7:HED3	2.53	0.44
21:3B:606:CL7:H41C	21:3B:606:CL7:H62C	1.65	0.44
21:3B:611:CL7:H141	21:3B:611:CL7:H161	1.65	0.44
21:3C:502:CL7:O1A	21:3C:503:CL7:H2	2.17	0.44
9:3K:21:VAL:HA	9:3K:24:MET:HG3	1.98	0.44
11:3M:13:LEU:HD12	11:3M:13:LEU:HA	1.80	0.44
21:31:404:CL7:H13	21:31:404:CL7:H102	1.51	0.44
21:33:507:CL7:H142	21:33:507:CL7:H111	1.85	0.44
21:33:511:CL7:H62C	21:33:511:CL7:H41C	1.63	0.44
20:34:71:TYR:OH	20:34:101:ILE:HB	2.17	0.44
20:34:88:LEU:HG	21:34:406:CL7:HED3	1.99	0.44
32:34:403:ZEX:H15	32:34:403:ZEX:H201	1.65	0.44
21:34:405:CL7:H62C	21:34:405:CL7:H41C	1.73	0.44
9:4K:21:VAL:HA	9:4K:24:MET:HG3	1.98	0.44
16:42:91:ALA:O	16:42:95:ILE:HG13	2.16	0.44
21:43:405:CL7:H92C	21:43:405:CL7:H61C	1.71	0.44
21:43:409:CL7:H62C	21:43:409:CL7:H102	1.52	0.44
21:43:417:CL7:H11C	21:43:417:CL7:HBA1	1.53	0.44
21:1A:407:CL7:HBA1	21:1A:407:CL7:H3A	1.55	0.44
2:1B:202:ASN:OD1	2:1B:204:THR:OG1	2.27	0.44
2:1B:357:ARG:NH2	4:1D:336:GLU:O	2.49	0.44
21:1B:607:CL7:HBA1	21:1B:607:CL7:H3A	1.26	0.44
21:12:501:CL7:H92C	21:12:501:CL7:H61C	1.75	0.44
18:11:67:VAL:HG13	21:11:405:CL7:HMA1	1.99	0.44
19:13:251:ALA:HB2	19:13:322:HIS:CD2	2.52	0.44
21:13:509:CL7:O1A	21:13:509:CL7:H2A	2.16	0.44
1:2A:104:GLU:O	1:2A:108:ASN:ND2	2.48	0.44
2:2B:303:ASP:N	2:2B:303:ASP:OD1	2.49	0.44
19:23:251:ALA:HB2	19:23:322:HIS:CD2	2.52	0.44
20:24:71:TYR:OH	20:24:101:ILE:HB	2.17	0.44
21:3A:407:CL7:HAA2	21:3A:407:CL7:HBD	1.99	0.44
21:32:505:CL7:CMD	32:32:520:ZEX:H163	2.47	0.44
25:33:521:SQD:H81	25:33:521:SQD:H45	1.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:34:157:SER:O	20:34:160:THR:HG22	2.17	0.44
3:4C:191:ALA:HA	3:4C:196:GLY:HA2	1.99	0.44
3:4C:388:ASP:OD1	3:4C:390:ASN:N	2.45	0.44
18:41:193:TYR:OH	18:41:210:ASP:OD2	2.35	0.44
4:1D:92:TRP:NE1	13:1X:13:SER:HB3	2.33	0.44
21:12:503:CL7:H3A	21:12:503:CL7:HBA1	1.85	0.44
21:12:508:CL7:HAA2	21:12:508:CL7:HBD	1.98	0.44
19:13:224:TRP:CZ3	19:13:228:VAL:HG21	2.53	0.44
20:14:289:VAL:HG22	21:14:410:CL7:HAB	2.00	0.44
3:2C:387:LEU:HD12	3:2C:392:LEU:HD21	1.98	0.44
16:22:189:TYR:O	16:22:198:PRO:HG3	2.16	0.44
21:21:408:CL7:C13	32:21:422:ZEX:H402	2.47	0.44
19:23:270:VAL:O	19:23:272:PRO:HD3	2.17	0.44
21:23:417:CL7:H11C	21:23:417:CL7:HBA1	1.53	0.44
32:24:420:ZEX:H15	32:24:420:ZEX:H201	1.81	0.44
1:3A:286:THR:OG1	21:3A:401:CL7:O1D	2.23	0.44
16:32:94:MET:CE	32:32:524:ZEX:H362	2.47	0.44
21:32:518:CL7:H121	19:43:75:TRP:HH2	1.81	0.44
19:33:128:ARG:HB3	21:33:514:CL7:HED1	1.99	0.44
21:4B:613:CL7:H62C	21:4B:613:CL7:H102	1.71	0.44
24:4B:622:LMG:H292	24:4B:622:LMG:HC91	1.71	0.44
18:41:67:VAL:HG13	21:41:405:CL7:HMA1	1.99	0.44
20:44:148:PHE:CZ	32:44:420:ZEX:O3	2.70	0.44
20:44:157:SER:O	20:44:160:THR:HG22	2.17	0.44
10:1L:15:ARG:HD2	25:2B:621:SQD:C24	2.46	0.44
20:14:88:LEU:HG	21:14:406:CL7:HED3	1.99	0.44
20:14:157:SER:O	20:14:160:THR:HG22	2.17	0.44
2:2B:443:PHE:O	2:2B:444:ARG:HG3	2.18	0.44
4:2D:203:ILE:HD13	4:2D:203:ILE:HA	1.80	0.44
21:23:408:CL7:H143	21:23:408:CL7:H162	1.81	0.44
21:23:409:CL7:H3A	21:23:409:CL7:HBA2	1.77	0.44
20:24:85:MET:HE2	20:24:85:MET:HB3	1.91	0.44
2:3B:443:PHE:O	2:3B:444:ARG:HG3	2.18	0.44
21:3B:614:CL7:H41C	21:3B:614:CL7:H62C	1.50	0.44
21:3C:509:CL7:H41C	21:3C:509:CL7:H62C	1.60	0.44
16:32:188:LYS:HB3	16:32:196:PHE:CD2	2.53	0.44
18:31:67:VAL:HG13	21:31:405:CL7:HMA1	1.99	0.44
21:33:517:CL7:HBA2	21:33:517:CL7:H3A	1.69	0.44
2:4B:443:PHE:O	2:4B:444:ARG:HG3	2.18	0.44
21:4B:610:CL7:H3A	21:4B:610:CL7:HBA1	1.50	0.44
21:4B:615:CL7:H62C	21:4B:615:CL7:H41C	1.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4E:16:SER:OG	5:4E:17:ILE:N	2.45	0.44
5:4E:19:TYR:HD1	5:4E:23:HIS:CD2	2.35	0.44
19:43:63:ASN:HB3	21:43:405:CL7:H2A	2.00	0.44
2:1B:52:LEU:HD21	2:1B:307:GLU:HG2	2.00	0.44
21:1B:606:CL7:C4A	21:1B:606:CL7:HBA2	2.46	0.44
21:12:510:CL7:H41C	21:12:510:CL7:H61C	1.54	0.44
21:12:517:CL7:H62C	21:12:517:CL7:H41C	1.41	0.44
21:11:410:CL7:H203	21:11:410:CL7:H161	1.73	0.44
20:14:155:PHE:CZ	21:14:408:CL7:HED3	2.52	0.44
2:2B:52:LEU:HD21	2:2B:307:GLU:HG2	2.00	0.44
2:2B:357:ARG:NH2	4:2D:336:GLU:O	2.49	0.44
21:2B:616:CL7:HBA2	21:2B:616:CL7:H11C	1.71	0.44
21:2C:502:CL7:O1A	21:2C:503:CL7:H2	2.17	0.44
21:2C:510:CL7:H72C	21:2C:510:CL7:H111	1.48	0.44
18:21:67:VAL:HG13	21:21:405:CL7:HMA1	1.99	0.44
4:3D:92:TRP:NE1	13:3X:13:SER:HB3	2.33	0.44
4:3D:328:MET:HG2	4:3D:332:ASP:HB2	2.00	0.44
16:32:123:SER:C	16:32:125:ALA:H	2.26	0.44
21:32:509:CL7:H62C	21:32:509:CL7:H93C	1.63	0.44
19:33:112:THR:HG23	19:33:113:LYS:H	1.82	0.44
5:4E:30:LEU:HD21	31:4F:101:HEM:HBB1	1.98	0.44
21:42:503:CL7:HBD	21:42:503:CL7:O1A	2.18	0.44
19:43:224:TRP:CZ3	19:43:228:VAL:HG21	2.53	0.44
21:43:404:CL7:H13	21:43:404:CL7:H101	1.75	0.44
21:43:410:CL7:H2A	21:43:410:CL7:O1A	2.16	0.44
21:12:505:CL7:CMD	32:12:520:ZEX:H163	2.47	0.44
21:12:512:CL7:HBA1	21:12:512:CL7:O1D	2.18	0.44
32:12:522:ZEX:H201	32:12:522:ZEX:H15	1.74	0.44
32:13:519:ZEX:H201	32:13:519:ZEX:H15	1.68	0.44
20:14:38:MET:HE3	20:14:38:MET:HB2	1.71	0.44
21:2B:615:CL7:H62C	21:2B:615:CL7:H41C	1.50	0.44
3:2C:48:TRP:O	21:2C:508:CL7:H2	2.18	0.44
9:2K:21:VAL:HA	9:2K:24:MET:HG3	1.98	0.44
16:22:94:MET:CE	32:22:524:ZEX:H362	2.47	0.44
19:23:112:THR:HG23	19:23:113:LYS:H	1.82	0.44
21:23:410:CL7:H2A	21:23:410:CL7:O1A	2.16	0.44
25:23:422:SQD:H161	25:23:422:SQD:H291	1.99	0.44
21:3B:604:CL7:H121	21:3B:604:CL7:H162	1.77	0.44
21:32:517:CL7:H3A	21:32:517:CL7:HBA1	1.48	0.44
32:32:519:ZEX:H15	32:32:519:ZEX:H201	1.80	0.44
19:33:224:TRP:CZ3	19:33:228:VAL:HG21	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:34:403:ZEX:H11	32:34:403:ZEX:H191	1.76	0.44
21:4A:407:CL7:H3A	21:4A:407:CL7:HBA1	1.55	0.44
21:4B:605:CL7:HAA2	21:4B:605:CL7:HBD	1.99	0.44
3:4C:48:TRP:O	21:4C:508:CL7:H2	2.17	0.44
21:42:514:CL7:HBA1	21:42:514:CL7:H3A	1.69	0.44
21:41:403:CL7:HAA2	21:41:403:CL7:HBD	1.99	0.44
21:43:405:CL7:H142	21:43:405:CL7:H112	1.77	0.44
2:1B:175:TRP:HA	2:1B:185:HIS:O	2.18	0.44
21:1B:604:CL7:HAA2	21:1B:604:CL7:HBD	1.99	0.44
3:1C:48:TRP:O	21:1C:508:CL7:H2	2.18	0.44
21:1C:505:CL7:H3A	21:1C:505:CL7:HBA1	1.63	0.44
21:1C:506:CL7:H11C	21:1C:506:CL7:HBA2	1.74	0.44
21:12:514:CL7:H3A	21:12:514:CL7:HBA1	1.69	0.44
18:11:152:ILE:HD11	21:11:410:CL7:H61C	2.00	0.44
20:14:148:PHE:CZ	32:14:420:ZEX:O3	2.70	0.44
1:2A:330:VAL:HG21	4:2D:327:TRP:CE2	2.53	0.44
18:21:111:PHE:HD1	18:21:115:ILE:HD12	1.83	0.44
19:23:63:ASN:HB3	21:23:405:CL7:H2A	2.00	0.44
2:3B:52:LEU:HD21	2:3B:307:GLU:HG2	2.00	0.44
2:3B:175:TRP:HA	2:3B:185:HIS:O	2.18	0.44
21:3B:608:CL7:HBC3	21:3B:608:CL7:HHD	2.00	0.44
21:3C:509:CL7:H141	21:3C:509:CL7:H162	1.70	0.44
21:32:503:CL7:HBD	21:32:503:CL7:O1A	2.17	0.44
18:31:152:ILE:HD11	21:31:410:CL7:H61C	2.00	0.44
21:31:403:CL7:HAA2	21:31:403:CL7:HBD	1.99	0.44
21:31:408:CL7:C13	32:31:422:ZEX:H402	2.47	0.44
21:33:504:CL7:H162	21:33:504:CL7:H141	1.80	0.44
32:33:520:ZEX:H191	32:33:520:ZEX:H11	1.52	0.44
21:34:412:CL7:O2A	21:34:412:CL7:H2A	2.18	0.44
21:4A:401:CL7:H41C	21:4A:401:CL7:H62C	1.48	0.44
21:4B:604:CL7:H62C	21:4B:604:CL7:H41C	1.73	0.44
21:4C:502:CL7:O1A	21:4C:503:CL7:H2	2.17	0.44
21:4C:508:CL7:H61C	21:4C:508:CL7:H41C	1.41	0.44
21:41:404:CL7:H202	21:41:411:CL7:HAB	1.99	0.44
19:43:270:VAL:O	19:43:272:PRO:HD3	2.17	0.44
21:44:412:CL7:H2A	21:44:412:CL7:O2A	2.18	0.44
32:44:420:ZEX:H15	32:44:420:ZEX:H201	1.82	0.44
21:1A:407:CL7:H161	21:1A:407:CL7:H141	1.84	0.44
3:1C:141:GLY:O	3:1C:145:THR:OG1	2.20	0.44
21:1C:509:CL7:HBA2	21:1C:509:CL7:H3A	1.63	0.44
4:1D:328:MET:HG2	4:1D:332:ASP:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:12:123:SER:C	16:12:125:ALA:H	2.26	0.44
19:13:231:TRP:NE1	21:13:506:CL7:OBD	2.47	0.44
20:14:124:ALA:HB2	21:14:415:CL7:C2C	2.47	0.44
1:2A:96:ILE:HG22	8:2I:1:MET:HE1	2.00	0.44
21:2B:611:CL7:H202	21:2B:611:CL7:H162	1.73	0.44
10:2L:28:LEU:HD23	10:2L:28:LEU:HA	1.88	0.44
16:22:42:ALA:O	16:22:46:THR:OG1	2.30	0.44
20:24:289:VAL:HG22	21:24:410:CL7:HAB	2.00	0.44
21:3B:603:CL7:H203	21:3B:609:CL7:H102	2.00	0.44
32:33:525:ZEX:H15	32:33:525:ZEX:H201	1.85	0.44
20:34:155:PHE:CZ	21:34:408:CL7:HED3	2.53	0.44
20:34:167:VAL:HG23	20:34:247:ALA:HB1	2.00	0.44
1:4A:330:VAL:HG21	4:4D:327:TRP:CE2	2.53	0.44
21:4A:407:CL7:HBD	21:4A:407:CL7:HAA2	2.00	0.44
2:4B:42:LEU:HD23	2:4B:42:LEU:HA	1.73	0.44
21:4B:613:CL7:H3A	21:4B:613:CL7:HBA1	1.60	0.44
3:4C:153:GLU:H	3:4C:153:GLU:CD	2.25	0.44
3:4C:171:GLN:O	3:4C:175:ILE:HG13	2.18	0.44
13:4X:36:LYS:HE2	13:4X:36:LYS:HB2	1.91	0.44
16:42:94:MET:CE	32:42:524:ZEX:H362	2.47	0.44
21:42:511:CL7:H91C	21:42:511:CL7:H111	1.81	0.44
18:41:140:LYS:O	18:41:144:ILE:HG13	2.17	0.44
19:43:112:THR:HG23	19:43:113:LYS:H	1.82	0.44
1:1A:330:VAL:HG21	4:1D:327:TRP:CE2	2.53	0.43
21:1A:407:CL7:HBD	21:1A:407:CL7:HAA2	2.00	0.43
21:1B:603:CL7:H203	21:1B:609:CL7:H102	2.00	0.43
9:1K:15:SER:O	9:1K:18:SER:OG	2.20	0.43
21:12:511:CL7:H41C	21:12:511:CL7:H61C	1.58	0.43
19:13:112:THR:HG23	19:13:113:LYS:N	2.33	0.43
21:13:504:CL7:H92C	21:13:504:CL7:H61C	1.71	0.43
21:13:507:CL7:H142	21:13:507:CL7:H111	1.85	0.43
1:2A:202:VAL:HG22	21:2A:401:CL7:C2B	2.48	0.43
4:2D:296:ASP:OD1	4:2D:296:ASP:N	2.50	0.43
16:22:313:PHE:CD2	32:22:519:ZEX:H30	2.53	0.43
18:21:152:ILE:HD11	21:21:410:CL7:H61C	2.00	0.43
18:21:313:LEU:O	18:21:317:THR:OG1	2.23	0.43
20:24:167:VAL:HG23	20:24:247:ALA:HB1	2.00	0.43
21:3C:507:CL7:H92C	21:3C:507:CL7:H61C	1.81	0.43
21:32:517:CL7:H193	21:32:517:CL7:H162	1.69	0.43
18:31:144:ILE:HG12	21:31:413:CL7:HMC2	2.00	0.43
21:33:507:CL7:H143	21:33:507:CL7:H162	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:33:520:ZEX:H31	32:33:520:ZEX:H401	1.79	0.43
21:34:412:CL7:H61C	21:34:412:CL7:H41C	1.76	0.43
1:4A:96:ILE:HG22	8:4I:1:MET:HE1	2.00	0.43
1:4A:202:VAL:HG22	21:4A:401:CL7:C2B	2.48	0.43
2:4B:303:ASP:OD1	2:4B:303:ASP:N	2.49	0.43
20:44:155:PHE:CZ	21:44:408:CL7:HED3	2.52	0.43
21:44:411:CL7:HED3	21:44:411:CL7:CGA	2.48	0.43
9:1K:21:VAL:HA	9:1K:24:MET:HG3	1.98	0.43
19:13:63:ASN:HB3	21:13:504:CL7:H2A	2.00	0.43
20:14:167:VAL:HG23	20:14:247:ALA:HB1	2.00	0.43
2:2B:202:ASN:OD1	2:2B:204:THR:OG1	2.27	0.43
2:2B:401:PHE:HB2	2:2B:406:LEU:O	2.18	0.43
3:2C:171:GLN:O	3:2C:175:ILE:HG13	2.18	0.43
21:2D:405:CL7:HAA2	21:2D:405:CL7:HBD	2.01	0.43
19:23:231:TRP:NE1	21:23:407:CL7:OBD	2.47	0.43
21:23:414:CL7:CHA	21:23:414:CL7:HBA2	2.46	0.43
20:24:148:PHE:CZ	32:24:420:ZEX:O3	2.70	0.43
20:24:230:GLU:OE1	20:24:230:GLU:N	2.38	0.43
21:24:406:CL7:H143	21:24:406:CL7:H111	1.80	0.43
22:3A:402:PHO:NC	22:3A:402:PHO:ND	2.66	0.43
2:3B:41:GLU:OE2	2:3B:61:PHE:N	2.35	0.43
25:3B:620:SQD:C24	10:4L:15:ARG:HD2	2.47	0.43
21:32:517:CL7:H2	19:43:40:PHE:CD1	2.53	0.43
1:4A:37:MET:HE2	1:4A:37:MET:HB3	1.95	0.43
2:4B:130:ILE:HG13	7:4H:12:LYS:HA	1.98	0.43
16:42:207:VAL:HA	32:42:520:ZEX:C38	2.37	0.43
20:44:88:LEU:HD23	20:44:88:LEU:HA	1.75	0.43
21:44:405:CL7:H2	21:44:406:CL7:H11C	2.00	0.43
1:1A:96:ILE:HG22	8:1I:1:MET:HE1	2.00	0.43
21:1B:608:CL7:H62C	21:1B:608:CL7:H41C	1.50	0.43
21:1B:611:CL7:HBC2	26:1B:623:LHG:H342	2.01	0.43
3:1C:171:GLN:O	3:1C:175:ILE:HG13	2.18	0.43
4:1D:323:GLY:O	4:1D:327:TRP:HD1	2.02	0.43
21:1D:405:CL7:HAA2	21:1D:405:CL7:HBD	2.01	0.43
16:12:188:LYS:HB3	16:12:196:PHE:CD2	2.53	0.43
16:12:208:MET:HE3	16:12:208:MET:HB3	1.85	0.43
21:12:518:CL7:H121	19:23:75:TRP:HH2	1.82	0.43
18:11:111:PHE:HD1	18:11:115:ILE:HD12	1.82	0.43
32:13:520:ZEX:H191	32:13:520:ZEX:H11	1.52	0.43
1:2A:93:LEU:HD21	21:2A:403:CL7:HAA1	2.00	0.43
1:2A:194:MET:HE2	1:2A:194:MET:HB3	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2C:191:ALA:HA	3:2C:196:GLY:HA2	1.99	0.43
21:2C:503:CL7:H112	21:2C:503:CL7:H151	1.75	0.43
21:2C:504:CL7:HBA2	21:2C:504:CL7:CHA	2.48	0.43
18:21:140:LYS:O	18:21:144:ILE:HG13	2.17	0.43
32:23:401:ZEX:H15	32:23:401:ZEX:H201	1.85	0.43
21:23:405:CL7:H92C	21:23:405:CL7:H61C	1.71	0.43
1:3A:104:GLU:O	1:3A:108:ASN:ND2	2.49	0.43
21:32:512:CL7:O1D	21:32:512:CL7:HBA1	2.18	0.43
21:31:410:CL7:H122	21:31:413:CL7:C3D	2.49	0.43
21:33:503:CL7:H121	21:33:509:CL7:H43C	2.00	0.43
21:33:509:CL7:H202	21:33:509:CL7:H161	1.78	0.43
21:4B:609:CL7:H62C	21:4B:609:CL7:H41C	1.50	0.43
21:4C:504:CL7:HBA2	21:4C:504:CL7:CHA	2.48	0.43
16:42:253:LEU:HA	16:42:253:LEU:HD23	1.82	0.43
21:41:408:CL7:C13	32:41:422:ZEX:H402	2.47	0.43
19:43:161:ALA:HA	19:43:166:VAL:HG13	2.00	0.43
1:1A:93:LEU:HD21	21:1A:403:CL7:HAA1	2.00	0.43
2:1B:303:ASP:OD1	2:1B:303:ASP:N	2.49	0.43
2:1B:443:PHE:O	2:1B:444:ARG:HG3	2.18	0.43
16:12:94:MET:CE	32:12:524:ZEX:H362	2.47	0.43
16:12:128:ARG:HB3	21:12:514:CL7:HED1	2.00	0.43
18:11:90:VAL:O	18:11:94:ILE:HG12	2.18	0.43
21:13:503:CL7:H121	21:13:509:CL7:H43C	2.00	0.43
21:13:507:CL7:H143	21:13:507:CL7:H162	1.81	0.43
32:13:522:ZEX:H391	32:13:522:ZEX:H27	1.81	0.43
21:14:405:CL7:H62C	21:14:405:CL7:H41C	1.73	0.43
21:14:406:CL7:H162	21:14:406:CL7:H202	1.73	0.43
21:2B:611:CL7:HBA2	21:2B:611:CL7:H11C	1.81	0.43
21:22:517:CL7:H193	21:22:517:CL7:H162	1.68	0.43
19:23:112:THR:HG23	19:23:113:LYS:N	2.33	0.43
19:23:161:ALA:HA	19:23:166:VAL:HG13	2.00	0.43
21:3B:605:CL7:HBA1	21:3B:605:CL7:H3A	1.78	0.43
3:3C:131:LEU:O	3:3C:134:SER:OG	2.27	0.43
4:3D:323:GLY:O	4:3D:327:TRP:HD1	2.02	0.43
16:32:31:HIS:ND1	21:32:509:CL7:H142	2.32	0.43
21:4B:608:CL7:HBA1	21:4B:608:CL7:H3A	1.26	0.43
32:42:522:ZEX:H201	32:42:522:ZEX:H15	1.74	0.43
21:43:409:CL7:H61C	21:43:409:CL7:H41C	1.53	0.43
21:1B:610:CL7:H162	21:1B:610:CL7:H202	1.73	0.43
3:1C:191:ALA:HA	3:1C:196:GLY:HA2	1.99	0.43
4:1D:242:THR:O	4:1D:242:THR:OG1	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:13:504:CL7:H62C	21:13:504:CL7:H41C	1.36	0.43
32:13:522:ZEX:H11	32:13:522:ZEX:H191	1.48	0.43
21:2A:401:CL7:H41C	21:2A:401:CL7:H62C	1.48	0.43
2:2B:175:TRP:HA	2:2B:185:HIS:O	2.18	0.43
21:2B:612:CL7:HBC2	26:2B:624:LHG:H342	2.01	0.43
21:2B:613:CL7:H62C	21:2B:613:CL7:H102	1.71	0.43
3:2C:68:HIS:CE1	3:2C:72:ILE:HD11	2.54	0.43
4:2D:323:GLY:O	4:2D:327:TRP:HD1	2.02	0.43
21:22:515:CL7:HMB1	32:22:520:ZEX:H202	2.01	0.43
32:23:420:ZEX:H27	32:23:420:ZEX:H30	1.76	0.43
32:24:403:ZEX:H25	32:24:403:ZEX:H28	1.64	0.43
21:24:405:CL7:H2	21:24:406:CL7:H11C	2.00	0.43
21:3B:611:CL7:HBC2	26:3B:623:LHG:H342	2.01	0.43
21:3D:405:CL7:HAA2	21:3D:405:CL7:HBD	2.01	0.43
21:32:501:CL7:H92C	21:32:501:CL7:H61C	1.75	0.43
21:31:404:CL7:H62C	21:31:404:CL7:H41C	1.62	0.43
19:33:267:ASN:OD1	19:33:269:VAL:N	2.39	0.43
21:33:505:CL7:H3A	21:33:505:CL7:HBA1	1.79	0.43
21:34:411:CL7:HED3	21:34:411:CL7:CGA	2.48	0.43
21:4B:613:CL7:H192	21:4B:613:CL7:H162	1.85	0.43
21:4C:503:CL7:H151	21:4C:503:CL7:H112	1.75	0.43
21:4D:405:CL7:HAA2	21:4D:405:CL7:HBD	2.01	0.43
16:42:188:LYS:HB3	16:42:196:PHE:CD2	2.53	0.43
21:41:416:CL7:HED3	21:41:416:CL7:HBD	1.71	0.43
21:43:413:CL7:H12C	21:43:413:CL7:H52C	1.86	0.43
1:1A:202:VAL:HG22	21:1A:401:CL7:C2B	2.48	0.43
21:1B:608:CL7:HBC3	21:1B:608:CL7:HHD	2.00	0.43
21:1C:506:CL7:H3A	21:1C:506:CL7:HBA1	1.76	0.43
16:12:168:ASP:HB3	16:12:171:VAL:HB	2.01	0.43
16:12:313:PHE:CD2	32:12:519:ZEX:H30	2.53	0.43
21:13:503:CL7:HAA2	21:13:503:CL7:HBD	2.01	0.43
20:14:85:MET:HE2	20:14:85:MET:HB3	1.91	0.43
4:2D:92:TRP:NE1	13:2X:13:SER:HB3	2.33	0.43
16:22:123:SER:C	16:22:125:ALA:H	2.26	0.43
16:22:164:HIS:ND1	16:22:164:HIS:O	2.52	0.43
16:22:188:LYS:HB3	16:22:196:PHE:CD2	2.53	0.43
21:24:412:CL7:H2A	21:24:412:CL7:O2A	2.18	0.43
1:3A:330:VAL:HG21	4:3D:327:TRP:CE2	2.53	0.43
2:3B:434:ARG:HG2	2:3B:439:SER:HB2	2.01	0.43
3:3C:170:MET:HG3	3:3C:268:PRO:HG3	2.01	0.43
3:3C:207:ASN:OD1	3:3C:208:VAL:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3F:45:ILE:HD13	6:3F:45:ILE:HA	1.87	0.43
8:3I:18:LEU:HD23	8:3I:18:LEU:HA	1.73	0.43
11:3M:17:ILE:HB	11:3M:18:PRO:HD3	2.00	0.43
16:32:128:ARG:HB3	21:32:514:CL7:HED1	2.00	0.43
32:31:422:ZEX:H391	32:31:422:ZEX:H27	1.76	0.43
19:33:75:TRP:CH2	21:42:518:CL7:H121	2.53	0.43
21:33:508:CL7:H102	21:33:508:CL7:H62C	1.52	0.43
2:4B:52:LEU:HD21	2:4B:307:GLU:HG2	2.00	0.43
3:4C:382:ARG:HA	3:4C:382:ARG:HD3	1.87	0.43
21:4C:509:CL7:H3A	21:4C:509:CL7:HBA2	1.63	0.43
16:42:123:SER:C	16:42:125:ALA:H	2.26	0.43
16:42:164:HIS:ND1	16:42:164:HIS:O	2.52	0.43
20:44:166:LEU:HA	20:44:166:LEU:HD23	1.78	0.43
20:44:289:VAL:HG22	21:44:410:CL7:HAB	1.99	0.43
1:1A:194:MET:HE2	1:1A:194:MET:HB3	1.85	0.43
2:1B:42:LEU:HA	2:1B:42:LEU:HD23	1.73	0.43
2:1B:434:ARG:HG2	2:1B:439:SER:HB2	2.01	0.43
3:1C:170:MET:HG3	3:1C:268:PRO:HG3	2.01	0.43
21:1C:510:CL7:H111	21:1C:510:CL7:H72C	1.48	0.43
16:12:31:HIS:ND1	21:12:509:CL7:H142	2.32	0.43
21:12:515:CL7:HMB1	32:12:520:ZEX:H202	2.01	0.43
19:13:167:TYR:OH	19:13:274:GLU:OE2	2.28	0.43
32:13:525:ZEX:H25	32:13:525:ZEX:H28	1.48	0.43
21:14:411:CL7:HED3	21:14:411:CL7:CGA	2.48	0.43
21:14:412:CL7:H2A	21:14:412:CL7:O2A	2.18	0.43
21:2B:604:CL7:H203	21:2B:610:CL7:H102	2.00	0.43
21:2B:605:CL7:HAA2	21:2B:605:CL7:HBD	1.99	0.43
21:2C:501:CL7:H3A	21:2C:501:CL7:HBA1	1.59	0.43
16:22:128:ARG:HB3	21:22:514:CL7:HED1	2.01	0.43
21:22:517:CL7:HBA1	21:22:517:CL7:H3A	1.48	0.43
21:21:409:CL7:OBD	32:21:421:ZEX:O3	2.25	0.43
2:3B:303:ASP:OD1	2:3B:303:ASP:N	2.49	0.43
2:3B:388:SER:HA	4:3D:343:GLU:OE2	2.19	0.43
21:31:406:CL7:H111	21:31:406:CL7:H142	1.76	0.43
19:33:112:THR:HG23	19:33:113:LYS:N	2.33	0.43
21:33:508:CL7:H3A	21:33:508:CL7:HBA2	1.77	0.43
1:4A:20:PHE:O	1:4A:23:SER:OG	2.29	0.43
3:4C:68:HIS:CE1	3:4C:72:ILE:HD11	2.54	0.43
4:4D:92:TRP:NE1	13:4X:13:SER:HB3	2.33	0.43
4:4D:323:GLY:O	4:4D:327:TRP:HD1	2.02	0.43
21:42:515:CL7:HMB1	32:42:520:ZEX:H202	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:52:ASN:HD21	18:41:91:PHE:HD1	1.67	0.43
18:41:152:ILE:HD11	21:41:410:CL7:H61C	2.00	0.43
21:41:410:CL7:H122	21:41:413:CL7:C3D	2.49	0.43
21:43:404:CL7:H121	21:43:410:CL7:H43C	2.00	0.43
21:43:410:CL7:H12C	21:43:410:CL7:HBA1	1.68	0.43
32:43:423:ZEX:H173	32:43:423:ZEX:H3	1.69	0.43
32:43:423:ZEX:H15	32:43:423:ZEX:H201	1.85	0.43
21:1A:407:CL7:H142	21:1A:407:CL7:H111	1.91	0.43
2:1B:388:SER:HA	4:1D:343:GLU:OE2	2.19	0.43
16:12:253:LEU:HD23	16:12:253:LEU:HA	1.82	0.43
21:12:518:CL7:H2A	21:12:518:CL7:O1D	2.19	0.43
19:13:40:PHE:CD1	21:22:517:CL7:H2	2.54	0.43
21:13:508:CL7:H3A	21:13:508:CL7:HBA2	1.77	0.43
20:14:71:TYR:OH	20:14:101:ILE:HB	2.17	0.43
21:2C:507:CL7:H61C	21:2C:507:CL7:H41C	1.77	0.43
30:2D:407:PL9:H321	30:2D:407:PL9:H28	1.78	0.43
16:22:168:ASP:HB3	16:22:171:VAL:HB	2.01	0.43
18:21:193:TYR:OH	18:21:210:ASP:OD2	2.35	0.43
21:21:406:CL7:H11C	32:21:422:ZEX:H173	2.00	0.43
21:23:410:CL7:H202	21:23:410:CL7:H161	1.78	0.43
1:3A:93:LEU:HD21	21:3A:403:CL7:HAA1	2.00	0.43
21:3B:609:CL7:H3A	21:3B:609:CL7:HBA1	1.50	0.43
27:3C:516:DGD:HB72	27:3C:516:DGD:HB42	1.58	0.43
21:32:511:CL7:C1B	32:32:524:ZEX:C17	2.97	0.43
18:31:72:LEU:HD11	21:31:404:CL7:HED3	2.01	0.43
18:31:111:PHE:HD1	18:31:115:ILE:HD12	1.83	0.43
21:31:407:CL7:HMA3	21:31:408:CL7:C2C	2.49	0.43
21:33:503:CL7:HBD	21:33:503:CL7:HAA2	2.01	0.43
32:33:522:ZEX:H15	32:33:522:ZEX:H201	1.85	0.43
21:42:511:CL7:C1B	32:42:524:ZEX:C17	2.97	0.43
21:42:516:CL7:H41C	21:42:516:CL7:H61C	1.33	0.43
18:41:111:PHE:HD1	18:41:115:ILE:HD12	1.83	0.43
19:43:112:THR:HG23	19:43:113:LYS:N	2.33	0.43
21:44:405:CL7:H41C	21:44:405:CL7:H62C	1.73	0.43
21:44:406:CL7:H3A	21:44:406:CL7:HBA1	1.62	0.43
2:1B:401:PHE:HB2	2:1B:406:LEU:O	2.18	0.43
30:1D:407:PL9:H321	30:1D:407:PL9:H28	1.78	0.43
21:11:410:CL7:H122	21:11:413:CL7:C3D	2.49	0.43
19:13:161:ALA:HA	19:13:166:VAL:HG13	2.00	0.43
32:13:522:ZEX:H15	32:13:522:ZEX:H201	1.85	0.43
32:14:403:ZEX:H401	32:14:403:ZEX:H31	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2A:407:CL7:HAA2	21:2A:407:CL7:HBD	2.00	0.43
21:2B:609:CL7:HBC3	21:2B:609:CL7:HHD	2.00	0.43
3:2C:170:MET:HG3	3:2C:268:PRO:HG3	2.01	0.43
5:2E:26:THR:HB	31:2F:101:HEM:HAB	2.01	0.43
11:2M:17:ILE:HB	11:2M:18:PRO:HD3	2.00	0.43
16:22:35:ILE:HG12	21:22:512:CL7:O1D	2.19	0.43
16:22:118:LEU:HD23	16:22:118:LEU:HA	1.90	0.43
18:21:252:LEU:O	18:21:256:ILE:HG13	2.19	0.43
21:24:411:CL7:HED3	21:24:411:CL7:CGA	2.48	0.43
1:3A:85:SER:HA	1:3A:109:GLY:HA3	2.01	0.43
2:3B:199:ASP:OD1	7:3H:61:ALA:HA	2.18	0.43
21:3B:612:CL7:H62C	21:3B:612:CL7:H102	1.71	0.43
3:3C:242:LEU:HD23	3:3C:242:LEU:HA	1.83	0.43
21:3C:501:CL7:H162	21:3C:501:CL7:H202	1.69	0.43
4:3D:296:ASP:N	4:3D:296:ASP:OD1	2.50	0.43
16:32:121:SER:OG	16:32:126:SER:OG	2.36	0.43
16:32:144:GLY:HA3	16:32:226:ILE:HG13	2.00	0.43
16:32:168:ASP:HB3	16:32:171:VAL:HB	2.01	0.43
16:32:313:PHE:CD2	32:32:519:ZEX:H30	2.53	0.43
18:31:90:VAL:O	18:31:94:ILE:HG12	2.18	0.43
19:33:11:TYR:HB3	19:33:15:SER:O	2.19	0.43
21:33:507:CL7:H101	21:33:507:CL7:H62C	1.64	0.43
21:33:516:CL7:H92C	21:33:516:CL7:H62C	1.83	0.43
2:4B:401:PHE:HB2	2:4B:406:LEU:O	2.18	0.43
3:4C:207:ASN:OD1	3:4C:208:VAL:N	2.52	0.43
21:4C:510:CL7:H72C	21:4C:510:CL7:H111	1.48	0.43
5:4E:26:THR:HB	31:4F:101:HEM:HAB	2.01	0.43
21:42:511:CL7:C2B	32:42:524:ZEX:H172	2.49	0.43
21:42:512:CL7:HBA1	21:42:512:CL7:O1D	2.18	0.43
19:43:202:ASN:HA	19:43:269:VAL:HG21	2.01	0.43
21:43:405:CL7:H41C	21:43:405:CL7:H62C	1.36	0.43
20:44:167:VAL:HG23	20:44:247:ALA:HB1	2.00	0.43
21:1C:502:CL7:H62C	21:1C:502:CL7:H41C	1.74	0.43
21:1C:510:CL7:H111	21:1C:510:CL7:H142	1.72	0.43
11:1M:17:ILE:HB	11:1M:18:PRO:HD3	2.00	0.43
18:11:144:ILE:HG12	21:11:413:CL7:HMC2	2.00	0.43
1:2A:331:MET:SD	4:2D:346:PRO:HB2	2.59	0.43
21:2C:510:CL7:H111	21:2C:510:CL7:H142	1.72	0.43
4:2D:328:MET:HG2	4:2D:332:ASP:HB2	2.00	0.43
21:21:407:CL7:HMA3	21:21:408:CL7:C2C	2.49	0.43
21:21:410:CL7:H122	21:21:413:CL7:C3D	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:23:404:CL7:H121	21:23:410:CL7:H43C	2.00	0.43
20:24:140:PRO:HD2	20:24:143:SER:OG	2.19	0.43
1:3A:97:TRP:CD1	1:3A:98:GLU:HG2	2.54	0.43
3:3C:48:TRP:O	21:3C:508:CL7:H2	2.18	0.43
3:3C:171:GLN:O	3:3C:175:ILE:HG13	2.18	0.43
16:32:164:HIS:ND1	16:32:164:HIS:O	2.52	0.43
21:32:503:CL7:H102	21:32:503:CL7:H13	1.67	0.43
21:31:402:CL7:HBA2	21:31:402:CL7:HBD	2.01	0.43
21:31:408:CL7:H193	21:31:408:CL7:H162	1.87	0.43
19:33:202:ASN:HA	19:33:269:VAL:HG21	2.01	0.43
21:33:502:CL7:H2	21:33:503:CL7:H193	2.01	0.43
20:34:85:MET:HE2	20:34:85:MET:HB3	1.91	0.43
20:34:88:LEU:HA	20:34:88:LEU:HD23	1.75	0.43
2:4B:177:SER:OG	2:4B:178:ASP:N	2.52	0.43
21:4B:609:CL7:HBC3	21:4B:609:CL7:HHD	2.00	0.43
3:4C:237:VAL:HG13	3:4C:301:TYR:HA	2.01	0.43
4:4D:296:ASP:N	4:4D:296:ASP:OD1	2.50	0.43
16:42:50:LEU:HD11	16:42:89:PHE:HB2	2.01	0.43
21:42:501:CL7:H162	21:42:501:CL7:H192	1.76	0.43
21:42:509:CL7:H93C	21:42:509:CL7:H62C	1.63	0.43
18:41:144:ILE:HG12	21:41:413:CL7:HMC2	2.00	0.43
21:41:407:CL7:HMA3	21:41:408:CL7:C2C	2.49	0.43
21:43:406:CL7:OBB	32:44:403:ZEX:H403	2.19	0.43
2:1B:199:ASP:OD1	7:1H:61:ALA:HA	2.18	0.42
2:1B:373:LYS:HE2	2:1B:373:LYS:HB2	1.88	0.42
21:1B:610:CL7:HBA2	21:1B:610:CL7:H11C	1.81	0.42
3:1C:207:ASN:OD1	3:1C:208:VAL:N	2.52	0.42
21:1C:505:CL7:HAA2	21:1C:505:CL7:CBD	2.49	0.42
21:11:405:CL7:HAA2	21:11:405:CL7:HBD	2.01	0.42
21:13:502:CL7:O1A	21:13:503:CL7:H12C	2.19	0.42
21:13:502:CL7:H2	21:13:503:CL7:H193	2.01	0.42
20:14:139:ALA:HA	20:14:140:PRO:HD3	1.88	0.42
21:14:405:CL7:H2	21:14:406:CL7:H11C	2.00	0.42
21:22:512:CL7:O1D	21:22:512:CL7:HBA1	2.18	0.42
21:21:403:CL7:H62C	21:21:403:CL7:H41C	1.87	0.42
21:23:403:CL7:H2	21:23:404:CL7:H193	2.01	0.42
21:23:404:CL7:HAA2	21:23:404:CL7:HBD	2.01	0.42
21:23:413:CL7:H62C	21:23:413:CL7:H41C	1.79	0.42
32:23:420:ZEX:H11	32:23:420:ZEX:H191	1.61	0.42
3:3C:237:VAL:HG13	3:3C:301:TYR:HA	2.01	0.42
15:3Z:40:ILE:HG23	15:3Z:41:TRP:HD1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:31:252:LEU:O	18:31:256:ILE:HG13	2.19	0.42
21:31:406:CL7:H11C	32:31:422:ZEX:H173	2.01	0.42
21:31:413:CL7:H2A	21:31:413:CL7:O1D	2.19	0.42
1:4A:85:SER:HA	1:4A:109:GLY:HA3	2.01	0.42
1:4A:331:MET:SD	4:4D:346:PRO:HB2	2.59	0.42
2:4B:41:GLU:OE2	2:4B:61:PHE:N	2.35	0.42
21:4C:505:CL7:HAA2	21:4C:505:CL7:CBD	2.49	0.42
16:42:144:GLY:HA3	16:42:226:ILE:HG13	2.00	0.42
16:42:313:PHE:CD2	32:42:519:ZEX:H30	2.53	0.42
21:41:406:CL7:H11C	32:41:422:ZEX:H173	2.00	0.42
19:43:11:TYR:HB3	19:43:15:SER:O	2.19	0.42
21:43:411:CL7:H41C	21:43:411:CL7:H61C	1.87	0.42
20:44:85:MET:HE2	20:44:85:MET:HB3	1.91	0.42
20:44:146:ALA:HA	20:44:149:ARG:HG3	2.00	0.42
1:1A:97:TRP:CD1	1:1A:98:GLU:HG2	2.54	0.42
3:1C:297:ILE:HB	21:1C:501:CL7:H43C	2.01	0.42
21:1C:504:CL7:HBA2	21:1C:504:CL7:CHA	2.48	0.42
5:1E:26:THR:HB	31:1F:101:HEM:HAB	2.01	0.42
21:12:511:CL7:H91C	21:12:511:CL7:H111	1.81	0.42
18:11:252:LEU:O	18:11:256:ILE:HG13	2.19	0.42
21:11:407:CL7:HMA3	21:11:408:CL7:C2C	2.49	0.42
1:2A:97:TRP:CD1	1:2A:98:GLU:HG2	2.54	0.42
1:2A:104:GLU:HG2	1:2A:108:ASN:HD21	1.84	0.42
3:2C:297:ILE:HB	21:2C:501:CL7:H43C	2.01	0.42
18:21:52:ASN:HD21	18:21:91:PHE:HD1	1.67	0.42
21:23:403:CL7:O1A	21:23:404:CL7:H12C	2.19	0.42
20:24:146:ALA:HA	20:24:149:ARG:HG3	2.00	0.42
2:3B:177:SER:OG	2:3B:178:ASP:N	2.52	0.42
3:3C:68:HIS:CE1	3:3C:72:ILE:HD11	2.54	0.42
21:3C:505:CL7:HAA2	21:3C:505:CL7:CBD	2.49	0.42
19:33:161:ALA:HA	19:33:166:VAL:HG13	2.00	0.42
21:33:502:CL7:O1A	21:33:503:CL7:H12C	2.19	0.42
20:34:166:LEU:HA	20:34:166:LEU:HD23	1.78	0.42
1:4A:93:LEU:HD21	21:4A:403:CL7:HAA1	2.00	0.42
22:4A:402:PHO:NC	22:4A:402:PHO:ND	2.66	0.42
21:4A:407:CL7:HHD	21:4A:407:CL7:HAC1	1.91	0.42
21:4B:604:CL7:H203	21:4B:610:CL7:H102	2.00	0.42
21:4B:608:CL7:HED3	21:4B:608:CL7:HBD	1.66	0.42
18:41:252:LEU:O	18:41:256:ILE:HG13	2.19	0.42
21:43:403:CL7:H2	21:43:404:CL7:H193	2.01	0.42
21:43:408:CL7:H143	21:43:408:CL7:H162	1.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:44:32:TRP:CD1	20:44:32:TRP:H	2.36	0.42
1:1A:331:MET:SD	4:1D:346:PRO:HB2	2.60	0.42
3:1C:131:LEU:O	3:1C:134:SER:OG	2.27	0.42
9:1K:42:VAL:HB	9:1K:45:LYS:HE2	2.01	0.42
16:12:164:HIS:ND1	16:12:164:HIS:O	2.52	0.42
21:11:406:CL7:H11C	32:11:422:ZEX:H173	2.01	0.42
21:11:413:CL7:H2A	21:11:413:CL7:O1D	2.19	0.42
19:13:75:TRP:HH2	21:22:518:CL7:H121	1.83	0.42
21:13:505:CL7:OBB	32:14:403:ZEX:H403	2.19	0.42
2:2B:388:SER:HA	4:2D:343:GLU:OE2	2.19	0.42
2:2B:434:ARG:HG2	2:2B:439:SER:HB2	2.01	0.42
4:2D:165:SER:OG	4:2D:166:TRP:N	2.53	0.42
9:2K:15:SER:O	9:2K:18:SER:OG	2.20	0.42
9:2K:30:PHE:O	9:2K:34:LEU:N	2.41	0.42
13:2X:29:ILE:O	13:2X:33:GLN:HG2	2.20	0.42
32:22:524:ZEX:H15	32:22:524:ZEX:H201	1.81	0.42
21:21:406:CL7:H111	21:21:406:CL7:H142	1.76	0.42
19:23:11:TYR:HB3	19:23:15:SER:O	2.19	0.42
21:23:410:CL7:H93C	21:23:410:CL7:H62C	1.78	0.42
20:24:32:TRP:CD1	20:24:32:TRP:H	2.36	0.42
1:3A:202:VAL:HG22	21:3A:401:CL7:C2B	2.48	0.42
21:3B:615:CL7:H3A	21:3B:615:CL7:HBA1	1.45	0.42
3:3C:476:GLU:CD	4:3D:244:SER:HG	2.22	0.42
21:3C:504:CL7:HBA2	21:3C:504:CL7:CHA	2.48	0.42
4:3D:188:HIS:HA	4:3D:293:ARG:HD2	2.01	0.42
9:3K:30:PHE:O	9:3K:34:LEU:N	2.41	0.42
9:3K:42:VAL:HB	9:3K:45:LYS:HE2	2.01	0.42
32:31:421:ZEX:H15	32:31:421:ZEX:H201	1.88	0.42
21:33:505:CL7:OBB	32:34:403:ZEX:H403	2.19	0.42
21:33:512:CL7:H62C	21:33:512:CL7:H41C	1.78	0.42
2:4B:199:ASP:OD2	2:4B:202:ASN:N	2.53	0.42
21:4B:607:CL7:C4A	21:4B:607:CL7:HBA2	2.46	0.42
3:4C:296:MET:HE1	3:4C:443:PHE:CD1	2.55	0.42
3:4C:297:ILE:HB	21:4C:501:CL7:H43C	2.01	0.42
21:4C:503:CL7:H162	21:4C:503:CL7:H141	1.62	0.42
11:4M:17:ILE:HB	11:4M:18:PRO:HD3	2.00	0.42
16:42:35:ILE:HG12	21:42:512:CL7:O1D	2.19	0.42
18:41:34:ILE:HA	21:41:413:CL7:HED1	2.02	0.42
1:1A:104:GLU:HG2	1:1A:108:ASN:HD21	1.85	0.42
21:1B:610:CL7:OBD	21:1B:612:CL7:H172	2.19	0.42
27:1C:516:DGD:HB72	27:1C:516:DGD:HB42	1.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:12:292:ASP:O	16:12:293:THR:OG1	2.38	0.42
22:2A:402:PHO:NC	22:2A:402:PHO:ND	2.66	0.42
21:2A:407:CL7:HBA1	21:2A:407:CL7:H3A	1.55	0.42
2:2B:48:SER:O	2:2B:50:PRO:HD3	2.20	0.42
3:2C:296:MET:HE1	3:2C:443:PHE:CD1	2.55	0.42
4:2D:28:PHE:O	4:2D:127:ARG:NH1	2.47	0.42
21:22:511:CL7:C2B	32:22:524:ZEX:H172	2.49	0.42
18:21:243:LYS:HE3	18:21:243:LYS:HB3	1.88	0.42
21:23:406:CL7:OBB	32:24:403:ZEX:H403	2.19	0.42
20:24:35:ASN:CG	21:24:411:CL7:HAB	2.45	0.42
1:3A:96:ILE:HG22	8:3I:1:MET:HE1	2.00	0.42
2:3B:357:ARG:NH2	4:3D:336:GLU:O	2.49	0.42
24:3B:621:LMG:HC91	24:3B:621:LMG:H292	1.71	0.42
3:3C:297:ILE:HB	21:3C:501:CL7:H43C	2.01	0.42
27:3C:516:DGD:HA51	27:3C:516:DGD:HA22	1.91	0.42
16:32:281:GLN:HG2	16:32:293:THR:HG22	2.01	0.42
16:32:292:ASP:O	16:32:293:THR:OG1	2.38	0.42
21:32:515:CL7:HMB1	32:32:520:ZEX:H202	2.01	0.42
21:32:518:CL7:H2A	21:32:518:CL7:O1D	2.19	0.42
18:31:151:LEU:HD23	18:31:151:LEU:HA	1.71	0.42
24:31:401:LMG:HC71	24:31:401:LMG:HC2	1.91	0.42
21:31:405:CL7:HBD	21:31:405:CL7:HAA2	2.02	0.42
21:31:418:CL7:H3A	21:31:418:CL7:HBA1	1.59	0.42
32:33:522:ZEX:H173	32:33:522:ZEX:H3	1.69	0.42
20:34:146:ALA:HA	20:34:149:ARG:HG3	2.00	0.42
1:4A:286:THR:OG1	21:4A:401:CL7:O1D	2.23	0.42
2:4B:48:SER:O	2:4B:50:PRO:HD3	2.19	0.42
2:4B:175:TRP:HA	2:4B:185:HIS:O	2.18	0.42
2:4B:199:ASP:OD1	7:4H:61:ALA:HA	2.18	0.42
3:4C:292:TYR:CD1	3:4C:450:PHE:HB2	2.55	0.42
13:4X:29:ILE:O	13:4X:33:GLN:HG2	2.20	0.42
21:42:503:CL7:H91C	21:42:503:CL7:H111	1.82	0.42
21:42:518:CL7:H2A	21:42:518:CL7:O1D	2.19	0.42
32:42:520:ZEX:H391	32:42:520:ZEX:H27	1.75	0.42
18:41:342:ASP:O	18:41:346:VAL:HG23	2.19	0.42
21:41:404:CL7:H41C	21:41:404:CL7:H62C	1.63	0.42
21:41:410:CL7:H8	21:41:410:CL7:H51C	1.63	0.42
19:43:213:PHE:O	19:43:216:SER:OG	2.35	0.42
21:43:409:CL7:C2D	32:43:420:ZEX:H162	2.50	0.42
4:1D:188:HIS:HA	4:1D:293:ARG:HD2	2.01	0.42
4:1D:298:VAL:CG2	10:1L:38:ASN:OXT	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:12:144:GLY:HA3	16:12:226:ILE:HG13	2.00	0.42
21:12:518:CL7:H121	19:23:75:TRP:CH2	2.55	0.42
18:11:72:LEU:HD11	21:11:404:CL7:HED3	2.01	0.42
21:2C:501:CL7:H202	21:2C:501:CL7:H162	1.70	0.42
21:2C:505:CL7:CBD	21:2C:505:CL7:HAA2	2.49	0.42
4:2D:83:SER:O	5:2E:69:ARG:HB2	2.20	0.42
4:2D:298:VAL:CG2	10:2L:38:ASN:OXT	2.68	0.42
16:22:50:LEU:HD11	16:22:89:PHE:HB2	2.01	0.42
16:22:144:GLY:HA3	16:22:226:ILE:HG13	2.00	0.42
18:21:90:VAL:O	18:21:94:ILE:HG12	2.18	0.42
21:21:405:CL7:HAA2	21:21:405:CL7:HBD	2.01	0.42
21:23:411:CL7:H112	21:23:411:CL7:H143	1.79	0.42
32:23:423:ZEX:H15	32:23:423:ZEX:H201	1.85	0.42
20:24:38:MET:HE3	20:24:38:MET:HB2	1.71	0.42
1:3A:104:GLU:HG2	1:3A:108:ASN:HD21	1.84	0.42
21:32:502:CL7:H2	21:32:503:CL7:C1	2.42	0.42
18:31:38:ALA:HB2	18:31:105:LEU:HB2	2.01	0.42
18:31:262:MET:HB3	21:31:402:CL7:H61C	2.01	0.42
21:33:508:CL7:C2D	32:33:519:ZEX:H162	2.50	0.42
32:33:519:ZEX:H27	32:33:519:ZEX:H30	1.76	0.42
1:4A:97:TRP:CD1	1:4A:98:GLU:HG2	2.54	0.42
1:4A:275:LEU:HD23	1:4A:275:LEU:HA	1.89	0.42
2:4B:100:SER:OG	2:4B:102:GLU:OE1	2.20	0.42
27:4C:516:DGD:HB42	27:4C:516:DGD:HB72	1.58	0.42
18:41:343:ILE:HD13	18:41:343:ILE:HA	1.86	0.42
21:41:418:CL7:H2A	21:41:418:CL7:HED3	2.01	0.42
20:44:140:PRO:HD2	20:44:143:SER:OG	2.19	0.42
1:1A:104:GLU:O	1:1A:108:ASN:ND2	2.48	0.42
2:1B:48:SER:O	2:1B:50:PRO:HD3	2.19	0.42
21:1B:615:CL7:H11C	21:1B:615:CL7:HBA2	1.71	0.42
25:1B:620:SQD:C24	10:2L:15:ARG:HD2	2.49	0.42
4:1D:83:SER:O	5:1E:69:ARG:HB2	2.20	0.42
4:1D:165:SER:OG	4:1D:166:TRP:N	2.53	0.42
16:12:121:SER:HG	16:12:126:SER:HG	1.65	0.42
21:12:511:CL7:C1B	32:12:524:ZEX:C17	2.97	0.42
21:12:516:CL7:HBA1	21:12:516:CL7:H3A	1.55	0.42
20:14:28:GLU:H	20:14:28:GLU:CD	2.28	0.42
20:14:88:LEU:HA	20:14:88:LEU:HD23	1.75	0.42
20:14:140:PRO:HD2	20:14:143:SER:OG	2.19	0.42
21:2B:611:CL7:OBD	21:2B:613:CL7:H172	2.19	0.42
3:2C:292:TYR:CD1	3:2C:450:PHE:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2C:507:CL7:H61C	21:2C:507:CL7:H92C	1.81	0.42
27:2C:516:DGD:HB42	27:2C:516:DGD:HB72	1.58	0.42
16:22:73:VAL:HG12	16:22:160:TRP:CZ3	2.54	0.42
21:22:515:CL7:H3A	21:22:515:CL7:HBA2	1.79	0.42
21:22:518:CL7:H8	21:22:518:CL7:H52C	1.84	0.42
21:22:518:CL7:O1D	21:22:518:CL7:H2A	2.19	0.42
18:21:34:ILE:HA	21:21:413:CL7:HED1	2.02	0.42
18:21:38:ALA:HB2	18:21:105:LEU:HB2	2.01	0.42
21:21:418:CL7:H2A	21:21:418:CL7:HED3	2.00	0.42
21:23:408:CL7:H101	21:23:408:CL7:H62C	1.64	0.42
21:24:415:CL7:H3A	21:24:415:CL7:HBA1	1.40	0.42
32:24:418:ZEX:H31	32:24:418:ZEX:H401	1.88	0.42
3:3C:296:MET:HE1	3:3C:443:PHE:CD1	2.55	0.42
4:3D:109:LEU:HD23	4:3D:109:LEU:HA	1.81	0.42
18:31:39:LEU:HD23	18:31:39:LEU:HA	1.93	0.42
19:33:253:LEU:HD23	19:33:253:LEU:HA	1.82	0.42
20:34:28:GLU:CD	20:34:28:GLU:H	2.28	0.42
1:4A:38:ILE:HB	1:4A:39:PRO:HD3	2.02	0.42
21:4B:612:CL7:HBC2	26:4B:624:LHG:H342	2.01	0.42
21:4B:613:CL7:H142	21:4B:613:CL7:H111	1.73	0.42
4:4D:83:SER:O	5:4E:69:ARG:HB2	2.20	0.42
4:4D:328:MET:HG2	4:4D:332:ASP:HB2	2.00	0.42
16:42:168:ASP:HB3	16:42:171:VAL:HB	2.01	0.42
21:42:503:CL7:H41C	21:42:503:CL7:H62C	1.78	0.42
21:43:410:CL7:H142	21:43:410:CL7:H111	1.64	0.42
1:1A:85:SER:HA	1:1A:109:GLY:HA3	2.01	0.42
1:1A:331:MET:HE2	4:1D:319:LEU:HB3	2.02	0.42
3:1C:68:HIS:CE1	3:1C:72:ILE:HD11	2.54	0.42
4:1D:296:ASP:N	4:1D:296:ASP:OD1	2.50	0.42
10:1L:28:LEU:HD23	10:1L:28:LEU:HA	1.88	0.42
16:12:111:ILE:HD12	16:12:111:ILE:HA	1.80	0.42
16:12:144:GLY:HA2	16:12:222:GLY:HA2	2.01	0.42
32:12:524:ZEX:H15	32:12:524:ZEX:H201	1.81	0.42
18:11:38:ALA:HB2	18:11:105:LEU:HB2	2.01	0.42
18:11:262:MET:HB3	21:11:402:CL7:H61C	2.02	0.42
19:13:169:PRO:HB3	19:13:272:PRO:HB3	2.02	0.42
32:13:525:ZEX:H15	32:13:525:ZEX:H201	1.85	0.42
20:14:35:ASN:CG	21:14:411:CL7:HAB	2.45	0.42
20:14:146:ALA:HA	20:14:149:ARG:HG3	2.00	0.42
21:14:411:CL7:H141	21:14:411:CL7:H162	1.70	0.42
2:2B:199:ASP:OD2	2:2B:202:ASN:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:199:ASP:OD1	7:2H:61:ALA:HA	2.18	0.42
21:2C:509:CL7:H41C	21:2C:509:CL7:H62C	1.60	0.42
21:22:516:CL7:H193	21:22:516:CL7:H162	1.75	0.42
18:21:342:ASP:O	18:21:346:VAL:HG23	2.19	0.42
19:23:327:LEU:HD23	19:23:327:LEU:HA	1.84	0.42
20:24:166:LEU:HA	20:24:166:LEU:HD23	1.78	0.42
1:3A:331:MET:SD	4:3D:346:PRO:HB2	2.59	0.42
2:3B:199:ASP:OD2	2:3B:202:ASN:N	2.53	0.42
3:3C:51:ASN:N	21:3C:508:CL7:O1A	2.53	0.42
21:3C:506:CL7:HBA1	21:3C:506:CL7:H3A	1.76	0.42
16:32:348:LEU:HD23	16:32:348:LEU:HA	1.64	0.42
18:31:290:PHE:CE2	18:31:294:PRO:HG3	2.55	0.42
19:33:63:ASN:HB3	21:33:504:CL7:H2A	2.00	0.42
2:4B:154:LEU:HD23	2:4B:154:LEU:HA	1.87	0.42
21:4B:611:CL7:OBD	21:4B:613:CL7:H172	2.19	0.42
4:4D:109:LEU:HA	4:4D:109:LEU:HD23	1.81	0.42
21:41:402:CL7:HBA2	21:41:402:CL7:HBD	2.01	0.42
21:43:404:CL7:HAA2	21:43:404:CL7:HBD	2.01	0.42
21:1B:605:CL7:HBA1	21:1B:605:CL7:H3A	1.78	0.42
3:1C:292:TYR:CD1	3:1C:450:PHE:HB2	2.55	0.42
3:1C:467:PHE:HE2	8:1I:31:ASN:HB2	1.85	0.42
15:1Z:40:ILE:HG23	15:1Z:41:TRP:HD1	1.84	0.42
18:11:34:ILE:HA	21:11:413:CL7:HED1	2.01	0.42
19:13:11:TYR:HB3	19:13:15:SER:O	2.19	0.42
32:13:520:ZEX:H401	32:13:520:ZEX:H31	1.79	0.42
1:2A:38:ILE:HB	1:2A:39:PRO:HD3	2.02	0.42
1:2A:331:MET:HE2	4:2D:319:LEU:HB3	2.02	0.42
21:2B:604:CL7:H192	21:2B:610:CL7:H122	2.01	0.42
3:2C:207:ASN:OD1	3:2C:208:VAL:N	2.52	0.42
4:2D:188:HIS:HA	4:2D:293:ARG:HD2	2.01	0.42
9:2K:42:VAL:HB	9:2K:45:LYS:HE2	2.01	0.42
16:22:255:LEU:O	16:22:259:VAL:HG23	2.20	0.42
20:24:304:ARG:CG	32:24:418:ZEX:H373	2.37	0.42
1:3A:37:MET:HE2	1:3A:37:MET:HB3	1.95	0.42
1:3A:154:THR:HG22	21:3A:401:CL7:C4	2.50	0.42
5:3E:26:THR:HB	31:3F:101:HEM:HAB	2.01	0.42
21:32:505:CL7:H41C	21:32:505:CL7:H62C	1.49	0.42
21:32:511:CL7:H91C	21:32:511:CL7:H111	1.81	0.42
21:32:517:CL7:H111	21:32:517:CL7:H142	1.80	0.42
21:31:410:CL7:H62C	21:31:410:CL7:H41C	1.76	0.42
21:33:503:CL7:H101	21:33:503:CL7:H13	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:33:525:ZEX:H25	32:33:525:ZEX:H28	1.49	0.42
21:34:405:CL7:H2	21:34:406:CL7:H11C	2.00	0.42
21:4A:407:CL7:H141	21:4A:407:CL7:H161	1.84	0.42
21:4B:604:CL7:H192	21:4B:610:CL7:H122	2.01	0.42
21:4C:503:CL7:H61C	21:4C:503:CL7:H41C	1.74	0.42
23:4C:515:8CT:C08	8:4I:24:ILE:HG22	2.50	0.42
21:42:516:CL7:HBA1	21:42:516:CL7:H12C	1.71	0.42
18:41:90:VAL:O	18:41:94:ILE:HG12	2.19	0.42
18:41:343:ILE:O	18:41:347:ILE:HG13	2.20	0.42
20:44:35:ASN:CG	21:44:411:CL7:HAB	2.45	0.42
1:1A:154:THR:HG22	21:1A:401:CL7:C4	2.50	0.42
25:1A:406:SQD:O9	25:1A:406:SQD:O4	2.25	0.42
2:1B:325:PHE:HA	21:1B:607:CL7:H43C	2.02	0.42
3:1C:237:VAL:HG13	3:1C:301:TYR:HA	2.01	0.42
4:1D:19:ASP:O	4:1D:23:ARG:HG3	2.20	0.42
16:12:50:LEU:HD11	16:12:89:PHE:HB2	2.01	0.42
21:12:511:CL7:C2B	32:12:524:ZEX:H172	2.49	0.42
18:11:290:PHE:CE2	18:11:294:PRO:HG3	2.55	0.42
21:11:402:CL7:HBA2	21:11:402:CL7:HBD	2.01	0.42
32:13:519:ZEX:H27	32:13:519:ZEX:H30	1.76	0.42
21:2B:613:CL7:H142	21:2B:613:CL7:H111	1.73	0.42
23:2C:515:8CT:C08	8:2I:24:ILE:HG22	2.50	0.42
18:21:293:ALA:HB3	24:21:401:LMG:H122	2.01	0.42
21:21:414:CL7:HMD2	20:34:258:PRO:HB2	1.99	0.42
21:23:409:CL7:C2D	32:23:420:ZEX:H162	2.50	0.42
21:23:418:CL7:HBA2	21:23:418:CL7:H3A	1.69	0.42
21:3C:503:CL7:H151	21:3C:503:CL7:H112	1.75	0.42
4:3D:19:ASP:O	4:3D:23:ARG:HG3	2.20	0.42
13:3X:29:ILE:O	13:3X:33:GLN:HG2	2.20	0.42
16:32:35:ILE:HG12	21:32:512:CL7:O1D	2.19	0.42
16:32:94:MET:CE	32:32:524:ZEX:C36	2.94	0.42
16:32:255:LEU:O	16:32:259:VAL:HG23	2.20	0.42
21:32:510:CL7:H162	21:32:510:CL7:H141	1.61	0.42
20:34:140:PRO:HD2	20:34:143:SER:OG	2.19	0.42
2:4B:194:ARG:HB3	2:4B:195:PRO:HD2	2.01	0.42
3:4C:170:MET:HG3	3:4C:268:PRO:HG3	2.01	0.42
16:42:73:VAL:HG12	16:42:160:TRP:CZ3	2.54	0.42
16:42:121:SER:OG	16:42:126:SER:OG	2.36	0.42
18:41:293:ALA:HB3	24:41:401:LMG:H122	2.01	0.42
21:41:403:CL7:H62C	21:41:403:CL7:H41C	1.87	0.42
21:41:408:CL7:H121	21:41:408:CL7:H161	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:41:410:CL7:HBA2	21:41:410:CL7:H11C	1.89	0.42
32:43:420:ZEX:H27	32:43:420:ZEX:H30	1.76	0.42
32:43:421:ZEX:H15	32:43:421:ZEX:H201	1.75	0.42
32:43:423:ZEX:H11	32:43:423:ZEX:H191	1.48	0.42
21:1B:602:CL7:H41C	21:1B:602:CL7:H61C	1.73	0.42
3:1C:388:ASP:OD1	3:1C:390:ASN:N	2.45	0.42
21:1C:509:CL7:H41C	21:1C:509:CL7:H62C	1.60	0.42
18:11:302:LEU:HD12	18:11:302:LEU:HA	1.92	0.42
19:13:202:ASN:HA	19:13:269:VAL:HG21	2.01	0.42
20:14:32:TRP:CD1	20:14:32:TRP:H	2.36	0.42
21:2A:407:CL7:HHD	21:2A:407:CL7:HAC1	1.91	0.42
2:2B:41:GLU:CD	2:2B:61:PHE:H	2.26	0.42
2:2B:178:ASP:OD1	2:2B:182:LEU:N	2.38	0.42
3:2C:237:VAL:HG13	3:2C:301:TYR:HA	2.01	0.42
16:22:292:ASP:O	16:22:293:THR:OG1	2.38	0.42
21:22:510:CL7:H41C	21:22:510:CL7:H61C	1.54	0.42
32:22:524:ZEX:H7	21:21:417:CL7:HED1	2.02	0.42
18:21:290:PHE:CE2	18:21:294:PRO:HG3	2.55	0.42
19:23:169:PRO:HB3	19:23:272:PRO:HB3	2.02	0.42
32:24:420:ZEX:H11	32:24:420:ZEX:H191	1.88	0.42
2:3B:401:PHE:HB2	2:3B:406:LEU:O	2.18	0.42
4:3D:298:VAL:CG2	10:3L:38:ASN:OXT	2.68	0.42
18:31:293:ALA:HB3	24:31:401:LMG:H122	2.01	0.42
19:33:169:PRO:HB3	19:33:272:PRO:HB3	2.02	0.42
1:4A:104:GLU:HG2	1:4A:108:ASN:HD21	1.85	0.42
2:4B:434:ARG:HG2	2:4B:439:SER:HB2	2.01	0.42
21:4B:607:CL7:HBA2	21:4B:607:CL7:H3A	1.70	0.42
4:4D:242:THR:O	4:4D:242:THR:OG1	2.37	0.42
16:42:111:ILE:HD12	16:42:111:ILE:HA	1.80	0.42
16:42:128:ARG:HB3	21:42:514:CL7:HED1	2.01	0.42
16:42:144:GLY:HA2	16:42:222:GLY:HA2	2.01	0.42
16:42:255:LEU:O	16:42:259:VAL:HG23	2.20	0.42
18:41:38:ALA:HB2	18:41:105:LEU:HB2	2.01	0.42
21:41:406:CL7:H111	21:41:406:CL7:H142	1.76	0.42
21:41:406:CL7:H8	21:41:406:CL7:H52C	1.90	0.42
21:43:409:CL7:H3A	21:43:409:CL7:HBA2	1.77	0.42
21:43:411:CL7:H112	21:43:411:CL7:H143	1.79	0.42
20:44:307:ASP:OD1	20:44:307:ASP:N	2.49	0.42
25:1B:620:SQD:H383	12:2T:12:CYS:HB3	2.02	0.41
16:12:73:VAL:HG12	16:12:160:TRP:CZ3	2.54	0.41
16:12:104:GLY:O	16:12:108:ILE:HG13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:12:503:CL7:H41C	21:12:503:CL7:H62C	1.78	0.41
21:12:509:CL7:H62C	21:12:509:CL7:H93C	1.63	0.41
18:11:52:ASN:HD21	18:11:91:PHE:HD1	1.67	0.41
18:11:343:ILE:O	18:11:347:ILE:HG13	2.20	0.41
2:2B:325:PHE:HA	21:2B:608:CL7:H43C	2.02	0.41
12:2T:14:ILE:HD13	12:2T:14:ILE:HA	1.90	0.41
18:21:144:ILE:HG12	21:21:413:CL7:HMC2	2.00	0.41
18:21:262:MET:HB3	21:21:402:CL7:H61C	2.01	0.41
19:23:202:ASN:HA	19:23:269:VAL:HG21	2.01	0.41
21:23:402:CL7:H162	21:23:402:CL7:H193	1.83	0.41
4:3D:158:MET:HE2	4:3D:158:MET:HB3	1.91	0.41
4:3D:270:MET:HE2	4:3D:270:MET:HB3	1.96	0.41
16:32:144:GLY:HA2	16:32:222:GLY:HA2	2.01	0.41
18:31:157:LEU:HD23	18:31:157:LEU:HA	1.84	0.41
18:31:313:LEU:O	18:31:317:THR:OG1	2.23	0.41
18:31:342:ASP:O	18:31:346:VAL:HG23	2.19	0.41
2:4B:172:PRO:HG3	21:4B:607:CL7:O1D	2.20	0.41
4:4D:165:SER:OG	4:4D:166:TRP:N	2.53	0.41
4:4D:298:VAL:CG2	10:4L:38:ASN:OXT	2.68	0.41
10:4L:14:ASN:OD1	10:4L:14:ASN:N	2.52	0.41
18:41:72:LEU:HD11	21:41:404:CL7:HED3	2.01	0.41
21:41:413:CL7:H2A	21:41:413:CL7:O1D	2.19	0.41
21:41:417:CL7:H3A	21:41:417:CL7:HBA1	1.70	0.41
21:43:403:CL7:O1A	21:43:404:CL7:H12C	2.19	0.41
1:1A:218:LEU:HD23	1:1A:218:LEU:HA	1.91	0.41
2:1B:177:SER:OG	2:1B:178:ASP:N	2.52	0.41
21:1C:506:CL7:HBC2	21:1C:507:CL7:H201	2.02	0.41
11:1M:13:LEU:HA	11:1M:13:LEU:HD12	1.80	0.41
13:1X:29:ILE:O	13:1X:33:GLN:HG2	2.20	0.41
16:12:35:ILE:HG12	21:12:512:CL7:O1D	2.19	0.41
21:11:418:CL7:H2A	21:11:418:CL7:HED3	2.01	0.41
20:14:232:VAL:HA	32:14:419:ZEX:H1	1.82	0.41
1:2A:154:THR:HG22	21:2A:401:CL7:C4	2.50	0.41
2:2B:42:LEU:HD23	2:2B:42:LEU:HA	1.73	0.41
2:2B:165:HIS:C	2:2B:165:HIS:CD2	2.98	0.41
21:2B:604:CL7:H93C	21:2B:604:CL7:H111	1.78	0.41
3:2C:128:ALA:O	3:2C:132:ILE:HG12	2.20	0.41
3:2C:467:PHE:HE2	8:2I:31:ASN:HB2	1.85	0.41
21:2C:508:CL7:H41C	21:2C:508:CL7:H61C	1.41	0.41
16:22:144:GLY:HA2	16:22:222:GLY:HA2	2.01	0.41
21:22:511:CL7:C1B	32:22:524:ZEX:C17	2.97	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:22:524:ZEX:C35	21:21:417:CL7:HBA2	2.49	0.41
18:21:72:LEU:HD11	21:21:404:CL7:HED3	2.01	0.41
21:21:403:CL7:H51C	21:21:404:CL7:H43C	2.02	0.41
21:21:413:CL7:O1D	21:21:413:CL7:H2A	2.19	0.41
20:24:88:LEU:HD23	20:24:88:LEU:HA	1.75	0.41
1:3A:331:MET:HE2	4:3D:319:LEU:HB3	2.02	0.41
2:3B:194:ARG:HB3	2:3B:195:PRO:HD2	2.01	0.41
20:34:32:TRP:CD1	20:34:32:TRP:H	2.36	0.41
20:34:35:ASN:CG	21:34:411:CL7:HAB	2.44	0.41
2:4B:325:PHE:HA	21:4B:608:CL7:H43C	2.02	0.41
21:4C:506:CL7:HBC2	21:4C:507:CL7:H201	2.02	0.41
15:4Z:40:ILE:HG23	15:4Z:41:TRP:HD1	1.84	0.41
16:42:98:PHE:CG	32:42:522:ZEX:H31	2.53	0.41
32:43:401:ZEX:H15	32:43:401:ZEX:H201	1.85	0.41
21:44:404:CL7:H3A	21:44:404:CL7:HBA1	1.27	0.41
2:1B:194:ARG:HB3	2:1B:195:PRO:HD2	2.01	0.41
16:12:281:GLN:HG2	16:12:293:THR:HG22	2.02	0.41
32:12:524:ZEX:H7	21:11:417:CL7:HED1	2.02	0.41
21:11:403:CL7:H51C	21:11:404:CL7:H43C	2.02	0.41
1:2A:85:SER:HA	1:2A:109:GLY:HA3	2.01	0.41
2:2B:172:PRO:HG3	21:2B:607:CL7:O1D	2.20	0.41
21:2B:607:CL7:H41C	21:2B:607:CL7:H62C	1.65	0.41
16:22:98:PHE:CG	32:22:522:ZEX:H31	2.53	0.41
21:22:518:CL7:H3A	21:22:518:CL7:HBA1	1.72	0.41
32:23:401:ZEX:H25	32:23:401:ZEX:H28	1.48	0.41
21:23:404:CL7:H13	21:23:404:CL7:H101	1.74	0.41
21:3B:603:CL7:H192	21:3B:609:CL7:H122	2.01	0.41
3:3C:467:PHE:HE2	8:3I:31:ASN:HB2	1.85	0.41
21:3C:506:CL7:HBC2	21:3C:507:CL7:H201	2.02	0.41
4:3D:182:LEU:HD23	4:3D:182:LEU:HA	1.80	0.41
18:31:339:LYS:HE3	18:31:339:LYS:HB2	1.93	0.41
21:33:501:CL7:H161	21:33:506:CL7:HMC1	2.02	0.41
21:33:504:CL7:H61C	21:33:504:CL7:H92C	1.71	0.41
20:34:201:LEU:O	20:34:203:PRO:HD3	2.21	0.41
21:34:411:CL7:H91C	21:34:411:CL7:H112	1.91	0.41
1:4A:323:ARG:HG3	4:4D:331:GLN:OE1	2.21	0.41
2:4B:388:SER:HA	4:4D:343:GLU:OE2	2.19	0.41
21:4B:616:CL7:HBA1	21:4B:616:CL7:H3A	1.45	0.41
21:4C:505:CL7:HBA1	21:4C:505:CL7:H3A	1.63	0.41
4:4D:188:HIS:HA	4:4D:293:ARG:HD2	2.01	0.41
16:42:104:GLY:O	16:42:108:ILE:HG13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:42:517:CL7:H142	21:42:517:CL7:H111	1.80	0.41
32:42:524:ZEX:H7	21:41:417:CL7:HED1	2.02	0.41
32:43:401:ZEX:H25	32:43:401:ZEX:H28	1.49	0.41
20:44:28:GLU:H	20:44:28:GLU:CD	2.28	0.41
32:44:420:ZEX:H11	32:44:420:ZEX:H191	1.88	0.41
2:1B:199:ASP:OD2	2:1B:202:ASN:N	2.53	0.41
21:1B:606:CL7:H62C	21:1B:606:CL7:H41C	1.65	0.41
21:1B:611:CL7:H141	21:1B:611:CL7:H161	1.65	0.41
3:1C:128:ALA:O	3:1C:132:ILE:HG12	2.20	0.41
3:1C:296:MET:HE1	3:1C:443:PHE:CD1	2.54	0.41
3:1C:382:ARG:HA	3:1C:382:ARG:HD3	1.87	0.41
18:11:342:ASP:O	18:11:346:VAL:HG23	2.19	0.41
21:13:501:CL7:H13	32:13:520:ZEX:H402	2.03	0.41
21:13:508:CL7:H142	21:13:508:CL7:H112	1.95	0.41
21:13:508:CL7:C2D	32:13:519:ZEX:H162	2.50	0.41
21:13:509:CL7:HBA1	21:13:509:CL7:H12C	1.68	0.41
20:14:166:LEU:HA	20:14:166:LEU:HD23	1.78	0.41
21:14:406:CL7:H162	21:14:406:CL7:H121	1.73	0.41
1:2A:323:ARG:HG3	4:2D:331:GLN:OE1	2.21	0.41
2:2B:41:GLU:OE2	2:2B:61:PHE:N	2.35	0.41
2:2B:194:ARG:HB3	2:2B:195:PRO:HD2	2.01	0.41
16:22:111:ILE:HD12	16:22:111:ILE:HA	1.80	0.41
16:22:281:GLN:HG2	16:22:293:THR:HG22	2.01	0.41
18:21:112:HIS:HE1	21:21:414:CL7:NC	2.18	0.41
21:21:410:CL7:HBA2	21:21:410:CL7:H11C	1.89	0.41
21:23:408:CL7:H142	21:23:408:CL7:H111	1.85	0.41
21:24:413:CL7:H142	21:24:413:CL7:H112	1.88	0.41
1:3A:150:PRO:O	1:3A:154:THR:HG23	2.20	0.41
1:3A:163:LEU:HD23	1:3A:163:LEU:HA	1.87	0.41
2:3B:325:PHE:HA	21:3B:607:CL7:H43C	2.02	0.41
3:3C:292:TYR:CD1	3:3C:450:PHE:HB2	2.55	0.41
4:3D:83:SER:O	5:3E:69:ARG:HB2	2.20	0.41
21:3D:404:CL7:H12C	22:3D:408:PHO:CAB	2.50	0.41
21:32:503:CL7:H41C	21:32:503:CL7:H62C	1.78	0.41
19:33:268:ASP:N	19:33:268:ASP:OD1	2.54	0.41
21:34:411:CL7:H162	21:34:411:CL7:H141	1.70	0.41
21:34:414:CL7:H62C	32:34:420:ZEX:H192	2.03	0.41
1:4A:173:PRO:HB2	1:4A:178:GLY:HA3	2.02	0.41
2:4B:165:HIS:CD2	2:4B:165:HIS:C	2.98	0.41
3:4C:48:TRP:CD1	3:4C:48:TRP:H	2.39	0.41
3:4C:128:ALA:O	3:4C:132:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4C:375:GLY:O	3:4C:379:GLU:HB2	2.21	0.41
4:4D:19:ASP:O	4:4D:23:ARG:HG3	2.20	0.41
21:4D:404:CL7:H12C	22:4D:408:PHO:CAB	2.50	0.41
5:4E:76:ILE:O	5:4E:80:THR:N	2.54	0.41
16:42:281:GLN:HG2	16:42:293:THR:HG22	2.01	0.41
16:42:292:ASP:O	16:42:293:THR:OG1	2.38	0.41
21:41:404:CL7:H193	21:41:404:CL7:H162	1.83	0.41
21:41:406:CL7:HBC2	32:41:422:ZEX:C19	2.51	0.41
21:41:409:CL7:OBD	32:41:421:ZEX:O3	2.25	0.41
20:44:230:GLU:OE1	20:44:230:GLU:N	2.37	0.41
2:1B:165:HIS:CD2	2:1B:165:HIS:C	2.98	0.41
21:1B:603:CL7:H192	21:1B:609:CL7:H122	2.01	0.41
3:1C:48:TRP:CD1	3:1C:48:TRP:H	2.39	0.41
16:12:255:LEU:O	16:12:259:VAL:HG23	2.20	0.41
21:12:505:CL7:H101	21:12:505:CL7:H62C	1.69	0.41
21:13:501:CL7:H161	21:13:506:CL7:HMC1	2.02	0.41
21:13:505:CL7:H41C	32:13:520:ZEX:H193	2.03	0.41
32:13:522:ZEX:H173	32:13:522:ZEX:H3	1.69	0.41
1:2A:150:PRO:O	1:2A:154:THR:HG23	2.20	0.41
21:2A:407:CL7:H141	21:2A:407:CL7:H161	1.84	0.41
2:2B:373:LYS:HB2	2:2B:373:LYS:HE2	1.88	0.41
3:2C:375:GLY:O	3:2C:379:GLU:HB2	2.21	0.41
21:2C:506:CL7:HBC2	21:2C:507:CL7:H201	2.02	0.41
4:2D:19:ASP:O	4:2D:23:ARG:HG3	2.20	0.41
21:22:517:CL7:H62C	21:22:517:CL7:H41C	1.42	0.41
18:21:343:ILE:O	18:21:347:ILE:HG13	2.20	0.41
21:21:406:CL7:H121	21:21:406:CL7:H162	1.83	0.41
21:21:410:CL7:H161	21:21:410:CL7:H203	1.73	0.41
21:23:402:CL7:H161	21:23:407:CL7:HMC1	2.02	0.41
21:23:406:CL7:H41C	32:23:421:ZEX:H193	2.03	0.41
21:23:409:CL7:H61C	21:23:409:CL7:H41C	1.53	0.41
16:32:73:VAL:HG12	16:32:160:TRP:CZ3	2.54	0.41
16:32:104:GLY:O	16:32:108:ILE:HG13	2.20	0.41
1:4A:331:MET:HE2	4:4D:319:LEU:HB3	2.02	0.41
10:4L:13:LEU:H	11:4M:29:THR:HG21	1.86	0.41
21:42:517:CL7:H62C	21:42:517:CL7:H41C	1.42	0.41
18:41:112:HIS:HE1	21:41:414:CL7:NC	2.18	0.41
18:41:262:MET:HB3	21:41:402:CL7:H61C	2.02	0.41
20:44:201:LEU:O	20:44:203:PRO:HD3	2.21	0.41
32:44:418:ZEX:H201	32:44:418:ZEX:H15	1.61	0.41
1:1A:63:ILE:HD12	1:1A:63:ILE:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:464:PHE:HB2	4:1D:279:TRP:CZ2	2.56	0.41
21:1B:614:CL7:H62C	21:1B:614:CL7:H41C	1.50	0.41
21:12:510:CL7:C2	32:12:519:ZEX:H181	2.51	0.41
21:12:510:CL7:HBD	21:12:510:CL7:HBA1	2.03	0.41
21:12:511:CL7:C1C	21:11:418:CL7:H161	2.51	0.41
19:13:109:TYR:HB2	21:22:505:CL7:CBA	2.50	0.41
21:13:507:CL7:H41C	21:13:507:CL7:H61C	1.62	0.41
21:13:509:CL7:H202	21:13:509:CL7:H161	1.78	0.41
21:13:510:CL7:H41C	21:13:510:CL7:H61C	1.87	0.41
20:14:201:LEU:O	20:14:203:PRO:HD3	2.21	0.41
21:2B:612:CL7:H141	21:2B:612:CL7:H161	1.66	0.41
5:2E:76:ILE:O	5:2E:80:THR:N	2.54	0.41
32:22:519:ZEX:H15	32:22:519:ZEX:H201	1.80	0.41
21:23:402:CL7:H13	32:23:421:ZEX:H402	2.03	0.41
20:24:28:GLU:H	20:24:28:GLU:CD	2.28	0.41
20:24:201:LEU:O	20:24:203:PRO:HD3	2.21	0.41
21:3A:407:CL7:H161	21:3A:407:CL7:H141	1.84	0.41
2:3B:48:SER:O	2:3B:50:PRO:HD3	2.19	0.41
2:3B:172:PRO:HG3	21:3B:606:CL7:O1D	2.20	0.41
2:3B:440:ASP:OD1	4:3D:302:ILE:HD11	2.21	0.41
21:3B:610:CL7:OBD	21:3B:612:CL7:H172	2.19	0.41
4:3D:165:SER:OG	4:3D:166:TRP:N	2.53	0.41
21:32:511:CL7:C2B	32:32:524:ZEX:H172	2.49	0.41
18:31:34:ILE:HA	21:31:413:CL7:HED1	2.01	0.41
18:31:173:ILE:HG13	18:31:177:ARG:HD2	2.02	0.41
18:31:343:ILE:O	18:31:347:ILE:HG13	2.20	0.41
21:33:516:CL7:HED2	32:34:403:ZEX:H172	2.02	0.41
20:34:50:LEU:HD13	20:34:124:ALA:HB1	2.02	0.41
1:4A:150:PRO:O	1:4A:154:THR:HG23	2.20	0.41
3:4C:51:ASN:N	21:4C:508:CL7:O1A	2.53	0.41
3:4C:467:PHE:HE2	8:4I:31:ASN:HB2	1.85	0.41
16:42:279:VAL:O	16:42:293:THR:OG1	2.32	0.41
18:41:173:ILE:HG13	18:41:177:ARG:HD2	2.02	0.41
18:41:313:LEU:O	18:41:317:THR:OG1	2.23	0.41
21:43:403:CL7:H93C	21:43:403:CL7:H61C	1.85	0.41
20:44:304:ARG:CG	32:44:418:ZEX:H373	2.37	0.41
32:44:419:ZEX:H31	32:44:419:ZEX:H401	1.94	0.41
1:1A:38:ILE:HB	1:1A:39:PRO:HD3	2.02	0.41
3:1C:288:LEU:HA	3:1C:288:LEU:HD23	1.86	0.41
23:1C:515:8CT:C08	8:1I:24:ILE:HG22	2.50	0.41
21:1D:404:CL7:H12C	22:1D:408:PHO:CAB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:52:PRO:HA	5:1E:55:TYR:CE2	2.56	0.41
21:12:515:CL7:HBA2	21:12:515:CL7:H3A	1.79	0.41
32:12:520:ZEX:H391	32:12:520:ZEX:H27	1.74	0.41
18:11:112:HIS:HE1	21:11:414:CL7:NC	2.18	0.41
18:11:293:ALA:HB3	24:11:401:LMG:H122	2.01	0.41
2:2B:177:SER:OG	2:2B:178:ASP:N	2.52	0.41
2:2B:460:LEU:HD12	2:2B:460:LEU:HA	1.93	0.41
3:2C:48:TRP:CD1	3:2C:48:TRP:H	2.39	0.41
3:2C:388:ASP:OD1	3:2C:390:ASN:N	2.45	0.41
15:2Z:40:ILE:HG23	15:2Z:41:TRP:HD1	1.84	0.41
21:22:510:CL7:HBD	21:22:510:CL7:HBA1	2.03	0.41
21:22:512:CL7:H161	21:22:512:CL7:H141	1.75	0.41
2:3B:464:PHE:HB2	4:3D:279:TRP:CZ2	2.56	0.41
21:3B:606:CL7:C4A	21:3B:606:CL7:HBA2	2.47	0.41
3:3C:156:SER:OG	3:3C:157:ASP:N	2.54	0.41
18:31:52:ASN:HD21	18:31:91:PHE:HD1	1.67	0.41
18:31:112:HIS:HE1	21:31:414:CL7:NC	2.18	0.41
21:31:403:CL7:H51C	21:31:404:CL7:H43C	2.02	0.41
21:31:418:CL7:H2A	21:31:418:CL7:HED3	2.00	0.41
19:33:231:TRP:NE1	21:33:506:CL7:OBD	2.47	0.41
2:4B:30:VAL:HG12	21:4B:606:CL7:HHD	2.03	0.41
21:4D:404:CL7:H61C	21:4D:404:CL7:H41C	1.67	0.41
25:42:521:SQD:O47	25:42:521:SQD:H1	2.21	0.41
18:41:82:GLY:HA2	18:41:169:TYR:HE1	1.86	0.41
18:41:151:LEU:CD1	21:41:413:CL7:H3A	2.50	0.41
21:43:403:CL7:C2D	21:43:404:CL7:H151	2.51	0.41
21:44:415:CL7:H3A	21:44:415:CL7:HBA1	1.40	0.41
21:1A:407:CL7:HHD	21:1A:407:CL7:HAC1	1.91	0.41
21:1C:507:CL7:H61C	21:1C:507:CL7:H92C	1.81	0.41
8:1I:21:PHE:O	8:1I:25:SER:OG	2.28	0.41
12:1T:14:ILE:HD13	12:1T:14:ILE:HA	1.90	0.41
21:11:406:CL7:H111	21:11:406:CL7:H142	1.76	0.41
20:14:50:LEU:HD13	20:14:124:ALA:HB1	2.02	0.41
21:14:404:CL7:H3A	21:14:404:CL7:HBA1	1.27	0.41
1:2A:173:PRO:HB2	1:2A:178:GLY:HA3	2.02	0.41
3:2C:51:ASN:N	21:2C:508:CL7:O1A	2.53	0.41
21:2C:505:CL7:H42C	21:2C:505:CL7:NC	2.36	0.41
10:2L:13:LEU:H	11:2M:29:THR:HG21	1.86	0.41
11:2M:25:LEU:HD23	11:2M:25:LEU:HA	1.91	0.41
21:22:501:CL7:H192	21:22:501:CL7:H162	1.76	0.41
18:21:343:ILE:HD13	18:21:343:ILE:HA	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:21:402:CL7:HBA2	21:21:402:CL7:HBD	2.01	0.41
21:21:406:CL7:HBC2	32:21:422:ZEX:C19	2.51	0.41
21:23:403:CL7:C2D	21:23:404:CL7:H151	2.51	0.41
32:23:420:ZEX:H201	32:23:420:ZEX:H15	1.68	0.41
32:23:421:ZEX:H191	32:23:421:ZEX:H11	1.52	0.41
20:24:50:LEU:HD13	20:24:124:ALA:HB1	2.02	0.41
20:24:258:PRO:HB2	21:31:414:CL7:HMD2	1.99	0.41
1:3A:75:ASN:HD21	4:3D:312:THR:HG21	1.86	0.41
3:3C:128:ALA:O	3:3C:132:ILE:HG12	2.20	0.41
21:3C:505:CL7:H42C	21:3C:505:CL7:NC	2.36	0.41
4:3D:84:LEU:HD13	4:3D:89:LEU:HD21	2.03	0.41
16:32:98:PHE:CG	32:32:522:ZEX:H31	2.53	0.41
16:32:148:LEU:HD23	16:32:148:LEU:HA	1.95	0.41
16:32:253:LEU:HD23	16:32:253:LEU:HA	1.83	0.41
21:32:505:CL7:H91C	21:32:505:CL7:H111	1.89	0.41
21:32:511:CL7:C1C	21:31:418:CL7:H161	2.51	0.41
21:32:514:CL7:H3A	21:32:514:CL7:HBA1	1.69	0.41
21:31:404:CL7:H162	21:31:404:CL7:H193	1.83	0.41
3:4C:288:LEU:HD23	3:4C:288:LEU:HA	1.86	0.41
16:42:281:GLN:HA	16:42:282:PRO:HD3	1.93	0.41
21:42:501:CL7:H72C	21:42:501:CL7:H41C	2.03	0.41
21:42:517:CL7:HBA1	21:42:517:CL7:H3A	1.48	0.41
18:41:198:PRO:HD3	21:41:420:CL7:HAB	2.02	0.41
21:41:403:CL7:H51C	21:41:404:CL7:H43C	2.02	0.41
19:43:169:PRO:HB3	19:43:272:PRO:HB3	2.02	0.41
21:43:402:CL7:H13	32:43:421:ZEX:H402	2.03	0.41
21:43:414:CL7:OBD	25:43:424:SQD:O2	2.30	0.41
1:1A:30:ILE:O	1:1A:34:GLY:HA3	2.21	0.41
1:1A:75:ASN:HD21	4:1D:312:THR:HG21	1.86	0.41
1:1A:150:PRO:O	1:1A:154:THR:HG23	2.20	0.41
2:1B:440:ASP:OD1	4:1D:302:ILE:HD11	2.21	0.41
21:1B:602:CL7:H61C	21:1B:602:CL7:H92C	1.88	0.41
21:1B:604:CL7:H92C	21:1B:604:CL7:H62C	1.86	0.41
27:1C:516:DGD:HA51	27:1C:516:DGD:HA22	1.91	0.41
5:1E:76:ILE:O	5:1E:80:THR:N	2.54	0.41
21:12:503:CL7:H91C	21:12:503:CL7:H111	1.82	0.41
21:12:505:CL7:H91C	21:12:505:CL7:H111	1.89	0.41
21:12:507:CL7:H142	21:12:507:CL7:H112	1.90	0.41
25:12:521:SQD:O47	25:12:521:SQD:H1	2.21	0.41
18:11:87:ASN:OD1	18:11:87:ASN:N	2.54	0.41
18:11:151:LEU:CD1	21:11:413:CL7:H3A	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:13:268:ASP:N	19:13:268:ASP:OD1	2.54	0.41
25:13:523:SQD:H201	21:22:506:CL7:H141	2.03	0.41
1:2A:28:LEU:HB2	25:2A:406:SQD:H102	2.03	0.41
1:2A:30:ILE:O	1:2A:34:GLY:HA3	2.21	0.41
2:2B:30:VAL:HG12	21:2B:606:CL7:HHD	2.03	0.41
2:2B:161:PHE:HB2	21:2B:607:CL7:CAB	2.51	0.41
3:2C:288:LEU:HA	3:2C:288:LEU:HD23	1.86	0.41
4:2D:56:SER:HB3	4:2D:78:SER:HB3	2.03	0.41
16:22:104:GLY:O	16:22:108:ILE:HG13	2.20	0.41
21:22:501:CL7:H92C	21:22:501:CL7:H61C	1.75	0.41
21:22:502:CL7:CMB	21:22:504:CL7:HAB	2.51	0.41
21:22:511:CL7:C1C	21:21:418:CL7:H161	2.51	0.41
18:21:82:GLY:HA2	18:21:169:TYR:HE1	1.86	0.41
18:21:198:PRO:HD3	21:21:420:CL7:HAB	2.02	0.41
18:21:261:LEU:O	18:21:265:ILE:HG13	2.21	0.41
32:21:421:ZEX:H15	32:21:421:ZEX:H201	1.88	0.41
21:3C:510:CL7:H111	21:3C:510:CL7:H142	1.72	0.41
5:3E:57:ASP:OD1	5:3E:57:ASP:N	2.54	0.41
10:3L:13:LEU:H	11:3M:29:THR:HG21	1.86	0.41
16:32:50:LEU:HD11	16:32:89:PHE:HB2	2.01	0.41
16:32:207:VAL:HG22	32:32:520:ZEX:H383	2.03	0.41
21:32:501:CL7:H41C	21:32:501:CL7:H72C	2.03	0.41
21:32:502:CL7:CMB	21:32:504:CL7:HAB	2.51	0.41
21:32:510:CL7:C2	32:32:519:ZEX:H181	2.51	0.41
18:31:198:PRO:HD3	21:31:420:CL7:HAB	2.02	0.41
21:31:403:CL7:H61C	21:31:403:CL7:H92C	1.92	0.41
21:33:505:CL7:H41C	32:33:520:ZEX:H193	2.03	0.41
32:33:519:ZEX:H191	32:33:519:ZEX:H11	1.61	0.41
32:33:519:ZEX:H201	32:33:519:ZEX:H15	1.68	0.41
20:34:232:VAL:HA	32:34:419:ZEX:H1	1.84	0.41
20:34:304:ARG:CG	32:34:418:ZEX:H373	2.37	0.41
1:4A:120:MET:SD	1:4A:159:LEU:HB2	2.61	0.41
2:4B:91:ILE:O	2:4B:94:ALA:HB3	2.21	0.41
2:4B:202:ASN:OD1	2:4B:204:THR:OG1	2.27	0.41
2:4B:464:PHE:HB2	4:4D:279:TRP:CZ2	2.56	0.41
3:4C:93:MET:HE1	3:4C:105:ALA:HB2	2.03	0.41
21:4C:501:CL7:H72C	21:4C:501:CL7:HMB3	2.02	0.41
10:4L:28:LEU:HD23	10:4L:28:LEU:HA	1.88	0.41
11:4M:13:LEU:HD12	11:4M:13:LEU:HA	1.80	0.41
32:42:522:ZEX:H162	32:42:522:ZEX:O3	2.21	0.41
18:41:87:ASN:OD1	18:41:87:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:41:250:GLY:O	18:41:254:THR:HG23	2.21	0.41
18:41:290:PHE:CE2	18:41:294:PRO:HG3	2.55	0.41
21:41:405:CL7:HAA2	21:41:405:CL7:HBD	2.02	0.41
32:41:422:ZEX:H15	32:41:422:ZEX:H201	1.82	0.41
32:41:422:ZEX:H373	32:41:422:ZEX:H23	1.87	0.41
21:43:406:CL7:H41C	32:43:421:ZEX:H193	2.03	0.41
21:43:411:CL7:H42C	32:43:420:ZEX:C17	2.51	0.41
20:44:50:LEU:HD13	20:44:124:ALA:HB1	2.02	0.41
20:44:138:ASP:N	20:44:138:ASP:OD1	2.53	0.41
20:44:232:VAL:HA	32:44:419:ZEX:H1	1.86	0.41
1:1A:28:LEU:HB2	25:1A:406:SQD:H102	2.03	0.41
1:1A:120:MET:SD	1:1A:159:LEU:HB2	2.61	0.41
21:1A:407:CL7:C4	30:1D:407:PL9:H211	2.51	0.41
2:1B:161:PHE:HB2	21:1B:606:CL7:CAB	2.51	0.41
2:1B:460:LEU:HD12	2:1B:460:LEU:HA	1.93	0.41
4:1D:56:SER:HB3	4:1D:78:SER:HB3	2.03	0.41
10:1L:13:LEU:H	11:1M:29:THR:HG21	1.86	0.41
16:12:98:PHE:CG	32:12:522:ZEX:H31	2.53	0.41
21:12:505:CL7:H43C	21:12:505:CL7:C4B	2.51	0.41
21:11:406:CL7:H162	21:11:406:CL7:H121	1.83	0.41
20:14:138:ASP:OD1	20:14:138:ASP:N	2.53	0.41
20:14:304:ARG:CG	32:14:418:ZEX:H373	2.37	0.41
21:14:413:CL7:H142	21:14:413:CL7:H112	1.88	0.41
1:2A:20:PHE:O	1:2A:23:SER:OG	2.29	0.41
1:2A:120:MET:SD	1:2A:159:LEU:HB2	2.61	0.41
18:21:202:CYS:C	18:21:204:PHE:H	2.29	0.41
21:3B:608:CL7:H41C	21:3B:608:CL7:H62C	1.50	0.41
3:3C:48:TRP:CD1	3:3C:48:TRP:H	2.39	0.41
4:3D:78:SER:HA	4:3D:171:SER:HB3	2.03	0.41
10:3L:15:ARG:HD2	25:4B:621:SQD:C24	2.50	0.41
16:32:281:GLN:HA	16:32:282:PRO:HD3	1.93	0.41
21:32:505:CL7:H101	21:32:505:CL7:H62C	1.69	0.41
21:32:505:CL7:H43C	21:32:505:CL7:C4B	2.51	0.41
21:32:516:CL7:H3A	21:32:516:CL7:HBA1	1.55	0.41
18:31:87:ASN:OD1	18:31:87:ASN:N	2.54	0.41
18:31:202:CYS:C	18:31:204:PHE:H	2.29	0.41
21:33:501:CL7:H13	32:33:520:ZEX:H402	2.03	0.41
20:34:59:VAL:HG21	21:34:412:CL7:HAC2	2.03	0.41
1:4A:30:ILE:O	1:4A:34:GLY:HA3	2.21	0.41
2:4B:440:ASP:OD1	4:4D:302:ILE:HD11	2.21	0.41
21:4C:508:CL7:H161	21:4C:508:CL7:H141	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:42:510:CL7:HBA1	21:42:510:CL7:HBD	2.03	0.41
21:44:405:CL7:HHD	21:44:405:CL7:HAC1	1.95	0.41
3:1C:156:SER:OG	3:1C:157:ASP:N	2.54	0.40
4:1D:84:LEU:HD13	4:1D:89:LEU:HD21	2.03	0.40
4:1D:109:LEU:HD23	4:1D:109:LEU:HA	1.81	0.40
16:12:94:MET:CE	32:12:524:ZEX:C36	2.95	0.40
21:12:510:CL7:H51C	21:12:510:CL7:HMA1	2.03	0.40
18:11:173:ILE:HG13	18:11:177:ARG:HD2	2.02	0.40
18:11:202:CYS:C	18:11:204:PHE:H	2.29	0.40
21:13:509:CL7:H142	21:13:509:CL7:H111	1.63	0.40
1:2A:218:LEU:HD23	1:2A:218:LEU:HA	1.91	0.40
2:2B:464:PHE:HB2	4:2D:279:TRP:CZ2	2.56	0.40
21:2B:603:CL7:H41C	21:2B:603:CL7:H61C	1.73	0.40
21:2B:606:CL7:HBA1	21:2B:606:CL7:H3A	1.78	0.40
3:2C:382:ARG:HA	3:2C:382:ARG:HD3	1.87	0.40
3:2C:405:ALA:O	3:2C:409:THR:HG23	2.21	0.40
9:2K:11:PRO:HB2	9:2K:14:PHE:HD2	1.86	0.40
21:22:505:CL7:HHD	21:22:505:CL7:HAC2	1.91	0.40
18:21:173:ILE:HG13	18:21:177:ARG:HD2	2.02	0.40
18:21:250:GLY:O	18:21:254:THR:HG23	2.21	0.40
21:23:417:CL7:HED2	32:24:403:ZEX:H172	2.02	0.40
20:24:137:ASN:O	20:24:149:ARG:NH1	2.54	0.40
2:3B:91:ILE:O	2:3B:94:ALA:HB3	2.21	0.40
21:3B:602:CL7:H61C	21:3B:602:CL7:H41C	1.73	0.40
21:3B:608:CL7:CHD	21:3B:609:CL7:H93C	2.50	0.40
3:3C:382:ARG:HA	3:3C:382:ARG:HD3	1.87	0.40
23:3C:515:8CT:C08	8:3I:24:ILE:HG22	2.50	0.40
4:3D:209:LEU:HD23	4:3D:209:LEU:HA	1.96	0.40
9:3K:25:PRO:O	9:3K:28:PRO:HD2	2.21	0.40
21:32:511:CL7:H43C	32:32:524:ZEX:H3	2.03	0.40
18:31:151:LEU:CD1	21:31:413:CL7:H3A	2.50	0.40
19:33:22:ASP:N	19:33:22:ASP:OD1	2.54	0.40
1:4A:154:THR:HG22	21:4A:401:CL7:C4	2.50	0.40
5:4E:57:ASP:OD1	5:4E:57:ASP:N	2.54	0.40
9:4K:42:VAL:HB	9:4K:45:LYS:HE2	2.01	0.40
16:42:271:PHE:CB	16:42:304:ARG:HH21	2.35	0.40
32:42:524:ZEX:C35	21:41:417:CL7:HBA2	2.49	0.40
18:41:206:ASP:HA	18:41:275:LEU:HB2	2.03	0.40
20:44:137:ASN:O	20:44:149:ARG:NH1	2.54	0.40
1:1A:323:ARG:HG3	4:1D:331:GLN:OE1	2.21	0.40
3:1C:375:GLY:O	3:1C:379:GLU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:405:ALA:O	3:1C:409:THR:HG23	2.21	0.40
21:1C:505:CL7:H42C	21:1C:505:CL7:NC	2.36	0.40
18:11:198:PRO:HD3	21:11:420:CL7:HAB	2.02	0.40
21:11:410:CL7:H62C	21:11:410:CL7:H41C	1.76	0.40
20:14:59:VAL:HG21	21:14:412:CL7:HAC2	2.03	0.40
21:14:414:CL7:H62C	32:14:420:ZEX:H192	2.03	0.40
1:2A:179:THR:O	1:2A:183:MET:HG3	2.22	0.40
1:2A:275:LEU:HD23	1:2A:275:LEU:HA	1.89	0.40
3:2C:93:MET:HE1	3:2C:105:ALA:HB2	2.03	0.40
3:2C:330:LEU:HD12	3:2C:352:TYR:N	2.37	0.40
21:2C:501:CL7:H72C	21:2C:501:CL7:HMB3	2.03	0.40
21:2C:502:CL7:H62C	21:2C:502:CL7:H41C	1.74	0.40
4:2D:109:LEU:HA	4:2D:109:LEU:HD23	1.81	0.40
10:2L:14:ASN:OD1	10:2L:14:ASN:N	2.52	0.40
16:22:271:PHE:CB	16:22:304:ARG:HH21	2.35	0.40
21:22:510:CL7:C2	32:22:519:ZEX:H181	2.51	0.40
18:21:87:ASN:OD1	18:21:87:ASN:N	2.54	0.40
18:21:151:LEU:CD1	21:21:413:CL7:H3A	2.50	0.40
20:24:152:TRP:HH2	21:24:411:CL7:H18	1.87	0.40
1:3A:82:VAL:HB	1:3A:174:LEU:HB2	2.03	0.40
21:3A:407:CL7:C4	30:3D:407:PL9:H211	2.51	0.40
2:3B:165:HIS:CD2	2:3B:165:HIS:C	2.98	0.40
3:3C:222:LEU:HD23	3:3C:222:LEU:HA	1.87	0.40
21:3C:501:CL7:HMB3	21:3C:501:CL7:H72C	2.03	0.40
5:3E:52:PRO:HA	5:3E:55:TYR:CE2	2.56	0.40
16:32:313:PHE:CG	32:32:519:ZEX:H32	2.57	0.40
21:32:510:CL7:HBD	21:32:510:CL7:HBA1	2.03	0.40
21:32:518:CL7:H121	19:43:75:TRP:CH2	2.55	0.40
32:32:524:ZEX:H7	21:31:417:CL7:HED1	2.02	0.40
18:31:168:ILE:H	18:31:168:ILE:HG13	1.73	0.40
18:31:261:LEU:O	18:31:265:ILE:HG13	2.21	0.40
1:4A:332:HIS:CG	1:4A:333:GLU:H	2.39	0.40
2:4B:373:LYS:HE2	2:4B:373:LYS:HB2	1.88	0.40
21:4B:609:CL7:CHD	21:4B:610:CL7:H93C	2.50	0.40
3:4C:330:LEU:HD12	3:4C:352:TYR:N	2.36	0.40
3:4C:477:TYR:CG	8:4I:32:PRO:HB3	2.56	0.40
21:4C:505:CL7:H42C	21:4C:505:CL7:NC	2.36	0.40
4:4D:203:ILE:HD13	4:4D:203:ILE:HA	1.80	0.40
9:4K:25:PRO:O	9:4K:28:PRO:HD2	2.21	0.40
21:42:505:CL7:H12C	32:42:520:ZEX:C17	2.51	0.40
32:42:519:ZEX:H31	32:42:519:ZEX:H401	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:41:408:CL7:H162	21:41:408:CL7:H193	1.87	0.40
21:43:402:CL7:H161	21:43:407:CL7:HMC1	2.02	0.40
21:43:417:CL7:HED2	32:44:403:ZEX:H172	2.02	0.40
21:44:414:CL7:H62C	32:44:420:ZEX:H192	2.03	0.40
2:1B:30:VAL:HG12	21:1B:605:CL7:HHD	2.03	0.40
21:1B:608:CL7:CHD	21:1B:609:CL7:H93C	2.50	0.40
21:12:515:CL7:H2A	21:12:515:CL7:O1D	2.22	0.40
21:13:502:CL7:C2D	21:13:503:CL7:H151	2.51	0.40
21:13:516:CL7:H62C	21:13:516:CL7:H92C	1.83	0.40
20:14:137:ASN:O	20:14:149:ARG:NH1	2.54	0.40
2:2B:91:ILE:O	2:2B:94:ALA:HB3	2.21	0.40
14:2Y:19:GLY:O	14:2Y:23:ILE:HG12	2.22	0.40
16:22:214:ILE:HD13	16:22:214:ILE:HA	1.98	0.40
21:22:501:CL7:H41C	21:22:501:CL7:H72C	2.03	0.40
21:22:505:CL7:H43C	21:22:505:CL7:C4B	2.51	0.40
21:22:505:CL7:H12C	32:22:520:ZEX:C17	2.51	0.40
19:23:97:LEU:HD23	19:23:97:LEU:HA	1.89	0.40
1:3A:302:PHE:O	1:3A:305:SER:OG	2.38	0.40
21:3B:604:CL7:HAB	21:3B:611:CL7:H193	2.04	0.40
21:3C:503:CL7:H61C	21:3C:503:CL7:H41C	1.74	0.40
5:3E:76:ILE:O	5:3E:80:THR:N	2.54	0.40
9:3K:11:PRO:HB2	9:3K:14:PHE:HD2	1.86	0.40
1:4A:63:ILE:HD12	1:4A:63:ILE:HA	1.88	0.40
1:4A:82:VAL:HB	1:4A:174:LEU:HB2	2.03	0.40
1:4A:161:TYR:HB3	1:4A:162:PRO:HD3	2.03	0.40
21:4B:605:CL7:H121	21:4B:605:CL7:H162	1.77	0.40
4:4D:56:SER:HB3	4:4D:78:SER:HB3	2.03	0.40
18:41:243:LYS:HB3	18:41:243:LYS:HE3	1.88	0.40
18:41:261:LEU:O	18:41:265:ILE:HG13	2.21	0.40
32:43:423:ZEX:H391	32:43:423:ZEX:H27	1.82	0.40
20:44:152:TRP:HH2	21:44:411:CL7:H18	1.87	0.40
32:44:403:ZEX:H401	32:44:403:ZEX:H31	1.75	0.40
1:1A:82:VAL:HB	1:1A:174:LEU:HB2	2.03	0.40
21:1C:507:CL7:H202	21:1C:507:CL7:H161	1.83	0.40
5:1E:57:ASP:OD1	5:1E:57:ASP:N	2.54	0.40
9:1K:11:PRO:HB2	9:1K:14:PHE:HD2	1.86	0.40
16:12:258:LEU:HD23	16:12:258:LEU:HA	1.94	0.40
32:12:520:ZEX:C11	25:23:424:SQD:H221	2.52	0.40
21:11:404:CL7:H41C	21:11:404:CL7:H62C	1.62	0.40
21:11:408:CL7:H193	21:11:408:CL7:H162	1.87	0.40
21:11:410:CL7:H13	21:11:410:CL7:H172	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:13:510:CL7:H101	21:13:510:CL7:H62C	1.83	0.40
21:13:516:CL7:HED2	32:14:403:ZEX:H172	2.02	0.40
1:2A:161:TYR:HB3	1:2A:162:PRO:HD3	2.03	0.40
21:2B:609:CL7:CHD	21:2B:610:CL7:H93C	2.50	0.40
26:2B:626:LHG:H202	30:2D:407:PL9:H212	2.03	0.40
21:2D:404:CL7:H12C	22:2D:408:PHO:CAB	2.50	0.40
9:2K:25:PRO:O	9:2K:28:PRO:HD2	2.21	0.40
21:21:408:CL7:H162	21:21:408:CL7:H193	1.87	0.40
19:23:72:ARG:HD3	21:23:402:CL7:O2D	2.22	0.40
1:3A:120:MET:SD	1:3A:159:LEU:HB2	2.61	0.40
1:3A:332:HIS:CG	1:3A:333:GLU:H	2.39	0.40
21:3A:401:CL7:H42C	21:3A:407:CL7:HHC	1.99	0.40
3:3C:93:MET:HE1	3:3C:105:ALA:HB2	2.03	0.40
3:3C:405:ALA:O	3:3C:409:THR:HG23	2.21	0.40
16:32:70:LEU:HG	21:32:503:CL7:CED	2.52	0.40
16:32:121:SER:HG	16:32:126:SER:HG	1.68	0.40
21:32:515:CL7:H2A	21:32:515:CL7:O1D	2.22	0.40
21:33:502:CL7:C2D	21:33:503:CL7:H151	2.51	0.40
6:4F:26:HIS:NE2	31:4F:101:HEM:NA	2.70	0.40
14:4Y:19:GLY:O	14:4Y:23:ILE:HG12	2.22	0.40
16:42:207:VAL:HG22	32:42:520:ZEX:H383	2.02	0.40
21:42:510:CL7:C2	32:42:519:ZEX:H181	2.51	0.40
21:42:515:CL7:H2A	21:42:515:CL7:O1D	2.22	0.40
21:43:406:CL7:HBA1	21:43:406:CL7:H3A	1.79	0.40
21:43:408:CL7:H111	21:43:408:CL7:H142	1.85	0.40
32:43:421:ZEX:H191	32:43:421:ZEX:H11	1.52	0.40
32:43:423:ZEX:H31	32:43:423:ZEX:H401	1.88	0.40
20:44:163:GLY:HA3	20:44:251:ILE:HG13	2.04	0.40
2:1B:172:PRO:HG3	21:1B:606:CL7:O1D	2.20	0.40
3:1C:476:GLU:CD	4:1D:244:SER:HG	2.22	0.40
4:1D:26:PHE:CD1	4:1D:27:VAL:HG13	2.57	0.40
16:12:207:VAL:HG22	32:12:520:ZEX:H383	2.03	0.40
16:12:313:PHE:CG	32:12:519:ZEX:H32	2.57	0.40
21:12:502:CL7:CMB	21:12:504:CL7:HAB	2.51	0.40
32:12:520:ZEX:H15	32:12:520:ZEX:H201	1.86	0.40
18:11:261:LEU:O	18:11:265:ILE:HG13	2.21	0.40
19:13:87:TYR:N	19:13:88:PRO:HD2	2.37	0.40
20:14:311:PRO:HA	20:14:312:PRO:HD2	1.99	0.40
3:2C:477:TYR:CG	8:2I:32:PRO:HB3	2.56	0.40
26:2D:409:LHG:H332	26:2D:409:LHG:H301	1.91	0.40
6:2F:26:HIS:NE2	31:2F:101:HEM:NA	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:22:515:CL7:H2A	21:22:515:CL7:O1D	2.22	0.40
25:22:521:SQD:O47	25:22:521:SQD:H1	2.21	0.40
32:22:522:ZEX:H162	32:22:522:ZEX:O3	2.21	0.40
21:21:404:CL7:H193	21:21:404:CL7:H162	1.83	0.40
19:23:253:LEU:HD23	19:23:253:LEU:HA	1.82	0.40
20:24:228:ASN:HB2	20:24:230:GLU:OE1	2.22	0.40
20:24:255:LYS:HD2	20:24:255:LYS:HA	1.91	0.40
1:3A:63:ILE:HD12	1:3A:63:ILE:HA	1.87	0.40
1:3A:173:PRO:HB2	1:3A:178:GLY:HA3	2.02	0.40
2:3B:161:PHE:HB2	21:3B:606:CL7:CAB	2.51	0.40
21:3B:604:CL7:H92C	21:3B:604:CL7:H62C	1.86	0.40
12:3T:12:CYS:HB3	25:4B:621:SQD:H383	2.04	0.40
16:32:271:PHE:CB	16:32:304:ARG:HH21	2.35	0.40
21:31:405:CL7:HBA1	21:31:405:CL7:H3A	1.71	0.40
21:31:406:CL7:HBC2	32:31:422:ZEX:C19	2.51	0.40
21:31:406:CL7:H8	21:31:406:CL7:H52C	1.90	0.40
19:33:171:ALA:HB1	19:33:175:ARG:NE	2.37	0.40
21:33:510:CL7:CAD	21:33:511:CL7:HAB	2.52	0.40
20:34:181:THR:O	20:34:196:GLN:HB3	2.22	0.40
20:34:228:ASN:HB2	20:34:230:GLU:OE1	2.22	0.40
1:4A:28:LEU:HB2	25:4A:406:SQD:H102	2.03	0.40
26:4B:626:LHG:H202	30:4D:407:PL9:H212	2.03	0.40
4:4D:278:LEU:HD23	4:4D:278:LEU:HA	1.86	0.40
30:4D:407:PL9:H321	30:4D:407:PL9:H28	1.78	0.40
5:4E:52:PRO:HA	5:4E:55:TYR:CE2	2.56	0.40
21:42:502:CL7:CMB	21:42:504:CL7:HAB	2.51	0.40
21:42:509:CL7:OBB	21:42:510:CL7:HBA2	2.22	0.40
19:43:57:LEU:HD23	19:43:57:LEU:HA	1.92	0.40
19:43:72:ARG:HD3	21:43:402:CL7:O2D	2.22	0.40
21:43:417:CL7:H92C	21:43:417:CL7:H62C	1.83	0.40
32:44:403:ZEX:H28	32:44:403:ZEX:H25	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	2A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	3A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	4A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
2	1B	477/506 (94%)	451 (94%)	26 (6%)	0	100	100
2	2B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	3B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	4B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
3	1C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	2C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	3C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	4C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
4	1D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	2D	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
4	3D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	4D	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
5	1E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	2E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	3E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	4E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
6	1F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	2F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	3F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	4F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
7	1H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	2H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	3H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	4H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
8	1I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	2I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	3I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	4I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
9	1K	35/45 (78%)	35 (100%)	0	0	100	100
9	2K	35/45 (78%)	35 (100%)	0	0	100	100
9	3K	35/45 (78%)	35 (100%)	0	0	100	100
9	4K	35/45 (78%)	35 (100%)	0	0	100	100
10	1L	34/38 (90%)	34 (100%)	0	0	100	100
10	2L	34/38 (90%)	34 (100%)	0	0	100	100
10	3L	34/38 (90%)	34 (100%)	0	0	100	100
10	4L	34/38 (90%)	34 (100%)	0	0	100	100
11	1M	29/34 (85%)	29 (100%)	0	0	100	100
11	2M	29/34 (85%)	29 (100%)	0	0	100	100
11	3M	29/34 (85%)	29 (100%)	0	0	100	100
11	4M	29/34 (85%)	29 (100%)	0	0	100	100
12	1T	26/46 (56%)	26 (100%)	0	0	100	100
12	2T	26/46 (56%)	26 (100%)	0	0	100	100
12	3T	26/46 (56%)	26 (100%)	0	0	100	100
12	4T	26/46 (56%)	26 (100%)	0	0	100	100
13	1X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	2X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	3X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	4X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
14	1Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	2Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	3Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	4Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
15	1Z	57/62 (92%)	57 (100%)	0	0	100	100
15	2Z	57/62 (92%)	57 (100%)	0	0	100	100
15	3Z	57/62 (92%)	57 (100%)	0	0	100	100
15	4Z	57/62 (92%)	57 (100%)	0	0	100	100
16	12	347/352 (99%)	325 (94%)	22 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	22	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	32	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	42	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
18	11	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
18	21	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
18	31	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
18	41	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
19	13	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	23	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	33	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	43	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
20	14	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	24	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	34	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	44	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
All	All	13020/14832 (88%)	12413 (95%)	599 (5%)	8 (0%)	49	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	13	4	TYR
19	23	4	TYR
19	33	4	TYR
19	43	4	TYR
18	11	202	CYS
18	21	202	CYS
18	31	202	CYS
18	41	202	CYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	232/292 (80%)	232 (100%)	0	100	100
1	2A	232/292 (80%)	232 (100%)	0	100	100
1	3A	232/292 (80%)	232 (100%)	0	100	100
1	4A	232/292 (80%)	232 (100%)	0	100	100
2	1B	395/418 (94%)	392 (99%)	3 (1%)	73	77
2	2B	395/418 (94%)	392 (99%)	3 (1%)	73	77
2	3B	395/418 (94%)	392 (99%)	3 (1%)	73	77
2	4B	395/418 (94%)	392 (99%)	3 (1%)	73	77
3	1C	322/378 (85%)	319 (99%)	3 (1%)	70	76
3	2C	322/378 (85%)	319 (99%)	3 (1%)	70	76
3	3C	322/378 (85%)	319 (99%)	3 (1%)	70	76
3	4C	322/378 (85%)	319 (99%)	3 (1%)	70	76
4	1D	265/284 (93%)	264 (100%)	1 (0%)	84	81
4	2D	265/284 (93%)	264 (100%)	1 (0%)	84	81
4	3D	265/284 (93%)	264 (100%)	1 (0%)	84	81
4	4D	265/284 (93%)	264 (100%)	1 (0%)	84	81
5	1E	57/71 (80%)	57 (100%)	0	100	100
5	2E	57/71 (80%)	57 (100%)	0	100	100
5	3E	57/71 (80%)	57 (100%)	0	100	100
5	4E	57/71 (80%)	57 (100%)	0	100	100
6	1F	25/84 (30%)	25 (100%)	0	100	100
6	2F	25/84 (30%)	25 (100%)	0	100	100
6	3F	25/84 (30%)	25 (100%)	0	100	100
6	4F	25/84 (30%)	25 (100%)	0	100	100
7	1H	55/57 (96%)	55 (100%)	0	100	100
7	2H	55/57 (96%)	55 (100%)	0	100	100
7	3H	55/57 (96%)	55 (100%)	0	100	100
7	4H	55/57 (96%)	55 (100%)	0	100	100
8	1I	30/30 (100%)	30 (100%)	0	100	100
8	2I	30/30 (100%)	30 (100%)	0	100	100
8	3I	30/30 (100%)	30 (100%)	0	100	100
8	4I	30/30 (100%)	30 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	1K	31/37 (84%)	30 (97%)	1 (3%)	34 58
9	2K	31/37 (84%)	30 (97%)	1 (3%)	34 58
9	3K	31/37 (84%)	30 (97%)	1 (3%)	34 58
9	4K	31/37 (84%)	30 (97%)	1 (3%)	34 58
10	1L	33/34 (97%)	33 (100%)	0	100 100
10	2L	33/34 (97%)	33 (100%)	0	100 100
10	3L	33/34 (97%)	33 (100%)	0	100 100
10	4L	33/34 (97%)	33 (100%)	0	100 100
11	1M	24/27 (89%)	24 (100%)	0	100 100
11	2M	24/27 (89%)	24 (100%)	0	100 100
11	3M	24/27 (89%)	24 (100%)	0	100 100
11	4M	24/27 (89%)	24 (100%)	0	100 100
12	1T	24/42 (57%)	24 (100%)	0	100 100
12	2T	24/42 (57%)	24 (100%)	0	100 100
12	3T	24/42 (57%)	24 (100%)	0	100 100
12	4T	24/42 (57%)	24 (100%)	0	100 100
13	1X	28/33 (85%)	28 (100%)	0	100 100
13	2X	28/33 (85%)	28 (100%)	0	100 100
13	3X	28/33 (85%)	28 (100%)	0	100 100
13	4X	28/33 (85%)	28 (100%)	0	100 100
14	1Y	18/31 (58%)	18 (100%)	0	100 100
14	2Y	18/31 (58%)	18 (100%)	0	100 100
14	3Y	18/31 (58%)	18 (100%)	0	100 100
14	4Y	18/31 (58%)	18 (100%)	0	100 100
15	1Z	43/46 (94%)	43 (100%)	0	100 100
15	2Z	43/46 (94%)	43 (100%)	0	100 100
15	3Z	43/46 (94%)	43 (100%)	0	100 100
15	4Z	43/46 (94%)	43 (100%)	0	100 100
16	12	276/278 (99%)	272 (99%)	4 (1%)	59 71
16	22	276/278 (99%)	272 (99%)	4 (1%)	59 71
16	32	276/278 (99%)	272 (99%)	4 (1%)	59 71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	42	276/278 (99%)	272 (99%)	4 (1%)	59	71
18	11	262/278 (94%)	259 (99%)	3 (1%)	65	74
18	21	262/278 (94%)	259 (99%)	3 (1%)	65	74
18	31	262/278 (94%)	259 (99%)	3 (1%)	65	74
18	41	262/278 (94%)	259 (99%)	3 (1%)	65	74
19	13	269/273 (98%)	266 (99%)	3 (1%)	65	74
19	23	269/273 (98%)	266 (99%)	3 (1%)	65	74
19	33	269/273 (98%)	266 (99%)	3 (1%)	65	74
19	43	269/273 (98%)	266 (99%)	3 (1%)	65	74
20	14	260/277 (94%)	256 (98%)	4 (2%)	57	70
20	24	260/277 (94%)	256 (98%)	4 (2%)	57	70
20	34	260/277 (94%)	256 (98%)	4 (2%)	57	70
20	44	260/277 (94%)	256 (98%)	4 (2%)	57	70
All	All	10596/11880 (89%)	10508 (99%)	88 (1%)	70	77

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1B	354	LEU
2	1B	373	LYS
2	1B	392	PHE
3	1C	218	LEU
3	1C	292	TYR
3	1C	432	VAL
4	1D	285	LEU
9	1K	45	LYS
16	12	62	GLN
16	12	263	PHE
16	12	274	GLU
16	12	294	LEU
18	11	66	LEU
18	11	143	TYR
18	11	202	CYS
19	13	4	TYR
19	13	263	PHE
19	13	286	VAL
20	14	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	14	101	ILE
20	14	193	THR
20	14	204	ILE
2	2B	354	LEU
2	2B	373	LYS
2	2B	392	PHE
3	2C	218	LEU
3	2C	292	TYR
3	2C	432	VAL
4	2D	285	LEU
9	2K	45	LYS
16	22	62	GLN
16	22	263	PHE
16	22	274	GLU
16	22	294	LEU
18	21	66	LEU
18	21	143	TYR
18	21	202	CYS
19	23	4	TYR
19	23	263	PHE
19	23	286	VAL
20	24	24	LEU
20	24	101	ILE
20	24	193	THR
20	24	204	ILE
2	3B	354	LEU
2	3B	373	LYS
2	3B	392	PHE
3	3C	218	LEU
3	3C	292	TYR
3	3C	432	VAL
4	3D	285	LEU
9	3K	45	LYS
16	32	62	GLN
16	32	263	PHE
16	32	274	GLU
16	32	294	LEU
18	31	66	LEU
18	31	143	TYR
18	31	202	CYS
19	33	4	TYR
19	33	263	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	33	286	VAL
20	34	24	LEU
20	34	101	ILE
20	34	193	THR
20	34	204	ILE
2	4B	354	LEU
2	4B	373	LYS
2	4B	392	PHE
3	4C	218	LEU
3	4C	292	TYR
3	4C	432	VAL
4	4D	285	LEU
9	4K	45	LYS
16	42	62	GLN
16	42	263	PHE
16	42	274	GLU
16	42	294	LEU
18	41	66	LEU
18	41	143	TYR
18	41	202	CYS
19	43	4	TYR
19	43	263	PHE
19	43	286	VAL
20	44	24	LEU
20	44	101	ILE
20	44	193	THR
20	44	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	75	ASN
1	1A	108	ASN
1	1A	303	ASN
1	1A	335	ASN
2	1B	9	HIS
2	1B	26	HIS
2	1B	122	HIS
2	1B	187	GLN
2	1B	224	HIS
2	1B	289	GLN
2	1B	394	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1C	68	HIS
4	1D	196	HIS
4	1D	337	ASN
4	1D	349	ASN
5	1E	23	HIS
16	12	62	GLN
18	11	166	HIS
19	13	2	GLN
19	13	34	GLN
19	13	54	ASN
20	14	195	HIS
20	14	227	ASN
20	14	280	ASN
1	2A	75	ASN
1	2A	108	ASN
1	2A	332	HIS
1	2A	335	ASN
2	2B	9	HIS
2	2B	26	HIS
2	2B	224	HIS
2	2B	289	GLN
2	2B	394	GLN
3	2C	68	HIS
4	2D	196	HIS
4	2D	337	ASN
4	2D	349	ASN
5	2E	23	HIS
16	22	62	GLN
16	22	145	HIS
18	21	166	HIS
18	21	331	HIS
19	23	2	GLN
19	23	34	GLN
19	23	320	GLN
20	24	195	HIS
20	24	227	ASN
20	24	275	ASN
20	24	280	ASN
1	3A	108	ASN
1	3A	303	ASN
1	3A	335	ASN
2	3B	9	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	3B	26	HIS
2	3B	187	GLN
2	3B	224	HIS
2	3B	289	GLN
2	3B	394	GLN
3	3C	68	HIS
4	3D	196	HIS
4	3D	349	ASN
5	3E	23	HIS
16	32	62	GLN
16	32	145	HIS
18	31	166	HIS
18	31	331	HIS
19	33	2	GLN
19	33	34	GLN
19	33	54	ASN
20	34	195	HIS
20	34	227	ASN
20	34	275	ASN
20	34	280	ASN
1	4A	75	ASN
1	4A	108	ASN
1	4A	303	ASN
1	4A	335	ASN
2	4B	9	HIS
2	4B	26	HIS
2	4B	224	HIS
2	4B	289	GLN
2	4B	394	GLN
3	4C	68	HIS
4	4D	196	HIS
4	4D	337	ASN
4	4D	349	ASN
5	4E	23	HIS
16	42	62	GLN
16	42	145	HIS
18	41	166	HIS
18	41	331	HIS
19	43	2	GLN
19	43	34	GLN
19	43	320	GLN
20	44	195	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	44	227	ASN
20	44	280	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 624 ligands modelled in this entry, 4 are monoatomic - leaving 620 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CL7	33	502	19	64,66,73	1.77	15 (23%)	71,104,113	2.40	22 (30%)
21	CL7	31	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	2C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	3C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.83	18 (35%)
25	SQD	32	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	22	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	23	404	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	23	415	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	3C	503	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	4B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
21	CL7	3B	616	2	51,53,73	1.97	19 (37%)	56,89,113	2.70	18 (32%)
21	CL7	1B	608	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	20 (25%)
21	CL7	33	513	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
32	ZEX	22	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	44	409	-	66,68,73	1.76	18 (27%)	74,107,113	2.67	24 (32%)
23	8CT	3C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
25	SQD	42	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	21	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.49	19 (25%)
21	CL7	31	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.40	21 (26%)
21	CL7	23	409	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
21	CL7	11	409	18	51,53,73	1.96	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	2B	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.33	20 (25%)
21	CL7	14	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	3C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.37	23 (28%)
21	CL7	31	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	24 (30%)
21	CL7	4D	405	4	51,53,73	1.96	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	13	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
21	CL7	43	410	19	71,73,73	1.69	16 (22%)	80,113,113	2.34	22 (27%)
32	ZEX	14	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.43	25 (45%)
26	LHG	2B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	2B	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.37	21 (26%)
21	CL7	31	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
21	CL7	34	414	20	59,61,73	1.84	18 (30%)	65,98,113	2.65	21 (32%)
21	CL7	21	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
23	8CT	2C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	32	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
27	DGD	1C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
30	PL9	4D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	34	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	14	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.45	25 (31%)
21	CL7	2B	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	32	517	16	71,73,73	1.68	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	2B	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
24	LMG	1B	621	-	51,51,55	0.25	0	59,59,63	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	41	412	18	51,53,73	1.95	16 (31%)	56,89,113	2.77	20 (35%)
32	ZEX	13	525	-	42,43,43	1.18	5 (11%)	55,60,60	2.44	18 (32%)
21	CL7	43	409	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	22 (27%)
32	ZEX	12	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.19	17 (30%)
32	ZEX	34	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	18 (32%)
32	ZEX	44	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
32	ZEX	34	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
24	LMG	1A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	1D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
21	CL7	22	501	16	71,73,73	1.68	17 (23%)	80,113,113	2.42	21 (26%)
21	CL7	1B	616	2	51,53,73	1.97	18 (35%)	56,89,113	2.69	18 (32%)
21	CL7	12	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
32	ZEX	12	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
26	LHG	14	401	-	48,48,48	0.29	0	51,54,54	0.34	0
21	CL7	2B	602	-	47,49,73	1.94	12 (25%)	51,84,113	2.87	18 (35%)
21	CL7	24	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	2C	506	3	66,68,73	1.76	17 (25%)	74,107,113	2.50	23 (31%)
24	LMG	4B	622	-	51,51,55	0.24	0	59,59,63	0.33	0
26	LHG	4B	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	4C	502	3	66,68,73	1.76	16 (24%)	74,107,113	2.45	19 (25%)
21	CL7	4C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	43	407	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	1C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.55	19 (27%)
24	LMG	3D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
26	LHG	3A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	23	418	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
21	CL7	44	417	20	48,50,73	1.93	14 (29%)	51,85,113	2.94	18 (35%)
25	SQD	3B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
22	PHO	4D	408	-	58,69,69	0.80	3 (5%)	56,99,99	1.27	5 (8%)
21	CL7	12	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.43	21 (26%)
21	CL7	1B	615	2	56,58,73	1.89	17 (30%)	62,95,113	2.68	21 (33%)
21	CL7	14	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	34	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.69	21 (37%)
21	CL7	41	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.34	23 (28%)
32	ZEX	12	522	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	17 (30%)
21	CL7	42	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.39	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	24	408	20	51,53,73	1.97	16 (31%)	56,89,113	2.69	21 (37%)
21	CL7	42	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
23	8CT	3C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
26	LHG	23	425	-	35,35,48	0.35	0	38,41,54	0.47	0
21	CL7	2B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	42	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.32	23 (28%)
21	CL7	34	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
21	CL7	42	516	16	71,73,73	1.70	16 (22%)	80,113,113	2.39	23 (28%)
24	LMG	3A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	3A	401	1	71,73,73	1.74	14 (19%)	80,113,113	2.47	25 (31%)
21	CL7	33	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)
21	CL7	44	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.88	21 (37%)
25	SQD	43	422	-	45,46,54	0.42	0	54,57,65	0.48	0
23	8CT	2K	101	-	40,41,41	4.75	25 (62%)	50,56,56	2.65	15 (30%)
21	CL7	12	518	16	71,73,73	1.69	13 (18%)	80,113,113	2.33	23 (28%)
21	CL7	3C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	13	512	19	61,63,73	1.84	19 (31%)	68,101,113	2.58	23 (33%)
23	8CT	44	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
32	ZEX	22	520	-	42,43,43	0.99	3 (7%)	55,60,60	2.18	17 (30%)
32	ZEX	32	520	-	42,43,43	0.97	3 (7%)	55,60,60	2.18	17 (30%)
32	ZEX	21	421	-	42,43,43	0.92	2 (4%)	55,60,60	2.23	20 (36%)
21	CL7	3C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	31	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.97	22 (43%)
21	CL7	31	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.70	19 (33%)
21	CL7	44	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	20 (35%)
32	ZEX	23	423	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	18 (32%)
21	CL7	2C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	2C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	3B	604	2	71,73,73	1.68	18 (25%)	80,113,113	2.32	23 (28%)
21	CL7	43	417	19	61,63,73	1.81	18 (29%)	68,101,113	2.56	25 (36%)
21	CL7	32	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	2B	615	2	66,68,73	1.79	18 (27%)	74,107,113	2.49	25 (33%)
21	CL7	13	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	24 (30%)
21	CL7	32	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.42	21 (26%)
26	LHG	44	401	-	48,48,48	0.28	0	51,54,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	ZEX	43	401	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
32	ZEX	32	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	17 (30%)
25	SQD	41	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	4C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.46	23 (28%)
23	8CT	2B	619	-	40,41,41	4.70	20 (50%)	50,56,56	2.67	20 (40%)
32	ZEX	23	420	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	2B	616	2	56,58,73	1.89	18 (32%)	62,95,113	2.69	21 (33%)
21	CL7	42	511	16	66,68,73	1.78	18 (27%)	74,107,113	2.40	21 (28%)
21	CL7	2D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
21	CL7	23	413	19	61,63,73	1.83	18 (29%)	68,101,113	2.58	22 (32%)
21	CL7	33	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.41	21 (26%)
21	CL7	2C	513	3	51,53,73	1.95	14 (27%)	56,89,113	2.91	19 (33%)
22	PHO	3D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.27	5 (8%)
21	CL7	32	513	16	51,53,73	1.96	15 (29%)	56,89,113	2.84	21 (37%)
21	CL7	43	415	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
24	LMG	3B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	1C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	33	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
23	8CT	1C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
32	ZEX	41	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	1C	510	3	71,73,73	1.69	14 (19%)	80,113,113	2.38	21 (26%)
21	CL7	43	406	19	71,73,73	1.70	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	3C	513	3	51,53,73	1.94	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	3B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
32	ZEX	32	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	21	410	-	71,73,73	1.69	16 (22%)	80,113,113	2.33	22 (27%)
25	SQD	4A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	23	416	-	47,49,73	1.93	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	3A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.60	23 (33%)
21	CL7	11	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
21	CL7	31	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	3C	509	3	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
32	ZEX	12	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	2C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.46	22 (27%)
21	CL7	3D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	8CT	4C	518	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	13	517	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
23	8CT	1D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
24	LMG	21	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	41	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.98	22 (43%)
32	ZEX	43	420	-	42,43,43	1.01	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	43	413	19	61,63,73	1.84	19 (31%)	68,101,113	2.58	23 (33%)
26	LHG	3D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	1B	611	2	71,73,73	1.69	17 (23%)	80,113,113	2.34	20 (25%)
21	CL7	11	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	1B	605	2	71,73,73	1.67	17 (23%)	80,113,113	2.40	20 (25%)
32	ZEX	23	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	32	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
21	CL7	23	402	19	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
23	8CT	3B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	14	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.68	25 (33%)
21	CL7	2C	502	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
26	LHG	1B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	32	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	22 (27%)
21	CL7	42	507	-	71,73,73	1.72	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	2A	401	1	71,73,73	1.73	13 (18%)	80,113,113	2.46	25 (31%)
23	8CT	1C	514	-	40,41,41	4.63	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	41	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	3B	602	2	66,68,73	1.78	17 (25%)	74,107,113	2.50	22 (29%)
21	CL7	41	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	19 (37%)
32	ZEX	42	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
32	ZEX	24	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
21	CL7	13	506	19	51,53,73	1.97	18 (35%)	56,89,113	2.75	19 (33%)
21	CL7	33	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.55	25 (36%)
21	CL7	4B	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	21 (28%)
21	CL7	13	509	19	71,73,73	1.68	16 (22%)	80,113,113	2.33	22 (27%)
21	CL7	3C	502	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
21	CL7	44	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.37	24 (30%)
21	CL7	1C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	22	513	16	51,53,73	1.97	14 (27%)	56,89,113	2.84	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	8CT	2C	514	-	40,41,41	4.65	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	32	504	-	51,53,73	1.99	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	14	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	4A	403	1	61,63,73	1.87	19 (31%)	68,101,113	2.61	23 (33%)
22	PHO	2D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.28	4 (7%)
21	CL7	1C	503	3	71,73,73	1.68	15 (21%)	80,113,113	2.40	21 (26%)
21	CL7	3C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	4B	602	-	47,49,73	1.94	13 (27%)	51,84,113	2.87	18 (35%)
23	8CT	4B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	23	411	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
30	PL9	1D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	21	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.45	23 (28%)
23	8CT	2D	406	-	40,41,41	4.63	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	43	402	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
25	SQD	21	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	42	512	16	71,73,73	1.69	14 (19%)	80,113,113	2.43	21 (26%)
27	DGD	2C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
32	ZEX	33	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
32	ZEX	44	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	18 (32%)
21	CL7	33	509	19	71,73,73	1.68	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	11	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	20 (39%)
23	8CT	1C	518	-	40,41,41	4.65	21 (52%)	50,56,56	2.71	20 (40%)
21	CL7	34	415	-	51,53,73	1.96	19 (37%)	56,89,113	2.87	20 (35%)
21	CL7	2B	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	31	420	18	51,53,73	1.95	13 (25%)	56,89,113	2.80	21 (37%)
21	CL7	21	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	21	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
21	CL7	3C	510	3	71,73,73	1.69	16 (22%)	80,113,113	2.38	21 (26%)
32	ZEX	34	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
23	8CT	34	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	4D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.48	22 (30%)
21	CL7	34	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.45	25 (31%)
21	CL7	23	408	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
21	CL7	43	412	19	71,73,73	1.68	18 (25%)	80,113,113	2.54	24 (30%)
21	CL7	42	501	16	71,73,73	1.67	16 (22%)	80,113,113	2.42	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	8CT	3C	515	-	40,41,41	4.64	20 (50%)	50,56,56	3.06	22 (44%)
21	CL7	24	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
21	CL7	2B	606	2	71,73,73	1.67	18 (25%)	80,113,113	2.39	20 (25%)
21	CL7	14	416	20	47,49,73	1.96	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	31	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	22	502	16	71,73,73	1.69	17 (23%)	80,113,113	2.35	23 (28%)
21	CL7	2B	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
23	8CT	3D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	44	406	20	71,73,73	1.70	15 (21%)	80,113,113	2.36	22 (27%)
21	CL7	33	508	19	71,73,73	1.71	18 (25%)	80,113,113	2.31	21 (26%)
21	CL7	3C	504	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	2B	612	2	71,73,73	1.70	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	4B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.32	22 (27%)
32	ZEX	24	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	3B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.47	21 (28%)
21	CL7	33	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.94	21 (41%)
21	CL7	34	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	42	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
21	CL7	4C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.50	23 (31%)
21	CL7	32	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
22	PHO	1D	408	-	58,69,69	0.80	4 (6%)	56,99,99	1.26	4 (7%)
32	ZEX	14	403	-	42,43,43	1.02	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	4C	510	3	71,73,73	1.69	14 (19%)	80,113,113	2.38	20 (25%)
21	CL7	42	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	13	510	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	44	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.44	21 (28%)
24	LMG	1D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	4B	606	2	71,73,73	1.68	18 (25%)	80,113,113	2.39	20 (25%)
21	CL7	13	513	-	51,53,73	1.98	17 (33%)	56,89,113	2.72	18 (32%)
21	CL7	2C	517	3	47,49,73	1.92	13 (27%)	51,84,113	2.88	19 (37%)
21	CL7	41	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	2A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.61	23 (33%)
21	CL7	24	414	20	59,61,73	1.85	18 (30%)	65,98,113	2.67	21 (32%)
21	CL7	14	415	-	51,53,73	1.97	20 (39%)	56,89,113	2.89	22 (39%)
32	ZEX	34	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	PHO	1A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.07	4 (7%)
23	8CT	4B	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	3B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.39	23 (28%)
23	8CT	14	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.77	21 (42%)
21	CL7	12	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	22	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	25 (31%)
21	CL7	33	514	-	51,53,73	1.99	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	22	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.37	22 (27%)
21	CL7	1B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.63	21 (30%)
21	CL7	4C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
23	8CT	2B	601	-	40,41,41	4.71	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	42	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.35	21 (26%)
21	CL7	12	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.73	19 (33%)
21	CL7	32	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
25	SQD	33	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
32	ZEX	33	519	-	42,43,43	1.01	3 (7%)	55,60,60	2.58	17 (30%)
23	8CT	1K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
21	CL7	32	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	22 (27%)
21	CL7	4B	616	2	56,58,73	1.90	17 (30%)	62,95,113	2.71	20 (32%)
21	CL7	13	505	19	71,73,73	1.69	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	4C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	41	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.86	21 (41%)
29	BCT	3D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
32	ZEX	24	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
26	LHG	34	401	-	48,48,48	0.28	0	51,54,54	0.34	0
32	ZEX	13	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	31	416	-	47,49,73	1.96	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	3D	405	4	51,53,73	1.95	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	3B	609	2	71,73,73	1.70	17 (23%)	80,113,113	2.33	20 (25%)
21	CL7	3B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	19 (27%)
21	CL7	41	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
32	ZEX	43	421	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	34	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.68	24 (32%)
29	BCT	2D	403	28	2,3,3	0.99	0	2,3,3	1.67	1 (50%)
21	CL7	32	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	33	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
21	CL7	13	511	19	71,73,73	1.68	17 (23%)	80,113,113	2.55	24 (30%)
21	CL7	1C	513	3	51,53,73	1.94	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	24	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.86	18 (35%)
32	ZEX	44	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
23	8CT	2C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	4C	504	-	61,63,73	1.85	16 (26%)	68,101,113	2.54	19 (27%)
21	CL7	31	410	-	71,73,73	1.71	17 (23%)	80,113,113	2.34	23 (28%)
21	CL7	4A	401	1	71,73,73	1.73	13 (18%)	80,113,113	2.47	25 (31%)
23	8CT	3K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.66	16 (32%)
24	LMG	11	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
23	8CT	24	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	41	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	14	414	20	59,61,73	1.84	17 (28%)	65,98,113	2.66	21 (32%)
21	CL7	41	415	-	47,49,73	1.95	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	2B	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
23	8CT	4C	515	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	13	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
21	CL7	1A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	31	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	44	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	43	403	19	64,66,73	1.78	17 (26%)	71,104,113	2.41	22 (30%)
25	SQD	43	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	13	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.32	21 (26%)
27	DGD	4C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
27	DGD	3B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
24	LMG	2D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	11	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
21	CL7	3C	512	3	47,49,73	1.92	12 (25%)	51,84,113	2.98	20 (39%)
21	CL7	13	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
25	SQD	2B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
21	CL7	22	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	33	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	24	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.71	20 (35%)
21	CL7	1B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	12	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	20 (35%)
21	CL7	44	407	-	47,49,73	1.95	13 (27%)	51,84,113	2.82	20 (39%)
21	CL7	1C	502	3	66,68,73	1.77	18 (27%)	74,107,113	2.45	19 (25%)
21	CL7	41	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.81	22 (39%)
21	CL7	43	408	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	22 (27%)
21	CL7	22	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	21 (37%)
32	ZEX	33	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	23	419	19	51,53,73	1.97	14 (27%)	56,89,113	2.74	20 (35%)
21	CL7	22	503	-	71,73,73	1.68	18 (25%)	80,113,113	2.51	25 (31%)
21	CL7	1B	610	-	71,73,73	1.68	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	43	414	-	51,53,73	1.98	18 (35%)	56,89,113	2.74	18 (32%)
21	CL7	32	503	-	71,73,73	1.68	17 (23%)	80,113,113	2.50	25 (31%)
21	CL7	4B	612	2	71,73,73	1.70	18 (25%)	80,113,113	2.36	20 (25%)
21	CL7	34	406	20	71,73,73	1.70	17 (23%)	80,113,113	2.35	21 (26%)
21	CL7	4B	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.69	18 (32%)
32	ZEX	42	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.18	17 (30%)
25	SQD	22	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
25	SQD	32	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	42	513	16	51,53,73	1.97	14 (27%)	56,89,113	2.84	21 (37%)
21	CL7	43	411	-	71,73,73	1.69	16 (22%)	80,113,113	2.37	24 (30%)
21	CL7	11	407	18	47,49,73	1.95	15 (31%)	51,84,113	2.86	20 (39%)
21	CL7	24	405	-	71,73,73	1.70	16 (22%)	80,113,113	2.46	26 (32%)
23	8CT	4D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.98	19 (38%)
21	CL7	2B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	20 (25%)
21	CL7	24	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.67	25 (33%)
21	CL7	23	405	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	4B	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
26	LHG	4A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
32	ZEX	42	524	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
23	8CT	4C	514	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	31	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	34	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	3B	608	2	71,73,73	1.69	19 (26%)	80,113,113	2.30	20 (25%)
21	CL7	1B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.37	23 (28%)
29	BCT	4D	403	28	2,3,3	0.99	0	2,3,3	1.66	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	24	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
26	LHG	24	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	13	502	19	64,66,73	1.77	15 (23%)	71,104,113	2.40	22 (30%)
21	CL7	4C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
32	ZEX	11	421	-	42,43,43	0.93	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	11	403	-	66,68,73	1.76	16 (24%)	74,107,113	2.51	22 (29%)
21	CL7	11	415	-	47,49,73	1.95	11 (23%)	51,84,113	2.97	20 (39%)
21	CL7	2B	614	2	61,63,73	1.84	19 (31%)	68,101,113	2.48	18 (26%)
26	LHG	13	524	-	35,35,48	0.34	0	38,41,54	0.47	0
29	BCT	1D	403	28	2,3,3	1.00	0	2,3,3	1.66	1 (50%)
21	CL7	21	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	22 (39%)
21	CL7	4C	508	3	71,73,73	1.70	16 (22%)	80,113,113	2.37	26 (32%)
21	CL7	11	405	-	51,53,73	1.97	17 (33%)	56,89,113	2.72	19 (33%)
21	CL7	4B	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	22 (32%)
22	PHO	3A	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.07	4 (7%)
27	DGD	2B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	21	419	-	51,53,73	1.97	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	21	413	-	47,49,73	1.94	13 (27%)	51,84,113	2.97	22 (43%)
32	ZEX	31	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.22	20 (36%)
21	CL7	33	517	19	56,58,73	1.88	15 (26%)	62,95,113	2.65	20 (32%)
21	CL7	41	405	-	51,53,73	1.97	17 (33%)	56,89,113	2.71	19 (33%)
32	ZEX	32	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	3B	614	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	24 (32%)
21	CL7	11	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.77	20 (35%)
23	8CT	2B	620	-	40,41,41	4.58	21 (52%)	50,56,56	2.91	18 (36%)
21	CL7	4C	512	3	47,49,73	1.92	14 (29%)	51,84,113	2.98	20 (39%)
21	CL7	3B	610	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	21 (26%)
21	CL7	3D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
32	ZEX	23	401	-	42,43,43	1.18	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	12	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
23	8CT	3A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
24	LMG	4D	410	-	33,33,55	0.29	0	41,41,63	0.33	0
21	CL7	21	416	-	47,49,73	1.95	13 (27%)	51,84,113	2.87	19 (37%)
21	CL7	12	513	16	51,53,73	1.96	15 (29%)	56,89,113	2.83	21 (37%)
21	CL7	13	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.92	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	ZEX	31	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	11	413	-	47,49,73	1.94	13 (27%)	51,84,113	2.98	22 (43%)
21	CL7	3B	615	2	56,58,73	1.89	18 (32%)	62,95,113	2.70	21 (33%)
21	CL7	1D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
23	8CT	3B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.24	21 (42%)
21	CL7	23	412	19	71,73,73	1.69	18 (25%)	80,113,113	2.55	24 (30%)
21	CL7	34	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.95	18 (35%)
21	CL7	14	407	-	47,49,73	1.95	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	42	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.65	19 (33%)
23	8CT	4B	619	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
24	LMG	2A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	4D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.61	20 (32%)
31	HEM	1F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
32	ZEX	43	423	-	42,43,43	1.01	4 (9%)	55,60,60	2.39	17 (30%)
21	CL7	3B	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.40	21 (26%)
25	SQD	33	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	32	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.73	19 (33%)
32	ZEX	21	422	-	42,43,43	0.95	2 (4%)	55,60,60	2.24	18 (32%)
21	CL7	12	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
21	CL7	21	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	18 (32%)
21	CL7	2B	611	-	71,73,73	1.68	16 (22%)	80,113,113	2.46	22 (27%)
21	CL7	14	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	19 (37%)
21	CL7	33	505	19	71,73,73	1.69	16 (22%)	80,113,113	2.39	21 (26%)
21	CL7	22	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.32	20 (25%)
21	CL7	31	403	-	66,68,73	1.76	16 (24%)	74,107,113	2.51	22 (29%)
23	8CT	4A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
32	ZEX	42	522	-	42,43,43	1.04	5 (11%)	55,60,60	2.47	15 (27%)
21	CL7	12	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	26 (32%)
21	CL7	34	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.36	23 (28%)
32	ZEX	44	419	-	42,43,43	0.98	3 (7%)	55,60,60	2.44	25 (45%)
23	8CT	4K	101	-	40,41,41	4.76	25 (62%)	50,56,56	2.66	16 (32%)
32	ZEX	14	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	1C	511	3	48,50,73	1.95	14 (29%)	51,85,113	2.83	18 (35%)
21	CL7	1C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	1B	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.32	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	24	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.87	21 (37%)
23	8CT	1B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	31	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.51	23 (28%)
21	CL7	43	418	19	56,58,73	1.88	16 (28%)	62,95,113	2.65	20 (32%)
21	CL7	12	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.41	21 (26%)
21	CL7	21	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	44	414	20	59,61,73	1.84	18 (30%)	65,98,113	2.66	21 (32%)
32	ZEX	33	520	-	42,43,43	0.92	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	3B	611	2	71,73,73	1.70	18 (25%)	80,113,113	2.34	20 (25%)
21	CL7	21	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.98	19 (37%)
25	SQD	23	422	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	21	404	-	71,73,73	1.71	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	31	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	1B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.78	17 (30%)
27	DGD	3C	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	22	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.63	19 (33%)
21	CL7	1B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	21	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
21	CL7	33	512	19	61,63,73	1.83	19 (31%)	68,101,113	2.59	23 (33%)
21	CL7	14	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	21 (37%)
21	CL7	21	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
22	PHO	4A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.08	4 (7%)
26	LHG	1D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
25	SQD	3A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	23	407	19	51,53,73	1.96	17 (33%)	56,89,113	2.75	19 (33%)
21	CL7	1D	405	4	51,53,73	1.96	18 (35%)	56,89,113	2.77	22 (39%)
21	CL7	21	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.87	20 (39%)
26	LHG	3B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	12	516	16	71,73,73	1.70	17 (23%)	80,113,113	2.39	24 (30%)
21	CL7	4C	503	3	71,73,73	1.68	15 (21%)	80,113,113	2.39	21 (26%)
24	LMG	31	401	-	51,51,55	0.22	0	59,59,63	0.42	1 (1%)
21	CL7	32	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
21	CL7	41	409	18	51,53,73	1.96	16 (31%)	56,89,113	2.72	20 (35%)
32	ZEX	22	524	-	42,43,43	1.03	3 (7%)	55,60,60	2.51	17 (30%)
31	HEM	2F	101	-	50,50,50	1.61	9 (18%)	66,82,82	1.81	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	34	411	20	71,73,73	1.68	16 (22%)	80,113,113	2.41	23 (28%)
21	CL7	44	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.33	21 (26%)
21	CL7	32	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.47	25 (31%)
25	SQD	23	424	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
25	SQD	12	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	22	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.43	21 (26%)
21	CL7	22	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
24	LMG	41	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	42	503	-	71,73,73	1.69	18 (25%)	80,113,113	2.50	24 (30%)
21	CL7	23	403	19	64,66,73	1.77	16 (25%)	71,104,113	2.41	22 (30%)
21	CL7	3B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	1C	517	3	47,49,73	1.93	13 (27%)	51,84,113	2.89	19 (37%)
21	CL7	4B	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
21	CL7	31	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
25	SQD	22	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	31	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.50	20 (27%)
32	ZEX	13	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	4C	513	3	51,53,73	1.95	14 (27%)	56,89,113	2.91	19 (33%)
26	LHG	2B	624	-	44,44,48	0.32	0	47,50,54	0.39	0
21	CL7	13	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.41	21 (26%)
21	CL7	1B	602	2	66,68,73	1.77	17 (25%)	74,107,113	2.51	21 (28%)
21	CL7	11	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	13	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	14	412	20	71,73,73	1.69	15 (21%)	80,113,113	2.38	25 (31%)
21	CL7	2C	503	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
27	DGD	4B	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
23	8CT	1B	618	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	24	413	20	66,68,73	1.77	17 (25%)	74,107,113	2.44	21 (28%)
21	CL7	33	510	-	71,73,73	1.69	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	34	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	3B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
25	SQD	13	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
25	SQD	1B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.53	1 (1%)
25	SQD	1A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
26	LHG	1B	625	-	48,48,48	0.30	0	51,54,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	23	406	19	71,73,73	1.69	17 (23%)	80,113,113	2.38	21 (26%)
26	LHG	2A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	24	417	20	48,50,73	1.94	13 (27%)	51,85,113	2.94	18 (35%)
32	ZEX	24	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	14	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.44	21 (28%)
21	CL7	42	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	20 (35%)
23	8CT	4B	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	22	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.37	22 (27%)
21	CL7	1C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	14	411	20	71,73,73	1.67	15 (21%)	80,113,113	2.41	23 (28%)
21	CL7	41	403	-	66,68,73	1.75	16 (24%)	74,107,113	2.51	22 (29%)
32	ZEX	41	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	43	404	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	11	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.43	20 (26%)
21	CL7	4B	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
25	SQD	42	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	3A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.45	21 (26%)
21	CL7	22	518	16	71,73,73	1.68	14 (19%)	80,113,113	2.33	23 (28%)
27	DGD	1B	624	-	63,63,67	0.83	2 (3%)	77,77,81	1.00	3 (3%)
26	LHG	1A	408	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	44	410	20	51,53,73	1.99	17 (33%)	56,89,113	2.71	19 (33%)
23	8CT	1B	626	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
31	HEM	3F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.81	15 (22%)
25	SQD	12	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	41	408	-	71,73,73	1.66	15 (21%)	80,113,113	2.51	23 (28%)
21	CL7	42	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.35	23 (28%)
21	CL7	23	414	-	51,53,73	1.98	17 (33%)	56,89,113	2.73	18 (32%)
21	CL7	1A	401	1	71,73,73	1.74	13 (18%)	80,113,113	2.46	25 (31%)
21	CL7	1C	507	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	24	412	20	71,73,73	1.69	17 (23%)	80,113,113	2.38	25 (31%)
21	CL7	4B	614	2	61,63,73	1.83	19 (31%)	68,101,113	2.47	18 (26%)
32	ZEX	22	522	-	42,43,43	1.04	3 (7%)	55,60,60	2.47	17 (30%)
31	HEM	4F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
23	8CT	3B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.76	19 (38%)
21	CL7	4C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	12	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.35	22 (27%)
21	CL7	3C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
21	CL7	2D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
21	CL7	13	518	19	51,53,73	1.97	14 (27%)	56,89,113	2.75	20 (35%)
21	CL7	2D	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	11	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
25	SQD	2A	406	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	21	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.96	19 (37%)
21	CL7	22	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	12	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	4B	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
30	PL9	3D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
26	LHG	2D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	12	511	16	66,68,73	1.78	16 (24%)	74,107,113	2.40	21 (28%)
21	CL7	1B	614	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	25 (33%)
23	8CT	2A	404	-	40,41,41	4.63	20 (50%)	50,56,56	2.97	20 (40%)
21	CL7	4B	611	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	41	418	18	71,73,73	1.67	15 (21%)	80,113,113	2.46	23 (28%)
24	LMG	2B	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	1B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	3B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	4A	407	-	71,73,73	1.67	17 (23%)	80,113,113	2.44	21 (26%)
26	LHG	43	425	-	35,35,48	0.34	0	38,41,54	0.47	0
21	CL7	41	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.49	19 (25%)
25	SQD	4B	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
21	CL7	12	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.78	19 (33%)
21	CL7	23	417	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
21	CL7	2C	505	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
21	CL7	31	407	18	47,49,73	1.94	14 (29%)	51,84,113	2.87	19 (37%)
21	CL7	44	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	2C	510	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	21 (26%)
21	CL7	22	511	16	66,68,73	1.78	16 (24%)	74,107,113	2.40	21 (28%)
21	CL7	1B	604	2	71,73,73	1.67	18 (25%)	80,113,113	2.32	23 (28%)
21	CL7	1C	512	3	47,49,73	1.93	13 (27%)	51,84,113	2.99	20 (39%)
21	CL7	3C	506	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CL7	11	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	22 (27%)
30	PL9	2D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	12	503	-	71,73,73	1.69	17 (23%)	80,113,113	2.51	25 (31%)
21	CL7	11	402	18	66,68,73	1.79	15 (22%)	74,107,113	2.50	19 (25%)
25	SQD	11	423	-	31,32,54	0.49	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	33	511	19	71,73,73	1.69	18 (25%)	80,113,113	2.55	24 (30%)
21	CL7	44	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.45	26 (32%)
21	CL7	11	411	-	51,53,73	1.98	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	2B	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	43	419	19	51,53,73	1.98	14 (27%)	56,89,113	2.74	20 (35%)
21	CL7	43	405	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	42	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.47	25 (31%)
21	CL7	42	510	16	71,73,73	1.68	18 (25%)	80,113,113	2.37	22 (27%)
23	8CT	2B	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
26	LHG	4D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	24	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	2C	509	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	1C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.35	22 (27%)
21	CL7	32	509	-	71,73,73	1.68	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	4B	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	2C	512	3	47,49,73	1.92	13 (27%)	51,84,113	2.97	20 (39%)
25	SQD	31	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
32	ZEX	11	422	-	42,43,43	0.96	2 (4%)	55,60,60	2.23	18 (32%)
23	8CT	1B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	1A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.62	23 (33%)
21	CL7	41	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.71	18 (32%)
21	CL7	33	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
26	LHG	4B	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	4B	615	2	66,68,73	1.78	18 (27%)	74,107,113	2.49	25 (33%)
21	CL7	41	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
22	PHO	2A	402	-	58,69,69	0.83	3 (5%)	56,99,99	1.08	4 (7%)
24	LMG	4A	405	-	50,50,55	0.24	0	58,58,63	0.41	0
21	CL7	22	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
26	LHG	3B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	11	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	SQD	13	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
23	8CT	1A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
23	8CT	3B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.66	20 (40%)
21	CL7	32	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	43	416	-	47,49,73	1.93	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	11	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	22 (39%)
26	LHG	33	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	13	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	2A	407	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	23	410	19	71,73,73	1.68	16 (22%)	80,113,113	2.33	22 (27%)
32	ZEX	14	420	-	42,43,43	1.01	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	12	507	-	71,73,73	1.72	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	2C	501	3	71,73,73	1.68	16 (22%)	80,113,113	2.35	21 (26%)
21	CL7	1B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	19 (27%)
21	CL7	21	412	18	51,53,73	1.95	16 (31%)	56,89,113	2.76	20 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	502	19	2/2/13/20	12/31/107/115	-
21	CL7	31	419	-	2/2/11/20	9/15/91/115	-
21	CL7	2C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	3C	511	3	2/2/10/20	5/12/88/115	-
25	SQD	32	521	-	-	7/45/65/69	0/1/1/1
21	CL7	22	507	-	2/2/15/20	20/39/115/115	-
21	CL7	23	404	-	2/2/15/20	20/39/115/115	-
21	CL7	23	415	-	2/2/11/20	5/15/91/115	-
21	CL7	3C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	4B	609	2	2/2/15/20	15/39/115/115	-
21	CL7	3B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	1B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	33	513	-	2/2/11/20	9/15/91/115	-
32	ZEX	22	519	-	-	11/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	44	409	-	2/2/14/20	17/33/109/115	-
23	8CT	3C	514	-	-	14/29/63/63	0/2/2/2
25	SQD	42	521	-	-	7/45/65/69	0/1/1/1
21	CL7	21	402	18	2/2/14/20	16/33/109/115	-
21	CL7	31	404	-	2/2/15/20	15/39/115/115	-
21	CL7	23	409	19	2/2/15/20	16/39/115/115	-
21	CL7	11	409	18	2/2/11/20	6/15/91/115	-
21	CL7	2B	610	2	2/2/15/20	14/39/115/115	-
21	CL7	14	406	20	2/2/15/20	24/39/115/115	-
21	CL7	3C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	31	418	18	2/2/15/20	22/39/115/115	-
21	CL7	4D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	13	507	-	2/2/15/20	15/39/115/115	-
21	CL7	43	410	19	2/2/15/20	17/39/115/115	-
32	ZEX	14	419	-	-	9/29/67/67	0/2/2/2
26	LHG	2B	626	-	-	6/53/53/53	-
21	CL7	2B	604	2	2/2/15/20	12/39/115/115	-
21	CL7	31	414	18	2/2/10/20	3/10/86/115	-
21	CL7	34	414	20	2/2/12/20	8/25/101/115	-
21	CL7	21	408	-	2/2/15/20	16/39/115/115	-
23	8CT	2C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	32	510	16	2/2/15/20	20/39/115/115	-
27	DGD	1C	516	-	-	9/51/91/95	0/2/2/2
30	PL9	4D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	34	404	20	2/2/15/20	14/39/115/115	-
21	CL7	14	405	-	2/2/15/20	18/39/115/115	-
21	CL7	2B	608	-	2/2/14/20	11/33/109/115	-
21	CL7	32	517	16	2/2/15/20	21/39/115/115	-
21	CL7	2B	617	2	2/2/11/20	4/15/91/115	-
24	LMG	1B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	41	412	18	2/2/11/20	10/15/91/115	-
32	ZEX	13	525	-	-	7/29/67/67	0/2/2/2
21	CL7	43	409	19	2/2/15/20	16/39/115/115	-
32	ZEX	12	520	-	-	6/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	34	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	44	403	-	-	10/29/67/67	0/2/2/2
32	ZEX	34	418	-	-	9/29/67/67	0/2/2/2
24	LMG	1A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	1D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	22	501	16	2/2/15/20	17/39/115/115	-
21	CL7	1B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	12	508	16	2/2/11/20	5/15/91/115	-
32	ZEX	12	524	-	-	11/29/67/67	0/2/2/2
26	LHG	14	401	-	-	8/53/53/53	-
21	CL7	2B	602	-	2/2/10/20	4/10/86/115	-
21	CL7	24	411	20	2/2/15/20	14/39/115/115	-
21	CL7	2C	506	3	2/2/14/20	15/33/109/115	-
24	LMG	4B	622	-	-	7/46/66/70	0/1/1/1
26	LHG	4B	626	-	-	6/53/53/53	-
21	CL7	4C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	4C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	43	407	19	2/2/11/20	13/15/91/115	-
21	CL7	1C	504	-	2/2/13/20	13/27/103/115	-
24	LMG	3D	410	-	-	5/28/48/70	0/1/1/1
26	LHG	3A	408	-	-	5/50/50/53	-
21	CL7	23	418	19	2/2/12/20	9/21/97/115	-
21	CL7	44	417	20	2/2/10/20	6/12/88/115	-
25	SQD	3B	620	-	-	5/49/69/69	0/1/1/1
22	PHO	4D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	12	512	16	2/2/15/20	18/39/115/115	-
21	CL7	1B	615	2	2/2/12/20	8/21/97/115	-
21	CL7	14	404	20	2/2/15/20	15/39/115/115	-
21	CL7	34	408	20	2/2/11/20	4/15/91/115	-
21	CL7	41	410	-	2/2/15/20	17/39/115/115	-
32	ZEX	12	522	-	-	6/29/67/67	0/2/2/2
21	CL7	42	506	16	2/2/15/20	14/39/115/115	-
21	CL7	24	408	20	2/2/11/20	4/15/91/115	-
21	CL7	42	509	-	2/2/15/20	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	3C	518	-	-	8/29/63/63	0/2/2/2
26	LHG	23	425	-	-	3/40/40/53	-
21	CL7	2B	605	2	2/2/15/20	17/39/115/115	-
21	CL7	42	518	16	2/2/15/20	12/39/115/115	-
21	CL7	34	413	20	2/2/14/20	7/33/109/115	-
21	CL7	42	516	16	2/2/15/20	16/39/115/115	-
24	LMG	3A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	3A	401	1	2/2/15/20	18/39/115/115	-
21	CL7	33	518	19	2/2/11/20	7/15/91/115	-
21	CL7	44	415	-	2/2/11/20	11/15/91/115	-
25	SQD	43	422	-	-	3/41/61/69	0/1/1/1
23	8CT	2K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	12	518	16	2/2/15/20	12/39/115/115	-
21	CL7	3C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	13	512	19	2/2/13/20	12/27/103/115	-
23	8CT	44	402	-	-	4/29/63/63	0/2/2/2
32	ZEX	22	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	32	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	21	421	-	-	14/29/67/67	0/2/2/2
21	CL7	3C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	31	413	-	2/2/10/20	2/10/86/115	-
21	CL7	31	405	-	2/2/11/20	10/15/91/115	-
21	CL7	44	408	20	2/2/11/20	4/15/91/115	-
32	ZEX	23	423	-	-	5/29/67/67	0/2/2/2
21	CL7	2C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	2C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	3B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	43	417	19	2/2/13/20	16/27/103/115	-
21	CL7	32	516	16	2/2/15/20	16/39/115/115	-
21	CL7	2B	615	2	2/2/14/20	14/33/109/115	-
21	CL7	13	501	19	2/2/15/20	21/39/115/115	-
21	CL7	32	512	16	2/2/15/20	18/39/115/115	-
26	LHG	44	401	-	-	8/53/53/53	-
32	ZEX	43	401	-	-	7/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	32	522	-	-	6/29/67/67	0/2/2/2
25	SQD	41	423	-	-	3/27/47/69	0/1/1/1
21	CL7	4C	507	-	2/2/15/20	17/39/115/115	-
23	8CT	2B	619	-	-	10/29/63/63	0/2/2/2
32	ZEX	23	420	-	-	10/29/67/67	0/2/2/2
21	CL7	2B	616	2	2/2/12/20	8/21/97/115	-
21	CL7	42	511	16	2/2/14/20	16/33/109/115	-
21	CL7	2D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	23	413	19	2/2/13/20	12/27/103/115	-
21	CL7	33	504	-	2/2/15/20	16/39/115/115	-
21	CL7	2C	513	3	2/2/11/20	8/15/91/115	-
22	PHO	3D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	32	513	16	2/2/11/20	8/15/91/115	-
21	CL7	43	415	-	2/2/11/20	5/15/91/115	-
24	LMG	3B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	1C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	33	503	-	2/2/15/20	20/39/115/115	-
23	8CT	1C	515	-	-	10/29/63/63	0/2/2/2
32	ZEX	41	422	-	-	6/29/67/67	0/2/2/2
21	CL7	1C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	43	406	19	2/2/15/20	14/39/115/115	-
21	CL7	3C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	3B	606	2	2/2/13/20	5/27/103/115	-
32	ZEX	32	524	-	-	11/29/67/67	0/2/2/2
21	CL7	21	410	-	2/2/15/20	17/39/115/115	-
25	SQD	4A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	23	416	-	2/2/10/20	0/10/86/115	-
21	CL7	3A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	11	419	-	2/2/11/20	9/15/91/115	-
21	CL7	31	409	18	2/2/11/20	6/15/91/115	-
21	CL7	3C	509	3	2/2/15/20	20/39/115/115	-
32	ZEX	12	519	-	-	11/29/67/67	0/2/2/2
21	CL7	2C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	3D	402	-	2/2/12/20	9/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	4C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	13	517	19	2/2/12/20	9/21/97/115	-
23	8CT	1D	406	-	-	10/29/63/63	0/2/2/2
24	LMG	21	401	-	-	5/46/66/70	0/1/1/1
21	CL7	41	413	-	2/2/10/20	2/10/86/115	-
32	ZEX	43	420	-	-	10/29/67/67	0/2/2/2
21	CL7	43	413	19	2/2/13/20	12/27/103/115	-
26	LHG	3D	409	-	-	7/53/53/53	-
21	CL7	1B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	11	416	-	2/2/10/20	4/10/86/115	-
21	CL7	1B	605	2	2/2/15/20	18/39/115/115	-
32	ZEX	23	421	-	-	10/29/67/67	0/2/2/2
21	CL7	32	515	-	2/2/11/20	8/15/91/115	-
21	CL7	23	402	19	2/2/15/20	21/39/115/115	-
23	8CT	3B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	14	409	-	2/2/14/20	17/33/109/115	-
21	CL7	2C	502	3	2/2/14/20	12/33/109/115	-
26	LHG	1B	623	-	-	3/49/49/53	-
21	CL7	32	502	16	2/2/15/20	17/39/115/115	-
21	CL7	42	507	-	2/2/15/20	20/39/115/115	-
21	CL7	2A	401	1	2/2/15/20	18/39/115/115	-
23	8CT	1C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	41	416	-	2/2/10/20	4/10/86/115	-
21	CL7	3B	602	2	2/2/14/20	9/33/109/115	-
21	CL7	41	414	18	2/2/10/20	3/10/86/115	-
32	ZEX	42	519	-	-	11/29/67/67	0/2/2/2
32	ZEX	24	419	-	-	9/29/67/67	0/2/2/2
21	CL7	13	506	19	2/2/11/20	13/15/91/115	-
21	CL7	33	516	19	2/2/13/20	16/27/103/115	-
21	CL7	4B	608	-	2/2/14/20	11/33/109/115	-
21	CL7	13	509	19	2/2/15/20	17/39/115/115	-
21	CL7	3C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	44	412	20	2/2/15/20	17/39/115/115	-
21	CL7	1C	508	3	2/2/15/20	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	22	513	16	2/2/11/20	8/15/91/115	-
23	8CT	2C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	32	504	-	2/2/11/20	6/15/91/115	-
21	CL7	14	410	20	2/2/11/20	9/15/91/115	-
21	CL7	4A	403	1	2/2/13/20	9/27/103/115	-
22	PHO	2D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
21	CL7	1C	503	3	2/2/15/20	19/39/115/115	-
21	CL7	3C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	4B	602	-	2/2/10/20	4/10/86/115	-
23	8CT	4B	618	-	-	7/29/63/63	0/2/2/2
21	CL7	23	411	-	2/2/15/20	15/39/115/115	-
30	PL9	1D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	21	418	18	2/2/15/20	22/39/115/115	-
23	8CT	2D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	43	402	19	2/2/15/20	21/39/115/115	-
25	SQD	21	423	-	-	3/27/47/69	0/1/1/1
21	CL7	42	512	16	2/2/15/20	18/39/115/115	-
27	DGD	2C	516	-	-	9/51/91/95	0/2/2/2
32	ZEX	33	525	-	-	7/29/67/67	0/2/2/2
32	ZEX	44	420	-	-	12/29/67/67	0/2/2/2
21	CL7	33	509	19	2/2/15/20	17/39/115/115	-
21	CL7	11	414	18	2/2/10/20	3/10/86/115	-
23	8CT	1C	518	-	-	8/29/63/63	0/2/2/2
21	CL7	34	415	-	2/2/11/20	11/15/91/115	-
21	CL7	2B	623	2	2/2/11/20	8/15/91/115	-
21	CL7	31	420	18	2/2/11/20	6/15/91/115	-
21	CL7	21	403	-	2/2/14/20	11/33/109/115	-
21	CL7	21	417	18	2/2/13/20	9/27/103/115	-
21	CL7	3C	510	3	2/2/15/20	22/39/115/115	-
32	ZEX	34	403	-	-	10/29/67/67	0/2/2/2
23	8CT	34	402	-	-	4/29/63/63	0/2/2/2
21	CL7	4D	404	4	2/2/13/20	13/31/107/115	-
21	CL7	34	405	-	2/2/15/20	18/39/115/115	-
21	CL7	23	408	-	2/2/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	43	412	19	2/2/15/20	19/39/115/115	-
21	CL7	42	501	16	2/2/15/20	17/39/115/115	-
23	8CT	3C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	24	404	20	2/2/15/20	15/39/115/115	-
21	CL7	2B	606	2	2/2/15/20	18/39/115/115	-
21	CL7	14	416	20	2/2/10/20	7/10/86/115	-
21	CL7	31	415	-	2/2/10/20	7/10/86/115	-
21	CL7	22	502	16	2/2/15/20	17/39/115/115	-
21	CL7	2B	607	2	2/2/13/20	5/27/103/115	-
23	8CT	3D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	44	406	20	2/2/15/20	24/39/115/115	-
21	CL7	33	508	19	2/2/15/20	16/39/115/115	-
21	CL7	3C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	2B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	4B	605	2	2/2/15/20	17/39/115/115	-
32	ZEX	24	418	-	-	9/29/67/67	0/2/2/2
21	CL7	3B	607	-	2/2/14/20	11/33/109/115	-
21	CL7	33	515	-	2/2/10/20	0/10/86/115	-
21	CL7	34	416	20	2/2/10/20	7/10/86/115	-
21	CL7	42	514	-	2/2/11/20	9/15/91/115	-
21	CL7	4C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	32	507	-	2/2/15/20	20/39/115/115	-
22	PHO	1D	408	-	1/1/17/22	8/37/103/103	0/5/6/6
32	ZEX	14	403	-	-	10/29/67/67	0/2/2/2
21	CL7	4C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	42	504	-	2/2/11/20	6/15/91/115	-
21	CL7	13	510	-	2/2/15/20	15/39/115/115	-
21	CL7	44	413	20	2/2/14/20	7/33/109/115	-
24	LMG	1D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	4B	606	2	2/2/15/20	18/39/115/115	-
21	CL7	13	513	-	2/2/11/20	9/15/91/115	-
21	CL7	2C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	41	406	18	2/2/14/20	13/36/112/115	-
21	CL7	2A	403	1	2/2/13/20	9/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	24	414	20	2/2/12/20	8/25/101/115	-
21	CL7	14	415	-	2/2/11/20	11/15/91/115	-
32	ZEX	34	419	-	-	9/29/67/67	0/2/2/2
22	PHO	1A	402	-	-	3/37/103/103	0/5/6/6
23	8CT	4B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	3B	612	2	2/2/15/20	17/39/115/115	-
23	8CT	14	402	-	-	4/29/63/63	0/2/2/2
21	CL7	12	517	16	2/2/15/20	21/39/115/115	-
21	CL7	22	505	16	2/2/15/20	18/39/115/115	-
21	CL7	33	514	-	2/2/11/20	5/15/91/115	-
21	CL7	22	510	16	2/2/15/20	20/39/115/115	-
21	CL7	1B	606	2	2/2/13/20	5/27/103/115	-
21	CL7	4C	511	3	2/2/10/20	5/12/88/115	-
23	8CT	2B	601	-	-	10/29/63/63	0/2/2/2
21	CL7	42	517	16	2/2/15/20	21/39/115/115	-
21	CL7	12	514	-	2/2/11/20	9/15/91/115	-
21	CL7	32	506	16	2/2/15/20	14/39/115/115	-
25	SQD	33	521	-	-	3/41/61/69	0/1/1/1
32	ZEX	33	519	-	-	10/29/67/67	0/2/2/2
23	8CT	1K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	32	518	16	2/2/15/20	12/39/115/115	-
21	CL7	4B	616	2	2/2/12/20	8/21/97/115	-
21	CL7	13	505	19	2/2/15/20	14/39/115/115	-
21	CL7	4C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	41	407	18	2/2/10/20	4/10/86/115	-
32	ZEX	24	420	-	-	12/29/67/67	0/2/2/2
26	LHG	34	401	-	-	8/53/53/53	-
32	ZEX	13	522	-	-	5/29/67/67	0/2/2/2
21	CL7	31	416	-	2/2/10/20	4/10/86/115	-
21	CL7	3D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	3B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	3B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	41	419	-	2/2/11/20	9/15/91/115	-
32	ZEX	43	421	-	-	10/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	34	409	-	2/2/14/20	17/33/109/115	-
21	CL7	32	508	16	2/2/11/20	5/15/91/115	-
21	CL7	33	501	19	2/2/15/20	21/39/115/115	-
21	CL7	13	511	19	2/2/15/20	19/39/115/115	-
21	CL7	1C	513	3	2/2/11/20	8/15/91/115	-
21	CL7	24	416	20	2/2/10/20	7/10/86/115	-
32	ZEX	44	418	-	-	9/29/67/67	0/2/2/2
23	8CT	2C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	4C	504	-	2/2/13/20	13/27/103/115	-
21	CL7	31	410	-	2/2/15/20	17/39/115/115	-
21	CL7	4A	401	1	2/2/15/20	18/39/115/115	-
23	8CT	3K	101	-	-	10/29/63/63	0/2/2/2
24	LMG	11	401	-	-	5/46/66/70	0/1/1/1
23	8CT	24	402	-	-	4/29/63/63	0/2/2/2
21	CL7	41	404	-	2/2/15/20	15/39/115/115	-
21	CL7	14	414	20	2/2/12/20	8/25/101/115	-
21	CL7	41	415	-	2/2/10/20	7/10/86/115	-
21	CL7	2B	613	2	2/2/15/20	17/39/115/115	-
23	8CT	4C	515	-	-	10/29/63/63	0/2/2/2
21	CL7	13	516	19	2/2/13/20	16/27/103/115	-
21	CL7	1A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	31	412	18	2/2/11/20	10/15/91/115	-
21	CL7	44	411	20	2/2/15/20	14/39/115/115	-
21	CL7	43	403	19	2/2/13/20	12/31/107/115	-
25	SQD	43	424	-	-	7/45/65/69	0/1/1/1
21	CL7	13	508	19	2/2/15/20	16/39/115/115	-
27	DGD	4C	516	-	-	9/51/91/95	0/2/2/2
27	DGD	3B	624	-	-	7/51/91/95	0/2/2/2
24	LMG	2D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	11	417	18	2/2/13/20	9/27/103/115	-
21	CL7	3C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	13	503	-	2/2/15/20	20/39/115/115	-
25	SQD	2B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	22	516	16	2/2/15/20	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	506	19	2/2/11/20	13/15/91/115	-
21	CL7	24	410	20	2/2/11/20	9/15/91/115	-
21	CL7	1B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	12	515	-	2/2/11/20	8/15/91/115	-
21	CL7	44	407	-	2/2/10/20	3/10/86/115	-
21	CL7	1C	502	3	2/2/14/20	12/33/109/115	-
21	CL7	41	420	18	2/2/11/20	6/15/91/115	-
21	CL7	43	408	-	2/2/15/20	15/39/115/115	-
21	CL7	22	515	-	2/2/11/20	8/15/91/115	-
32	ZEX	33	522	-	-	5/29/67/67	0/2/2/2
21	CL7	23	419	19	2/2/11/20	7/15/91/115	-
21	CL7	22	503	-	2/2/15/20	17/39/115/115	-
21	CL7	1B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	43	414	-	2/2/11/20	9/15/91/115	-
21	CL7	32	503	-	2/2/15/20	17/39/115/115	-
21	CL7	4B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	34	406	20	2/2/15/20	24/39/115/115	-
21	CL7	4B	617	2	2/2/11/20	4/15/91/115	-
32	ZEX	42	520	-	-	6/29/67/67	0/2/2/2
25	SQD	22	523	-	-	0/36/56/69	0/1/1/1
25	SQD	32	523	-	-	0/36/56/69	0/1/1/1
21	CL7	42	513	16	2/2/11/20	8/15/91/115	-
21	CL7	43	411	-	2/2/15/20	16/39/115/115	-
21	CL7	11	407	18	2/2/10/20	4/10/86/115	-
21	CL7	24	405	-	2/2/15/20	18/39/115/115	-
23	8CT	4D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	2B	609	2	2/2/15/20	15/39/115/115	-
21	CL7	24	409	-	2/2/14/20	17/33/109/115	-
21	CL7	23	405	-	2/2/15/20	16/39/115/115	-
21	CL7	4B	623	2	2/2/11/20	8/15/91/115	-
26	LHG	4A	408	-	-	5/50/50/53	-
32	ZEX	42	524	-	-	11/29/67/67	0/2/2/2
23	8CT	4C	514	-	-	14/29/63/63	0/2/2/2
21	CL7	31	406	18	2/2/14/20	13/36/112/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	34	410	20	2/2/11/20	9/15/91/115	-
21	CL7	3B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	1B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	24	407	-	2/2/10/20	3/10/86/115	-
26	LHG	24	401	-	-	8/53/53/53	-
21	CL7	13	502	19	2/2/13/20	12/31/107/115	-
21	CL7	4C	505	3	2/2/15/20	16/39/115/115	-
32	ZEX	11	421	-	-	14/29/67/67	0/2/2/2
21	CL7	11	403	-	2/2/14/20	11/33/109/115	-
21	CL7	11	415	-	2/2/10/20	7/10/86/115	-
21	CL7	2B	614	2	2/2/13/20	5/27/103/115	-
26	LHG	13	524	-	-	3/40/40/53	-
21	CL7	21	420	18	2/2/11/20	6/15/91/115	-
21	CL7	4C	508	3	2/2/15/20	17/39/115/115	-
21	CL7	11	405	-	2/2/11/20	10/15/91/115	-
21	CL7	4B	607	2	2/2/13/20	5/27/103/115	-
22	PHO	3A	402	-	-	3/37/103/103	0/5/6/6
27	DGD	2B	625	-	-	7/51/91/95	0/2/2/2
21	CL7	21	419	-	2/2/11/20	9/15/91/115	-
21	CL7	21	413	-	2/2/10/20	2/10/86/115	-
32	ZEX	31	421	-	-	14/29/67/67	0/2/2/2
21	CL7	33	517	19	2/2/12/20	9/21/97/115	-
21	CL7	41	405	-	2/2/11/20	10/15/91/115	-
32	ZEX	32	519	-	-	11/29/67/67	0/2/2/2
21	CL7	3B	614	2	2/2/14/20	14/33/109/115	-
21	CL7	11	412	18	2/2/11/20	10/15/91/115	-
23	8CT	2B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	4C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	3B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	3D	404	4	2/2/13/20	13/31/107/115	-
32	ZEX	23	401	-	-	7/29/67/67	0/2/2/2
21	CL7	12	510	16	2/2/15/20	20/39/115/115	-
23	8CT	3A	404	-	-	5/29/63/63	0/2/2/2
24	LMG	4D	410	-	-	6/28/48/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	21	416	-	2/2/10/20	4/10/86/115	-
21	CL7	12	513	16	2/2/11/20	8/15/91/115	-
21	CL7	13	515	-	2/2/10/20	0/10/86/115	-
32	ZEX	31	422	-	-	6/29/67/67	0/2/2/2
21	CL7	11	413	-	2/2/10/20	2/10/86/115	-
21	CL7	3B	615	2	2/2/12/20	8/21/97/115	-
21	CL7	1D	404	4	2/2/13/20	13/31/107/115	-
23	8CT	3B	626	-	-	10/29/63/63	0/2/2/2
21	CL7	23	412	19	2/2/15/20	19/39/115/115	-
21	CL7	34	417	20	2/2/10/20	6/12/88/115	-
21	CL7	14	407	-	2/2/10/20	3/10/86/115	-
21	CL7	42	508	16	2/2/11/20	5/15/91/115	-
23	8CT	4B	619	-	-	10/29/63/63	0/2/2/2
24	LMG	2A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	4D	402	-	2/2/12/20	9/21/97/115	-
31	HEM	1F	101	-	-	8/14/54/54	-
32	ZEX	43	423	-	-	5/29/67/67	0/2/2/2
21	CL7	3B	605	2	2/2/15/20	18/39/115/115	-
25	SQD	33	523	-	-	7/45/65/69	0/1/1/1
21	CL7	32	514	-	2/2/11/20	9/15/91/115	-
32	ZEX	21	422	-	-	6/29/67/67	0/2/2/2
21	CL7	12	506	16	2/2/15/20	14/39/115/115	-
21	CL7	21	405	-	2/2/11/20	10/15/91/115	-
21	CL7	2B	611	-	2/2/15/20	11/39/115/115	-
21	CL7	14	417	20	2/2/10/20	6/12/88/115	-
21	CL7	33	505	19	2/2/15/20	14/39/115/115	-
21	CL7	22	509	-	2/2/15/20	16/39/115/115	-
21	CL7	31	403	-	2/2/14/20	11/33/109/115	-
23	8CT	4A	404	-	-	5/29/63/63	0/2/2/2
32	ZEX	42	522	-	-	6/29/67/67	0/2/2/2
21	CL7	12	505	16	2/2/15/20	18/39/115/115	-
21	CL7	34	412	20	2/2/15/20	17/39/115/115	-
32	ZEX	44	419	-	-	9/29/67/67	0/2/2/2
23	8CT	4K	101	-	-	10/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	14	418	-	-	9/29/67/67	0/2/2/2
21	CL7	1C	511	3	2/2/10/20	5/12/88/115	-
21	CL7	1C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	1B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	24	415	-	2/2/11/20	11/15/91/115	-
23	8CT	1B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	31	408	-	2/2/15/20	16/39/115/115	-
21	CL7	43	418	19	2/2/12/20	9/21/97/115	-
21	CL7	12	501	16	2/2/15/20	17/39/115/115	-
21	CL7	21	406	18	2/2/14/20	13/36/112/115	-
21	CL7	44	414	20	2/2/12/20	8/25/101/115	-
32	ZEX	33	520	-	-	10/29/67/67	0/2/2/2
21	CL7	3B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	21	414	18	2/2/10/20	3/10/86/115	-
25	SQD	23	422	-	-	3/41/61/69	0/1/1/1
21	CL7	21	404	-	2/2/15/20	15/39/115/115	-
21	CL7	31	411	-	2/2/11/20	7/15/91/115	-
21	CL7	1B	622	2	2/2/11/20	8/15/91/115	-
27	DGD	3C	516	-	-	9/51/91/95	0/2/2/2
21	CL7	22	508	16	2/2/11/20	5/15/91/115	-
21	CL7	1B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	21	411	-	2/2/11/20	7/15/91/115	-
21	CL7	33	512	19	2/2/13/20	12/27/103/115	-
21	CL7	14	408	20	2/2/11/20	4/15/91/115	-
21	CL7	21	409	18	2/2/11/20	6/15/91/115	-
22	PHO	4A	402	-	-	3/37/103/103	0/5/6/6
26	LHG	1D	409	-	-	7/53/53/53	-
25	SQD	3A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	23	407	19	2/2/11/20	13/15/91/115	-
21	CL7	1D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	21	407	18	2/2/10/20	4/10/86/115	-
26	LHG	3B	623	-	-	3/49/49/53	-
21	CL7	12	516	16	2/2/15/20	16/39/115/115	-
21	CL7	4C	503	3	2/2/15/20	19/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	31	401	-	-	5/46/66/70	0/1/1/1
21	CL7	32	501	16	2/2/15/20	17/39/115/115	-
21	CL7	41	409	18	2/2/11/20	6/15/91/115	-
32	ZEX	22	524	-	-	11/29/67/67	0/2/2/2
31	HEM	2F	101	-	-	8/14/54/54	-
21	CL7	34	411	20	2/2/15/20	14/39/115/115	-
21	CL7	44	404	20	2/2/15/20	14/39/115/115	-
21	CL7	32	505	16	2/2/15/20	18/39/115/115	-
25	SQD	23	424	-	-	7/45/65/69	0/1/1/1
25	SQD	12	521	-	-	7/45/65/69	0/1/1/1
21	CL7	22	512	16	2/2/15/20	18/39/115/115	-
21	CL7	22	514	-	2/2/11/20	9/15/91/115	-
24	LMG	41	401	-	-	5/46/66/70	0/1/1/1
21	CL7	42	503	-	2/2/15/20	17/39/115/115	-
21	CL7	23	403	19	2/2/13/20	12/31/107/115	-
21	CL7	3B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	1C	517	3	2/2/10/20	5/10/86/115	-
21	CL7	4B	610	2	2/2/15/20	14/39/115/115	-
21	CL7	31	417	18	2/2/13/20	9/27/103/115	-
25	SQD	22	521	-	-	7/45/65/69	0/1/1/1
21	CL7	31	402	18	2/2/14/20	16/33/109/115	-
32	ZEX	13	520	-	-	10/29/67/67	0/2/2/2
21	CL7	4C	513	3	2/2/11/20	8/15/91/115	-
26	LHG	2B	624	-	-	3/49/49/53	-
21	CL7	13	504	-	2/2/15/20	16/39/115/115	-
21	CL7	1B	602	2	2/2/14/20	9/33/109/115	-
21	CL7	11	404	-	2/2/15/20	15/39/115/115	-
21	CL7	13	514	-	2/2/11/20	5/15/91/115	-
21	CL7	14	412	20	2/2/15/20	17/39/115/115	-
21	CL7	2C	503	3	2/2/15/20	19/39/115/115	-
27	DGD	4B	625	-	-	7/51/91/95	0/2/2/2
23	8CT	1B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	24	413	20	2/2/14/20	7/33/109/115	-
21	CL7	33	510	-	2/2/15/20	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	34	407	-	2/2/10/20	3/10/86/115	-
21	CL7	3B	622	2	2/2/11/20	8/15/91/115	-
25	SQD	13	521	-	-	3/41/61/69	0/1/1/1
25	SQD	1B	620	-	-	5/49/69/69	0/1/1/1
25	SQD	1A	406	-	-	3/29/49/69	0/1/1/1
26	LHG	1B	625	-	-	6/53/53/53	-
21	CL7	23	406	19	2/2/15/20	14/39/115/115	-
26	LHG	2A	408	-	-	5/50/50/53	-
21	CL7	24	417	20	2/2/10/20	6/12/88/115	-
32	ZEX	24	403	-	-	10/29/67/67	0/2/2/2
21	CL7	14	413	20	2/2/14/20	7/33/109/115	-
21	CL7	42	515	-	2/2/11/20	8/15/91/115	-
23	8CT	4B	620	-	-	4/29/63/63	0/2/2/2
21	CL7	22	506	16	2/2/15/20	14/39/115/115	-
21	CL7	1C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	14	411	20	2/2/15/20	14/39/115/115	-
21	CL7	41	403	-	2/2/14/20	11/33/109/115	-
32	ZEX	41	421	-	-	14/29/67/67	0/2/2/2
21	CL7	43	404	-	2/2/15/20	20/39/115/115	-
21	CL7	11	406	18	2/2/14/20	13/36/112/115	-
21	CL7	4B	603	2	2/2/14/20	9/33/109/115	-
25	SQD	42	523	-	-	0/36/56/69	0/1/1/1
21	CL7	3A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	22	518	16	2/2/15/20	12/39/115/115	-
27	DGD	1B	624	-	-	7/51/91/95	0/2/2/2
26	LHG	1A	408	-	-	5/50/50/53	-
21	CL7	44	410	20	2/2/11/20	9/15/91/115	-
23	8CT	1B	626	-	-	10/29/63/63	0/2/2/2
31	HEM	3F	101	-	-	8/14/54/54	-
25	SQD	12	523	-	-	0/36/56/69	0/1/1/1
21	CL7	41	408	-	2/2/15/20	16/39/115/115	-
21	CL7	42	502	16	2/2/15/20	17/39/115/115	-
21	CL7	23	414	-	2/2/11/20	9/15/91/115	-
21	CL7	1A	401	1	2/2/15/20	18/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	1C	507	-	2/2/15/20	17/39/115/115	-
21	CL7	24	412	20	2/2/15/20	17/39/115/115	-
21	CL7	4B	614	2	2/2/13/20	5/27/103/115	-
32	ZEX	22	522	-	-	6/29/67/67	0/2/2/2
31	HEM	4F	101	-	-	8/14/54/54	-
23	8CT	3B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	4C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	12	502	16	2/2/15/20	17/39/115/115	-
21	CL7	3C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	2D	404	4	2/2/13/20	13/31/107/115	-
21	CL7	13	518	19	2/2/11/20	7/15/91/115	-
21	CL7	2D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	11	410	-	2/2/15/20	17/39/115/115	-
25	SQD	2A	406	-	-	3/29/49/69	0/1/1/1
21	CL7	21	415	-	2/2/10/20	7/10/86/115	-
21	CL7	22	517	16	2/2/15/20	21/39/115/115	-
21	CL7	12	509	-	2/2/15/20	16/39/115/115	-
21	CL7	4B	604	2	2/2/15/20	12/39/115/115	-
30	PL9	3D	407	-	-	9/53/73/73	0/1/1/1
26	LHG	2D	409	-	-	7/53/53/53	-
21	CL7	12	511	16	2/2/14/20	16/33/109/115	-
21	CL7	1B	614	2	2/2/14/20	14/33/109/115	-
23	8CT	2A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	4B	611	-	2/2/15/20	11/39/115/115	-
21	CL7	41	418	18	2/2/15/20	22/39/115/115	-
24	LMG	2B	622	-	-	7/46/66/70	0/1/1/1
21	CL7	1B	607	-	2/2/14/20	11/33/109/115	-
21	CL7	3B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	4A	407	-	2/2/15/20	16/39/115/115	-
26	LHG	43	425	-	-	3/40/40/53	-
21	CL7	41	402	18	2/2/14/20	16/33/109/115	-
25	SQD	4B	621	-	-	5/49/69/69	0/1/1/1
21	CL7	12	504	-	2/2/11/20	6/15/91/115	-
21	CL7	23	417	19	2/2/13/20	16/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2C	505	3	2/2/15/20	16/39/115/115	-
21	CL7	31	407	18	2/2/10/20	4/10/86/115	-
21	CL7	44	416	20	2/2/10/20	7/10/86/115	-
21	CL7	2C	510	3	2/2/15/20	22/39/115/115	-
21	CL7	22	511	16	2/2/14/20	16/33/109/115	-
21	CL7	1B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	1C	512	3	2/2/10/20	4/10/86/115	-
21	CL7	3C	506	3	2/2/14/20	15/33/109/115	-
21	CL7	11	418	18	2/2/15/20	22/39/115/115	-
30	PL9	2D	407	-	-	9/53/73/73	0/1/1/1
21	CL7	12	503	-	2/2/15/20	17/39/115/115	-
21	CL7	11	402	18	2/2/14/20	16/33/109/115	-
25	SQD	11	423	-	-	3/27/47/69	0/1/1/1
21	CL7	33	511	19	2/2/15/20	19/39/115/115	-
21	CL7	44	405	-	2/2/15/20	18/39/115/115	-
21	CL7	11	411	-	2/2/11/20	7/15/91/115	-
21	CL7	2B	603	2	2/2/14/20	9/33/109/115	-
21	CL7	43	419	19	2/2/11/20	7/15/91/115	-
21	CL7	43	405	-	2/2/15/20	16/39/115/115	-
21	CL7	42	505	16	2/2/15/20	18/39/115/115	-
21	CL7	42	510	16	2/2/15/20	20/39/115/115	-
23	8CT	2B	618	-	-	7/29/63/63	0/2/2/2
26	LHG	4D	409	-	-	7/53/53/53	-
21	CL7	24	406	20	2/2/15/20	24/39/115/115	-
21	CL7	2C	509	3	2/2/15/20	20/39/115/115	-
21	CL7	1C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	32	509	-	2/2/15/20	16/39/115/115	-
21	CL7	4B	613	2	2/2/15/20	17/39/115/115	-
21	CL7	2C	512	3	2/2/10/20	4/10/86/115	-
25	SQD	31	423	-	-	3/27/47/69	0/1/1/1
32	ZEX	11	422	-	-	6/29/67/67	0/2/2/2
23	8CT	1B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	1A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	41	411	-	2/2/11/20	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	33	507	-	2/2/15/20	15/39/115/115	-
26	LHG	4B	624	-	-	3/49/49/53	-
21	CL7	4B	615	2	2/2/14/20	14/33/109/115	-
21	CL7	41	417	18	2/2/13/20	9/27/103/115	-
22	PHO	2A	402	-	-	3/37/103/103	0/5/6/6
24	LMG	4A	405	-	2/2/8/8	8/45/65/70	0/1/1/1
21	CL7	22	504	-	2/2/11/20	6/15/91/115	-
26	LHG	3B	625	-	-	6/53/53/53	-
21	CL7	11	408	-	2/2/15/20	16/39/115/115	-
25	SQD	13	523	-	-	7/45/65/69	0/1/1/1
23	8CT	1A	404	-	-	5/29/63/63	0/2/2/2
23	8CT	3B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	32	511	16	2/2/14/20	16/33/109/115	-
21	CL7	43	416	-	2/2/10/20	0/10/86/115	-
21	CL7	11	420	18	2/2/11/20	6/15/91/115	-
26	LHG	33	524	-	-	3/40/40/53	-
32	ZEX	13	519	-	-	10/29/67/67	0/2/2/2
21	CL7	2A	407	-	2/2/15/20	16/39/115/115	-
21	CL7	23	410	19	2/2/15/20	17/39/115/115	-
32	ZEX	14	420	-	-	12/29/67/67	0/2/2/2
21	CL7	12	507	-	2/2/15/20	20/39/115/115	-
21	CL7	2C	501	3	2/2/15/20	20/39/115/115	-
21	CL7	1B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	21	412	18	2/2/11/20	10/15/91/115	-

All (8119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2B	601	8CT	C02-C03	14.85	1.60	1.34
23	1B	626	8CT	C02-C03	14.83	1.60	1.34
23	4B	619	8CT	C02-C03	14.82	1.60	1.34
23	4B	601	8CT	C02-C03	14.80	1.60	1.34
23	3B	626	8CT	C02-C03	14.80	1.60	1.34
23	3B	618	8CT	C02-C03	14.79	1.60	1.34
23	1B	618	8CT	C02-C03	14.76	1.60	1.34
23	2B	619	8CT	C02-C03	14.73	1.60	1.34
23	2C	518	8CT	C02-C03	14.63	1.59	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4C	518	8CT	C02-C03	14.60	1.59	1.34
23	3C	518	8CT	C02-C03	14.58	1.59	1.34
23	1C	518	8CT	C02-C03	14.58	1.59	1.34
23	3A	404	8CT	C02-C03	14.56	1.59	1.34
23	1A	404	8CT	C02-C03	14.54	1.59	1.34
23	2C	514	8CT	C02-C03	14.54	1.59	1.34
23	3C	514	8CT	C02-C03	14.51	1.59	1.34
23	3K	101	8CT	C02-C03	14.51	1.59	1.34
23	2A	404	8CT	C02-C03	14.51	1.59	1.34
23	1C	514	8CT	C02-C03	14.51	1.59	1.34
23	4C	514	8CT	C02-C03	14.51	1.59	1.34
23	1K	101	8CT	C02-C03	14.50	1.59	1.34
23	4K	101	8CT	C02-C03	14.50	1.59	1.34
23	4A	404	8CT	C02-C03	14.49	1.59	1.34
23	2K	101	8CT	C02-C03	14.43	1.59	1.34
23	24	402	8CT	C02-C03	14.43	1.59	1.34
23	34	402	8CT	C02-C03	14.43	1.59	1.34
23	14	402	8CT	C02-C03	14.42	1.59	1.34
23	44	402	8CT	C02-C03	14.42	1.59	1.34
23	2B	618	8CT	C02-C03	14.30	1.59	1.34
23	3B	617	8CT	C02-C03	14.27	1.59	1.34
23	2D	406	8CT	C02-C03	14.27	1.59	1.34
23	1B	617	8CT	C02-C03	14.27	1.59	1.34
23	4B	618	8CT	C02-C03	14.27	1.59	1.34
23	3B	619	8CT	C02-C03	14.27	1.59	1.34
23	1B	619	8CT	C02-C03	14.26	1.59	1.34
23	4B	620	8CT	C02-C03	14.26	1.59	1.34
23	4D	406	8CT	C02-C03	14.25	1.59	1.34
23	2B	620	8CT	C02-C03	14.23	1.59	1.34
23	1D	406	8CT	C02-C03	14.22	1.59	1.34
23	3D	406	8CT	C02-C03	14.19	1.59	1.34
23	1C	515	8CT	C02-C03	14.07	1.58	1.34
23	4C	515	8CT	C02-C03	14.07	1.58	1.34
23	3C	515	8CT	C02-C03	14.02	1.58	1.34
23	2C	515	8CT	C02-C03	14.02	1.58	1.34
23	1K	101	8CT	C32-C31	13.73	1.59	1.32
23	2K	101	8CT	C32-C31	13.72	1.59	1.32
23	3K	101	8CT	C32-C31	13.72	1.59	1.32
23	4K	101	8CT	C32-C31	13.70	1.59	1.32
23	2D	406	8CT	C32-C31	13.49	1.59	1.32
23	3D	406	8CT	C32-C31	13.48	1.59	1.32
23	2B	619	8CT	C32-C31	13.48	1.59	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1B	618	8CT	C32-C31	13.44	1.59	1.32
23	2A	404	8CT	C32-C31	13.43	1.59	1.32
23	1D	406	8CT	C32-C31	13.43	1.59	1.32
23	2C	518	8CT	C32-C31	13.43	1.59	1.32
23	3C	518	8CT	C32-C31	13.43	1.59	1.32
23	4B	619	8CT	C32-C31	13.42	1.59	1.32
23	4D	406	8CT	C32-C31	13.42	1.59	1.32
23	3B	618	8CT	C32-C31	13.41	1.59	1.32
23	1A	404	8CT	C32-C31	13.41	1.59	1.32
23	4A	404	8CT	C32-C31	13.41	1.59	1.32
23	1C	518	8CT	C32-C31	13.40	1.59	1.32
23	4C	518	8CT	C32-C31	13.40	1.59	1.32
23	3A	404	8CT	C32-C31	13.39	1.59	1.32
23	3C	514	8CT	C32-C31	13.35	1.59	1.32
23	2B	601	8CT	C32-C31	13.34	1.59	1.32
23	2C	514	8CT	C32-C31	13.33	1.58	1.32
23	3B	626	8CT	C32-C31	13.32	1.58	1.32
23	4B	601	8CT	C32-C31	13.32	1.58	1.32
23	2C	515	8CT	C32-C31	13.31	1.58	1.32
23	3C	515	8CT	C32-C31	13.31	1.58	1.32
23	4C	514	8CT	C32-C31	13.31	1.58	1.32
23	4B	618	8CT	C32-C31	13.31	1.58	1.32
23	4C	515	8CT	C32-C31	13.30	1.58	1.32
23	1B	626	8CT	C32-C31	13.30	1.58	1.32
23	1C	514	8CT	C32-C31	13.29	1.58	1.32
23	3B	617	8CT	C32-C31	13.29	1.58	1.32
23	1B	617	8CT	C32-C31	13.28	1.58	1.32
23	1C	515	8CT	C32-C31	13.27	1.58	1.32
23	2B	618	8CT	C32-C31	13.27	1.58	1.32
23	14	402	8CT	C32-C31	13.21	1.58	1.32
23	44	402	8CT	C32-C31	13.21	1.58	1.32
23	3B	619	8CT	C32-C31	13.20	1.58	1.32
23	1B	619	8CT	C32-C31	13.20	1.58	1.32
23	4B	620	8CT	C32-C31	13.20	1.58	1.32
23	34	402	8CT	C32-C31	13.20	1.58	1.32
23	2B	620	8CT	C32-C31	13.19	1.58	1.32
23	24	402	8CT	C32-C31	13.17	1.58	1.32
23	2B	618	8CT	C34-C35	-9.94	1.33	1.54
23	3B	617	8CT	C34-C35	-9.94	1.33	1.54
23	1B	617	8CT	C34-C35	-9.92	1.33	1.54
23	4B	618	8CT	C34-C35	-9.92	1.33	1.54
23	1C	515	8CT	C34-C35	-9.82	1.34	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2C	514	8CT	C34-C35	-9.79	1.34	1.54
23	3C	514	8CT	C34-C35	-9.79	1.34	1.54
23	2C	515	8CT	C34-C35	-9.79	1.34	1.54
23	3C	515	8CT	C34-C35	-9.79	1.34	1.54
23	4C	515	8CT	C34-C35	-9.79	1.34	1.54
23	4C	514	8CT	C34-C35	-9.77	1.34	1.54
23	1C	514	8CT	C34-C35	-9.74	1.34	1.54
23	1A	404	8CT	C34-C35	-9.54	1.34	1.54
23	4A	404	8CT	C34-C35	-9.54	1.34	1.54
23	3A	404	8CT	C34-C35	-9.53	1.34	1.54
23	2A	404	8CT	C34-C35	-9.52	1.34	1.54
23	3C	518	8CT	C34-C35	-9.40	1.34	1.54
23	3B	619	8CT	C34-C35	-9.37	1.34	1.54
23	1C	518	8CT	C34-C35	-9.37	1.34	1.54
23	4C	518	8CT	C34-C35	-9.37	1.34	1.54
23	2C	518	8CT	C34-C35	-9.35	1.34	1.54
23	1K	101	8CT	C34-C35	-9.35	1.34	1.54
23	2K	101	8CT	C34-C35	-9.34	1.34	1.54
23	3K	101	8CT	C34-C35	-9.34	1.35	1.54
23	4K	101	8CT	C34-C35	-9.34	1.35	1.54
23	4B	620	8CT	C34-C35	-9.32	1.35	1.54
23	1B	626	8CT	C34-C35	-9.32	1.35	1.54
23	2B	619	8CT	C34-C35	-9.32	1.35	1.54
23	2B	601	8CT	C34-C35	-9.31	1.35	1.54
23	3B	626	8CT	C34-C35	-9.31	1.35	1.54
23	2B	620	8CT	C34-C35	-9.31	1.35	1.54
23	1B	619	8CT	C34-C35	-9.30	1.35	1.54
23	4B	601	8CT	C34-C35	-9.30	1.35	1.54
23	1B	618	8CT	C34-C35	-9.24	1.35	1.54
23	4B	619	8CT	C34-C35	-9.24	1.35	1.54
23	3B	618	8CT	C34-C35	-9.23	1.35	1.54
23	2D	406	8CT	C34-C35	-9.20	1.35	1.54
23	44	402	8CT	C34-C35	-9.20	1.35	1.54
23	24	402	8CT	C34-C35	-9.19	1.35	1.54
23	14	402	8CT	C34-C35	-9.19	1.35	1.54
23	1D	406	8CT	C34-C35	-9.19	1.35	1.54
23	4D	406	8CT	C34-C35	-9.19	1.35	1.54
23	3D	406	8CT	C34-C35	-9.18	1.35	1.54
23	34	402	8CT	C34-C35	-9.15	1.35	1.54
23	2C	515	8CT	C04-C03	-8.00	1.42	1.53
23	1C	515	8CT	C04-C03	-8.00	1.42	1.53
23	4C	515	8CT	C04-C03	-8.00	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3C	515	8CT	C04-C03	-7.99	1.42	1.53
23	4B	619	8CT	C04-C03	-7.99	1.42	1.53
23	2B	619	8CT	C04-C03	-7.96	1.42	1.53
23	1B	618	8CT	C04-C03	-7.95	1.42	1.53
23	3B	618	8CT	C04-C03	-7.93	1.42	1.53
23	14	402	8CT	C04-C03	-7.70	1.43	1.53
23	24	402	8CT	C04-C03	-7.69	1.43	1.53
23	34	402	8CT	C04-C03	-7.69	1.43	1.53
23	44	402	8CT	C04-C03	-7.67	1.43	1.53
23	4C	518	8CT	C04-C03	-7.65	1.43	1.53
23	4A	404	8CT	C04-C03	-7.65	1.43	1.53
23	1A	404	8CT	C04-C03	-7.64	1.43	1.53
23	3A	404	8CT	C04-C03	-7.63	1.43	1.53
23	1B	617	8CT	C04-C03	-7.61	1.43	1.53
23	4B	618	8CT	C04-C03	-7.61	1.43	1.53
23	2C	518	8CT	C04-C03	-7.61	1.43	1.53
23	2B	618	8CT	C04-C03	-7.61	1.43	1.53
23	3B	617	8CT	C04-C03	-7.61	1.43	1.53
23	3C	518	8CT	C04-C03	-7.60	1.43	1.53
23	2A	404	8CT	C04-C03	-7.60	1.43	1.53
23	1C	518	8CT	C04-C03	-7.60	1.43	1.53
23	1B	619	8CT	C04-C03	-7.55	1.43	1.53
23	3B	619	8CT	C04-C03	-7.52	1.43	1.53
23	3K	101	8CT	C04-C03	-7.49	1.43	1.53
23	2B	620	8CT	C04-C03	-7.49	1.43	1.53
23	4B	620	8CT	C04-C03	-7.48	1.43	1.53
23	4K	101	8CT	C04-C03	-7.47	1.43	1.53
23	2K	101	8CT	C04-C03	-7.43	1.43	1.53
23	1K	101	8CT	C04-C03	-7.41	1.43	1.53
23	2C	514	8CT	C04-C03	-7.29	1.43	1.53
23	3C	514	8CT	C04-C03	-7.27	1.43	1.53
23	4C	514	8CT	C04-C03	-7.23	1.43	1.53
23	1C	514	8CT	C04-C03	-7.22	1.43	1.53
23	3D	406	8CT	C04-C03	-7.02	1.44	1.53
23	1D	406	8CT	C04-C03	-7.00	1.44	1.53
23	4D	406	8CT	C04-C03	-7.00	1.44	1.53
23	2D	406	8CT	C04-C03	-6.99	1.44	1.53
23	4B	601	8CT	C04-C03	-6.84	1.44	1.53
23	1B	626	8CT	C04-C03	-6.83	1.44	1.53
23	2B	601	8CT	C04-C03	-6.81	1.44	1.53
23	24	402	8CT	C05-C06	-6.77	1.35	1.52
23	44	402	8CT	C05-C06	-6.77	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	34	402	8CT	C05-C06	-6.77	1.35	1.52
23	3B	626	8CT	C04-C03	-6.74	1.44	1.53
23	14	402	8CT	C05-C06	-6.72	1.36	1.52
23	4B	620	8CT	C05-C06	-6.59	1.36	1.52
23	2B	620	8CT	C05-C06	-6.58	1.36	1.52
23	3B	619	8CT	C05-C06	-6.57	1.36	1.52
23	1B	619	8CT	C05-C06	-6.56	1.36	1.52
23	2C	514	8CT	C05-C06	-6.54	1.36	1.52
23	3C	514	8CT	C05-C06	-6.54	1.36	1.52
23	4A	404	8CT	C05-C06	-6.53	1.36	1.52
23	2A	404	8CT	C05-C06	-6.52	1.36	1.52
23	1C	514	8CT	C05-C06	-6.51	1.36	1.52
23	2B	619	8CT	C05-C06	-6.51	1.36	1.52
23	4C	514	8CT	C05-C06	-6.51	1.36	1.52
23	1C	515	8CT	C05-C06	-6.51	1.36	1.52
23	4C	515	8CT	C05-C06	-6.51	1.36	1.52
23	2C	515	8CT	C05-C06	-6.51	1.36	1.52
23	3C	515	8CT	C05-C06	-6.50	1.36	1.52
23	1A	404	8CT	C05-C06	-6.50	1.36	1.52
23	4B	601	8CT	C05-C06	-6.50	1.36	1.52
23	3D	406	8CT	C05-C06	-6.48	1.36	1.52
23	3B	618	8CT	C05-C06	-6.48	1.36	1.52
23	1D	406	8CT	C05-C06	-6.48	1.36	1.52
23	3B	626	8CT	C05-C06	-6.47	1.36	1.52
23	1B	618	8CT	C05-C06	-6.47	1.36	1.52
23	3A	404	8CT	C05-C06	-6.47	1.36	1.52
23	4B	619	8CT	C05-C06	-6.47	1.36	1.52
23	1B	617	8CT	C05-C06	-6.47	1.36	1.52
23	1B	626	8CT	C05-C06	-6.46	1.36	1.52
23	4D	406	8CT	C05-C06	-6.46	1.36	1.52
23	2B	601	8CT	C05-C06	-6.45	1.36	1.52
23	2D	406	8CT	C05-C06	-6.45	1.36	1.52
23	2B	618	8CT	C05-C06	-6.45	1.36	1.52
23	4B	618	8CT	C05-C06	-6.44	1.36	1.52
23	1K	101	8CT	C05-C06	-6.42	1.36	1.52
23	4K	101	8CT	C05-C06	-6.42	1.36	1.52
23	3B	617	8CT	C05-C06	-6.41	1.36	1.52
23	3K	101	8CT	C05-C06	-6.41	1.36	1.52
23	2K	101	8CT	C05-C06	-6.39	1.36	1.52
23	1C	518	8CT	C05-C06	-6.29	1.37	1.52
23	2C	518	8CT	C05-C06	-6.29	1.37	1.52
23	3C	518	8CT	C05-C06	-6.29	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4C	518	8CT	C05-C06	-6.27	1.37	1.52
23	3K	101	8CT	C15-C16	5.96	1.58	1.45
23	4K	101	8CT	C15-C16	5.96	1.58	1.45
23	2K	101	8CT	C15-C16	5.93	1.58	1.45
23	1K	101	8CT	C15-C16	5.93	1.58	1.45
23	2B	601	8CT	C15-C16	5.85	1.58	1.45
23	3B	626	8CT	C15-C16	5.85	1.58	1.45
23	1B	626	8CT	C15-C16	5.85	1.58	1.45
23	2B	618	8CT	C15-C16	5.85	1.58	1.45
23	4B	618	8CT	C15-C16	5.83	1.58	1.45
23	4B	601	8CT	C15-C16	5.82	1.58	1.45
23	3B	617	8CT	C15-C16	5.82	1.58	1.45
23	1B	617	8CT	C15-C16	5.79	1.58	1.45
23	2C	515	8CT	C15-C16	5.71	1.58	1.45
23	1C	515	8CT	C15-C16	5.69	1.58	1.45
23	4C	515	8CT	C15-C16	5.69	1.58	1.45
23	3C	515	8CT	C15-C16	5.68	1.58	1.45
23	3C	514	8CT	C15-C16	5.66	1.58	1.45
23	4C	514	8CT	C15-C16	5.64	1.58	1.45
23	4C	518	8CT	C15-C16	5.63	1.58	1.45
23	2C	514	8CT	C15-C16	5.63	1.58	1.45
23	2C	518	8CT	C15-C16	5.62	1.58	1.45
23	3C	518	8CT	C15-C16	5.62	1.58	1.45
23	2B	620	8CT	C15-C16	5.61	1.58	1.45
23	3B	618	8CT	C15-C16	5.61	1.58	1.45
23	1C	514	8CT	C15-C16	5.61	1.58	1.45
23	1B	618	8CT	C15-C16	5.60	1.58	1.45
23	4B	619	8CT	C15-C16	5.60	1.58	1.45
23	1D	406	8CT	C15-C16	5.60	1.58	1.45
23	3B	619	8CT	C15-C16	5.60	1.58	1.45
23	2B	619	8CT	C15-C16	5.60	1.58	1.45
23	1C	518	8CT	C15-C16	5.58	1.57	1.45
23	4D	406	8CT	C15-C16	5.57	1.57	1.45
23	2D	406	8CT	C15-C16	5.57	1.57	1.45
23	3D	406	8CT	C15-C16	5.57	1.57	1.45
23	1B	619	8CT	C15-C16	5.55	1.57	1.45
23	4B	620	8CT	C15-C16	5.54	1.57	1.45
23	2B	619	8CT	C11-C12	5.46	1.57	1.45
23	1B	618	8CT	C11-C12	5.45	1.57	1.45
23	4B	619	8CT	C11-C12	5.45	1.57	1.45
23	2A	404	8CT	C15-C16	5.43	1.57	1.45
23	3B	618	8CT	C11-C12	5.43	1.57	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4A	404	8CT	C15-C16	5.42	1.57	1.45
23	1A	404	8CT	C15-C16	5.41	1.57	1.45
23	14	402	8CT	C34-C33	5.37	1.65	1.52
23	44	402	8CT	C34-C33	5.37	1.65	1.52
23	24	402	8CT	C34-C33	5.37	1.65	1.52
23	3A	404	8CT	C15-C16	5.37	1.57	1.45
23	34	402	8CT	C34-C33	5.34	1.65	1.52
23	14	402	8CT	C15-C16	5.32	1.57	1.45
23	4B	601	8CT	C05-C04	5.31	1.66	1.54
23	24	402	8CT	C15-C16	5.31	1.57	1.45
23	44	402	8CT	C15-C16	5.30	1.57	1.45
23	2B	601	8CT	C05-C04	5.29	1.66	1.54
23	34	402	8CT	C15-C16	5.29	1.57	1.45
23	2K	101	8CT	C11-C12	5.28	1.57	1.45
23	3K	101	8CT	C11-C12	5.28	1.57	1.45
23	1B	626	8CT	C05-C04	5.28	1.66	1.54
23	3B	626	8CT	C05-C04	5.27	1.66	1.54
21	2B	607	CL7	CHD-C4C	5.27	1.48	1.38
21	1B	606	CL7	CHD-C4C	5.26	1.48	1.38
23	1K	101	8CT	C11-C12	5.26	1.57	1.45
23	4K	101	8CT	C11-C12	5.26	1.57	1.45
23	4B	601	8CT	C35-C30	5.26	1.71	1.56
30	2D	407	PL9	C3-C4	-5.25	1.40	1.49
30	3D	407	PL9	C3-C4	-5.25	1.40	1.49
30	1D	407	PL9	C3-C4	-5.25	1.40	1.49
30	4D	407	PL9	C3-C4	-5.25	1.40	1.49
21	31	414	CL7	CHD-C4C	5.24	1.48	1.38
23	1B	626	8CT	C35-C30	5.24	1.71	1.56
21	3B	606	CL7	CHD-C4C	5.24	1.48	1.38
23	2B	601	8CT	C35-C30	5.24	1.71	1.56
23	3B	626	8CT	C35-C30	5.24	1.71	1.56
21	4B	607	CL7	CHD-C4C	5.22	1.48	1.38
21	11	414	CL7	CHD-C4C	5.21	1.48	1.38
21	41	414	CL7	CHD-C4C	5.21	1.48	1.38
23	2B	601	8CT	C11-C12	5.19	1.57	1.45
23	3B	626	8CT	C11-C12	5.19	1.57	1.45
23	3B	618	8CT	C34-C33	5.19	1.64	1.52
21	21	414	CL7	CHD-C4C	5.18	1.48	1.38
23	2B	619	8CT	C34-C33	5.18	1.64	1.52
23	4B	619	8CT	C34-C33	5.17	1.64	1.52
21	2D	402	CL7	CHD-C4C	5.17	1.48	1.38
21	3D	402	CL7	CHD-C4C	5.17	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	101	8CT	C05-C04	5.17	1.66	1.54
23	3K	101	8CT	C05-C04	5.17	1.66	1.54
23	1B	626	8CT	C11-C12	5.16	1.57	1.45
23	3B	619	8CT	C34-C33	5.16	1.64	1.52
23	2B	620	8CT	C34-C33	5.16	1.64	1.52
23	1B	618	8CT	C34-C33	5.16	1.64	1.52
21	1A	401	CL7	CHC-C1C	5.16	1.48	1.38
23	1B	619	8CT	C34-C33	5.16	1.64	1.52
23	4B	620	8CT	C34-C33	5.16	1.64	1.52
23	3D	406	8CT	C34-C33	5.15	1.64	1.52
23	1D	406	8CT	C34-C33	5.15	1.64	1.52
23	4B	601	8CT	C11-C12	5.15	1.57	1.45
21	1D	402	CL7	CHD-C4C	5.14	1.48	1.38
21	4D	402	CL7	CHD-C4C	5.14	1.48	1.38
23	1K	101	8CT	C05-C04	5.14	1.66	1.54
23	4K	101	8CT	C05-C04	5.14	1.66	1.54
23	2D	406	8CT	C34-C33	5.13	1.64	1.52
23	4D	406	8CT	C34-C33	5.12	1.64	1.52
21	4A	401	CL7	CHC-C1C	5.12	1.48	1.38
21	42	513	CL7	CHD-C4C	5.12	1.48	1.38
21	22	513	CL7	CHD-C4C	5.11	1.48	1.38
21	32	513	CL7	CHD-C4C	5.11	1.48	1.38
21	2A	401	CL7	CHC-C1C	5.11	1.48	1.38
21	3A	401	CL7	CHC-C1C	5.11	1.48	1.38
21	11	416	CL7	CHD-C4C	5.10	1.48	1.38
21	4B	623	CL7	CHD-C4C	5.10	1.48	1.38
21	12	513	CL7	CHD-C4C	5.09	1.48	1.38
21	31	416	CL7	CHD-C4C	5.09	1.48	1.38
21	3B	622	CL7	CHD-C4C	5.07	1.48	1.38
21	21	416	CL7	CHD-C4C	5.06	1.48	1.38
21	21	404	CL7	CHD-C4C	5.06	1.48	1.38
21	2B	623	CL7	CHD-C4C	5.06	1.48	1.38
21	31	404	CL7	CHD-C4C	5.05	1.48	1.38
21	41	416	CL7	CHD-C4C	5.05	1.48	1.38
21	12	515	CL7	CHD-C4C	5.05	1.48	1.38
21	42	514	CL7	CHD-C4C	5.05	1.48	1.38
21	34	411	CL7	CHD-C4C	5.05	1.48	1.38
21	13	506	CL7	CHD-C4C	5.04	1.48	1.38
21	13	517	CL7	CHD-C4C	5.04	1.48	1.38
23	4D	406	8CT	C05-C04	5.04	1.65	1.54
21	23	418	CL7	CHD-C4C	5.03	1.48	1.38
21	13	518	CL7	CHD-C4C	5.03	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	43	419	CL7	CHD-C4C	5.03	1.48	1.38
23	1K	101	8CT	C35-C30	5.03	1.70	1.56
23	4K	101	8CT	C35-C30	5.03	1.70	1.56
23	3D	406	8CT	C05-C04	5.03	1.65	1.54
23	1C	518	8CT	C11-C12	5.03	1.56	1.45
21	31	410	CL7	CHD-C4C	5.02	1.48	1.38
23	2C	518	8CT	C11-C12	5.02	1.56	1.45
23	3C	518	8CT	C11-C12	5.02	1.56	1.45
21	1B	622	CL7	CHD-C4C	5.02	1.48	1.38
21	23	407	CL7	CHD-C4C	5.02	1.48	1.38
23	3A	404	8CT	C34-C33	5.02	1.64	1.52
23	1D	406	8CT	C05-C04	5.02	1.65	1.54
23	2A	404	8CT	C34-C33	5.02	1.64	1.52
21	33	518	CL7	CHD-C4C	5.02	1.48	1.38
23	1B	619	8CT	C05-C04	5.02	1.65	1.54
23	4A	404	8CT	C34-C33	5.02	1.64	1.52
23	2D	406	8CT	C05-C04	5.01	1.65	1.54
21	43	407	CL7	CHD-C4C	5.01	1.48	1.38
21	14	417	CL7	CHB-C1B	5.01	1.50	1.39
23	1A	404	8CT	C34-C33	5.01	1.64	1.52
23	4K	101	8CT	C14-C13	5.01	1.59	1.43
23	4B	620	8CT	C05-C04	5.01	1.65	1.54
23	2K	101	8CT	C35-C30	5.01	1.70	1.56
23	3K	101	8CT	C35-C30	5.01	1.70	1.56
21	33	516	CL7	CHD-C4C	5.00	1.48	1.38
21	14	411	CL7	CHD-C4C	5.00	1.48	1.38
21	21	419	CL7	CHC-C1C	5.00	1.48	1.38
21	43	419	CL7	CHC-C1C	5.00	1.48	1.38
23	3B	619	8CT	C05-C04	5.00	1.65	1.54
21	23	419	CL7	CHD-C4C	5.00	1.48	1.38
21	33	506	CL7	CHD-C4C	5.00	1.48	1.38
21	2B	623	CL7	CHC-C1C	5.00	1.48	1.38
21	3B	622	CL7	CHC-C1C	5.00	1.48	1.38
21	24	417	CL7	CHB-C1B	5.00	1.50	1.39
21	34	417	CL7	CHB-C1B	5.00	1.50	1.39
21	32	515	CL7	CHD-C4C	5.00	1.48	1.38
21	11	404	CL7	CHD-C4C	5.00	1.48	1.38
21	23	417	CL7	CHD-C4C	5.00	1.48	1.38
21	41	404	CL7	CHD-C4C	5.00	1.48	1.38
23	1B	617	8CT	C05-C04	5.00	1.65	1.54
23	4B	618	8CT	C05-C04	5.00	1.65	1.54
21	22	515	CL7	CHD-C4C	5.00	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	21	408	CL7	CHD-C4C	5.00	1.48	1.38
21	31	408	CL7	CHD-C4C	5.00	1.48	1.38
21	22	514	CL7	CHD-C4C	4.99	1.48	1.38
21	32	514	CL7	CHD-C4C	4.99	1.48	1.38
21	4B	623	CL7	CHC-C1C	4.99	1.48	1.38
21	21	411	CL7	CHD-C4C	4.99	1.48	1.38
21	1B	601	CL7	CHD-C4C	4.99	1.48	1.38
21	11	411	CL7	CHD-C4C	4.99	1.48	1.38
21	33	517	CL7	CHD-C4C	4.99	1.48	1.38
23	4C	518	8CT	C11-C12	4.99	1.56	1.45
21	21	419	CL7	CHD-C4C	4.99	1.48	1.38
21	44	411	CL7	CHD-C4C	4.99	1.48	1.38
21	1B	609	CL7	CHD-C4C	4.99	1.48	1.38
21	24	411	CL7	CHD-C4C	4.99	1.48	1.38
21	42	515	CL7	CHD-C4C	4.99	1.48	1.38
21	13	516	CL7	CHD-C4C	4.99	1.48	1.38
21	43	417	CL7	CHD-C4C	4.99	1.48	1.38
21	4C	517	CL7	CHD-C4C	4.98	1.48	1.38
21	41	410	CL7	CHD-C4C	4.98	1.48	1.38
21	44	417	CL7	CHB-C1B	4.98	1.50	1.39
21	1C	517	CL7	CHD-C4C	4.98	1.48	1.38
21	12	514	CL7	CHD-C4C	4.98	1.48	1.38
23	2B	618	8CT	C05-C04	4.98	1.65	1.54
23	3B	617	8CT	C05-C04	4.98	1.65	1.54
23	2K	101	8CT	C14-C13	4.98	1.58	1.43
21	21	417	CL7	CHD-C4C	4.98	1.48	1.38
23	3K	101	8CT	C14-C13	4.98	1.58	1.43
21	13	502	CL7	CHD-C4C	4.98	1.48	1.38
21	2C	517	CL7	CHD-C4C	4.97	1.48	1.38
21	3C	517	CL7	CHD-C4C	4.97	1.48	1.38
21	2B	610	CL7	CHD-C4C	4.97	1.48	1.38
21	3B	609	CL7	CHD-C4C	4.97	1.48	1.38
23	2B	620	8CT	C05-C04	4.97	1.65	1.54
21	21	420	CL7	CHC-C1C	4.97	1.48	1.38
21	11	419	CL7	CHD-C4C	4.97	1.48	1.38
21	41	419	CL7	CHD-C4C	4.97	1.48	1.38
21	11	408	CL7	CHD-C4C	4.97	1.48	1.38
21	23	419	CL7	CHC-C1C	4.97	1.48	1.38
21	33	518	CL7	CHC-C1C	4.97	1.48	1.38
21	41	408	CL7	CHD-C4C	4.97	1.48	1.38
21	1A	401	CL7	CHD-C4C	4.97	1.48	1.38
21	41	419	CL7	CHC-C1C	4.96	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	43	418	CL7	CHD-C4C	4.96	1.48	1.38
23	2B	601	8CT	C34-C33	4.96	1.64	1.52
21	43	403	CL7	CHD-C4C	4.96	1.48	1.38
21	1B	622	CL7	CHC-C1C	4.96	1.48	1.38
23	1K	101	8CT	C14-C13	4.96	1.58	1.43
21	2B	602	CL7	CHD-C4C	4.96	1.48	1.38
21	3B	601	CL7	CHD-C4C	4.96	1.48	1.38
21	4B	610	CL7	CHD-C4C	4.96	1.48	1.38
21	11	420	CL7	CHC-C1C	4.96	1.48	1.38
21	3A	401	CL7	CHD-C4C	4.96	1.48	1.38
21	41	420	CL7	CHC-C1C	4.96	1.48	1.38
21	4B	602	CL7	CHD-C4C	4.96	1.48	1.38
21	41	411	CL7	CHD-C4C	4.96	1.48	1.38
21	13	518	CL7	CHC-C1C	4.96	1.48	1.38
21	11	415	CL7	CHC-C1C	4.95	1.48	1.38
21	41	415	CL7	CHC-C1C	4.95	1.48	1.38
21	31	411	CL7	CHD-C4C	4.95	1.48	1.38
21	21	415	CL7	CHC-C1C	4.95	1.48	1.38
21	12	518	CL7	CHD-C4C	4.95	1.48	1.38
21	31	419	CL7	CHD-C4C	4.95	1.48	1.38
21	2A	401	CL7	CHD-C4C	4.95	1.48	1.38
21	11	405	CL7	CHD-C4C	4.95	1.48	1.38
21	31	419	CL7	CHC-C1C	4.95	1.48	1.38
21	11	415	CL7	CHD-C4C	4.95	1.48	1.38
23	3B	626	8CT	C34-C33	4.95	1.64	1.52
21	24	412	CL7	CHD-C4C	4.95	1.48	1.38
21	11	419	CL7	CHC-C1C	4.95	1.48	1.38
21	14	412	CL7	CHD-C4C	4.95	1.48	1.38
23	4C	518	8CT	C05-C04	4.94	1.65	1.54
21	21	410	CL7	CHD-C4C	4.94	1.48	1.38
23	1C	518	8CT	C34-C33	4.94	1.64	1.52
23	4C	518	8CT	C34-C33	4.94	1.64	1.52
21	3C	505	CL7	CHD-C4C	4.94	1.48	1.38
21	22	518	CL7	CHD-C4C	4.94	1.48	1.38
21	3C	510	CL7	CHD-C4C	4.94	1.48	1.38
21	32	518	CL7	CHD-C4C	4.94	1.48	1.38
21	31	415	CL7	CHC-C1C	4.94	1.48	1.38
21	2C	511	CL7	CHC-C1C	4.94	1.48	1.38
21	31	415	CL7	CHD-C4C	4.93	1.48	1.38
21	31	416	CL7	CHC-C1C	4.93	1.48	1.38
23	4B	601	8CT	C34-C33	4.93	1.64	1.52
21	32	504	CL7	CHD-C4C	4.93	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	420	CL7	CHC-C1C	4.93	1.48	1.38
21	11	410	CL7	CHD-C4C	4.93	1.48	1.38
21	4A	401	CL7	CHD-C4C	4.93	1.48	1.38
21	44	408	CL7	CHD-C4C	4.93	1.48	1.38
23	2C	518	8CT	C34-C33	4.93	1.64	1.52
21	34	408	CL7	CHD-C4C	4.93	1.48	1.38
21	42	518	CL7	CHD-C4C	4.93	1.48	1.38
21	23	403	CL7	CHD-C4C	4.93	1.48	1.38
23	3C	518	8CT	C34-C33	4.93	1.64	1.52
23	2K	101	8CT	C28-C26	4.93	1.56	1.45
21	21	415	CL7	CHD-C4C	4.92	1.48	1.38
21	21	405	CL7	CHD-C4C	4.92	1.48	1.38
23	1K	101	8CT	C28-C26	4.92	1.56	1.45
21	41	417	CL7	CHD-C4C	4.92	1.47	1.38
21	1C	511	CL7	CHC-C1C	4.92	1.47	1.38
21	2A	407	CL7	CHD-C4C	4.92	1.47	1.38
21	11	416	CL7	CHC-C1C	4.92	1.47	1.38
21	31	417	CL7	CHD-C4C	4.92	1.47	1.38
21	41	416	CL7	CHC-C1C	4.92	1.47	1.38
23	1B	626	8CT	C34-C33	4.92	1.64	1.52
21	2B	608	CL7	CHD-C4C	4.92	1.47	1.38
21	3B	607	CL7	CHD-C4C	4.92	1.47	1.38
21	24	416	CL7	CHC-C1C	4.92	1.47	1.38
21	34	416	CL7	CHC-C1C	4.92	1.47	1.38
21	22	504	CL7	CHD-C4C	4.91	1.47	1.38
21	1C	510	CL7	CHD-C4C	4.91	1.47	1.38
21	33	502	CL7	CHD-C4C	4.91	1.47	1.38
23	2C	518	8CT	C05-C04	4.91	1.65	1.54
23	3C	518	8CT	C05-C04	4.91	1.65	1.54
21	41	415	CL7	CHD-C4C	4.91	1.47	1.38
21	41	417	CL7	CHC-C1C	4.91	1.47	1.38
21	41	405	CL7	CHD-C4C	4.91	1.47	1.38
21	4C	510	CL7	CHD-C4C	4.90	1.47	1.38
21	11	417	CL7	CHD-C4C	4.90	1.47	1.38
21	14	408	CL7	CHD-C4C	4.90	1.47	1.38
21	23	402	CL7	CHD-C4C	4.90	1.47	1.38
21	33	501	CL7	CHD-C4C	4.90	1.47	1.38
23	14	402	8CT	C05-C04	4.90	1.65	1.54
21	1C	504	CL7	CHD-C4C	4.90	1.47	1.38
21	12	504	CL7	CHD-C4C	4.90	1.47	1.38
21	2C	505	CL7	CHD-C4C	4.90	1.47	1.38
21	21	417	CL7	CHC-C1C	4.90	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3K	101	8CT	C28-C26	4.90	1.56	1.45
21	2C	510	CL7	CHD-C4C	4.90	1.47	1.38
21	2C	513	CL7	CHD-C4C	4.90	1.47	1.38
21	24	409	CL7	CHD-C4C	4.90	1.47	1.38
21	34	409	CL7	CHD-C4C	4.90	1.47	1.38
21	11	414	CL7	CHC-C1C	4.90	1.47	1.38
21	41	414	CL7	CHC-C1C	4.90	1.47	1.38
23	2B	619	8CT	C05-C04	4.89	1.65	1.54
21	1B	607	CL7	CHD-C4C	4.89	1.47	1.38
21	4B	608	CL7	CHD-C4C	4.89	1.47	1.38
21	1C	505	CL7	CHD-C4C	4.89	1.47	1.38
21	4C	505	CL7	CHD-C4C	4.89	1.47	1.38
23	4A	404	8CT	C05-C04	4.89	1.65	1.54
21	21	404	CL7	CHC-C1C	4.89	1.47	1.38
21	41	404	CL7	CHC-C1C	4.89	1.47	1.38
21	44	412	CL7	CHD-C4C	4.89	1.47	1.38
21	34	412	CL7	CHD-C4C	4.89	1.47	1.38
21	13	501	CL7	CHD-C4C	4.89	1.47	1.38
21	43	402	CL7	CHD-C4C	4.89	1.47	1.38
23	2A	404	8CT	C05-C04	4.89	1.65	1.54
23	34	402	8CT	C05-C04	4.89	1.65	1.54
21	14	416	CL7	CHC-C1C	4.89	1.47	1.38
21	3A	407	CL7	CHD-C4C	4.89	1.47	1.38
23	1C	518	8CT	C05-C04	4.88	1.65	1.54
21	31	405	CL7	CHD-C4C	4.88	1.47	1.38
21	24	408	CL7	CHD-C4C	4.88	1.47	1.38
21	11	404	CL7	CHC-C1C	4.88	1.47	1.38
21	4C	504	CL7	CHC-C1C	4.88	1.47	1.38
21	4C	511	CL7	CHC-C1C	4.88	1.47	1.38
21	44	416	CL7	CHC-C1C	4.88	1.47	1.38
21	33	514	CL7	CHD-C4C	4.88	1.47	1.38
23	24	402	8CT	C05-C04	4.88	1.65	1.54
21	43	414	CL7	CHD-C4C	4.88	1.47	1.38
21	1C	506	CL7	CHD-C4C	4.88	1.47	1.38
21	4C	506	CL7	CHD-C4C	4.88	1.47	1.38
21	4C	513	CL7	CHD-C4C	4.87	1.47	1.38
21	42	504	CL7	CHD-C4C	4.87	1.47	1.38
23	4B	601	8CT	C14-C13	4.87	1.58	1.43
23	3B	618	8CT	C05-C04	4.87	1.65	1.54
23	4K	101	8CT	C28-C26	4.87	1.56	1.45
21	1A	407	CL7	CHD-C4C	4.87	1.47	1.38
21	31	414	CL7	CHC-C1C	4.87	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3C	513	CL7	CHD-C4C	4.87	1.47	1.38
21	14	409	CL7	CHD-C4C	4.87	1.47	1.38
21	3C	511	CL7	CHC-C1C	4.87	1.47	1.38
21	44	409	CL7	CHD-C4C	4.87	1.47	1.38
21	2C	506	CL7	CHD-C4C	4.87	1.47	1.38
21	3C	506	CL7	CHD-C4C	4.87	1.47	1.38
31	4F	101	HEM	FE-NB	4.87	2.09	1.94
23	44	402	8CT	C05-C04	4.86	1.65	1.54
21	11	417	CL7	CHC-C1C	4.86	1.47	1.38
21	3B	616	CL7	CHD-C4C	4.86	1.47	1.38
21	22	508	CL7	CHD-C4C	4.86	1.47	1.38
21	32	508	CL7	CHD-C4C	4.86	1.47	1.38
23	3B	617	8CT	C11-C12	4.86	1.56	1.45
23	1B	617	8CT	C11-C12	4.86	1.56	1.45
21	13	514	CL7	CHD-C4C	4.86	1.47	1.38
21	21	414	CL7	CHC-C1C	4.86	1.47	1.38
23	1B	618	8CT	C05-C04	4.85	1.65	1.54
23	4B	619	8CT	C05-C04	4.85	1.65	1.54
21	12	507	CL7	CHD-C4C	4.85	1.47	1.38
21	24	405	CL7	CHD-C4C	4.85	1.47	1.38
21	34	405	CL7	CHD-C4C	4.85	1.47	1.38
23	2B	618	8CT	C11-C12	4.85	1.56	1.45
21	21	416	CL7	CHC-C1C	4.85	1.47	1.38
21	24	417	CL7	CHC-C1C	4.85	1.47	1.38
21	34	417	CL7	CHC-C1C	4.85	1.47	1.38
21	42	508	CL7	CHD-C4C	4.85	1.47	1.38
21	4C	504	CL7	CHD-C4C	4.85	1.47	1.38
21	2C	504	CL7	CHD-C4C	4.85	1.47	1.38
21	21	411	CL7	CHC-C1C	4.85	1.47	1.38
21	3C	504	CL7	CHD-C4C	4.85	1.47	1.38
21	42	507	CL7	CHD-C4C	4.85	1.47	1.38
21	31	417	CL7	CHC-C1C	4.85	1.47	1.38
23	1A	404	8CT	C05-C04	4.85	1.65	1.54
21	22	507	CL7	CHD-C4C	4.85	1.47	1.38
21	32	507	CL7	CHD-C4C	4.85	1.47	1.38
21	41	409	CL7	CHD-C4C	4.85	1.47	1.38
21	21	413	CL7	CHB-C1B	4.85	1.50	1.39
21	41	402	CL7	CHD-C4C	4.85	1.47	1.38
21	1C	513	CL7	CHD-C4C	4.85	1.47	1.38
21	14	417	CL7	CHC-C1C	4.85	1.47	1.38
21	4A	407	CL7	CHD-C4C	4.85	1.47	1.38
23	1B	626	8CT	C14-C13	4.85	1.58	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2B	601	8CT	C14-C13	4.85	1.58	1.43
23	3B	626	8CT	C14-C13	4.85	1.58	1.43
23	2C	515	8CT	C05-C04	4.85	1.65	1.54
21	11	402	CL7	CHD-C4C	4.85	1.47	1.38
21	23	410	CL7	CHC-C1C	4.84	1.47	1.38
23	2C	514	8CT	C05-C04	4.84	1.65	1.54
21	21	412	CL7	CHB-C1B	4.84	1.50	1.39
23	1C	515	8CT	C05-C04	4.84	1.65	1.54
23	4C	515	8CT	C05-C04	4.84	1.65	1.54
31	3F	101	HEM	FE-NB	4.84	2.09	1.94
21	41	411	CL7	CHC-C1C	4.84	1.47	1.38
21	13	513	CL7	CHD-C4C	4.84	1.47	1.38
23	3A	404	8CT	C05-C04	4.84	1.65	1.54
23	2K	101	8CT	C34-C33	4.84	1.64	1.52
21	31	413	CL7	CHB-C1B	4.84	1.50	1.39
21	23	415	CL7	CHD-C4C	4.84	1.47	1.38
21	3C	510	CL7	CHC-C1C	4.84	1.47	1.38
21	31	404	CL7	CHC-C1C	4.84	1.47	1.38
21	31	411	CL7	CHC-C1C	4.84	1.47	1.38
21	23	414	CL7	CHD-C4C	4.84	1.47	1.38
21	33	513	CL7	CHD-C4C	4.84	1.47	1.38
21	14	405	CL7	CHD-C4C	4.83	1.47	1.38
21	1C	504	CL7	CHC-C1C	4.83	1.47	1.38
21	2B	617	CL7	CHD-C4C	4.83	1.47	1.38
21	43	415	CL7	CHD-C4C	4.83	1.47	1.38
21	24	416	CL7	CHD-C4C	4.83	1.47	1.38
21	42	506	CL7	CHD-C4C	4.83	1.47	1.38
21	1B	601	CL7	CHC-C1C	4.83	1.47	1.38
21	13	509	CL7	CHC-C1C	4.83	1.47	1.38
21	43	410	CL7	CHC-C1C	4.83	1.47	1.38
21	31	412	CL7	CHB-C1B	4.83	1.50	1.39
21	11	415	CL7	CHB-C1B	4.83	1.50	1.39
21	41	415	CL7	CHB-C1B	4.83	1.50	1.39
21	12	508	CL7	CHD-C4C	4.82	1.47	1.38
21	2C	513	CL7	CHC-C1C	4.82	1.47	1.38
23	3C	514	8CT	C05-C04	4.82	1.65	1.54
21	2C	504	CL7	CHC-C1C	4.82	1.47	1.38
21	3C	504	CL7	CHC-C1C	4.82	1.47	1.38
21	33	509	CL7	CHC-C1C	4.82	1.47	1.38
21	3B	616	CL7	CHC-C1C	4.82	1.47	1.38
21	2B	614	CL7	CHD-C4C	4.82	1.47	1.38
21	22	518	CL7	CHC-C1C	4.82	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	409	CL7	CHD-C4C	4.82	1.47	1.38
21	2D	404	CL7	CHD-C4C	4.82	1.47	1.38
31	1F	101	HEM	FE-NB	4.82	2.09	1.94
21	1B	616	CL7	CHD-C4C	4.82	1.47	1.38
21	4B	617	CL7	CHD-C4C	4.82	1.47	1.38
23	4B	618	8CT	C11-C12	4.82	1.56	1.45
23	3C	515	8CT	C11-C12	4.82	1.56	1.45
31	2F	101	HEM	FE-NB	4.82	2.09	1.94
21	11	413	CL7	CHB-C1B	4.82	1.50	1.39
21	41	413	CL7	CHB-C1B	4.82	1.50	1.39
23	4C	515	8CT	C14-C13	4.82	1.58	1.43
21	21	409	CL7	CHD-C4C	4.82	1.47	1.38
21	31	409	CL7	CHD-C4C	4.82	1.47	1.38
21	31	415	CL7	CHB-C1B	4.82	1.50	1.39
21	21	402	CL7	CHD-C4C	4.82	1.47	1.38
21	41	412	CL7	CHB-C1B	4.81	1.50	1.39
21	1B	616	CL7	CHC-C1C	4.81	1.47	1.38
21	4B	617	CL7	CHC-C1C	4.81	1.47	1.38
21	21	415	CL7	CHB-C1B	4.81	1.50	1.39
21	11	418	CL7	CHD-C4C	4.81	1.47	1.38
21	2B	617	CL7	CHC-C1C	4.81	1.47	1.38
21	22	501	CL7	CHD-C4C	4.81	1.47	1.38
23	4K	101	8CT	C34-C33	4.81	1.63	1.52
23	3C	515	8CT	C05-C04	4.81	1.65	1.54
21	13	515	CL7	CHD-C4C	4.81	1.47	1.38
21	1C	510	CL7	CHC-C1C	4.81	1.47	1.38
21	4C	510	CL7	CHC-C1C	4.81	1.47	1.38
21	12	518	CL7	CHC-C1C	4.81	1.47	1.38
21	4B	602	CL7	CHC-C1C	4.81	1.47	1.38
23	4C	515	8CT	C11-C12	4.81	1.56	1.45
21	44	405	CL7	CHD-C4C	4.80	1.47	1.38
21	4A	403	CL7	CHC-C1C	4.80	1.47	1.38
21	34	416	CL7	CHD-C4C	4.80	1.47	1.38
21	41	407	CL7	CHD-C4C	4.80	1.47	1.38
23	1C	515	8CT	C14-C13	4.80	1.58	1.43
21	32	501	CL7	CHD-C4C	4.80	1.47	1.38
21	11	412	CL7	CHB-C1B	4.80	1.50	1.39
21	31	410	CL7	CHC-C1C	4.80	1.47	1.38
21	21	407	CL7	CHD-C4C	4.80	1.47	1.38
23	1C	514	8CT	C05-C04	4.80	1.65	1.54
23	4C	514	8CT	C05-C04	4.80	1.65	1.54
21	21	418	CL7	CHD-C4C	4.80	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3C	513	CL7	CHC-C1C	4.80	1.47	1.38
21	24	408	CL7	CHC-C1C	4.80	1.47	1.38
21	34	408	CL7	CHC-C1C	4.80	1.47	1.38
21	11	410	CL7	CHC-C1C	4.80	1.47	1.38
21	41	410	CL7	CHC-C1C	4.80	1.47	1.38
21	13	508	CL7	CHD-C4C	4.80	1.47	1.38
21	23	403	CL7	CHC-C1C	4.79	1.47	1.38
21	4C	513	CL7	CHC-C1C	4.79	1.47	1.38
23	1K	101	8CT	C34-C33	4.79	1.63	1.52
23	2C	515	8CT	C14-C13	4.79	1.58	1.43
21	14	408	CL7	CHC-C1C	4.79	1.47	1.38
21	14	416	CL7	CHD-C4C	4.79	1.47	1.38
21	44	408	CL7	CHC-C1C	4.79	1.47	1.38
21	44	416	CL7	CHD-C4C	4.79	1.47	1.38
21	11	411	CL7	CHC-C1C	4.79	1.47	1.38
21	22	506	CL7	CHD-C4C	4.79	1.47	1.38
21	3A	403	CL7	CHC-C1C	4.79	1.47	1.38
21	32	506	CL7	CHD-C4C	4.79	1.47	1.38
21	13	502	CL7	CHC-C1C	4.79	1.47	1.38
21	32	518	CL7	CHC-C1C	4.79	1.47	1.38
21	44	417	CL7	CHD-C4C	4.79	1.47	1.38
23	3C	518	8CT	C35-C30	4.79	1.69	1.56
21	2B	602	CL7	CHC-C1C	4.79	1.47	1.38
21	3B	601	CL7	CHC-C1C	4.79	1.47	1.38
23	1B	617	8CT	C35-C30	4.79	1.69	1.56
23	4B	618	8CT	C35-C30	4.79	1.69	1.56
23	2D	406	8CT	C11-C12	4.79	1.56	1.45
21	43	403	CL7	CHC-C1C	4.79	1.47	1.38
21	43	414	CL7	CHC-C1C	4.79	1.47	1.38
21	42	501	CL7	CHD-C4C	4.79	1.47	1.38
21	32	511	CL7	CHD-C4C	4.79	1.47	1.38
21	32	502	CL7	CHB-C1B	4.79	1.50	1.39
21	1B	613	CL7	CHD-C4C	4.79	1.47	1.38
21	33	502	CL7	CHC-C1C	4.79	1.47	1.38
21	4B	614	CL7	CHD-C4C	4.79	1.47	1.38
21	2C	510	CL7	CHC-C1C	4.79	1.47	1.38
21	23	409	CL7	CHD-C4C	4.79	1.47	1.38
21	33	508	CL7	CHD-C4C	4.79	1.47	1.38
23	2C	514	8CT	C34-C33	4.79	1.63	1.52
23	3C	514	8CT	C34-C33	4.79	1.63	1.52
23	1B	617	8CT	C14-C13	4.78	1.58	1.43
23	4B	618	8CT	C14-C13	4.78	1.58	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3K	101	8CT	C34-C33	4.78	1.63	1.52
21	1D	404	CL7	CHD-C4C	4.78	1.47	1.38
21	4D	404	CL7	CHD-C4C	4.78	1.47	1.38
23	3C	515	8CT	C14-C13	4.78	1.58	1.43
21	22	502	CL7	CHB-C1B	4.78	1.50	1.39
21	31	402	CL7	CHD-C4C	4.78	1.47	1.38
21	23	416	CL7	CHC-C1C	4.78	1.47	1.38
21	33	515	CL7	CHC-C1C	4.78	1.47	1.38
21	11	407	CL7	CHD-C4C	4.78	1.47	1.38
21	21	409	CL7	CHC-C1C	4.78	1.47	1.38
21	43	416	CL7	CHC-C1C	4.78	1.47	1.38
23	1C	515	8CT	C11-C12	4.78	1.56	1.45
21	42	518	CL7	CHC-C1C	4.78	1.47	1.38
23	2B	618	8CT	C14-C13	4.78	1.58	1.43
21	1C	511	CL7	CHD-C4C	4.78	1.47	1.38
21	44	417	CL7	CHC-C1C	4.78	1.47	1.38
23	1D	406	8CT	C14-C13	4.77	1.58	1.43
21	12	511	CL7	CHD-C4C	4.77	1.47	1.38
21	21	420	CL7	CHD-C4C	4.77	1.47	1.38
21	31	420	CL7	CHD-C4C	4.77	1.47	1.38
21	12	502	CL7	CHB-C1B	4.77	1.50	1.39
21	42	502	CL7	CHB-C1B	4.77	1.50	1.39
21	23	416	CL7	CHD-C4C	4.77	1.47	1.38
21	3B	613	CL7	CHD-C4C	4.77	1.47	1.38
21	33	515	CL7	CHD-C4C	4.77	1.47	1.38
21	14	406	CL7	CHC-C1C	4.77	1.47	1.38
23	2C	514	8CT	C35-C30	4.77	1.69	1.56
23	3C	514	8CT	C35-C30	4.77	1.69	1.56
23	3B	617	8CT	C14-C13	4.77	1.58	1.43
23	2C	515	8CT	C11-C12	4.77	1.56	1.45
21	12	506	CL7	CHD-C4C	4.77	1.47	1.38
21	14	404	CL7	CHC-C1C	4.77	1.47	1.38
21	31	402	CL7	CHC-C1C	4.77	1.47	1.38
21	41	420	CL7	CHD-C4C	4.77	1.47	1.38
23	1C	518	8CT	C35-C30	4.77	1.69	1.56
23	4C	518	8CT	C35-C30	4.77	1.69	1.56
21	1A	403	CL7	CHC-C1C	4.77	1.47	1.38
23	2D	406	8CT	C14-C13	4.77	1.58	1.43
21	2A	403	CL7	CHC-C1C	4.77	1.47	1.38
23	1C	514	8CT	C34-C33	4.77	1.63	1.52
21	11	420	CL7	CHD-C4C	4.76	1.47	1.38
21	14	413	CL7	CHD-C4C	4.76	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	404	CL7	CHD-C4C	4.76	1.47	1.38
21	44	413	CL7	CHD-C4C	4.76	1.47	1.38
21	3C	507	CL7	CHD-C4C	4.76	1.47	1.38
23	4C	514	8CT	C35-C30	4.76	1.69	1.56
21	3D	404	CL7	CHD-C4C	4.76	1.47	1.38
21	42	511	CL7	CHD-C4C	4.76	1.47	1.38
21	12	501	CL7	CHD-C4C	4.76	1.47	1.38
21	24	404	CL7	CHC-C1C	4.76	1.47	1.38
21	43	409	CL7	CHD-C4C	4.76	1.47	1.38
21	24	417	CL7	CHD-C4C	4.76	1.47	1.38
21	11	409	CL7	CHC-C1C	4.76	1.47	1.38
21	31	413	CL7	CHD-C4C	4.76	1.47	1.38
21	41	409	CL7	CHC-C1C	4.76	1.47	1.38
21	1C	507	CL7	CHD-C4C	4.76	1.47	1.38
21	1C	513	CL7	CHC-C1C	4.76	1.47	1.38
21	22	511	CL7	CHD-C4C	4.76	1.47	1.38
21	31	407	CL7	CHD-C4C	4.76	1.47	1.38
21	4C	507	CL7	CHD-C4C	4.76	1.47	1.38
21	41	418	CL7	CHD-C4C	4.76	1.47	1.38
21	2B	603	CL7	CHD-C4C	4.76	1.47	1.38
21	11	412	CL7	CHD-C4C	4.76	1.47	1.38
21	41	412	CL7	CHD-C4C	4.76	1.47	1.38
21	21	402	CL7	CHC-C1C	4.76	1.47	1.38
21	4B	609	CL7	CHD-C4C	4.76	1.47	1.38
21	11	413	CL7	CHD-C4C	4.76	1.47	1.38
21	2B	604	CL7	CHD-C4C	4.76	1.47	1.38
21	3B	603	CL7	CHD-C4C	4.76	1.47	1.38
21	23	414	CL7	CHC-C1C	4.76	1.47	1.38
21	33	513	CL7	CHC-C1C	4.76	1.47	1.38
23	3D	406	8CT	C11-C12	4.76	1.56	1.45
21	43	416	CL7	CHD-C4C	4.76	1.47	1.38
23	4D	406	8CT	C14-C13	4.75	1.58	1.43
21	14	404	CL7	CHD-C4C	4.75	1.47	1.38
21	4B	604	CL7	CHD-C4C	4.75	1.47	1.38
21	13	515	CL7	CHC-C1C	4.75	1.47	1.38
21	21	412	CL7	CHD-C4C	4.75	1.47	1.38
21	4C	511	CL7	CHD-C4C	4.75	1.47	1.38
23	1D	406	8CT	C11-C12	4.75	1.56	1.45
23	4C	514	8CT	C34-C33	4.75	1.63	1.52
21	12	510	CL7	CHD-C4C	4.75	1.47	1.38
21	2B	615	CL7	CHD-C4C	4.75	1.47	1.38
21	4B	604	CL7	CHC-C1C	4.75	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4D	406	8CT	C35-C30	4.75	1.69	1.56
23	3C	514	8CT	C11-C12	4.75	1.56	1.45
23	3D	406	8CT	C14-C13	4.75	1.58	1.43
21	13	513	CL7	CHC-C1C	4.75	1.47	1.38
21	22	512	CL7	CHC-C1C	4.75	1.47	1.38
21	32	512	CL7	CHC-C1C	4.75	1.47	1.38
23	1D	406	8CT	C35-C30	4.75	1.69	1.56
21	31	409	CL7	CHC-C1C	4.75	1.47	1.38
23	1B	619	8CT	C11-C12	4.75	1.56	1.45
23	4B	620	8CT	C11-C12	4.75	1.56	1.45
23	2C	518	8CT	C14-C13	4.75	1.58	1.43
21	34	406	CL7	CHC-C1C	4.75	1.47	1.38
21	34	413	CL7	CHD-C4C	4.75	1.47	1.38
23	2C	518	8CT	C35-C30	4.75	1.69	1.56
21	14	417	CL7	CHD-C4C	4.75	1.47	1.38
21	44	404	CL7	CHD-C4C	4.75	1.47	1.38
21	11	407	CL7	CHC-C1C	4.74	1.47	1.38
21	24	406	CL7	CHC-C1C	4.74	1.47	1.38
23	2B	618	8CT	C35-C30	4.74	1.69	1.56
23	3B	617	8CT	C35-C30	4.74	1.69	1.56
21	31	418	CL7	CHD-C4C	4.74	1.47	1.38
21	11	408	CL7	CHC-C1C	4.74	1.47	1.38
23	3D	406	8CT	C35-C30	4.74	1.69	1.56
21	31	408	CL7	CHC-C1C	4.74	1.47	1.38
21	2C	511	CL7	CHD-C4C	4.74	1.47	1.38
21	3C	511	CL7	CHD-C4C	4.74	1.47	1.38
21	41	408	CL7	CHC-C1C	4.74	1.47	1.38
21	41	413	CL7	CHD-C4C	4.74	1.47	1.38
21	11	412	CL7	CHC-C1C	4.74	1.47	1.38
21	41	412	CL7	CHC-C1C	4.74	1.47	1.38
21	41	403	CL7	CHD-C4C	4.74	1.47	1.38
21	22	510	CL7	CHD-C4C	4.74	1.47	1.38
21	21	410	CL7	CHC-C1C	4.74	1.47	1.38
23	3B	619	8CT	C11-C12	4.74	1.56	1.45
21	11	402	CL7	CHC-C1C	4.74	1.47	1.38
21	24	404	CL7	CHD-C4C	4.74	1.47	1.38
21	34	417	CL7	CHD-C4C	4.74	1.47	1.38
21	41	402	CL7	CHC-C1C	4.74	1.47	1.38
21	44	406	CL7	CHC-C1C	4.74	1.47	1.38
21	2C	501	CL7	CHC-C1C	4.74	1.47	1.38
21	1B	608	CL7	CHD-C4C	4.73	1.47	1.38
23	2D	406	8CT	C35-C30	4.73	1.69	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	33	504	CL7	CHC-C1C	4.73	1.47	1.38
21	21	416	CL7	CHB-C1B	4.73	1.50	1.39
21	31	416	CL7	CHB-C1B	4.73	1.50	1.39
21	23	413	CL7	CHD-C4C	4.73	1.47	1.38
21	24	413	CL7	CHD-C4C	4.73	1.47	1.38
21	31	419	CL7	CHB-C1B	4.73	1.50	1.39
23	1C	514	8CT	C35-C30	4.73	1.69	1.56
23	2C	514	8CT	C11-C12	4.73	1.56	1.45
23	4D	406	8CT	C11-C12	4.73	1.56	1.45
21	12	509	CL7	CHC-C1C	4.73	1.47	1.38
21	12	512	CL7	CHC-C1C	4.73	1.47	1.38
21	22	511	CL7	CHC-C1C	4.73	1.47	1.38
21	42	509	CL7	CHC-C1C	4.73	1.47	1.38
21	42	512	CL7	CHC-C1C	4.73	1.47	1.38
21	13	504	CL7	CHC-C1C	4.73	1.47	1.38
21	14	407	CL7	CHC-C1C	4.73	1.47	1.38
21	3B	614	CL7	CHD-C4C	4.73	1.47	1.38
21	43	404	CL7	CHC-C1C	4.73	1.47	1.38
21	43	405	CL7	CHC-C1C	4.73	1.47	1.38
21	44	407	CL7	CHC-C1C	4.73	1.47	1.38
21	21	413	CL7	CHD-C4C	4.73	1.47	1.38
21	31	407	CL7	CHC-C1C	4.73	1.47	1.38
21	31	412	CL7	CHD-C4C	4.73	1.47	1.38
21	21	405	CL7	CHC-C1C	4.72	1.47	1.38
21	31	403	CL7	CHD-C4C	4.72	1.47	1.38
23	1C	518	8CT	C14-C13	4.72	1.58	1.43
21	3B	603	CL7	CHC-C1C	4.72	1.47	1.38
21	13	507	CL7	CHD-C4C	4.72	1.47	1.38
21	2C	502	CL7	CHD-C4C	4.72	1.47	1.38
21	31	412	CL7	CHC-C1C	4.72	1.47	1.38
21	42	502	CL7	CHD-C4C	4.72	1.47	1.38
23	2B	620	8CT	C11-C12	4.72	1.56	1.45
21	4B	603	CL7	CHD-C4C	4.72	1.47	1.38
21	44	404	CL7	CHC-C1C	4.72	1.47	1.38
21	1C	501	CL7	CHC-C1C	4.72	1.47	1.38
21	22	509	CL7	CHC-C1C	4.72	1.47	1.38
21	4C	501	CL7	CHC-C1C	4.72	1.47	1.38
21	22	509	CL7	CHD-C4C	4.72	1.47	1.38
21	4C	506	CL7	CHC-C1C	4.72	1.47	1.38
21	32	502	CL7	CHD-C4C	4.72	1.47	1.38
21	32	517	CL7	CHC-C1C	4.72	1.47	1.38
21	1B	603	CL7	CHC-C1C	4.72	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1A	407	CL7	CHC-C1C	4.72	1.47	1.38
21	34	404	CL7	CHC-C1C	4.72	1.47	1.38
23	4C	514	8CT	C11-C12	4.72	1.56	1.45
21	2B	609	CL7	CHD-C4C	4.72	1.47	1.38
21	24	411	CL7	CHC-C1C	4.72	1.47	1.38
21	1B	603	CL7	CHD-C4C	4.72	1.47	1.38
21	1B	614	CL7	CHD-C4C	4.72	1.47	1.38
21	2C	506	CL7	CHC-C1C	4.72	1.47	1.38
21	24	405	CL7	CHC-C1C	4.72	1.47	1.38
21	3C	506	CL7	CHC-C1C	4.72	1.47	1.38
21	4B	615	CL7	CHD-C4C	4.72	1.47	1.38
21	43	413	CL7	CHD-C4C	4.72	1.47	1.38
21	12	504	CL7	CHC-C1C	4.71	1.47	1.38
21	42	511	CL7	CHC-C1C	4.71	1.47	1.38
21	11	403	CL7	CHD-C4C	4.71	1.47	1.38
21	14	411	CL7	CHC-C1C	4.71	1.47	1.38
21	42	510	CL7	CHD-C4C	4.71	1.47	1.38
21	32	510	CL7	CHD-C4C	4.71	1.47	1.38
21	23	404	CL7	CHC-C1C	4.71	1.47	1.38
21	32	503	CL7	CHC-C1C	4.71	1.47	1.38
21	33	503	CL7	CHC-C1C	4.71	1.47	1.38
21	42	517	CL7	CHC-C1C	4.71	1.47	1.38
23	4C	518	8CT	C14-C13	4.71	1.58	1.43
21	14	405	CL7	CHB-C1B	4.71	1.50	1.39
21	21	408	CL7	CHC-C1C	4.71	1.47	1.38
21	24	407	CL7	CHC-C1C	4.71	1.47	1.38
21	42	516	CL7	CHC-C1C	4.71	1.47	1.38
21	32	511	CL7	CHC-C1C	4.71	1.47	1.38
21	12	509	CL7	CHD-C4C	4.71	1.47	1.38
21	42	509	CL7	CHD-C4C	4.71	1.47	1.38
21	41	407	CL7	CHC-C1C	4.71	1.47	1.38
21	32	516	CL7	CHC-C1C	4.71	1.47	1.38
21	13	512	CL7	CHD-C4C	4.71	1.47	1.38
21	34	411	CL7	CHC-C1C	4.71	1.47	1.38
21	11	405	CL7	CHC-C1C	4.71	1.47	1.38
21	41	405	CL7	CHC-C1C	4.71	1.47	1.38
21	2B	615	CL7	CHC-C1C	4.71	1.47	1.38
23	3C	518	8CT	C14-C13	4.70	1.58	1.43
21	24	415	CL7	CHC-C1C	4.70	1.47	1.38
21	34	415	CL7	CHC-C1C	4.70	1.47	1.38
21	12	503	CL7	CHC-C1C	4.70	1.47	1.38
21	3C	501	CL7	CHC-C1C	4.70	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	615	CL7	CHD-C4C	4.70	1.47	1.38
21	3C	502	CL7	CHD-C4C	4.70	1.47	1.38
21	24	405	CL7	CHB-C1B	4.70	1.50	1.39
21	14	415	CL7	CHC-C1C	4.70	1.47	1.38
21	4B	603	CL7	CHC-C1C	4.70	1.47	1.38
21	4B	616	CL7	CHD-C4C	4.70	1.47	1.38
21	11	419	CL7	CHB-C1B	4.70	1.49	1.39
21	42	512	CL7	CHB-C1B	4.70	1.49	1.39
21	41	419	CL7	CHB-C1B	4.70	1.49	1.39
21	1C	502	CL7	CHC-C1C	4.70	1.47	1.38
21	13	503	CL7	CHC-C1C	4.70	1.47	1.38
21	3C	502	CL7	CHC-C1C	4.70	1.47	1.38
23	1C	514	8CT	C11-C12	4.70	1.56	1.45
21	22	502	CL7	CHD-C4C	4.70	1.47	1.38
21	22	503	CL7	CHC-C1C	4.70	1.47	1.38
21	32	509	CL7	CHC-C1C	4.70	1.47	1.38
21	44	411	CL7	CHC-C1C	4.70	1.47	1.38
21	1C	503	CL7	CHD-C4C	4.70	1.47	1.38
21	42	505	CL7	CHB-C1B	4.70	1.49	1.39
21	1B	602	CL7	CHD-C4C	4.70	1.47	1.38
21	41	404	CL7	CHB-C1B	4.70	1.49	1.39
21	4D	405	CL7	CHD-C4C	4.70	1.47	1.38
23	4A	404	8CT	C11-C12	4.70	1.56	1.45
21	32	516	CL7	CHD-C4C	4.69	1.47	1.38
21	44	415	CL7	CHC-C1C	4.69	1.47	1.38
21	11	416	CL7	CHB-C1B	4.69	1.49	1.39
21	41	416	CL7	CHB-C1B	4.69	1.49	1.39
21	23	408	CL7	CHD-C4C	4.69	1.47	1.38
21	33	507	CL7	CHD-C4C	4.69	1.47	1.38
21	33	501	CL7	CHC-C1C	4.69	1.47	1.38
21	2B	604	CL7	CHC-C1C	4.69	1.47	1.38
21	2C	507	CL7	CHD-C4C	4.69	1.47	1.38
21	33	512	CL7	CHD-C4C	4.69	1.47	1.38
21	21	404	CL7	CHB-C1B	4.69	1.49	1.39
21	31	404	CL7	CHB-C1B	4.69	1.49	1.39
21	22	516	CL7	CHC-C1C	4.69	1.47	1.38
21	21	419	CL7	CHB-C1B	4.69	1.49	1.39
21	1D	405	CL7	CHD-C4C	4.69	1.47	1.38
21	21	407	CL7	CHC-C1C	4.69	1.47	1.38
21	3B	608	CL7	CHD-C4C	4.69	1.47	1.38
21	3B	602	CL7	CHD-C4C	4.69	1.47	1.38
21	34	405	CL7	CHC-C1C	4.69	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2A	407	CL7	CHC-C1C	4.69	1.47	1.38
21	3A	407	CL7	CHC-C1C	4.69	1.47	1.38
21	2B	605	CL7	CHD-C4C	4.69	1.47	1.38
21	22	504	CL7	CHC-C1C	4.69	1.47	1.38
21	2D	405	CL7	CHD-C4C	4.69	1.47	1.38
21	1C	502	CL7	CHD-C4C	4.68	1.47	1.38
21	22	517	CL7	CHC-C1C	4.68	1.47	1.38
21	4C	502	CL7	CHD-C4C	4.68	1.47	1.38
21	34	405	CL7	CHB-C1B	4.68	1.49	1.39
21	12	502	CL7	CHD-C4C	4.68	1.47	1.38
21	12	511	CL7	CHC-C1C	4.68	1.47	1.38
21	21	412	CL7	CHC-C1C	4.68	1.47	1.38
21	34	412	CL7	CHC-C1C	4.68	1.47	1.38
21	44	412	CL7	CHC-C1C	4.68	1.47	1.38
21	23	405	CL7	CHC-C1C	4.68	1.47	1.38
21	2B	603	CL7	CHC-C1C	4.68	1.47	1.38
21	3B	602	CL7	CHC-C1C	4.68	1.47	1.38
21	12	512	CL7	CHB-C1B	4.68	1.49	1.39
21	2D	402	CL7	CHC-C1C	4.68	1.47	1.38
21	2B	612	CL7	CHD-C4C	4.68	1.47	1.38
21	1C	506	CL7	CHC-C1C	4.68	1.47	1.38
21	32	504	CL7	CHC-C1C	4.68	1.47	1.38
21	43	408	CL7	CHD-C4C	4.68	1.47	1.38
21	2C	503	CL7	CHC-C1C	4.68	1.47	1.38
21	3C	503	CL7	CHC-C1C	4.68	1.47	1.38
21	4B	612	CL7	CHD-C4C	4.68	1.47	1.38
23	2A	404	8CT	C11-C12	4.68	1.56	1.45
21	31	405	CL7	CHC-C1C	4.68	1.47	1.38
21	2C	503	CL7	CHD-C4C	4.68	1.47	1.38
21	3C	503	CL7	CHD-C4C	4.68	1.47	1.38
21	34	407	CL7	CHC-C1C	4.68	1.47	1.38
21	41	420	CL7	CHB-C1B	4.68	1.49	1.39
21	1B	615	CL7	CHD-C4C	4.67	1.47	1.38
21	12	517	CL7	CHC-C1C	4.67	1.47	1.38
21	14	405	CL7	CHC-C1C	4.67	1.47	1.38
21	44	405	CL7	CHC-C1C	4.67	1.47	1.38
21	24	409	CL7	CHB-C1B	4.67	1.49	1.39
21	1D	402	CL7	CHC-C1C	4.67	1.47	1.38
21	12	516	CL7	CHC-C1C	4.67	1.47	1.38
21	31	420	CL7	CHB-C1B	4.67	1.49	1.39
21	42	515	CL7	CHB-C1B	4.67	1.49	1.39
21	14	410	CL7	CHD-C4C	4.67	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	410	CL7	CHD-C4C	4.67	1.47	1.38
21	42	504	CL7	CHC-C1C	4.67	1.47	1.38
21	13	501	CL7	CHC-C1C	4.67	1.47	1.38
21	14	406	CL7	CHD-C4C	4.67	1.47	1.38
21	2B	616	CL7	CHD-C4C	4.67	1.47	1.38
21	23	411	CL7	CHD-C4C	4.67	1.47	1.38
21	33	510	CL7	CHD-C4C	4.67	1.47	1.38
21	32	505	CL7	CHB-C1B	4.67	1.49	1.39
21	24	406	CL7	CHD-C4C	4.67	1.47	1.38
21	32	509	CL7	CHD-C4C	4.67	1.47	1.38
21	34	406	CL7	CHD-C4C	4.67	1.47	1.38
23	2K	101	8CT	C24-C25	4.67	1.57	1.43
23	3K	101	8CT	C24-C25	4.67	1.57	1.43
21	2C	509	CL7	CHD-C4C	4.67	1.47	1.38
21	1C	503	CL7	CHC-C1C	4.67	1.47	1.38
21	4C	503	CL7	CHC-C1C	4.67	1.47	1.38
21	24	414	CL7	CHD-C4C	4.67	1.47	1.38
21	14	409	CL7	CHB-C1B	4.67	1.49	1.39
21	4C	508	CL7	CHD-C4C	4.67	1.47	1.38
21	42	503	CL7	CHC-C1C	4.67	1.47	1.38
21	1B	604	CL7	CHD-C4C	4.67	1.47	1.38
21	2C	508	CL7	CHD-C4C	4.67	1.47	1.38
21	21	406	CL7	CHC-C1C	4.67	1.47	1.38
21	21	403	CL7	CHD-C4C	4.67	1.47	1.38
21	13	510	CL7	CHD-C4C	4.67	1.47	1.38
21	24	415	CL7	CHD-C4C	4.67	1.47	1.38
21	31	406	CL7	CHD-C4C	4.67	1.47	1.38
21	43	411	CL7	CHD-C4C	4.67	1.47	1.38
21	32	512	CL7	CHB-C1B	4.67	1.49	1.39
21	12	516	CL7	CHD-C4C	4.66	1.47	1.38
23	4C	515	8CT	C34-C33	4.66	1.63	1.52
21	3D	402	CL7	CHC-C1C	4.66	1.47	1.38
21	4B	605	CL7	CHB-C1B	4.66	1.49	1.39
21	4D	402	CL7	CHC-C1C	4.66	1.47	1.38
23	1K	101	8CT	C24-C25	4.66	1.57	1.43
23	4K	101	8CT	C24-C25	4.66	1.57	1.43
21	33	510	CL7	CHC-C1C	4.66	1.47	1.38
21	4B	606	CL7	CHC-C1C	4.66	1.47	1.38
21	44	405	CL7	CHB-C1B	4.66	1.49	1.39
21	3B	611	CL7	CHD-C4C	4.66	1.47	1.38
21	34	409	CL7	CHB-C1B	4.66	1.49	1.39
21	1B	613	CL7	CHC-C1C	4.66	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	605	CL7	CHD-C4C	4.66	1.47	1.38
21	2B	606	CL7	CHC-C1C	4.66	1.47	1.38
21	3B	614	CL7	CHC-C1C	4.65	1.47	1.38
21	4C	503	CL7	CHD-C4C	4.65	1.47	1.38
21	22	516	CL7	CHD-C4C	4.65	1.47	1.38
21	11	420	CL7	CHB-C1B	4.65	1.49	1.39
21	14	406	CL7	CHB-C1B	4.65	1.49	1.39
21	44	406	CL7	CHB-C1B	4.65	1.49	1.39
21	11	406	CL7	CHD-C4C	4.65	1.47	1.38
21	44	410	CL7	CHC-C1C	4.65	1.47	1.38
21	4A	407	CL7	CHC-C1C	4.65	1.47	1.38
21	1B	614	CL7	CHC-C1C	4.65	1.47	1.38
21	4B	615	CL7	CHC-C1C	4.65	1.47	1.38
21	22	505	CL7	CHC-C1C	4.65	1.47	1.38
21	23	417	CL7	CHC-C1C	4.65	1.47	1.38
21	32	505	CL7	CHC-C1C	4.65	1.47	1.38
21	11	404	CL7	CHB-C1B	4.65	1.49	1.39
21	42	513	CL7	CHC-C1C	4.65	1.47	1.38
21	22	515	CL7	CHB-C1B	4.65	1.49	1.39
21	32	515	CL7	CHB-C1B	4.65	1.49	1.39
21	3B	605	CL7	CHC-C1C	4.65	1.47	1.38
23	1C	515	8CT	C34-C33	4.65	1.63	1.52
21	2C	502	CL7	CHC-C1C	4.65	1.47	1.38
21	4C	502	CL7	CHC-C1C	4.65	1.47	1.38
23	2C	515	8CT	C34-C33	4.65	1.63	1.52
23	3C	515	8CT	C34-C33	4.65	1.63	1.52
23	3A	404	8CT	C11-C12	4.65	1.55	1.45
21	12	513	CL7	CHC-C1C	4.65	1.47	1.38
21	1B	607	CL7	CHC-C1C	4.65	1.47	1.38
21	21	413	CL7	CHC-C1C	4.65	1.47	1.38
21	31	413	CL7	CHC-C1C	4.65	1.47	1.38
21	4B	608	CL7	CHC-C1C	4.65	1.47	1.38
21	24	410	CL7	CHD-C4C	4.64	1.47	1.38
21	34	410	CL7	CHD-C4C	4.64	1.47	1.38
21	12	505	CL7	CHB-C1B	4.64	1.49	1.39
21	11	403	CL7	CHB-C1B	4.64	1.49	1.39
21	41	403	CL7	CHB-C1B	4.64	1.49	1.39
21	11	413	CL7	CHC-C1C	4.64	1.47	1.38
21	41	413	CL7	CHC-C1C	4.64	1.47	1.38
21	12	505	CL7	CHC-C1C	4.64	1.47	1.38
21	42	505	CL7	CHC-C1C	4.64	1.47	1.38
21	1B	606	CL7	CHC-C1C	4.64	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	607	CL7	CHC-C1C	4.64	1.47	1.38
21	14	412	CL7	CHC-C1C	4.64	1.47	1.38
21	24	412	CL7	CHC-C1C	4.64	1.47	1.38
21	43	402	CL7	CHC-C1C	4.64	1.47	1.38
21	14	415	CL7	CHD-C4C	4.64	1.47	1.38
21	44	415	CL7	CHD-C4C	4.64	1.47	1.38
23	1A	404	8CT	C11-C12	4.64	1.55	1.45
21	1C	508	CL7	CHD-C4C	4.64	1.47	1.38
21	24	406	CL7	CHB-C1B	4.64	1.49	1.39
21	34	406	CL7	CHB-C1B	4.64	1.49	1.39
23	3B	617	8CT	C34-C33	4.64	1.63	1.52
21	1B	602	CL7	CHC-C1C	4.64	1.47	1.38
21	3D	405	CL7	CHD-C4C	4.64	1.47	1.38
21	13	505	CL7	CHC-C1C	4.63	1.47	1.38
21	43	406	CL7	CHC-C1C	4.63	1.47	1.38
21	43	410	CL7	CHD-C4C	4.63	1.47	1.38
21	44	407	CL7	CHB-C1B	4.63	1.49	1.39
21	12	508	CL7	CHB-C1B	4.63	1.49	1.39
21	42	508	CL7	CHB-C1B	4.63	1.49	1.39
21	1C	512	CL7	CHD-C4C	4.63	1.47	1.38
21	34	415	CL7	CHD-C4C	4.63	1.47	1.38
21	43	418	CL7	CHC-C1C	4.63	1.47	1.38
21	24	407	CL7	CHB-C1B	4.63	1.49	1.39
21	1C	509	CL7	CHD-C4C	4.63	1.47	1.38
21	4C	509	CL7	CHD-C4C	4.63	1.47	1.38
21	21	403	CL7	CHB-C1B	4.63	1.49	1.39
21	31	403	CL7	CHB-C1B	4.63	1.49	1.39
21	2B	614	CL7	CHC-C1C	4.63	1.47	1.38
21	44	409	CL7	CHB-C1B	4.63	1.49	1.39
21	22	517	CL7	CHD-C4C	4.63	1.47	1.38
21	2B	605	CL7	CHB-C1B	4.63	1.49	1.39
21	3B	604	CL7	CHB-C1B	4.63	1.49	1.39
23	2C	515	8CT	C24-C25	4.63	1.57	1.43
23	3C	515	8CT	C24-C25	4.63	1.57	1.43
21	33	514	CL7	CHC-C1C	4.63	1.47	1.38
21	4B	606	CL7	CHD-C4C	4.63	1.47	1.38
21	1B	604	CL7	CHB-C1B	4.63	1.49	1.39
21	22	505	CL7	CHB-C1B	4.63	1.49	1.39
21	23	415	CL7	CHC-C1C	4.63	1.47	1.38
21	3C	508	CL7	CHD-C4C	4.63	1.47	1.38
21	1B	611	CL7	CHD-C4C	4.63	1.47	1.38
21	22	513	CL7	CHC-C1C	4.63	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2B	602	CL7	CHB-C1B	4.63	1.49	1.39
21	3B	601	CL7	CHB-C1B	4.63	1.49	1.39
23	1C	515	8CT	C24-C25	4.63	1.57	1.43
23	4C	515	8CT	C24-C25	4.63	1.57	1.43
21	21	406	CL7	CHB-C1B	4.63	1.49	1.39
21	2B	606	CL7	CHD-C4C	4.63	1.47	1.38
21	3B	605	CL7	CHD-C4C	4.63	1.47	1.38
21	32	513	CL7	CHC-C1C	4.63	1.47	1.38
21	31	406	CL7	CHC-C1C	4.63	1.47	1.38
21	33	505	CL7	CHC-C1C	4.63	1.47	1.38
21	3B	604	CL7	CHD-C4C	4.62	1.47	1.38
21	21	420	CL7	CHB-C1B	4.62	1.49	1.39
21	23	405	CL7	CHD-C4C	4.62	1.47	1.38
21	44	407	CL7	CHD-C4C	4.62	1.47	1.38
21	42	516	CL7	CHD-C4C	4.62	1.47	1.38
21	22	512	CL7	CHB-C1B	4.62	1.49	1.39
21	3C	512	CL7	CHD-C4C	4.62	1.47	1.38
21	1B	605	CL7	CHC-C1C	4.62	1.47	1.38
21	23	402	CL7	CHC-C1C	4.62	1.47	1.38
21	23	418	CL7	CHC-C1C	4.62	1.47	1.38
21	33	509	CL7	CHD-C4C	4.62	1.47	1.38
21	22	508	CL7	CHB-C1B	4.62	1.49	1.39
21	32	508	CL7	CHB-C1B	4.62	1.49	1.39
21	11	406	CL7	CHC-C1C	4.62	1.47	1.38
21	13	504	CL7	CHD-C4C	4.62	1.47	1.38
21	24	410	CL7	CHC-C1C	4.62	1.47	1.38
21	34	410	CL7	CHC-C1C	4.62	1.47	1.38
21	41	406	CL7	CHC-C1C	4.62	1.47	1.38
21	41	406	CL7	CHD-C4C	4.62	1.47	1.38
21	34	407	CL7	CHB-C1B	4.62	1.49	1.39
21	43	411	CL7	CHC-C1C	4.62	1.47	1.38
21	41	406	CL7	CHB-C1B	4.62	1.49	1.39
21	12	515	CL7	CHB-C1B	4.62	1.49	1.39
21	14	414	CL7	CHD-C4C	4.62	1.47	1.38
21	44	406	CL7	CHD-C4C	4.62	1.47	1.38
21	44	414	CL7	CHD-C4C	4.62	1.47	1.38
21	1B	601	CL7	CHB-C1B	4.62	1.49	1.39
21	4B	602	CL7	CHB-C1B	4.62	1.49	1.39
21	23	406	CL7	CHC-C1C	4.62	1.47	1.38
21	13	516	CL7	CHC-C1C	4.61	1.47	1.38
21	43	417	CL7	CHC-C1C	4.61	1.47	1.38
21	43	416	CL7	CHB-C1B	4.61	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	416	CL7	CHB-C1B	4.61	1.49	1.39
21	1C	507	CL7	CHC-C1C	4.61	1.47	1.38
21	13	510	CL7	CHC-C1C	4.61	1.47	1.38
21	14	410	CL7	CHC-C1C	4.61	1.47	1.38
21	4B	616	CL7	CHB-C1B	4.61	1.49	1.39
23	1B	617	8CT	C34-C33	4.61	1.63	1.52
23	4B	618	8CT	C34-C33	4.61	1.63	1.52
21	23	411	CL7	CHC-C1C	4.61	1.47	1.38
23	2B	618	8CT	C34-C33	4.61	1.63	1.52
21	3C	509	CL7	CHD-C4C	4.61	1.47	1.38
21	14	407	CL7	CHB-C1B	4.61	1.49	1.39
21	23	410	CL7	CHD-C4C	4.61	1.47	1.38
21	41	402	CL7	CHB-C1B	4.61	1.49	1.39
21	3B	612	CL7	CHD-C4C	4.61	1.47	1.38
21	33	517	CL7	CHC-C1C	4.61	1.47	1.38
21	11	406	CL7	CHB-C1B	4.61	1.49	1.39
21	14	413	CL7	CHC-C1C	4.61	1.47	1.38
21	33	511	CL7	CHC-C1C	4.61	1.47	1.38
21	4B	614	CL7	CHC-C1C	4.61	1.47	1.38
21	1C	503	CL7	CHB-C1B	4.61	1.49	1.39
21	1B	605	CL7	CHD-C4C	4.61	1.47	1.38
21	34	414	CL7	CHD-C4C	4.61	1.47	1.38
21	22	518	CL7	CHB-C1B	4.61	1.49	1.39
21	42	517	CL7	CHD-C4C	4.60	1.47	1.38
21	12	507	CL7	CHB-C1B	4.60	1.49	1.39
21	13	514	CL7	CHC-C1C	4.60	1.47	1.38
21	33	511	CL7	CHD-C4C	4.60	1.47	1.38
21	43	415	CL7	CHC-C1C	4.60	1.47	1.38
21	1C	501	CL7	CHB-C1B	4.60	1.49	1.39
21	2C	501	CL7	CHB-C1B	4.60	1.49	1.39
21	3C	501	CL7	CHB-C1B	4.60	1.49	1.39
21	12	517	CL7	CHD-C4C	4.60	1.47	1.38
21	2B	607	CL7	CHC-C1C	4.60	1.47	1.38
21	3B	606	CL7	CHC-C1C	4.60	1.47	1.38
21	4B	611	CL7	CHC-C1C	4.60	1.47	1.38
21	2B	608	CL7	CHC-C1C	4.60	1.47	1.38
21	3B	607	CL7	CHC-C1C	4.60	1.47	1.38
21	13	514	CL7	CHB-C1B	4.60	1.49	1.39
21	31	402	CL7	CHB-C1B	4.60	1.49	1.39
21	34	413	CL7	CHC-C1C	4.60	1.47	1.38
21	3D	402	CL7	CHB-C1B	4.60	1.49	1.39
21	13	517	CL7	CHC-C1C	4.60	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	407	CL7	CHD-C4C	4.60	1.47	1.38
21	23	412	CL7	CHD-C4C	4.60	1.47	1.38
21	4A	401	CL7	CHB-C1B	4.60	1.49	1.39
21	1B	615	CL7	CHB-C1B	4.60	1.49	1.39
21	4C	512	CL7	CHD-C4C	4.60	1.47	1.38
21	2B	616	CL7	CHB-C1B	4.60	1.49	1.39
21	13	511	CL7	CHD-C4C	4.59	1.47	1.38
21	21	406	CL7	CHD-C4C	4.59	1.47	1.38
21	1B	612	CL7	CHD-C4C	4.59	1.47	1.38
21	4B	613	CL7	CHD-C4C	4.59	1.47	1.38
21	33	515	CL7	CHB-C1B	4.59	1.49	1.39
23	1A	404	8CT	C14-C13	4.59	1.57	1.43
23	4A	404	8CT	C14-C13	4.59	1.57	1.43
21	12	510	CL7	CHC-C1C	4.59	1.47	1.38
21	43	405	CL7	CHD-C4C	4.59	1.47	1.38
23	2A	404	8CT	C14-C13	4.59	1.57	1.43
21	3C	513	CL7	CHB-C1B	4.59	1.49	1.39
21	22	501	CL7	CHC-C1C	4.59	1.47	1.38
21	34	407	CL7	CHD-C4C	4.59	1.47	1.38
21	1C	508	CL7	CHC-C1C	4.59	1.47	1.38
21	33	516	CL7	CHC-C1C	4.59	1.47	1.38
21	23	415	CL7	CHB-C1B	4.59	1.49	1.39
21	32	517	CL7	CHD-C4C	4.59	1.47	1.38
21	33	507	CL7	CHB-C1B	4.59	1.49	1.39
21	21	402	CL7	CHB-C1B	4.58	1.49	1.39
21	33	514	CL7	CHB-C1B	4.58	1.49	1.39
21	11	405	CL7	CHB-C1B	4.58	1.49	1.39
21	4C	511	CL7	CHB-C1B	4.58	1.49	1.39
21	31	406	CL7	CHB-C1B	4.58	1.49	1.39
21	3B	613	CL7	CHC-C1C	4.58	1.47	1.38
21	12	518	CL7	CHB-C1B	4.58	1.49	1.39
21	42	518	CL7	CHB-C1B	4.58	1.49	1.39
21	13	509	CL7	CHD-C4C	4.58	1.47	1.38
21	33	508	CL7	CHB-C1B	4.58	1.49	1.39
21	13	506	CL7	CHB-C1B	4.58	1.49	1.39
23	1C	514	8CT	C14-C13	4.58	1.57	1.43
21	13	507	CL7	CHB-C1B	4.58	1.49	1.39
21	24	416	CL7	CHB-C1B	4.58	1.49	1.39
21	32	518	CL7	CHB-C1B	4.58	1.49	1.39
21	2C	511	CL7	CHB-C1B	4.58	1.49	1.39
21	3C	511	CL7	CHB-C1B	4.58	1.49	1.39
21	1B	610	CL7	CHC-C1C	4.58	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2C	512	CL7	CHD-C4C	4.58	1.47	1.38
21	23	404	CL7	CHD-C4C	4.58	1.47	1.38
21	23	412	CL7	CHC-C1C	4.58	1.47	1.38
21	33	503	CL7	CHD-C4C	4.58	1.47	1.38
21	2C	513	CL7	CHB-C1B	4.58	1.49	1.39
21	3C	503	CL7	CHB-C1B	4.58	1.49	1.39
21	3B	615	CL7	CHB-C1B	4.58	1.49	1.39
21	3B	610	CL7	CHC-C1C	4.58	1.47	1.38
21	1C	513	CL7	CHB-C1B	4.58	1.49	1.39
21	23	416	CL7	CHB-C1B	4.58	1.49	1.39
21	4C	513	CL7	CHB-C1B	4.58	1.49	1.39
21	44	413	CL7	CHC-C1C	4.57	1.47	1.38
21	13	515	CL7	CHB-C1B	4.57	1.49	1.39
21	13	511	CL7	CHC-C1C	4.57	1.47	1.38
23	3A	404	8CT	C14-C13	4.57	1.57	1.43
21	22	507	CL7	CHB-C1B	4.57	1.49	1.39
21	32	507	CL7	CHB-C1B	4.57	1.49	1.39
23	3B	618	8CT	C35-C30	4.57	1.69	1.56
21	34	416	CL7	CHB-C1B	4.57	1.49	1.39
21	4D	402	CL7	CHB-C1B	4.57	1.49	1.39
23	4C	514	8CT	C14-C13	4.57	1.57	1.43
21	43	404	CL7	CHD-C4C	4.57	1.47	1.38
21	14	416	CL7	CHB-C1B	4.57	1.49	1.39
21	2C	509	CL7	CHC-C1C	4.57	1.47	1.38
21	22	506	CL7	CHC-C1C	4.57	1.47	1.38
21	43	412	CL7	CHD-C4C	4.57	1.47	1.38
23	1C	515	8CT	C35-C30	4.57	1.69	1.56
21	1B	605	CL7	CHB-C1B	4.57	1.49	1.39
21	11	402	CL7	CHB-C1B	4.57	1.49	1.39
21	41	405	CL7	CHB-C1B	4.57	1.49	1.39
21	24	407	CL7	CHD-C4C	4.57	1.47	1.38
21	1D	402	CL7	CHB-C1B	4.57	1.49	1.39
21	42	507	CL7	CHB-C1B	4.57	1.49	1.39
21	2C	503	CL7	CHB-C1B	4.57	1.49	1.39
21	2A	401	CL7	CHB-C1B	4.57	1.49	1.39
21	43	408	CL7	CHB-C1B	4.57	1.49	1.39
21	24	413	CL7	CHC-C1C	4.57	1.47	1.38
23	4C	515	8CT	C35-C30	4.56	1.69	1.56
21	42	506	CL7	CHC-C1C	4.56	1.47	1.38
23	2C	515	8CT	C35-C30	4.56	1.69	1.56
21	23	407	CL7	CHB-C1B	4.56	1.49	1.39
21	4C	501	CL7	CHB-C1B	4.56	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4C	503	CL7	CHB-C1B	4.56	1.49	1.39
21	1D	405	CL7	CHB-C1B	4.56	1.49	1.39
23	2B	619	8CT	C14-C13	4.56	1.57	1.43
23	1B	618	8CT	C35-C30	4.56	1.69	1.56
23	4B	619	8CT	C35-C30	4.56	1.69	1.56
21	12	506	CL7	CHC-C1C	4.56	1.47	1.38
21	43	407	CL7	CHB-C1B	4.56	1.49	1.39
21	13	512	CL7	CHC-C1C	4.56	1.47	1.38
21	43	413	CL7	CHC-C1C	4.56	1.47	1.38
21	2D	402	CL7	CHB-C1B	4.56	1.49	1.39
21	21	405	CL7	CHB-C1B	4.56	1.49	1.39
21	31	405	CL7	CHB-C1B	4.56	1.49	1.39
23	2B	619	8CT	C35-C30	4.56	1.69	1.56
23	3C	514	8CT	C14-C13	4.56	1.57	1.43
21	4C	507	CL7	CHC-C1C	4.56	1.47	1.38
21	11	414	CL7	CHB-C1B	4.56	1.49	1.39
21	41	414	CL7	CHB-C1B	4.56	1.49	1.39
23	1A	404	8CT	C35-C30	4.56	1.69	1.56
23	3A	404	8CT	C35-C30	4.56	1.69	1.56
21	43	415	CL7	CHB-C1B	4.56	1.49	1.39
21	44	410	CL7	CHB-C1B	4.56	1.49	1.39
21	33	504	CL7	CHD-C4C	4.56	1.47	1.38
23	1B	618	8CT	C14-C13	4.55	1.57	1.43
23	4B	619	8CT	C14-C13	4.55	1.57	1.43
21	21	414	CL7	CHB-C1B	4.55	1.49	1.39
21	32	515	CL7	CHC-C1C	4.55	1.47	1.38
21	43	404	CL7	CHB-C1B	4.55	1.49	1.39
21	2B	613	CL7	CHD-C4C	4.55	1.47	1.38
21	2C	508	CL7	CHC-C1C	4.55	1.47	1.38
21	3C	508	CL7	CHC-C1C	4.55	1.47	1.38
21	1B	609	CL7	CHC-C1C	4.55	1.47	1.38
21	13	505	CL7	CHD-C4C	4.55	1.47	1.38
21	43	406	CL7	CHD-C4C	4.55	1.47	1.38
21	3B	605	CL7	CHB-C1B	4.55	1.49	1.39
21	23	406	CL7	CHD-C4C	4.55	1.47	1.38
21	33	505	CL7	CHD-C4C	4.55	1.47	1.38
23	2C	514	8CT	C14-C13	4.55	1.57	1.43
21	1B	611	CL7	CHB-C1B	4.55	1.49	1.39
23	2A	404	8CT	C35-C30	4.55	1.69	1.56
23	3C	515	8CT	C35-C30	4.55	1.69	1.56
21	1C	511	CL7	CHB-C1B	4.55	1.49	1.39
21	12	515	CL7	CHC-C1C	4.55	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	14	402	8CT	C35-C30	4.55	1.69	1.56
23	44	402	8CT	C35-C30	4.55	1.69	1.56
21	13	503	CL7	CHD-C4C	4.55	1.47	1.38
23	44	402	8CT	C14-C13	4.55	1.57	1.43
21	2B	609	CL7	CHC-C1C	4.55	1.47	1.38
21	3B	608	CL7	CHC-C1C	4.55	1.47	1.38
21	1A	403	CL7	CHD-C4C	4.55	1.47	1.38
21	32	501	CL7	CHC-C1C	4.55	1.47	1.38
23	3B	618	8CT	C14-C13	4.55	1.57	1.43
21	32	506	CL7	CHC-C1C	4.54	1.47	1.38
21	3A	401	CL7	CHB-C1B	4.54	1.49	1.39
21	4D	405	CL7	CHB-C1B	4.54	1.49	1.39
21	1A	401	CL7	CHB-C1B	4.54	1.49	1.39
21	43	409	CL7	CHB-C1B	4.54	1.49	1.39
21	43	412	CL7	CHC-C1C	4.54	1.47	1.38
21	14	414	CL7	CHB-C1B	4.54	1.49	1.39
21	23	409	CL7	CHB-C1B	4.54	1.49	1.39
21	22	505	CL7	CHD-C4C	4.54	1.47	1.38
21	1C	517	CL7	CHB-C1B	4.54	1.49	1.39
21	3B	610	CL7	CHD-C4C	4.54	1.47	1.38
21	42	510	CL7	CHC-C1C	4.54	1.47	1.38
21	2B	610	CL7	CHC-C1C	4.54	1.47	1.38
21	3B	609	CL7	CHC-C1C	4.54	1.47	1.38
21	4C	508	CL7	CHC-C1C	4.54	1.47	1.38
21	4C	517	CL7	CHB-C1B	4.54	1.49	1.39
21	33	512	CL7	CHC-C1C	4.53	1.47	1.38
21	24	410	CL7	CHB-C1B	4.53	1.49	1.39
21	34	410	CL7	CHB-C1B	4.53	1.49	1.39
23	14	402	8CT	C14-C13	4.53	1.57	1.43
21	1C	509	CL7	CHC-C1C	4.53	1.47	1.38
21	4C	509	CL7	CHC-C1C	4.53	1.47	1.38
21	4B	612	CL7	CHB-C1B	4.53	1.49	1.39
21	1B	608	CL7	CHC-C1C	4.53	1.47	1.38
21	4B	609	CL7	CHC-C1C	4.53	1.47	1.38
21	21	411	CL7	CHB-C1B	4.53	1.49	1.39
21	12	516	CL7	CHB-C1B	4.53	1.49	1.39
21	42	516	CL7	CHB-C1B	4.53	1.49	1.39
21	2C	507	CL7	CHC-C1C	4.53	1.47	1.38
21	22	510	CL7	CHC-C1C	4.53	1.47	1.38
21	3C	507	CL7	CHC-C1C	4.53	1.47	1.38
21	32	510	CL7	CHC-C1C	4.53	1.47	1.38
21	2C	517	CL7	CHB-C1B	4.53	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	22	516	CL7	CHB-C1B	4.53	1.49	1.39
21	21	409	CL7	CHB-C1B	4.53	1.49	1.39
23	24	402	8CT	C14-C13	4.53	1.57	1.43
23	34	402	8CT	C14-C13	4.53	1.57	1.43
23	24	402	8CT	C35-C30	4.53	1.69	1.56
23	34	402	8CT	C35-C30	4.53	1.69	1.56
21	21	408	CL7	CHB-C1B	4.53	1.49	1.39
21	31	408	CL7	CHB-C1B	4.53	1.49	1.39
21	12	505	CL7	CHD-C4C	4.53	1.47	1.38
21	2D	405	CL7	CHB-C1B	4.53	1.49	1.39
21	3D	405	CL7	CHB-C1B	4.53	1.49	1.39
21	4B	610	CL7	CHC-C1C	4.53	1.47	1.38
21	4B	611	CL7	CHD-C4C	4.53	1.47	1.38
21	23	408	CL7	CHB-C1B	4.53	1.49	1.39
21	3B	611	CL7	CHB-C1B	4.53	1.49	1.39
21	4B	606	CL7	CHB-C1B	4.53	1.49	1.39
21	3C	517	CL7	CHB-C1B	4.52	1.49	1.39
23	4A	404	8CT	C35-C30	4.52	1.69	1.56
21	44	408	CL7	CHB-C1B	4.52	1.49	1.39
21	23	404	CL7	CHB-C1B	4.52	1.49	1.39
21	24	414	CL7	CHB-C1B	4.52	1.49	1.39
21	34	414	CL7	CHB-C1B	4.52	1.49	1.39
21	2A	403	CL7	CHD-C4C	4.52	1.47	1.38
21	3A	403	CL7	CHD-C4C	4.52	1.47	1.38
21	1A	407	CL7	CHB-C1B	4.52	1.49	1.39
21	3C	509	CL7	CHC-C1C	4.52	1.47	1.38
21	23	413	CL7	CHC-C1C	4.52	1.47	1.38
21	2B	612	CL7	CHB-C1B	4.52	1.49	1.39
21	33	506	CL7	CHB-C1B	4.52	1.49	1.39
21	12	501	CL7	CHC-C1C	4.52	1.47	1.38
21	42	501	CL7	CHC-C1C	4.52	1.47	1.38
21	12	511	CL7	CHB-C1B	4.52	1.49	1.39
21	11	411	CL7	CHB-C1B	4.52	1.49	1.39
21	1C	505	CL7	CHC-C1C	4.51	1.47	1.38
21	4C	505	CL7	CHC-C1C	4.51	1.47	1.38
21	41	409	CL7	CHB-C1B	4.51	1.49	1.39
21	42	505	CL7	CHD-C4C	4.51	1.47	1.38
21	12	513	CL7	CHB-C1B	4.51	1.49	1.39
21	11	409	CL7	CHB-C1B	4.51	1.49	1.39
21	1C	512	CL7	CHB-C1B	4.51	1.49	1.39
21	13	508	CL7	CHB-C1B	4.51	1.49	1.39
21	4C	512	CL7	CHB-C1B	4.51	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	43	406	CL7	CHB-C1B	4.51	1.49	1.39
21	31	411	CL7	CHB-C1B	4.51	1.49	1.39
21	13	503	CL7	CHB-C1B	4.51	1.49	1.39
21	42	515	CL7	CHC-C1C	4.51	1.47	1.38
21	22	513	CL7	CHB-C1B	4.51	1.49	1.39
21	41	418	CL7	CHB-C1B	4.51	1.49	1.39
21	33	503	CL7	CHB-C1B	4.51	1.49	1.39
21	2B	611	CL7	CHC-C1C	4.51	1.47	1.38
21	24	414	CL7	CHC-C1C	4.51	1.47	1.38
21	2B	606	CL7	CHB-C1B	4.51	1.49	1.39
21	3A	407	CL7	CHB-C1B	4.51	1.49	1.39
21	12	514	CL7	CHB-C1B	4.51	1.49	1.39
21	4B	603	CL7	CHB-C1B	4.51	1.49	1.39
21	4C	508	CL7	CHB-C1B	4.51	1.49	1.39
21	41	411	CL7	CHB-C1B	4.51	1.49	1.39
21	14	410	CL7	CHB-C1B	4.50	1.49	1.39
21	32	505	CL7	CHD-C4C	4.50	1.47	1.38
21	11	418	CL7	CHC-C1C	4.50	1.47	1.38
23	1B	619	8CT	C14-C13	4.50	1.57	1.43
23	4B	620	8CT	C14-C13	4.50	1.57	1.43
21	13	505	CL7	CHB-C1B	4.50	1.49	1.39
21	24	408	CL7	CHB-C1B	4.50	1.49	1.39
21	34	408	CL7	CHB-C1B	4.50	1.49	1.39
21	4B	609	CL7	CHB-C1B	4.50	1.49	1.39
23	1K	101	8CT	C18-C17	4.50	1.57	1.43
21	2B	611	CL7	CHD-C4C	4.50	1.47	1.38
21	2B	609	CL7	CHB-C1B	4.50	1.49	1.39
21	31	403	CL7	CHC-C1C	4.50	1.47	1.38
21	44	414	CL7	CHB-C1B	4.50	1.49	1.39
21	23	406	CL7	CHB-C1B	4.50	1.49	1.39
21	14	408	CL7	CHB-C1B	4.50	1.49	1.39
21	3B	608	CL7	CHB-C1B	4.50	1.49	1.39
21	24	415	CL7	CHB-C1B	4.50	1.49	1.39
21	14	415	CL7	CHB-C1B	4.50	1.49	1.39
21	33	505	CL7	CHB-C1B	4.50	1.49	1.39
21	2C	505	CL7	CHC-C1C	4.50	1.47	1.38
21	3C	505	CL7	CHC-C1C	4.50	1.47	1.38
21	31	414	CL7	CHB-C1B	4.50	1.49	1.39
23	3B	626	8CT	C24-C25	4.49	1.57	1.43
21	1C	508	CL7	CHB-C1B	4.49	1.49	1.39
21	4A	401	CL7	O2D-CGD	4.49	1.44	1.33
23	2B	601	8CT	C24-C25	4.49	1.57	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4A	403	CL7	CHD-C4C	4.49	1.47	1.38
23	1B	626	8CT	C24-C25	4.49	1.57	1.43
21	1B	610	CL7	CHD-C4C	4.49	1.47	1.38
21	2A	407	CL7	CHB-C1B	4.49	1.49	1.39
21	31	418	CL7	CHC-C1C	4.49	1.47	1.38
21	2B	603	CL7	CHB-C1B	4.49	1.49	1.39
21	31	409	CL7	CHB-C1B	4.49	1.49	1.39
21	22	514	CL7	CHB-C1B	4.49	1.49	1.39
21	32	514	CL7	CHB-C1B	4.49	1.49	1.39
21	32	516	CL7	CHB-C1B	4.49	1.49	1.39
21	11	408	CL7	CHB-C1B	4.49	1.49	1.39
21	22	506	CL7	CHB-C1B	4.49	1.49	1.39
21	32	506	CL7	CHB-C1B	4.49	1.49	1.39
21	41	408	CL7	CHB-C1B	4.49	1.49	1.39
21	1D	405	CL7	CHC-C1C	4.49	1.47	1.38
21	22	515	CL7	CHC-C1C	4.48	1.47	1.38
21	1B	602	CL7	CHB-C1B	4.48	1.49	1.39
21	2C	508	CL7	CHB-C1B	4.48	1.49	1.39
21	3C	508	CL7	CHB-C1B	4.48	1.49	1.39
21	21	403	CL7	CHC-C1C	4.48	1.47	1.38
21	32	517	CL7	CHB-C1B	4.48	1.49	1.39
21	31	418	CL7	CHB-C1B	4.48	1.49	1.39
21	2C	504	CL7	CHB-C1B	4.48	1.49	1.39
21	42	511	CL7	CHB-C1B	4.48	1.49	1.39
23	2B	620	8CT	C14-C13	4.48	1.57	1.43
23	3B	619	8CT	C14-C13	4.48	1.57	1.43
21	1C	504	CL7	CHB-C1B	4.48	1.49	1.39
21	1C	505	CL7	CHB-C1B	4.48	1.49	1.39
21	4C	505	CL7	CHB-C1B	4.48	1.49	1.39
21	22	511	CL7	CHB-C1B	4.48	1.49	1.39
21	32	511	CL7	CHB-C1B	4.48	1.49	1.39
21	4A	407	CL7	CHB-C1B	4.48	1.49	1.39
21	14	409	CL7	CHC-C1C	4.48	1.47	1.38
23	4K	101	8CT	C18-C17	4.48	1.57	1.43
21	32	503	CL7	CHD-C4C	4.48	1.47	1.38
21	44	414	CL7	CHC-C1C	4.48	1.47	1.38
21	32	514	CL7	CHC-C1C	4.48	1.47	1.38
21	3C	505	CL7	CHB-C1B	4.47	1.49	1.39
21	3C	517	CL7	CHC-C1C	4.47	1.47	1.38
21	11	418	CL7	CHB-C1B	4.47	1.49	1.39
21	2C	512	CL7	CHB-C1B	4.47	1.49	1.39
21	3C	512	CL7	CHB-C1B	4.47	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	513	CL7	CHB-C1B	4.47	1.49	1.39
21	1C	517	CL7	CHC-C1C	4.47	1.47	1.38
21	4C	517	CL7	CHC-C1C	4.47	1.47	1.38
21	12	503	CL7	CHD-C4C	4.47	1.47	1.38
21	11	403	CL7	CHC-C1C	4.47	1.47	1.38
21	42	503	CL7	CHD-C4C	4.47	1.47	1.38
21	13	504	CL7	CHB-C1B	4.47	1.49	1.39
21	43	405	CL7	CHB-C1B	4.47	1.49	1.39
21	41	403	CL7	CHC-C1C	4.47	1.47	1.38
21	2C	505	CL7	CHB-C1B	4.47	1.49	1.39
21	44	412	CL7	CHB-C1B	4.47	1.49	1.39
23	44	402	8CT	C11-C12	4.47	1.55	1.45
21	32	504	CL7	CHB-C1B	4.47	1.49	1.39
21	2C	512	CL7	CHC-C1C	4.47	1.47	1.38
23	2D	406	8CT	C24-C25	4.47	1.57	1.43
21	2C	517	CL7	CHC-C1C	4.47	1.47	1.38
21	21	418	CL7	CHC-C1C	4.47	1.47	1.38
21	24	412	CL7	CHB-C1B	4.47	1.49	1.39
21	34	414	CL7	CHC-C1C	4.47	1.47	1.38
21	2A	401	CL7	O2D-CGD	4.46	1.44	1.33
21	12	506	CL7	CHB-C1B	4.46	1.49	1.39
21	42	506	CL7	CHB-C1B	4.46	1.49	1.39
21	42	517	CL7	CHB-C1B	4.46	1.49	1.39
21	22	517	CL7	CHB-C1B	4.46	1.49	1.39
21	4D	405	CL7	CHC-C1C	4.46	1.47	1.38
21	22	502	CL7	CHC-C1C	4.46	1.47	1.38
21	14	414	CL7	CHC-C1C	4.46	1.47	1.38
23	4B	601	8CT	C24-C25	4.46	1.57	1.43
23	2K	101	8CT	C18-C17	4.46	1.57	1.43
23	3K	101	8CT	C18-C17	4.46	1.57	1.43
21	1C	512	CL7	CHC-C1C	4.46	1.47	1.38
21	4C	512	CL7	CHC-C1C	4.46	1.47	1.38
21	3B	602	CL7	CHB-C1B	4.46	1.49	1.39
21	1A	401	CL7	O2D-CGD	4.46	1.44	1.33
21	42	514	CL7	CHB-C1B	4.46	1.49	1.39
23	4D	406	8CT	C24-C25	4.46	1.57	1.43
21	4C	501	CL7	CHD-C4C	4.46	1.47	1.38
21	32	502	CL7	CHC-C1C	4.46	1.47	1.38
23	24	402	8CT	C11-C12	4.46	1.55	1.45
23	3D	406	8CT	C24-C25	4.46	1.57	1.43
21	1B	608	CL7	CHB-C1B	4.46	1.49	1.39
21	41	418	CL7	CHC-C1C	4.46	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3A	401	CL7	O2D-CGD	4.46	1.44	1.33
23	14	402	8CT	C11-C12	4.46	1.55	1.45
21	32	513	CL7	CHB-C1B	4.45	1.49	1.39
21	44	415	CL7	CHB-C1B	4.45	1.49	1.39
21	23	414	CL7	CHB-C1B	4.45	1.49	1.39
21	13	518	CL7	CHB-C1B	4.45	1.49	1.39
21	2D	405	CL7	CHC-C1C	4.45	1.47	1.38
21	3D	405	CL7	CHC-C1C	4.45	1.47	1.38
21	12	503	CL7	CHB-C1B	4.45	1.49	1.39
21	4D	404	CL7	CHB-C1B	4.45	1.49	1.39
21	12	517	CL7	CHB-C1B	4.45	1.49	1.39
21	3B	609	CL7	CHB-C1B	4.45	1.49	1.39
21	43	414	CL7	CHB-C1B	4.45	1.49	1.39
21	12	514	CL7	CHC-C1C	4.45	1.47	1.38
21	33	508	CL7	CHC-C1C	4.45	1.47	1.38
21	42	514	CL7	CHC-C1C	4.45	1.47	1.38
21	32	509	CL7	CHB-C1B	4.45	1.49	1.39
21	13	508	CL7	CHC-C1C	4.45	1.47	1.38
21	22	503	CL7	CHB-C1B	4.45	1.49	1.39
21	14	412	CL7	CHB-C1B	4.45	1.49	1.39
21	23	409	CL7	CHC-C1C	4.45	1.47	1.38
21	3C	501	CL7	CHD-C4C	4.45	1.47	1.38
21	1C	510	CL7	CHB-C1B	4.45	1.49	1.39
21	4C	510	CL7	CHB-C1B	4.45	1.49	1.39
21	21	418	CL7	CHB-C1B	4.44	1.49	1.39
23	34	402	8CT	C11-C12	4.44	1.55	1.45
21	3C	512	CL7	CHC-C1C	4.44	1.47	1.38
21	2C	510	CL7	CHB-C1B	4.44	1.49	1.39
21	3C	510	CL7	CHB-C1B	4.44	1.49	1.39
21	4C	504	CL7	CHB-C1B	4.44	1.49	1.39
21	12	502	CL7	CHC-C1C	4.44	1.47	1.38
21	42	502	CL7	CHC-C1C	4.44	1.47	1.38
21	43	402	CL7	CHB-C1B	4.44	1.49	1.39
21	42	507	CL7	CHC-C1C	4.44	1.47	1.38
21	3C	502	CL7	CHB-C1B	4.44	1.49	1.39
21	34	415	CL7	CHB-C1B	4.44	1.49	1.39
21	12	504	CL7	CHB-C1B	4.44	1.49	1.39
21	23	419	CL7	CHB-C1B	4.44	1.49	1.39
21	3C	504	CL7	CHB-C1B	4.44	1.49	1.39
21	33	518	CL7	CHB-C1B	4.44	1.49	1.39
21	13	513	CL7	CHB-C1B	4.44	1.49	1.39
21	23	402	CL7	CHB-C1B	4.44	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	33	501	CL7	CHB-C1B	4.44	1.49	1.39
21	2B	610	CL7	CHB-C1B	4.44	1.49	1.39
21	2C	502	CL7	CHB-C1B	4.44	1.49	1.39
21	3D	404	CL7	CHB-C1B	4.44	1.49	1.39
21	41	407	CL7	CHB-C1B	4.44	1.49	1.39
21	24	409	CL7	CHC-C1C	4.44	1.47	1.38
21	34	409	CL7	CHC-C1C	4.44	1.47	1.38
21	4B	610	CL7	CHB-C1B	4.44	1.49	1.39
21	33	504	CL7	CHB-C1B	4.44	1.49	1.39
21	44	409	CL7	CHC-C1C	4.44	1.47	1.38
23	2C	518	8CT	C24-C25	4.43	1.57	1.43
21	2B	611	CL7	CHB-C1B	4.43	1.49	1.39
21	1A	403	CL7	CHB-C1B	4.43	1.49	1.39
21	42	509	CL7	CHB-C1B	4.43	1.49	1.39
23	3B	619	8CT	C35-C30	4.43	1.68	1.56
23	1B	619	8CT	C35-C30	4.43	1.68	1.56
23	4B	620	8CT	C35-C30	4.43	1.68	1.56
23	1D	406	8CT	C24-C25	4.43	1.57	1.43
21	1D	404	CL7	CHB-C1B	4.43	1.49	1.39
21	23	405	CL7	CHB-C1B	4.43	1.49	1.39
23	4D	406	8CT	C28-C26	4.43	1.55	1.45
21	22	503	CL7	CHD-C4C	4.43	1.47	1.38
21	43	409	CL7	CHC-C1C	4.43	1.47	1.38
21	42	504	CL7	CHB-C1B	4.43	1.49	1.39
23	2D	406	8CT	C28-C26	4.43	1.55	1.45
23	3D	406	8CT	C28-C26	4.43	1.55	1.45
21	21	407	CL7	CHB-C1B	4.43	1.49	1.39
21	31	407	CL7	CHB-C1B	4.43	1.49	1.39
21	34	412	CL7	CHB-C1B	4.43	1.49	1.39
21	22	504	CL7	CHB-C1B	4.43	1.49	1.39
21	1C	509	CL7	CHB-C1B	4.43	1.49	1.39
21	22	514	CL7	CHC-C1C	4.42	1.47	1.38
21	13	501	CL7	CHB-C1B	4.42	1.49	1.39
21	43	419	CL7	CHB-C1B	4.42	1.49	1.39
21	1C	502	CL7	CHB-C1B	4.42	1.49	1.39
21	4C	502	CL7	CHB-C1B	4.42	1.49	1.39
23	4C	518	8CT	C24-C25	4.42	1.57	1.43
23	1C	518	8CT	C24-C25	4.42	1.57	1.43
21	1C	501	CL7	CHD-C4C	4.42	1.47	1.38
21	2C	501	CL7	CHD-C4C	4.42	1.47	1.38
21	12	510	CL7	CHB-C1B	4.42	1.49	1.39
21	42	510	CL7	CHB-C1B	4.42	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	509	CL7	CHB-C1B	4.42	1.49	1.39
21	32	510	CL7	CHB-C1B	4.42	1.49	1.39
21	33	513	CL7	CHB-C1B	4.41	1.49	1.39
21	4C	509	CL7	CHB-C1B	4.41	1.49	1.39
21	3A	403	CL7	CHB-C1B	4.41	1.49	1.39
21	22	510	CL7	CHB-C1B	4.41	1.49	1.39
21	22	509	CL7	CHB-C1B	4.41	1.49	1.39
21	2D	404	CL7	CHB-C1B	4.41	1.49	1.39
21	4B	611	CL7	CHB-C1B	4.41	1.49	1.39
23	3C	518	8CT	C24-C25	4.41	1.57	1.43
21	12	507	CL7	CHC-C1C	4.41	1.46	1.38
21	22	501	CL7	CHB-C1B	4.41	1.49	1.39
21	32	501	CL7	CHB-C1B	4.41	1.49	1.39
21	31	410	CL7	CHB-C1B	4.41	1.49	1.39
21	3B	616	CL7	CHB-C1B	4.41	1.49	1.39
21	43	417	CL7	CHB-C1B	4.41	1.49	1.39
21	23	417	CL7	CHB-C1B	4.40	1.49	1.39
21	33	516	CL7	CHB-C1B	4.40	1.49	1.39
21	12	512	CL7	CHD-C4C	4.40	1.46	1.38
21	3B	610	CL7	CHB-C1B	4.40	1.49	1.39
21	22	512	CL7	CHD-C4C	4.40	1.46	1.38
21	32	503	CL7	CHB-C1B	4.40	1.49	1.39
23	2B	620	8CT	C35-C30	4.40	1.68	1.56
21	4A	403	CL7	CHB-C1B	4.40	1.49	1.39
21	13	509	CL7	CHB-C1B	4.40	1.49	1.39
21	41	410	CL7	CHB-C1B	4.40	1.49	1.39
21	1C	506	CL7	CHB-C1B	4.40	1.49	1.39
21	3C	509	CL7	CHB-C1B	4.40	1.49	1.39
21	4C	506	CL7	CHB-C1B	4.40	1.49	1.39
21	42	503	CL7	CHB-C1B	4.40	1.49	1.39
21	12	501	CL7	CHB-C1B	4.39	1.49	1.39
21	42	501	CL7	CHB-C1B	4.39	1.49	1.39
21	12	508	CL7	CHC-C1C	4.39	1.46	1.38
21	1B	609	CL7	CHB-C1B	4.39	1.49	1.39
21	11	410	CL7	CHB-C1B	4.39	1.49	1.39
21	1B	610	CL7	CHB-C1B	4.39	1.49	1.39
21	23	410	CL7	CHB-C1B	4.39	1.49	1.39
21	13	516	CL7	CHB-C1B	4.39	1.49	1.39
21	22	507	CL7	CHC-C1C	4.39	1.46	1.38
21	32	507	CL7	CHC-C1C	4.39	1.46	1.38
23	1D	406	8CT	C28-C26	4.39	1.55	1.45
21	23	408	CL7	CHC-C1C	4.39	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	33	507	CL7	CHC-C1C	4.39	1.46	1.38
21	22	508	CL7	CHC-C1C	4.39	1.46	1.38
21	32	508	CL7	CHC-C1C	4.39	1.46	1.38
21	11	407	CL7	CHB-C1B	4.38	1.49	1.39
23	1B	626	8CT	C18-C17	4.38	1.57	1.43
23	4B	601	8CT	C18-C17	4.38	1.57	1.43
21	11	417	CL7	CHB-C1B	4.38	1.49	1.39
21	34	404	CL7	CHB-C1B	4.38	1.49	1.39
21	2A	403	CL7	CHB-C1B	4.38	1.49	1.39
21	2C	506	CL7	CHB-C1B	4.38	1.49	1.39
21	3C	506	CL7	CHB-C1B	4.38	1.49	1.39
21	4B	617	CL7	CHB-C1B	4.38	1.49	1.39
21	1B	616	CL7	CHB-C1B	4.38	1.49	1.39
21	2D	404	CL7	CHC-C1C	4.38	1.46	1.38
21	42	512	CL7	CHD-C4C	4.38	1.46	1.38
21	32	512	CL7	CHD-C4C	4.37	1.46	1.38
21	2B	617	CL7	CHB-C1B	4.37	1.49	1.39
21	13	517	CL7	CHB-C1B	4.37	1.49	1.39
21	13	507	CL7	CHC-C1C	4.37	1.46	1.38
21	43	408	CL7	CHC-C1C	4.37	1.46	1.38
21	4B	612	CL7	CHC-C1C	4.37	1.46	1.38
21	1D	404	CL7	CHC-C1C	4.37	1.46	1.38
21	4D	404	CL7	CHC-C1C	4.37	1.46	1.38
21	21	417	CL7	CHB-C1B	4.36	1.49	1.39
21	31	417	CL7	CHB-C1B	4.36	1.49	1.39
21	2B	612	CL7	CHC-C1C	4.36	1.46	1.38
21	3B	611	CL7	CHC-C1C	4.36	1.46	1.38
21	33	512	CL7	CHB-C1B	4.36	1.49	1.39
21	43	410	CL7	CHB-C1B	4.36	1.49	1.39
21	1B	611	CL7	CHC-C1C	4.36	1.46	1.38
21	2C	509	CL7	CHB-C1B	4.36	1.49	1.39
21	21	410	CL7	CHB-C1B	4.36	1.49	1.39
21	3D	404	CL7	CHC-C1C	4.36	1.46	1.38
21	14	404	CL7	CHB-C1B	4.35	1.49	1.39
21	44	404	CL7	CHB-C1B	4.35	1.49	1.39
21	1B	622	CL7	CHB-C1B	4.35	1.49	1.39
21	4B	623	CL7	CHB-C1B	4.35	1.49	1.39
21	33	509	CL7	CHB-C1B	4.35	1.49	1.39
23	2B	601	8CT	C18-C17	4.34	1.56	1.43
23	3B	626	8CT	C18-C17	4.34	1.56	1.43
21	42	508	CL7	CHC-C1C	4.34	1.46	1.38
21	2B	623	CL7	CHB-C1B	4.34	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	622	CL7	CHB-C1B	4.34	1.49	1.39
21	43	412	CL7	CHB-C1B	4.34	1.49	1.39
21	2B	613	CL7	CHB-C1B	4.34	1.49	1.39
21	41	417	CL7	CHB-C1B	4.34	1.49	1.39
21	23	411	CL7	CHB-C1B	4.34	1.49	1.39
21	33	510	CL7	CHB-C1B	4.34	1.49	1.39
21	14	413	CL7	CHB-C1B	4.34	1.49	1.39
21	44	413	CL7	CHB-C1B	4.34	1.49	1.39
21	24	404	CL7	CHB-C1B	4.33	1.49	1.39
21	1B	607	CL7	CHB-C1B	4.33	1.49	1.39
21	23	412	CL7	CHB-C1B	4.33	1.49	1.39
21	24	413	CL7	CHB-C1B	4.33	1.49	1.39
21	34	413	CL7	CHB-C1B	4.33	1.49	1.39
21	1B	612	CL7	CHB-C1B	4.33	1.49	1.39
21	13	512	CL7	CHB-C1B	4.33	1.49	1.39
23	2A	404	8CT	C24-C25	4.32	1.56	1.43
23	3A	404	8CT	C24-C25	4.32	1.56	1.43
21	43	418	CL7	CHB-C1B	4.32	1.49	1.39
21	23	418	CL7	CHB-C1B	4.32	1.49	1.39
21	33	517	CL7	CHB-C1B	4.32	1.49	1.39
23	1A	404	8CT	C24-C25	4.32	1.56	1.43
23	34	402	8CT	C24-C25	4.32	1.56	1.43
23	4A	404	8CT	C24-C25	4.32	1.56	1.43
21	4B	605	CL7	CHC-C1C	4.32	1.46	1.38
23	2C	515	8CT	C28-C26	4.32	1.55	1.45
21	2B	605	CL7	CHC-C1C	4.32	1.46	1.38
21	3B	604	CL7	CHC-C1C	4.32	1.46	1.38
23	1B	618	8CT	C28-C26	4.31	1.55	1.45
21	13	511	CL7	CHB-C1B	4.31	1.49	1.39
21	23	403	CL7	CHB-C1B	4.31	1.49	1.39
21	43	413	CL7	CHB-C1B	4.31	1.49	1.39
23	14	402	8CT	C24-C25	4.31	1.56	1.43
23	44	402	8CT	C24-C25	4.31	1.56	1.43
21	33	511	CL7	CHB-C1B	4.31	1.49	1.39
21	1B	604	CL7	CHC-C1C	4.31	1.46	1.38
23	2C	514	8CT	C24-C25	4.31	1.56	1.43
21	33	502	CL7	CHB-C1B	4.30	1.49	1.39
21	2B	608	CL7	CHB-C1B	4.30	1.49	1.39
21	3B	607	CL7	CHB-C1B	4.30	1.49	1.39
21	23	413	CL7	CHB-C1B	4.30	1.49	1.39
21	3B	612	CL7	CHB-C1B	4.30	1.49	1.39
23	1B	618	8CT	C24-C25	4.30	1.56	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4B	619	8CT	C24-C25	4.30	1.56	1.43
21	43	403	CL7	CHB-C1B	4.29	1.49	1.39
21	4B	613	CL7	CHC-C1C	4.29	1.46	1.38
23	1C	514	8CT	C24-C25	4.29	1.56	1.43
23	4C	514	8CT	C24-C25	4.29	1.56	1.43
23	3B	618	8CT	C28-C26	4.29	1.55	1.45
23	3B	618	8CT	C24-C25	4.29	1.56	1.43
21	2B	604	CL7	CHB-C1B	4.29	1.49	1.39
23	2B	620	8CT	C24-C25	4.29	1.56	1.43
23	3B	619	8CT	C24-C25	4.29	1.56	1.43
23	24	402	8CT	C24-C25	4.29	1.56	1.43
21	13	510	CL7	CHB-C1B	4.29	1.49	1.39
21	43	411	CL7	CHB-C1B	4.29	1.49	1.39
23	1B	619	8CT	C24-C25	4.28	1.56	1.43
23	3C	515	8CT	C28-C26	4.28	1.55	1.45
23	4C	515	8CT	C28-C26	4.28	1.55	1.45
23	3C	514	8CT	C24-C25	4.28	1.56	1.43
21	4B	608	CL7	CHB-C1B	4.28	1.49	1.39
21	13	502	CL7	CHB-C1B	4.28	1.49	1.39
23	4B	619	8CT	C28-C26	4.27	1.55	1.45
23	1C	515	8CT	C18-C17	4.27	1.56	1.43
21	4B	613	CL7	CHB-C1B	4.27	1.49	1.39
21	4B	604	CL7	CHB-C1B	4.27	1.49	1.39
23	3B	626	8CT	C28-C26	4.27	1.55	1.45
23	2C	515	8CT	C18-C17	4.27	1.56	1.43
21	1B	603	CL7	CHB-C1B	4.27	1.49	1.39
23	1C	515	8CT	C28-C26	4.27	1.55	1.45
23	4B	601	8CT	C28-C26	4.26	1.55	1.45
21	3B	603	CL7	CHB-C1B	4.26	1.49	1.39
23	2B	619	8CT	C28-C26	4.26	1.55	1.45
21	2B	613	CL7	CHC-C1C	4.26	1.46	1.38
21	3B	612	CL7	CHC-C1C	4.26	1.46	1.38
23	4B	620	8CT	C24-C25	4.26	1.56	1.43
23	1B	617	8CT	C24-C25	4.25	1.56	1.43
23	4B	618	8CT	C24-C25	4.25	1.56	1.43
23	2B	619	8CT	C24-C25	4.25	1.56	1.43
21	3B	606	CL7	CHB-C1B	4.25	1.48	1.39
21	1B	613	CL7	CHB-C1B	4.25	1.48	1.39
23	2B	601	8CT	C28-C26	4.24	1.55	1.45
23	4C	515	8CT	C18-C17	4.24	1.56	1.43
21	4B	614	CL7	CHB-C1B	4.24	1.48	1.39
21	1C	507	CL7	CHB-C1B	4.24	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2C	507	CL7	CHB-C1B	4.23	1.48	1.39
21	3C	507	CL7	CHB-C1B	4.23	1.48	1.39
21	2B	614	CL7	CHB-C1B	4.23	1.48	1.39
21	4B	607	CL7	CHB-C1B	4.23	1.48	1.39
23	4D	406	8CT	C18-C17	4.23	1.56	1.43
21	1B	612	CL7	CHC-C1C	4.23	1.46	1.38
23	3C	515	8CT	C18-C17	4.22	1.56	1.43
23	2B	618	8CT	C24-C25	4.22	1.56	1.43
23	3B	617	8CT	C24-C25	4.22	1.56	1.43
23	1B	626	8CT	C28-C26	4.22	1.55	1.45
21	2B	607	CL7	CHB-C1B	4.22	1.48	1.39
23	34	402	8CT	C28-C26	4.21	1.55	1.45
23	4B	619	8CT	C18-C17	4.21	1.56	1.43
21	4C	507	CL7	CHB-C1B	4.21	1.48	1.39
23	14	402	8CT	C28-C26	4.21	1.55	1.45
23	44	402	8CT	C28-C26	4.21	1.55	1.45
23	2B	619	8CT	C18-C17	4.21	1.56	1.43
23	2D	406	8CT	C18-C17	4.21	1.56	1.43
23	1D	406	8CT	C18-C17	4.20	1.56	1.43
23	1B	618	8CT	C18-C17	4.20	1.56	1.43
23	3B	618	8CT	C18-C17	4.20	1.56	1.43
23	2C	514	8CT	C28-C26	4.20	1.55	1.45
21	1B	606	CL7	CHB-C1B	4.20	1.48	1.39
21	3B	613	CL7	CHB-C1B	4.20	1.48	1.39
21	13	506	CL7	CHC-C1C	4.19	1.46	1.38
21	4B	616	CL7	CHC-C1C	4.19	1.46	1.38
21	43	407	CL7	CHC-C1C	4.19	1.46	1.38
23	1C	518	8CT	C28-C26	4.19	1.54	1.45
21	2B	615	CL7	CHB-C1B	4.19	1.48	1.39
21	3B	614	CL7	CHB-C1B	4.19	1.48	1.39
23	3D	406	8CT	C18-C17	4.19	1.56	1.43
21	23	407	CL7	CHC-C1C	4.18	1.46	1.38
21	33	506	CL7	CHC-C1C	4.18	1.46	1.38
21	1B	614	CL7	CHB-C1B	4.18	1.48	1.39
21	4B	615	CL7	CHB-C1B	4.18	1.48	1.39
23	24	402	8CT	C28-C26	4.18	1.54	1.45
23	4C	514	8CT	C28-C26	4.17	1.54	1.45
23	3C	514	8CT	C28-C26	4.17	1.54	1.45
23	1B	617	8CT	C18-C17	4.17	1.56	1.43
23	4B	618	8CT	C18-C17	4.17	1.56	1.43
23	2B	618	8CT	C18-C17	4.17	1.56	1.43
23	3B	617	8CT	C18-C17	4.17	1.56	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2C	518	8CT	C18-C17	4.16	1.56	1.43
23	4C	518	8CT	C18-C17	4.16	1.56	1.43
21	2B	616	CL7	CHC-C1C	4.16	1.46	1.38
23	3C	518	8CT	C28-C26	4.16	1.54	1.45
23	2C	518	8CT	C28-C26	4.16	1.54	1.45
23	1C	518	8CT	C18-C17	4.15	1.56	1.43
23	4C	518	8CT	C28-C26	4.15	1.54	1.45
23	1B	617	8CT	C28-C26	4.15	1.54	1.45
23	2B	618	8CT	C28-C26	4.14	1.54	1.45
23	1C	514	8CT	C18-C17	4.14	1.56	1.43
23	2C	514	8CT	C18-C17	4.14	1.56	1.43
23	1C	514	8CT	C28-C26	4.14	1.54	1.45
23	4C	514	8CT	C18-C17	4.14	1.56	1.43
23	3C	518	8CT	C18-C17	4.14	1.56	1.43
23	3C	514	8CT	C18-C17	4.14	1.56	1.43
21	1B	615	CL7	CHC-C1C	4.13	1.46	1.38
23	3B	619	8CT	C28-C26	4.13	1.54	1.45
23	4B	618	8CT	C28-C26	4.12	1.54	1.45
21	3B	615	CL7	CHC-C1C	4.12	1.46	1.38
23	4A	404	8CT	C28-C26	4.12	1.54	1.45
23	2C	518	8CT	C06-C07	4.12	1.65	1.52
23	3C	518	8CT	C06-C07	4.12	1.65	1.52
23	1B	619	8CT	C28-C26	4.11	1.54	1.45
23	3B	617	8CT	C28-C26	4.11	1.54	1.45
23	4A	404	8CT	C18-C17	4.10	1.56	1.43
23	2B	620	8CT	C28-C26	4.10	1.54	1.45
23	1C	518	8CT	C06-C07	4.10	1.65	1.52
23	1A	404	8CT	C28-C26	4.10	1.54	1.45
23	3A	404	8CT	C18-C17	4.10	1.56	1.43
23	1A	404	8CT	C18-C17	4.10	1.56	1.43
23	2A	404	8CT	C28-C26	4.10	1.54	1.45
23	3A	404	8CT	C28-C26	4.10	1.54	1.45
23	4B	620	8CT	C28-C26	4.09	1.54	1.45
23	4C	518	8CT	C06-C07	4.09	1.65	1.52
23	34	402	8CT	C18-C17	4.09	1.56	1.43
23	2A	404	8CT	C18-C17	4.09	1.56	1.43
23	14	402	8CT	C18-C17	4.08	1.56	1.43
23	44	402	8CT	C18-C17	4.08	1.56	1.43
27	3B	624	DGD	O1G-C1A	4.07	1.45	1.33
27	1B	624	DGD	O1G-C1A	4.07	1.45	1.33
27	4B	625	DGD	O1G-C1A	4.07	1.45	1.33
23	24	402	8CT	C18-C17	4.07	1.56	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2B	625	DGD	O1G-C1A	4.06	1.45	1.33
23	4B	620	8CT	C18-C17	4.04	1.56	1.43
23	2B	620	8CT	C18-C17	4.02	1.55	1.43
23	3B	619	8CT	C18-C17	4.02	1.55	1.43
23	1B	619	8CT	C18-C17	4.01	1.55	1.43
27	4C	516	DGD	O1G-C1A	4.00	1.45	1.33
27	1C	516	DGD	O2G-C1B	4.00	1.45	1.34
27	4C	516	DGD	O2G-C1B	3.99	1.45	1.34
27	2C	516	DGD	O2G-C1B	3.99	1.45	1.34
27	3C	516	DGD	O2G-C1B	3.98	1.45	1.34
27	1C	516	DGD	O1G-C1A	3.98	1.45	1.33
27	2C	516	DGD	O1G-C1A	3.98	1.45	1.33
27	3C	516	DGD	O1G-C1A	3.98	1.45	1.33
23	1A	404	8CT	C06-C07	3.96	1.64	1.52
23	3A	404	8CT	C06-C07	3.94	1.64	1.52
21	44	411	CL7	CHB-C1B	3.94	1.48	1.39
21	14	411	CL7	CHB-C1B	3.94	1.48	1.39
23	2A	404	8CT	C06-C07	3.94	1.64	1.52
23	4A	404	8CT	C06-C07	3.94	1.64	1.52
23	3C	515	8CT	C06-C07	3.92	1.64	1.52
23	1C	515	8CT	C06-C07	3.92	1.64	1.52
23	4C	515	8CT	C06-C07	3.92	1.64	1.52
21	3B	602	CL7	O2A-CGA	3.92	1.44	1.33
23	4K	101	8CT	C23-C21	3.92	1.54	1.45
23	4B	618	8CT	C06-C07	3.92	1.64	1.52
23	2C	515	8CT	C06-C07	3.91	1.64	1.52
23	2B	618	8CT	C06-C07	3.90	1.64	1.52
21	24	411	CL7	CHB-C1B	3.90	1.48	1.39
21	34	411	CL7	CHB-C1B	3.90	1.48	1.39
23	4B	601	8CT	C06-C07	3.90	1.64	1.52
23	2K	101	8CT	C23-C21	3.90	1.54	1.45
23	3K	101	8CT	C23-C21	3.90	1.54	1.45
21	2B	603	CL7	O2A-CGA	3.90	1.44	1.33
21	4B	603	CL7	O2A-CGA	3.90	1.44	1.33
23	1C	515	8CT	C23-C21	3.89	1.54	1.45
23	4C	515	8CT	C23-C21	3.89	1.54	1.45
23	1B	617	8CT	C06-C07	3.89	1.64	1.52
23	3D	406	8CT	C06-C07	3.89	1.64	1.52
21	3A	401	CL7	C2A-C1A	3.89	1.56	1.50
23	1K	101	8CT	C23-C21	3.88	1.54	1.45
23	3B	617	8CT	C06-C07	3.87	1.64	1.52
21	1B	602	CL7	O2A-CGA	3.87	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3C	515	8CT	C23-C21	3.87	1.54	1.45
23	4D	406	8CT	C06-C07	3.87	1.64	1.52
23	2B	601	8CT	C06-C07	3.87	1.64	1.52
23	3B	626	8CT	C06-C07	3.87	1.64	1.52
23	2B	619	8CT	C06-C07	3.87	1.64	1.52
23	3B	618	8CT	C06-C07	3.87	1.64	1.52
23	2C	515	8CT	C23-C21	3.87	1.54	1.45
23	1B	626	8CT	C06-C07	3.86	1.64	1.52
23	1K	101	8CT	C06-C07	3.86	1.64	1.52
21	2A	401	CL7	O2A-CGA	3.85	1.44	1.33
23	1B	618	8CT	C06-C07	3.85	1.64	1.52
23	4B	619	8CT	C06-C07	3.85	1.64	1.52
23	1D	406	8CT	C06-C07	3.85	1.64	1.52
23	2K	101	8CT	C06-C07	3.85	1.64	1.52
23	3K	101	8CT	C06-C07	3.85	1.64	1.52
23	2D	406	8CT	C06-C07	3.85	1.64	1.52
21	1A	401	CL7	O2A-CGA	3.84	1.44	1.33
21	1A	401	CL7	C2A-C1A	3.84	1.56	1.50
23	4K	101	8CT	C06-C07	3.84	1.64	1.52
21	4A	401	CL7	O2A-CGA	3.83	1.44	1.33
23	2B	620	8CT	C06-C07	3.83	1.64	1.52
21	3A	401	CL7	O2A-CGA	3.82	1.44	1.33
21	2A	401	CL7	C2A-C1A	3.82	1.56	1.50
23	1B	619	8CT	C06-C07	3.82	1.64	1.52
23	4B	620	8CT	C06-C07	3.82	1.64	1.52
23	24	402	8CT	C06-C07	3.82	1.64	1.52
23	34	402	8CT	C06-C07	3.82	1.64	1.52
23	3B	619	8CT	C06-C07	3.82	1.64	1.52
21	1C	504	CL7	C2A-C1A	3.82	1.56	1.50
21	4C	504	CL7	C2A-C1A	3.82	1.56	1.50
31	1F	101	HEM	FE-NC	3.81	2.08	1.95
31	3F	101	HEM	FE-NC	3.80	2.08	1.95
23	4B	601	8CT	C23-C21	3.80	1.54	1.45
23	44	402	8CT	C06-C07	3.80	1.64	1.52
23	14	402	8CT	C06-C07	3.79	1.64	1.52
31	4F	101	HEM	FE-NC	3.78	2.08	1.95
23	1C	514	8CT	C06-C07	3.78	1.64	1.52
23	4C	514	8CT	C06-C07	3.78	1.64	1.52
23	3C	514	8CT	C06-C07	3.78	1.64	1.52
23	2C	514	8CT	C06-C07	3.78	1.64	1.52
31	3F	101	HEM	C1B-NB	-3.78	1.33	1.40
31	2F	101	HEM	FE-NC	3.77	2.07	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2C	504	CL7	C2A-C1A	3.77	1.56	1.50
21	3C	504	CL7	C2A-C1A	3.77	1.56	1.50
21	4A	401	CL7	C2A-C1A	3.76	1.56	1.50
27	1B	624	DGD	O2G-C1B	3.76	1.44	1.34
31	1F	101	HEM	C1B-NB	-3.75	1.33	1.40
23	1B	626	8CT	C23-C21	3.75	1.54	1.45
23	2B	601	8CT	C23-C21	3.75	1.54	1.45
23	3B	626	8CT	C23-C21	3.75	1.54	1.45
31	4F	101	HEM	C1B-NB	-3.74	1.33	1.40
23	14	402	8CT	C23-C21	3.74	1.54	1.45
23	34	402	8CT	C23-C21	3.73	1.54	1.45
23	4D	406	8CT	C23-C21	3.73	1.54	1.45
27	3B	624	DGD	O2G-C1B	3.72	1.44	1.34
23	24	402	8CT	C23-C21	3.71	1.53	1.45
31	2F	101	HEM	C1B-NB	-3.71	1.33	1.40
27	2B	625	DGD	O2G-C1B	3.71	1.44	1.34
23	44	402	8CT	C23-C21	3.71	1.53	1.45
31	1F	101	HEM	C4D-ND	-3.70	1.33	1.40
31	4F	101	HEM	C4D-ND	-3.70	1.33	1.40
27	4B	625	DGD	O2G-C1B	3.70	1.44	1.34
23	2D	406	8CT	C23-C21	3.70	1.53	1.45
23	3D	406	8CT	C23-C21	3.70	1.53	1.45
23	1D	406	8CT	C23-C21	3.69	1.53	1.45
31	3F	101	HEM	C4D-ND	-3.67	1.34	1.40
21	11	411	CL7	O2A-CGA	3.67	1.43	1.30
21	21	411	CL7	O2A-CGA	3.67	1.43	1.30
31	2F	101	HEM	C4D-ND	-3.67	1.34	1.40
21	41	411	CL7	O2A-CGA	3.66	1.43	1.30
21	11	402	CL7	C2A-C1A	3.66	1.56	1.50
21	31	411	CL7	O2A-CGA	3.66	1.43	1.30
21	31	402	CL7	C2A-C1A	3.66	1.56	1.50
21	11	420	CL7	O2A-CGA	3.64	1.43	1.30
21	41	420	CL7	O2A-CGA	3.64	1.43	1.30
21	31	420	CL7	O2A-CGA	3.63	1.42	1.30
21	31	419	CL7	O2A-CGA	3.62	1.42	1.30
21	21	419	CL7	O2A-CGA	3.62	1.42	1.30
21	21	420	CL7	O2A-CGA	3.62	1.42	1.30
21	21	402	CL7	C2A-C1A	3.61	1.56	1.50
21	13	518	CL7	O2A-CGA	3.61	1.42	1.30
21	23	419	CL7	O2A-CGA	3.61	1.42	1.30
21	33	518	CL7	O2A-CGA	3.61	1.42	1.30
21	42	514	CL7	O2A-CGA	3.61	1.42	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	32	514	CL7	O2A-CGA	3.61	1.42	1.30
21	11	419	CL7	O2A-CGA	3.60	1.42	1.30
21	41	419	CL7	O2A-CGA	3.60	1.42	1.30
21	31	412	CL7	O2A-CGA	3.60	1.42	1.30
21	43	419	CL7	O2A-CGA	3.60	1.42	1.30
21	11	412	CL7	O2A-CGA	3.60	1.42	1.30
21	41	412	CL7	O2A-CGA	3.60	1.42	1.30
21	43	414	CL7	O2A-CGA	3.60	1.42	1.30
21	12	515	CL7	O2A-CGA	3.60	1.42	1.30
21	1B	614	CL7	O2A-CGA	3.59	1.43	1.33
21	4B	615	CL7	O2A-CGA	3.59	1.43	1.33
21	1B	622	CL7	O2A-CGA	3.59	1.42	1.30
21	4B	623	CL7	O2A-CGA	3.59	1.42	1.30
21	22	515	CL7	O2A-CGA	3.59	1.42	1.30
21	32	515	CL7	O2A-CGA	3.59	1.42	1.30
21	21	412	CL7	O2A-CGA	3.59	1.42	1.30
23	1C	518	8CT	C23-C21	3.59	1.53	1.45
21	42	515	CL7	O2A-CGA	3.59	1.42	1.30
21	41	402	CL7	C2A-C1A	3.59	1.56	1.50
23	2C	518	8CT	C23-C21	3.58	1.53	1.45
21	34	408	CL7	O2A-CGA	3.58	1.42	1.30
21	12	514	CL7	O2A-CGA	3.58	1.42	1.30
21	2B	615	CL7	O2A-CGA	3.58	1.43	1.33
21	3B	614	CL7	O2A-CGA	3.58	1.43	1.33
21	22	514	CL7	O2A-CGA	3.58	1.42	1.30
21	31	405	CL7	O2A-CGA	3.57	1.42	1.30
21	23	414	CL7	O2A-CGA	3.57	1.42	1.30
21	33	513	CL7	O2A-CGA	3.57	1.42	1.30
21	2B	623	CL7	O2A-CGA	3.57	1.42	1.30
21	3B	622	CL7	O2A-CGA	3.57	1.42	1.30
21	32	508	CL7	O2A-CGA	3.57	1.42	1.30
21	12	508	CL7	O2A-CGA	3.57	1.42	1.30
21	11	405	CL7	O2A-CGA	3.56	1.42	1.30
21	41	405	CL7	O2A-CGA	3.56	1.42	1.30
21	14	408	CL7	O2A-CGA	3.56	1.42	1.30
21	43	415	CL7	O2A-CGA	3.56	1.42	1.30
21	23	415	CL7	O2A-CGA	3.56	1.42	1.30
21	12	504	CL7	O2A-CGA	3.56	1.42	1.30
23	2A	404	8CT	C23-C21	3.56	1.53	1.45
21	13	513	CL7	O2A-CGA	3.56	1.42	1.30
21	42	508	CL7	O2A-CGA	3.55	1.42	1.30
23	2C	514	8CT	C23-C21	3.55	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3C	518	8CT	C23-C21	3.55	1.53	1.45
21	44	408	CL7	O2A-CGA	3.55	1.42	1.30
21	22	508	CL7	O2A-CGA	3.55	1.42	1.30
23	4C	518	8CT	C23-C21	3.55	1.53	1.45
21	21	405	CL7	O2A-CGA	3.55	1.42	1.30
21	22	504	CL7	O2A-CGA	3.55	1.42	1.30
21	32	504	CL7	O2A-CGA	3.55	1.42	1.30
21	23	415	CL7	C2A-C1A	3.54	1.56	1.50
21	33	514	CL7	C2A-C1A	3.54	1.56	1.50
21	14	417	CL7	O2D-CGD	3.54	1.41	1.33
21	31	419	CL7	O2D-CGD	3.54	1.41	1.33
21	13	514	CL7	O2A-CGA	3.54	1.42	1.30
21	4B	617	CL7	O2A-CGA	3.54	1.42	1.30
21	24	408	CL7	O2A-CGA	3.54	1.42	1.30
23	1C	514	8CT	C23-C21	3.54	1.53	1.45
23	4C	514	8CT	C23-C21	3.54	1.53	1.45
21	24	417	CL7	O2D-CGD	3.54	1.41	1.33
21	21	409	CL7	O2A-CGA	3.54	1.42	1.30
21	3B	616	CL7	O2A-CGA	3.54	1.42	1.30
21	4D	405	CL7	O2A-CGA	3.53	1.42	1.30
21	11	409	CL7	O2A-CGA	3.53	1.42	1.30
21	41	409	CL7	O2A-CGA	3.53	1.42	1.30
23	3A	404	8CT	C23-C21	3.53	1.53	1.45
21	44	410	CL7	O2A-CGA	3.53	1.42	1.30
21	14	410	CL7	O2A-CGA	3.53	1.42	1.30
21	42	504	CL7	O2A-CGA	3.53	1.42	1.30
21	24	410	CL7	O2A-CGA	3.53	1.42	1.30
21	44	417	CL7	O2D-CGD	3.53	1.41	1.33
21	33	514	CL7	O2A-CGA	3.53	1.42	1.30
21	1B	616	CL7	O2A-CGA	3.53	1.42	1.30
21	11	412	CL7	C2A-C1A	3.52	1.56	1.50
23	4A	404	8CT	C23-C21	3.52	1.53	1.45
21	2A	403	CL7	O2A-CGA	3.52	1.43	1.33
21	3D	405	CL7	O2A-CGA	3.52	1.42	1.30
21	1A	403	CL7	O2A-CGA	3.52	1.43	1.33
23	3C	514	8CT	C23-C21	3.52	1.53	1.45
21	34	410	CL7	O2A-CGA	3.52	1.42	1.30
21	2B	617	CL7	O2A-CGA	3.51	1.42	1.30
21	43	415	CL7	C2A-C1A	3.51	1.56	1.50
21	31	409	CL7	O2A-CGA	3.51	1.42	1.30
23	1A	404	8CT	C23-C21	3.51	1.53	1.45
21	2D	405	CL7	O2A-CGA	3.51	1.42	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1D	405	CL7	O2A-CGA	3.51	1.42	1.30
21	14	415	CL7	O2A-CGA	3.51	1.42	1.30
21	24	415	CL7	O2A-CGA	3.49	1.42	1.30
21	34	415	CL7	O2A-CGA	3.49	1.42	1.30
21	3A	403	CL7	O2A-CGA	3.49	1.43	1.33
21	34	417	CL7	O2D-CGD	3.49	1.41	1.33
21	4A	403	CL7	O2A-CGA	3.49	1.43	1.33
21	1C	513	CL7	O2A-CGA	3.49	1.42	1.30
21	2C	513	CL7	O2A-CGA	3.49	1.42	1.30
21	3C	513	CL7	O2A-CGA	3.49	1.42	1.30
21	21	419	CL7	O2D-CGD	3.49	1.41	1.33
21	11	419	CL7	O2D-CGD	3.49	1.41	1.33
21	41	419	CL7	O2D-CGD	3.49	1.41	1.33
21	44	415	CL7	O2A-CGA	3.48	1.42	1.30
21	4C	513	CL7	O2A-CGA	3.48	1.42	1.30
21	34	416	CL7	O2D-CGD	3.48	1.41	1.33
21	41	416	CL7	O2D-CGD	3.48	1.41	1.33
21	13	514	CL7	C2A-C1A	3.47	1.56	1.50
21	1B	614	CL7	C2A-C1A	3.47	1.56	1.50
21	21	416	CL7	O2D-CGD	3.46	1.41	1.33
21	13	506	CL7	O2A-CGA	3.46	1.42	1.30
21	21	412	CL7	C2A-C1A	3.46	1.56	1.50
21	31	412	CL7	C2A-C1A	3.46	1.56	1.50
21	41	412	CL7	C2A-C1A	3.46	1.56	1.50
21	21	415	CL7	O2D-CGD	3.46	1.41	1.33
21	23	407	CL7	O2A-CGA	3.46	1.42	1.30
21	14	408	CL7	C2A-C1A	3.46	1.56	1.50
21	11	415	CL7	O2D-CGD	3.45	1.41	1.33
21	41	415	CL7	O2D-CGD	3.45	1.41	1.33
21	31	416	CL7	O2D-CGD	3.45	1.41	1.33
21	11	416	CL7	O2D-CGD	3.45	1.41	1.33
21	44	408	CL7	C2A-C1A	3.45	1.56	1.50
21	43	407	CL7	O2A-CGA	3.45	1.42	1.30
21	14	416	CL7	O2D-CGD	3.45	1.41	1.33
21	21	411	CL7	O2D-CGD	3.45	1.41	1.33
21	31	411	CL7	O2D-CGD	3.45	1.41	1.33
21	44	416	CL7	O2D-CGD	3.45	1.41	1.33
21	42	513	CL7	O2A-CGA	3.45	1.42	1.30
21	2B	615	CL7	C2A-C1A	3.44	1.56	1.50
21	3B	614	CL7	C2A-C1A	3.44	1.56	1.50
21	11	411	CL7	O2D-CGD	3.44	1.41	1.33
21	24	408	CL7	C2A-C1A	3.44	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	408	CL7	C2A-C1A	3.44	1.56	1.50
21	24	416	CL7	O2D-CGD	3.44	1.41	1.33
21	1C	508	CL7	O2A-CGA	3.44	1.43	1.33
21	31	415	CL7	O2D-CGD	3.44	1.41	1.33
21	2C	508	CL7	O2A-CGA	3.43	1.43	1.33
21	33	506	CL7	O2A-CGA	3.42	1.42	1.30
21	22	512	CL7	C4C-C3C	-3.42	1.39	1.45
21	32	512	CL7	C4C-C3C	-3.42	1.39	1.45
21	12	512	CL7	C4C-C3C	-3.42	1.39	1.45
21	41	411	CL7	O2D-CGD	3.42	1.41	1.33
21	21	407	CL7	O2D-CGD	3.42	1.41	1.33
21	31	407	CL7	O2D-CGD	3.42	1.41	1.33
21	4B	615	CL7	C2A-C1A	3.42	1.56	1.50
21	22	513	CL7	O2A-CGA	3.42	1.42	1.30
21	32	513	CL7	O2A-CGA	3.42	1.42	1.30
23	1B	618	8CT	C23-C21	3.41	1.53	1.45
23	3B	619	8CT	C23-C21	3.41	1.53	1.45
21	42	512	CL7	C4C-C3C	-3.41	1.39	1.45
21	4C	508	CL7	O2A-CGA	3.41	1.43	1.33
21	11	407	CL7	O2D-CGD	3.41	1.41	1.33
21	43	414	CL7	C2A-C1A	3.41	1.56	1.50
23	1B	619	8CT	C23-C21	3.41	1.53	1.45
23	4B	620	8CT	C23-C21	3.41	1.53	1.45
21	3C	508	CL7	O2A-CGA	3.41	1.43	1.33
21	43	419	CL7	O2D-CGD	3.41	1.41	1.33
21	41	407	CL7	O2D-CGD	3.40	1.41	1.33
21	12	513	CL7	O2A-CGA	3.40	1.42	1.30
23	4B	619	8CT	C23-C21	3.40	1.53	1.45
21	33	506	CL7	C2A-C1A	3.40	1.56	1.50
21	31	402	CL7	O2A-CGA	3.40	1.43	1.33
23	2B	620	8CT	C23-C21	3.39	1.53	1.45
23	2B	619	8CT	C23-C21	3.39	1.53	1.45
23	3B	618	8CT	C23-C21	3.39	1.53	1.45
21	23	414	CL7	C2A-C1A	3.39	1.55	1.50
21	1C	513	CL7	O2D-CGD	3.39	1.41	1.33
21	11	412	CL7	O2D-CGD	3.38	1.41	1.33
21	31	412	CL7	O2D-CGD	3.38	1.41	1.33
21	33	518	CL7	O2D-CGD	3.38	1.41	1.33
21	41	412	CL7	O2D-CGD	3.38	1.41	1.33
21	2B	602	CL7	O2D-CGD	3.38	1.41	1.33
21	1B	601	CL7	O2D-CGD	3.38	1.41	1.33
21	4B	602	CL7	O2D-CGD	3.38	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	24	420	ZEX	C21-C26	-3.37	1.49	1.53
21	2C	513	CL7	O2D-CGD	3.37	1.41	1.33
21	21	412	CL7	O2D-CGD	3.37	1.41	1.33
21	11	402	CL7	O2A-CGA	3.37	1.43	1.33
21	41	402	CL7	O2A-CGA	3.37	1.43	1.33
21	43	407	CL7	C2A-C1A	3.37	1.55	1.50
32	14	420	ZEX	C21-C26	-3.37	1.49	1.53
22	2D	408	PHO	C4D-CHA	3.37	1.45	1.39
22	1D	408	PHO	C4D-CHA	3.37	1.45	1.39
22	4D	408	PHO	C4D-CHA	3.37	1.45	1.39
21	31	417	CL7	O2A-CGA	3.37	1.43	1.33
21	4B	613	CL7	C4C-C3C	-3.36	1.39	1.45
21	21	417	CL7	O2A-CGA	3.36	1.43	1.33
21	13	518	CL7	O2D-CGD	3.36	1.41	1.33
21	21	402	CL7	O2A-CGA	3.36	1.43	1.33
21	22	514	CL7	O2D-CGD	3.35	1.41	1.33
21	32	514	CL7	O2D-CGD	3.35	1.41	1.33
21	3B	601	CL7	O2D-CGD	3.35	1.41	1.33
21	42	514	CL7	O2D-CGD	3.35	1.41	1.33
32	34	420	ZEX	C21-C26	-3.35	1.49	1.53
21	13	513	CL7	C2A-C1A	3.35	1.55	1.50
21	1C	504	CL7	O2D-CGD	3.35	1.41	1.33
21	4C	504	CL7	O2D-CGD	3.35	1.41	1.33
21	21	414	CL7	O2D-CGD	3.35	1.41	1.33
21	31	414	CL7	O2D-CGD	3.35	1.41	1.33
21	11	414	CL7	O2D-CGD	3.35	1.41	1.33
21	41	414	CL7	O2D-CGD	3.35	1.41	1.33
21	3C	513	CL7	O2D-CGD	3.34	1.41	1.33
21	33	513	CL7	C2A-C1A	3.34	1.55	1.50
21	12	514	CL7	O2D-CGD	3.34	1.41	1.33
21	13	512	CL7	O2A-CGA	3.34	1.43	1.33
21	43	413	CL7	O2A-CGA	3.34	1.43	1.33
21	11	417	CL7	O2A-CGA	3.34	1.43	1.33
21	41	417	CL7	O2A-CGA	3.34	1.43	1.33
21	11	413	CL7	O2D-CGD	3.34	1.41	1.33
21	21	413	CL7	O2D-CGD	3.34	1.41	1.33
21	23	419	CL7	O2D-CGD	3.34	1.41	1.33
21	41	413	CL7	O2D-CGD	3.34	1.41	1.33
21	43	418	CL7	O2D-CGD	3.34	1.41	1.33
21	24	413	CL7	C2A-C1A	3.33	1.55	1.50
32	44	420	ZEX	C21-C26	-3.33	1.49	1.53
21	23	418	CL7	O2D-CGD	3.33	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	33	517	CL7	O2D-CGD	3.33	1.41	1.33
21	3C	504	CL7	O2D-CGD	3.33	1.41	1.33
21	13	510	CL7	O2D-CGD	3.33	1.41	1.33
21	43	411	CL7	O2D-CGD	3.33	1.41	1.33
21	4C	513	CL7	O2D-CGD	3.33	1.41	1.33
21	3B	612	CL7	C4C-C3C	-3.33	1.39	1.45
21	23	411	CL7	O2D-CGD	3.33	1.41	1.33
21	33	510	CL7	O2D-CGD	3.33	1.41	1.33
21	2C	504	CL7	O2D-CGD	3.32	1.41	1.33
21	32	511	CL7	C2A-C1A	3.32	1.55	1.50
21	42	511	CL7	C2A-C1A	3.32	1.55	1.50
21	34	413	CL7	O2D-CGD	3.32	1.41	1.33
21	12	505	CL7	C4C-C3C	-3.32	1.39	1.45
21	13	512	CL7	C2A-C1A	3.32	1.55	1.50
21	42	511	CL7	O2A-CGA	3.32	1.43	1.33
21	22	511	CL7	O2A-CGA	3.32	1.43	1.33
21	11	418	CL7	C4C-C3C	-3.32	1.39	1.45
21	41	418	CL7	C4C-C3C	-3.32	1.39	1.45
21	12	506	CL7	O2D-CGD	3.32	1.41	1.33
21	3C	504	CL7	O2A-CGA	3.32	1.43	1.33
21	23	413	CL7	O2A-CGA	3.32	1.43	1.33
21	33	512	CL7	O2A-CGA	3.32	1.43	1.33
21	13	506	CL7	C2A-C1A	3.32	1.55	1.50
21	42	501	CL7	O2D-CGD	3.32	1.41	1.33
21	23	407	CL7	C2A-C1A	3.31	1.55	1.50
21	31	410	CL7	O2D-CGD	3.31	1.41	1.33
21	31	413	CL7	O2D-CGD	3.31	1.41	1.33
21	2B	623	CL7	O2D-CGD	3.31	1.41	1.33
21	14	405	CL7	O2A-CGA	3.31	1.43	1.33
21	21	420	CL7	O2D-CGD	3.31	1.41	1.33
21	41	409	CL7	O2D-CGD	3.31	1.41	1.33
21	24	409	CL7	C2A-C1A	3.31	1.55	1.50
21	34	409	CL7	C2A-C1A	3.31	1.55	1.50
21	34	413	CL7	C2A-C1A	3.31	1.55	1.50
21	44	413	CL7	C2A-C1A	3.31	1.55	1.50
21	2B	613	CL7	C4C-C3C	-3.31	1.39	1.45
21	12	511	CL7	C2A-C1A	3.31	1.55	1.50
21	44	404	CL7	O2A-CGA	3.31	1.43	1.33
22	3D	408	PHO	C4D-CHA	3.31	1.44	1.39
21	1B	622	CL7	O2D-CGD	3.31	1.41	1.33
21	12	510	CL7	O2D-CGD	3.31	1.41	1.33
21	11	410	CL7	O2A-CGA	3.31	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	501	CL7	O2D-CGD	3.31	1.41	1.33
21	14	413	CL7	O2D-CGD	3.31	1.41	1.33
21	44	413	CL7	O2D-CGD	3.31	1.41	1.33
21	31	410	CL7	C2A-C1A	3.31	1.55	1.50
21	21	402	CL7	O2D-CGD	3.30	1.41	1.33
21	32	501	CL7	O2D-CGD	3.30	1.41	1.33
21	44	405	CL7	O2A-CGA	3.30	1.43	1.33
21	31	420	CL7	O2D-CGD	3.30	1.41	1.33
21	31	410	CL7	O2A-CGA	3.30	1.43	1.33
21	34	404	CL7	O2A-CGA	3.30	1.43	1.33
21	14	409	CL7	C2A-C1A	3.30	1.55	1.50
21	44	409	CL7	C2A-C1A	3.30	1.55	1.50
21	22	510	CL7	O2D-CGD	3.30	1.41	1.33
21	23	413	CL7	C2A-C1A	3.30	1.55	1.50
21	33	512	CL7	C2A-C1A	3.30	1.55	1.50
21	24	405	CL7	O2A-CGA	3.30	1.43	1.33
21	22	518	CL7	O2A-CGA	3.30	1.43	1.33
21	32	518	CL7	O2A-CGA	3.30	1.43	1.33
21	21	409	CL7	O2D-CGD	3.30	1.41	1.33
21	22	513	CL7	C2A-C1A	3.30	1.55	1.50
21	32	511	CL7	O2A-CGA	3.30	1.43	1.33
21	13	517	CL7	O2D-CGD	3.30	1.41	1.33
21	4C	504	CL7	O2A-CGA	3.30	1.43	1.33
21	12	511	CL7	O2A-CGA	3.29	1.43	1.33
21	22	505	CL7	C4C-C3C	-3.29	1.39	1.45
21	32	505	CL7	C4C-C3C	-3.29	1.39	1.45
21	24	406	CL7	O2A-CGA	3.29	1.43	1.33
21	42	518	CL7	O2A-CGA	3.29	1.43	1.33
21	2C	502	CL7	O2D-CGD	3.29	1.41	1.33
21	3C	502	CL7	O2D-CGD	3.29	1.41	1.33
32	32	522	ZEX	C1-C6	-3.29	1.49	1.53
21	33	504	CL7	C2A-C1A	3.29	1.55	1.50
21	22	501	CL7	O2D-CGD	3.29	1.41	1.33
21	14	404	CL7	O2A-CGA	3.29	1.42	1.33
21	14	407	CL7	O2D-CGD	3.29	1.41	1.33
23	4B	618	8CT	C23-C21	3.29	1.53	1.45
21	32	510	CL7	O2D-CGD	3.29	1.41	1.33
21	12	507	CL7	O2A-CGA	3.29	1.42	1.33
32	12	522	ZEX	C1-C6	-3.29	1.49	1.53
21	1C	502	CL7	O2D-CGD	3.29	1.41	1.33
21	11	402	CL7	O2D-CGD	3.29	1.41	1.33
21	4C	502	CL7	O2D-CGD	3.29	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	409	CL7	O2D-CGD	3.28	1.41	1.33
21	2C	503	CL7	O2A-CGA	3.28	1.42	1.33
21	3C	503	CL7	O2A-CGA	3.28	1.42	1.33
21	43	413	CL7	C2A-C1A	3.28	1.55	1.50
21	13	515	CL7	O2D-CGD	3.28	1.41	1.33
23	1B	617	8CT	C23-C21	3.28	1.53	1.45
21	33	515	CL7	O2D-CGD	3.28	1.41	1.33
21	4B	623	CL7	O2D-CGD	3.28	1.41	1.33
21	24	404	CL7	O2A-CGA	3.28	1.42	1.33
21	41	404	CL7	O2D-CGD	3.28	1.41	1.33
21	44	404	CL7	O2D-CGD	3.28	1.41	1.33
21	24	404	CL7	O2D-CGD	3.28	1.41	1.33
21	34	406	CL7	O2A-CGA	3.28	1.42	1.33
21	14	404	CL7	O2D-CGD	3.28	1.41	1.33
21	33	503	CL7	C4C-C3C	-3.28	1.39	1.45
21	3B	622	CL7	O2D-CGD	3.28	1.41	1.33
21	24	413	CL7	O2D-CGD	3.28	1.41	1.33
21	34	405	CL7	O2A-CGA	3.28	1.42	1.33
21	42	513	CL7	C2A-C1A	3.28	1.55	1.50
21	31	405	CL7	O2D-CGD	3.28	1.41	1.33
21	41	402	CL7	O2D-CGD	3.28	1.41	1.33
21	1B	612	CL7	C4C-C3C	-3.28	1.39	1.45
21	4C	511	CL7	O2D-CGD	3.28	1.41	1.33
21	23	416	CL7	O2D-CGD	3.28	1.41	1.33
21	23	419	CL7	C2A-C1A	3.28	1.55	1.50
21	21	418	CL7	C4C-C3C	-3.28	1.39	1.45
21	31	418	CL7	C4C-C3C	-3.28	1.39	1.45
21	44	407	CL7	O2D-CGD	3.27	1.41	1.33
21	31	402	CL7	O2D-CGD	3.27	1.41	1.33
21	13	509	CL7	O2D-CGD	3.27	1.41	1.33
21	42	506	CL7	O2D-CGD	3.27	1.41	1.33
21	41	410	CL7	O2A-CGA	3.27	1.42	1.33
21	42	502	CL7	O2A-CGA	3.27	1.42	1.33
21	42	517	CL7	O2A-CGA	3.27	1.42	1.33
21	1C	504	CL7	O2A-CGA	3.27	1.42	1.33
21	12	518	CL7	O2A-CGA	3.27	1.42	1.33
21	21	410	CL7	O2A-CGA	3.27	1.42	1.33
21	2D	402	CL7	O2D-CGD	3.27	1.41	1.33
21	21	410	CL7	O2D-CGD	3.27	1.41	1.33
21	3D	402	CL7	O2D-CGD	3.27	1.41	1.33
21	4C	507	CL7	C4C-C3C	-3.27	1.39	1.45
21	34	407	CL7	O2D-CGD	3.27	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	406	CL7	O2A-CGA	3.27	1.42	1.33
21	42	510	CL7	O2D-CGD	3.27	1.41	1.33
21	32	502	CL7	O2A-CGA	3.27	1.42	1.33
21	23	405	CL7	C2A-C1A	3.27	1.55	1.50
21	4D	402	CL7	O2D-CGD	3.27	1.41	1.33
21	2A	407	CL7	C4C-C3C	-3.27	1.39	1.45
21	23	404	CL7	C4C-C3C	-3.27	1.39	1.45
21	43	404	CL7	C4C-C3C	-3.27	1.39	1.45
21	22	502	CL7	O2A-CGA	3.27	1.42	1.33
21	2C	504	CL7	O2A-CGA	3.27	1.42	1.33
21	22	506	CL7	O2D-CGD	3.27	1.41	1.33
21	42	511	CL7	O2D-CGD	3.26	1.41	1.33
21	11	410	CL7	O2D-CGD	3.26	1.41	1.33
21	21	405	CL7	O2D-CGD	3.26	1.41	1.33
21	41	410	CL7	O2D-CGD	3.26	1.41	1.33
21	32	506	CL7	O2D-CGD	3.26	1.41	1.33
21	34	405	CL7	O2D-CGD	3.26	1.41	1.33
21	22	511	CL7	O2D-CGD	3.26	1.41	1.33
21	31	409	CL7	O2D-CGD	3.26	1.41	1.33
21	11	404	CL7	O2D-CGD	3.26	1.41	1.33
21	32	511	CL7	O2D-CGD	3.26	1.41	1.33
21	14	413	CL7	C2A-C1A	3.26	1.55	1.50
21	22	511	CL7	C2A-C1A	3.26	1.55	1.50
21	11	420	CL7	O2D-CGD	3.26	1.41	1.33
21	41	420	CL7	O2D-CGD	3.26	1.41	1.33
21	14	406	CL7	O2A-CGA	3.26	1.42	1.33
21	31	420	CL7	C2A-C1A	3.26	1.55	1.50
21	42	505	CL7	C4C-C3C	-3.26	1.39	1.45
21	34	404	CL7	O2D-CGD	3.26	1.41	1.33
21	1D	402	CL7	O2D-CGD	3.26	1.41	1.33
21	3A	407	CL7	C4C-C3C	-3.26	1.39	1.45
21	1C	503	CL7	O2A-CGA	3.26	1.42	1.33
21	4C	503	CL7	O2A-CGA	3.26	1.42	1.33
21	22	511	CL7	C4C-C3C	-3.26	1.39	1.45
21	13	503	CL7	C4C-C3C	-3.26	1.39	1.45
21	1B	622	CL7	C2A-C1A	3.26	1.55	1.50
23	3B	617	8CT	C23-C21	3.26	1.52	1.45
21	32	513	CL7	C2A-C1A	3.25	1.55	1.50
21	14	405	CL7	O2D-CGD	3.25	1.41	1.33
21	12	502	CL7	O2A-CGA	3.25	1.42	1.33
21	3C	507	CL7	C4C-C3C	-3.25	1.39	1.45
21	12	503	CL7	C4C-C3C	-3.25	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	410	CL7	C2A-C1A	3.25	1.55	1.50
21	41	410	CL7	C2A-C1A	3.25	1.55	1.50
21	11	405	CL7	O2D-CGD	3.25	1.41	1.33
21	13	518	CL7	C2A-C1A	3.25	1.55	1.50
21	43	419	CL7	C2A-C1A	3.25	1.55	1.50
21	3C	510	CL7	O2D-CGD	3.25	1.41	1.33
21	22	507	CL7	O2A-CGA	3.25	1.42	1.33
21	32	507	CL7	O2A-CGA	3.25	1.42	1.33
21	32	506	CL7	O2A-CGA	3.25	1.42	1.33
23	2B	618	8CT	C23-C21	3.25	1.52	1.45
21	43	416	CL7	O2D-CGD	3.25	1.41	1.33
21	14	410	CL7	C2A-C1A	3.25	1.55	1.50
21	2D	402	CL7	C2A-C1A	3.25	1.55	1.50
21	3D	402	CL7	C2A-C1A	3.25	1.55	1.50
21	23	410	CL7	O2D-CGD	3.25	1.41	1.33
21	22	505	CL7	O2D-CGD	3.25	1.41	1.33
21	31	404	CL7	O2D-CGD	3.25	1.41	1.33
21	2B	623	CL7	C2A-C1A	3.25	1.55	1.50
21	3B	622	CL7	C2A-C1A	3.25	1.55	1.50
21	1C	510	CL7	O2D-CGD	3.25	1.41	1.33
21	2C	510	CL7	O2D-CGD	3.25	1.41	1.33
21	4C	510	CL7	O2D-CGD	3.25	1.41	1.33
21	22	504	CL7	O2D-CGD	3.24	1.41	1.33
21	33	506	CL7	O2D-CGD	3.24	1.41	1.33
21	1D	402	CL7	C2A-C1A	3.24	1.55	1.50
21	22	517	CL7	O2A-CGA	3.24	1.42	1.33
21	41	405	CL7	O2D-CGD	3.24	1.41	1.33
21	42	507	CL7	O2A-CGA	3.24	1.42	1.33
21	3C	511	CL7	O2D-CGD	3.24	1.41	1.33
21	2C	502	CL7	O2A-CGA	3.24	1.42	1.33
21	11	419	CL7	C2A-C1A	3.24	1.55	1.50
21	41	419	CL7	C2A-C1A	3.24	1.55	1.50
21	13	504	CL7	C2A-C1A	3.24	1.55	1.50
21	43	405	CL7	C2A-C1A	3.24	1.55	1.50
21	24	407	CL7	O2D-CGD	3.24	1.41	1.33
21	12	517	CL7	O2A-CGA	3.24	1.42	1.33
21	21	404	CL7	O2D-CGD	3.24	1.41	1.33
21	33	518	CL7	C2A-C1A	3.24	1.55	1.50
21	12	506	CL7	O2A-CGA	3.24	1.42	1.33
21	4D	402	CL7	C2A-C1A	3.24	1.55	1.50
21	1C	511	CL7	O2D-CGD	3.24	1.41	1.33
21	1B	613	CL7	C4C-C3C	-3.24	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	43	410	CL7	O2D-CGD	3.24	1.41	1.33
21	13	506	CL7	O2D-CGD	3.23	1.41	1.33
21	32	504	CL7	O2D-CGD	3.23	1.41	1.33
21	12	513	CL7	C2A-C1A	3.23	1.55	1.50
21	11	403	CL7	C2A-C1A	3.23	1.55	1.50
21	12	518	CL7	O2D-CGD	3.23	1.41	1.33
21	1C	507	CL7	C4C-C3C	-3.23	1.39	1.45
21	24	405	CL7	O2D-CGD	3.23	1.41	1.33
21	42	511	CL7	C4C-C3C	-3.23	1.39	1.45
21	22	518	CL7	O2D-CGD	3.23	1.41	1.33
21	2C	511	CL7	O2D-CGD	3.23	1.41	1.33
21	32	517	CL7	O2A-CGA	3.23	1.42	1.33
21	4B	614	CL7	C4C-C3C	-3.23	1.39	1.45
21	12	511	CL7	O2D-CGD	3.23	1.41	1.33
21	42	518	CL7	O2D-CGD	3.23	1.41	1.33
21	21	410	CL7	C2A-C1A	3.23	1.55	1.50
21	32	518	CL7	O2D-CGD	3.23	1.41	1.33
21	31	419	CL7	C2A-C1A	3.23	1.55	1.50
21	1B	610	CL7	O2A-CGA	3.23	1.42	1.33
21	2C	510	CL7	O2A-CGA	3.22	1.42	1.33
21	3C	510	CL7	O2A-CGA	3.22	1.42	1.33
21	31	403	CL7	C2A-C1A	3.22	1.55	1.50
21	42	515	CL7	O2D-CGD	3.22	1.41	1.33
21	3B	610	CL7	O2A-CGA	3.22	1.42	1.33
21	3B	609	CL7	O2D-CGD	3.22	1.41	1.33
21	2B	614	CL7	C4C-C3C	-3.22	1.39	1.45
21	22	503	CL7	C4C-C3C	-3.22	1.39	1.45
21	23	405	CL7	C4C-C3C	-3.22	1.39	1.45
21	3B	613	CL7	C4C-C3C	-3.22	1.39	1.45
21	42	504	CL7	O2D-CGD	3.22	1.41	1.33
21	33	517	CL7	O2A-CGA	3.22	1.42	1.33
21	31	408	CL7	O2D-CGD	3.22	1.41	1.33
21	4C	510	CL7	O2A-CGA	3.22	1.42	1.33
21	12	504	CL7	O2D-CGD	3.22	1.41	1.33
21	33	509	CL7	O2D-CGD	3.22	1.41	1.33
21	1C	502	CL7	O2A-CGA	3.22	1.42	1.33
21	4C	502	CL7	O2A-CGA	3.22	1.42	1.33
32	22	522	ZEX	C1-C6	-3.22	1.49	1.53
21	13	517	CL7	O2A-CGA	3.22	1.42	1.33
21	11	408	CL7	O2D-CGD	3.22	1.41	1.33
21	14	412	CL7	O2A-CGA	3.22	1.42	1.33
21	44	412	CL7	O2A-CGA	3.22	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	403	CL7	C2A-C1A	3.22	1.55	1.50
21	13	501	CL7	O2D-CGD	3.22	1.41	1.33
21	44	413	CL7	O2A-CGA	3.22	1.42	1.33
21	33	516	CL7	O2A-CGA	3.22	1.42	1.33
21	42	506	CL7	O2A-CGA	3.22	1.42	1.33
21	13	504	CL7	C4C-C3C	-3.22	1.39	1.45
21	2C	507	CL7	C4C-C3C	-3.22	1.39	1.45
23	4C	514	8CT	C07-C02	-3.22	1.44	1.51
21	1C	505	CL7	O2D-CGD	3.22	1.41	1.33
21	24	411	CL7	O2D-CGD	3.22	1.41	1.33
21	43	418	CL7	O2A-CGA	3.22	1.42	1.33
21	44	405	CL7	O2D-CGD	3.22	1.41	1.33
32	42	522	ZEX	C1-C6	-3.22	1.49	1.53
21	14	406	CL7	C2A-C1A	3.22	1.55	1.50
21	22	515	CL7	O2D-CGD	3.22	1.41	1.33
21	2B	608	CL7	C4C-C3C	-3.22	1.39	1.45
21	3B	607	CL7	C4C-C3C	-3.22	1.39	1.45
21	43	407	CL7	O2D-CGD	3.22	1.41	1.33
21	4B	611	CL7	O2A-CGA	3.21	1.42	1.33
21	1C	510	CL7	O2A-CGA	3.21	1.42	1.33
21	4B	623	CL7	C2A-C1A	3.21	1.55	1.50
21	4C	505	CL7	O2D-CGD	3.21	1.41	1.33
21	11	420	CL7	C2A-C1A	3.21	1.55	1.50
21	41	420	CL7	C2A-C1A	3.21	1.55	1.50
21	23	407	CL7	O2D-CGD	3.21	1.41	1.33
21	32	505	CL7	O2D-CGD	3.21	1.41	1.33
21	22	509	CL7	O2D-CGD	3.21	1.41	1.33
21	32	509	CL7	O2D-CGD	3.21	1.41	1.33
21	3C	502	CL7	O2A-CGA	3.21	1.42	1.33
21	12	509	CL7	O2D-CGD	3.21	1.41	1.33
21	21	406	CL7	O2D-CGD	3.21	1.41	1.33
21	42	509	CL7	O2D-CGD	3.21	1.41	1.33
21	4A	407	CL7	C4C-C3C	-3.21	1.39	1.45
21	44	406	CL7	C2A-C1A	3.21	1.55	1.50
21	4B	608	CL7	C4C-C3C	-3.21	1.39	1.45
21	11	406	CL7	O2D-CGD	3.21	1.41	1.33
21	41	406	CL7	O2D-CGD	3.21	1.41	1.33
21	3B	615	CL7	O2A-CGA	3.21	1.42	1.33
21	2B	615	CL7	O2D-CGD	3.21	1.41	1.33
21	24	406	CL7	C2A-C1A	3.21	1.55	1.50
21	34	406	CL7	C2A-C1A	3.21	1.55	1.50
21	23	418	CL7	O2A-CGA	3.21	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1C	501	CL7	O2A-CGA	3.21	1.42	1.33
21	14	413	CL7	O2A-CGA	3.21	1.42	1.33
21	4C	501	CL7	O2A-CGA	3.21	1.42	1.33
21	21	408	CL7	O2D-CGD	3.21	1.41	1.33
21	12	508	CL7	O2D-CGD	3.21	1.41	1.33
21	42	508	CL7	O2D-CGD	3.21	1.41	1.33
21	1A	407	CL7	C4C-C3C	-3.21	1.39	1.45
21	24	413	CL7	O2A-CGA	3.21	1.42	1.33
21	34	413	CL7	O2A-CGA	3.21	1.42	1.33
21	13	516	CL7	O2A-CGA	3.21	1.42	1.33
21	2C	501	CL7	O2A-CGA	3.21	1.42	1.33
21	42	513	CL7	O2D-CGD	3.20	1.41	1.33
21	12	516	CL7	O2A-CGA	3.20	1.42	1.33
21	23	402	CL7	O2D-CGD	3.20	1.41	1.33
21	33	501	CL7	O2D-CGD	3.20	1.41	1.33
21	22	506	CL7	O2A-CGA	3.20	1.42	1.33
21	22	513	CL7	O2D-CGD	3.20	1.41	1.33
21	32	513	CL7	O2D-CGD	3.20	1.41	1.33
21	2C	505	CL7	O2D-CGD	3.20	1.41	1.33
21	3C	505	CL7	O2D-CGD	3.20	1.41	1.33
21	31	403	CL7	O2D-CGD	3.20	1.41	1.33
21	22	501	CL7	C2A-C1A	3.20	1.55	1.50
21	32	501	CL7	C2A-C1A	3.20	1.55	1.50
21	42	501	CL7	C2A-C1A	3.20	1.55	1.50
21	43	402	CL7	O2D-CGD	3.20	1.41	1.33
21	22	503	CL7	C2A-C1A	3.20	1.55	1.50
21	22	508	CL7	O2D-CGD	3.20	1.41	1.33
21	32	508	CL7	O2D-CGD	3.20	1.41	1.33
23	1B	619	8CT	C07-C02	-3.20	1.44	1.51
21	44	410	CL7	C2A-C1A	3.20	1.55	1.50
21	1B	607	CL7	C4C-C3C	-3.20	1.39	1.45
21	11	403	CL7	O2D-CGD	3.20	1.41	1.33
21	13	514	CL7	O2D-CGD	3.20	1.41	1.33
21	42	503	CL7	C4C-C3C	-3.20	1.39	1.45
21	24	414	CL7	O2A-CGA	3.20	1.42	1.33
21	42	505	CL7	O2D-CGD	3.20	1.41	1.33
21	23	415	CL7	O2D-CGD	3.20	1.41	1.33
21	33	514	CL7	O2D-CGD	3.20	1.41	1.33
21	12	503	CL7	C2A-C1A	3.19	1.55	1.50
21	42	503	CL7	C2A-C1A	3.19	1.55	1.50
21	1B	609	CL7	O2D-CGD	3.19	1.41	1.33
21	4B	610	CL7	O2D-CGD	3.19	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3C	517	CL7	O2D-CGD	3.19	1.41	1.33
21	4B	616	CL7	O2D-CGD	3.19	1.41	1.33
21	24	412	CL7	O2A-CGA	3.19	1.42	1.33
21	12	515	CL7	O2D-CGD	3.19	1.41	1.33
21	2B	605	CL7	C4C-C3C	-3.19	1.39	1.45
21	1B	615	CL7	O2A-CGA	3.19	1.42	1.33
21	43	415	CL7	O2D-CGD	3.19	1.41	1.33
21	12	513	CL7	O2D-CGD	3.19	1.41	1.33
21	23	417	CL7	O2A-CGA	3.19	1.42	1.33
21	32	515	CL7	O2D-CGD	3.19	1.41	1.33
21	2B	611	CL7	O2A-CGA	3.19	1.42	1.33
21	1C	517	CL7	O2D-CGD	3.19	1.41	1.33
21	12	505	CL7	O2D-CGD	3.19	1.41	1.33
21	4C	517	CL7	O2D-CGD	3.19	1.41	1.33
21	1D	402	CL7	O2A-CGA	3.19	1.42	1.33
21	1B	604	CL7	C4C-C3C	-3.19	1.39	1.45
21	12	511	CL7	C4C-C3C	-3.19	1.39	1.45
21	4B	605	CL7	C4C-C3C	-3.19	1.39	1.45
21	34	410	CL7	C2A-C1A	3.19	1.55	1.50
21	43	409	CL7	O2A-CGA	3.19	1.42	1.33
21	1B	614	CL7	O2D-CGD	3.19	1.41	1.33
21	2C	509	CL7	O2D-CGD	3.19	1.41	1.33
21	3C	501	CL7	C4C-C3C	-3.19	1.39	1.45
21	34	411	CL7	O2D-CGD	3.19	1.41	1.33
21	22	516	CL7	O2A-CGA	3.19	1.42	1.33
21	32	516	CL7	O2A-CGA	3.19	1.42	1.33
21	31	406	CL7	O2D-CGD	3.19	1.41	1.33
21	12	501	CL7	C2A-C1A	3.19	1.55	1.50
23	4B	620	8CT	C07-C02	-3.19	1.44	1.51
21	4B	616	CL7	O2A-CGA	3.19	1.42	1.33
21	1B	615	CL7	O2D-CGD	3.19	1.41	1.33
21	3C	501	CL7	O2A-CGA	3.19	1.42	1.33
21	14	411	CL7	O2D-CGD	3.18	1.41	1.33
21	23	409	CL7	O2A-CGA	3.18	1.42	1.33
21	33	508	CL7	O2A-CGA	3.18	1.42	1.33
21	43	417	CL7	O2A-CGA	3.18	1.42	1.33
21	2B	611	CL7	C4C-C3C	-3.18	1.39	1.45
21	13	508	CL7	O2A-CGA	3.18	1.42	1.33
21	3B	604	CL7	C4C-C3C	-3.18	1.39	1.45
21	2B	616	CL7	O2D-CGD	3.18	1.41	1.33
21	3B	615	CL7	O2D-CGD	3.18	1.41	1.33
21	21	403	CL7	O2A-CGA	3.18	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	403	CL7	O2A-CGA	3.18	1.42	1.33
21	13	502	CL7	C2A-C1A	3.18	1.55	1.50
21	1A	407	CL7	O2D-CGD	3.18	1.41	1.33
21	2B	616	CL7	O2A-CGA	3.18	1.42	1.33
21	32	503	CL7	C2A-C1A	3.18	1.55	1.50
21	33	502	CL7	O2A-CGA	3.18	1.42	1.33
21	4B	609	CL7	O2A-CGA	3.18	1.42	1.33
21	23	403	CL7	C2A-C1A	3.18	1.55	1.50
21	33	502	CL7	C2A-C1A	3.18	1.55	1.50
21	3B	605	CL7	C4C-C3C	-3.18	1.39	1.45
21	31	406	CL7	O2A-CGA	3.18	1.42	1.33
21	44	414	CL7	O2A-CGA	3.18	1.42	1.33
21	32	503	CL7	C4C-C3C	-3.18	1.39	1.45
21	34	414	CL7	O2A-CGA	3.18	1.42	1.33
21	32	511	CL7	C4C-C3C	-3.18	1.39	1.45
21	33	510	CL7	O2A-CGA	3.18	1.42	1.33
21	33	504	CL7	O2D-CGD	3.18	1.40	1.33
21	43	411	CL7	O2A-CGA	3.17	1.42	1.33
21	4B	615	CL7	O2D-CGD	3.17	1.40	1.33
21	24	412	CL7	C4C-C3C	-3.17	1.39	1.45
21	13	507	CL7	O2A-CGA	3.17	1.42	1.33
21	1B	610	CL7	C4C-C3C	-3.17	1.39	1.45
21	4B	606	CL7	C4C-C3C	-3.17	1.39	1.45
21	4B	611	CL7	C4C-C3C	-3.17	1.39	1.45
21	2B	610	CL7	O2D-CGD	3.17	1.40	1.33
21	21	420	CL7	C2A-C1A	3.17	1.55	1.50
23	2C	514	8CT	C07-C02	-3.17	1.44	1.51
23	3C	514	8CT	C07-C02	-3.17	1.44	1.51
21	42	516	CL7	O2A-CGA	3.17	1.42	1.33
21	21	403	CL7	C2A-C1A	3.17	1.55	1.50
21	32	516	CL7	O2D-CGD	3.17	1.40	1.33
21	11	403	CL7	O2A-CGA	3.17	1.42	1.33
21	41	403	CL7	O2A-CGA	3.17	1.42	1.33
23	1C	514	8CT	C07-C02	-3.17	1.44	1.51
21	33	510	CL7	C4C-C3C	-3.17	1.39	1.45
21	3B	608	CL7	O2D-CGD	3.17	1.40	1.33
21	34	412	CL7	O2A-CGA	3.17	1.42	1.33
23	3B	619	8CT	C07-C02	-3.17	1.44	1.51
21	13	504	CL7	O2D-CGD	3.17	1.40	1.33
21	43	405	CL7	O2D-CGD	3.17	1.40	1.33
23	2B	620	8CT	C07-C02	-3.17	1.44	1.51
23	3B	617	8CT	C07-C02	-3.17	1.44	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	412	CL7	C4C-C3C	-3.17	1.39	1.45
21	44	412	CL7	C4C-C3C	-3.17	1.39	1.45
21	14	414	CL7	O2A-CGA	3.17	1.42	1.33
21	11	417	CL7	O2D-CGD	3.17	1.40	1.33
21	33	504	CL7	C4C-C3C	-3.17	1.39	1.45
21	41	408	CL7	O2D-CGD	3.17	1.40	1.33
21	34	412	CL7	C4C-C3C	-3.17	1.39	1.45
21	2D	402	CL7	O2A-CGA	3.17	1.42	1.33
21	3D	402	CL7	O2A-CGA	3.17	1.42	1.33
21	21	419	CL7	C2A-C1A	3.17	1.55	1.50
21	3B	608	CL7	O2A-CGA	3.17	1.42	1.33
23	2B	601	8CT	C19-C20	3.16	1.53	1.43
21	23	408	CL7	O2A-CGA	3.16	1.42	1.33
21	33	507	CL7	O2A-CGA	3.16	1.42	1.33
21	21	403	CL7	O2D-CGD	3.16	1.40	1.33
21	3B	610	CL7	C4C-C3C	-3.16	1.39	1.45
21	11	404	CL7	O2A-CGA	3.16	1.42	1.33
32	23	401	ZEX	C1-C6	-3.16	1.49	1.53
21	4C	501	CL7	C4C-C3C	-3.16	1.39	1.45
21	3B	614	CL7	O2D-CGD	3.16	1.40	1.33
21	43	405	CL7	C4C-C3C	-3.16	1.39	1.45
21	13	502	CL7	O2A-CGA	3.16	1.42	1.33
21	23	411	CL7	O2A-CGA	3.16	1.42	1.33
21	43	403	CL7	O2A-CGA	3.16	1.42	1.33
21	4D	402	CL7	O2A-CGA	3.16	1.42	1.33
21	41	403	CL7	O2D-CGD	3.16	1.40	1.33
21	4C	509	CL7	O2D-CGD	3.16	1.40	1.33
21	2A	407	CL7	O2D-CGD	3.16	1.40	1.33
21	3A	407	CL7	O2D-CGD	3.16	1.40	1.33
21	43	408	CL7	O2A-CGA	3.16	1.42	1.33
21	41	406	CL7	O2A-CGA	3.16	1.42	1.33
21	21	408	CL7	O2A-CGA	3.16	1.42	1.33
21	31	408	CL7	O2A-CGA	3.16	1.42	1.33
21	1C	509	CL7	O2D-CGD	3.16	1.40	1.33
21	4A	407	CL7	O2D-CGD	3.16	1.40	1.33
21	44	411	CL7	O2D-CGD	3.16	1.40	1.33
21	11	408	CL7	O2A-CGA	3.16	1.42	1.33
21	3C	509	CL7	O2D-CGD	3.16	1.40	1.33
21	3B	610	CL7	C4C-NC	-3.16	1.33	1.37
21	2B	606	CL7	O2D-CGD	3.16	1.40	1.33
21	3B	605	CL7	O2D-CGD	3.16	1.40	1.33
21	22	516	CL7	O2D-CGD	3.15	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	609	CL7	O2D-CGD	3.15	1.40	1.33
21	1B	605	CL7	O2D-CGD	3.15	1.40	1.33
21	43	403	CL7	C2A-C1A	3.15	1.55	1.50
21	13	510	CL7	O2A-CGA	3.15	1.42	1.33
21	2C	517	CL7	O2D-CGD	3.15	1.40	1.33
21	23	403	CL7	O2A-CGA	3.15	1.42	1.33
21	3C	505	CL7	O2A-CGA	3.15	1.42	1.33
21	1C	501	CL7	C4C-C3C	-3.15	1.39	1.45
23	1B	617	8CT	C07-C02	-3.15	1.44	1.51
23	4B	618	8CT	C07-C02	-3.15	1.44	1.51
21	1B	608	CL7	O2A-CGA	3.15	1.42	1.33
21	2C	505	CL7	O2A-CGA	3.15	1.42	1.33
21	13	510	CL7	C4C-C3C	-3.15	1.39	1.45
21	42	516	CL7	O2D-CGD	3.15	1.40	1.33
21	42	512	CL7	C2A-C1A	3.15	1.55	1.50
21	44	410	CL7	O2D-CGD	3.15	1.40	1.33
21	1B	608	CL7	O2D-CGD	3.15	1.40	1.33
21	24	414	CL7	O2D-CGD	3.15	1.40	1.33
21	12	512	CL7	O2A-CGA	3.15	1.42	1.33
21	42	512	CL7	O2A-CGA	3.15	1.42	1.33
21	41	404	CL7	O2A-CGA	3.15	1.42	1.33
23	1B	626	8CT	C19-C20	3.15	1.53	1.43
23	4B	601	8CT	C19-C20	3.15	1.53	1.43
21	2C	509	CL7	C4C-C3C	-3.15	1.39	1.45
23	2B	618	8CT	C07-C02	-3.15	1.44	1.51
21	23	405	CL7	O2D-CGD	3.15	1.40	1.33
21	23	411	CL7	C4C-C3C	-3.15	1.39	1.45
21	21	406	CL7	O2A-CGA	3.15	1.42	1.33
21	1B	614	CL7	C4C-C3C	-3.14	1.39	1.45
21	43	411	CL7	C4C-C3C	-3.14	1.39	1.45
21	4B	606	CL7	O2D-CGD	3.14	1.40	1.33
21	2B	604	CL7	O2D-CGD	3.14	1.40	1.33
32	14	419	ZEX	C21-C26	-3.14	1.49	1.53
32	44	419	ZEX	C21-C26	-3.14	1.49	1.53
21	4B	615	CL7	C4C-C3C	-3.14	1.39	1.45
21	44	414	CL7	C4C-C3C	-3.14	1.39	1.45
21	1B	610	CL7	C4C-NC	-3.14	1.33	1.37
21	2B	612	CL7	C4C-NC	-3.14	1.33	1.37
21	4B	611	CL7	C4C-NC	-3.14	1.33	1.37
21	32	504	CL7	C2A-C1A	3.14	1.55	1.50
21	13	513	CL7	O2D-CGD	3.14	1.40	1.33
21	41	408	CL7	O2A-CGA	3.14	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	512	CL7	C2A-C1A	3.14	1.55	1.50
21	33	513	CL7	O2D-CGD	3.14	1.40	1.33
21	14	409	CL7	O2A-CGA	3.14	1.42	1.33
21	41	418	CL7	O2A-CGA	3.14	1.42	1.33
21	2B	609	CL7	O2A-CGA	3.14	1.42	1.33
21	1C	503	CL7	O2D-CGD	3.14	1.40	1.33
21	24	410	CL7	C2A-C1A	3.14	1.55	1.50
21	4B	612	CL7	C4C-C3C	-3.14	1.39	1.45
21	21	404	CL7	O2A-CGA	3.14	1.42	1.33
21	12	516	CL7	O2D-CGD	3.14	1.40	1.33
21	22	512	CL7	O2A-CGA	3.14	1.42	1.33
21	32	512	CL7	O2A-CGA	3.14	1.42	1.33
21	21	418	CL7	O2A-CGA	3.14	1.42	1.33
23	3B	626	8CT	C19-C20	3.14	1.53	1.43
21	1C	505	CL7	O2A-CGA	3.14	1.42	1.33
21	4C	505	CL7	O2A-CGA	3.14	1.42	1.33
23	4K	101	8CT	C07-C02	-3.13	1.44	1.51
21	2B	609	CL7	O2D-CGD	3.13	1.40	1.33
21	31	417	CL7	O2D-CGD	3.13	1.40	1.33
23	3K	101	8CT	C19-C20	3.13	1.53	1.43
21	41	417	CL7	O2D-CGD	3.13	1.40	1.33
23	1K	101	8CT	C19-C20	3.13	1.53	1.43
21	24	414	CL7	C4C-C3C	-3.13	1.39	1.45
21	12	518	CL7	C2A-C1A	3.13	1.55	1.50
21	1B	607	CL7	O2A-CGA	3.13	1.42	1.33
23	2K	101	8CT	C19-C20	3.13	1.53	1.43
21	1B	603	CL7	O2D-CGD	3.13	1.40	1.33
21	4B	604	CL7	O2D-CGD	3.13	1.40	1.33
23	14	402	8CT	C07-C02	-3.13	1.44	1.51
32	13	525	ZEX	C1-C6	-3.13	1.49	1.53
32	33	525	ZEX	C1-C6	-3.13	1.49	1.53
32	43	401	ZEX	C1-C6	-3.13	1.49	1.53
21	11	406	CL7	O2A-CGA	3.12	1.42	1.33
21	2B	606	CL7	C4C-C3C	-3.12	1.39	1.45
21	4C	503	CL7	O2D-CGD	3.12	1.40	1.33
21	33	511	CL7	O2D-CGD	3.12	1.40	1.33
21	22	506	CL7	C2A-C1A	3.12	1.55	1.50
21	32	518	CL7	C2A-C1A	3.12	1.55	1.50
23	24	402	8CT	C07-C02	-3.12	1.44	1.51
23	34	402	8CT	C07-C02	-3.12	1.44	1.51
21	21	417	CL7	O2D-CGD	3.12	1.40	1.33
21	31	404	CL7	O2A-CGA	3.12	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2B	615	CL7	C4C-C3C	-3.12	1.39	1.45
21	3B	614	CL7	C4C-C3C	-3.12	1.39	1.45
21	34	410	CL7	O2D-CGD	3.12	1.40	1.33
21	43	414	CL7	O2D-CGD	3.12	1.40	1.33
32	24	419	ZEX	C21-C26	-3.12	1.49	1.53
21	1B	605	CL7	C4C-C3C	-3.12	1.39	1.45
21	24	409	CL7	O2A-CGA	3.12	1.42	1.33
21	34	409	CL7	O2A-CGA	3.12	1.42	1.33
21	2B	617	CL7	O2D-CGD	3.12	1.40	1.33
21	3B	616	CL7	O2D-CGD	3.12	1.40	1.33
21	23	414	CL7	O2D-CGD	3.12	1.40	1.33
21	34	414	CL7	C4C-C3C	-3.12	1.39	1.45
21	14	414	CL7	O2D-CGD	3.12	1.40	1.33
21	2D	404	CL7	C4C-C3C	-3.12	1.39	1.45
21	1C	509	CL7	C4C-C3C	-3.12	1.39	1.45
21	4C	508	CL7	C4C-C3C	-3.12	1.39	1.45
21	44	409	CL7	O2A-CGA	3.12	1.42	1.33
21	34	414	CL7	O2D-CGD	3.12	1.40	1.33
21	42	504	CL7	C2A-C1A	3.11	1.55	1.50
21	11	409	CL7	C2A-C1A	3.11	1.55	1.50
21	23	412	CL7	C4C-C3C	-3.11	1.39	1.45
21	11	418	CL7	O2A-CGA	3.11	1.42	1.33
21	23	402	CL7	C4C-C3C	-3.11	1.39	1.45
21	42	506	CL7	C2A-C1A	3.11	1.55	1.50
23	4K	101	8CT	C19-C20	3.11	1.53	1.43
21	2B	610	CL7	O2A-CGA	3.11	1.42	1.33
21	12	517	CL7	O2D-CGD	3.11	1.40	1.33
21	13	511	CL7	O2D-CGD	3.11	1.40	1.33
21	43	412	CL7	O2D-CGD	3.11	1.40	1.33
21	4B	610	CL7	O2A-CGA	3.11	1.42	1.33
21	3B	603	CL7	O2D-CGD	3.11	1.40	1.33
21	2C	501	CL7	C4C-C3C	-3.11	1.39	1.45
21	14	410	CL7	O2D-CGD	3.11	1.40	1.33
21	2B	612	CL7	C4C-C3C	-3.11	1.39	1.45
21	31	418	CL7	O2A-CGA	3.11	1.42	1.33
21	43	404	CL7	O2A-CGA	3.11	1.42	1.33
21	2B	611	CL7	O2D-CGD	3.11	1.40	1.33
21	3B	610	CL7	O2D-CGD	3.11	1.40	1.33
21	4C	513	CL7	C2A-C1A	3.10	1.55	1.50
21	1C	511	CL7	C4C-C3C	-3.10	1.39	1.45
21	3B	611	CL7	C4C-C3C	-3.10	1.39	1.45
21	1B	616	CL7	O2D-CGD	3.10	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	617	CL7	O2D-CGD	3.10	1.40	1.33
21	22	504	CL7	C2A-C1A	3.10	1.55	1.50
21	4B	611	CL7	O2D-CGD	3.10	1.40	1.33
21	2B	608	CL7	O2A-CGA	3.10	1.42	1.33
21	3B	607	CL7	O2A-CGA	3.10	1.42	1.33
21	13	511	CL7	O2A-CGA	3.10	1.42	1.33
21	33	501	CL7	C4C-C3C	-3.10	1.39	1.45
21	12	504	CL7	C2A-C1A	3.10	1.55	1.50
21	1B	611	CL7	C4C-C3C	-3.10	1.39	1.45
21	4B	608	CL7	O2A-CGA	3.10	1.42	1.33
21	3B	606	CL7	O2A-CGA	3.10	1.42	1.33
21	33	503	CL7	O2A-CGA	3.10	1.42	1.33
21	13	502	CL7	O2D-CGD	3.10	1.40	1.33
21	43	403	CL7	O2D-CGD	3.10	1.40	1.33
21	4B	603	CL7	O2D-CGD	3.10	1.40	1.33
21	33	503	CL7	C2A-C1A	3.10	1.55	1.50
21	42	517	CL7	O2D-CGD	3.10	1.40	1.33
21	44	414	CL7	O2D-CGD	3.10	1.40	1.33
21	14	414	CL7	C4C-C3C	-3.10	1.39	1.45
21	11	406	CL7	C2A-C1A	3.10	1.55	1.50
21	13	501	CL7	C4C-C3C	-3.10	1.39	1.45
21	4C	509	CL7	C4C-C3C	-3.10	1.39	1.45
21	43	402	CL7	C4C-C3C	-3.10	1.39	1.45
21	24	410	CL7	O2D-CGD	3.09	1.40	1.33
21	23	404	CL7	O2A-CGA	3.09	1.42	1.33
21	4B	607	CL7	O2A-CGA	3.09	1.42	1.33
21	42	518	CL7	C2A-C1A	3.09	1.55	1.50
23	1C	515	8CT	C07-C02	-3.09	1.44	1.51
23	4C	515	8CT	C07-C02	-3.09	1.44	1.51
21	23	412	CL7	O2A-CGA	3.09	1.42	1.33
21	2C	503	CL7	O2D-CGD	3.09	1.40	1.33
21	3C	503	CL7	O2D-CGD	3.09	1.40	1.33
21	22	512	CL7	C2A-C1A	3.09	1.55	1.50
21	32	512	CL7	C2A-C1A	3.09	1.55	1.50
21	42	514	CL7	C2A-C1A	3.09	1.55	1.50
21	22	514	CL7	C2A-C1A	3.09	1.55	1.50
21	32	514	CL7	C2A-C1A	3.09	1.55	1.50
21	2C	506	CL7	C4C-C3C	-3.09	1.39	1.45
21	32	517	CL7	O2D-CGD	3.09	1.40	1.33
21	3B	611	CL7	C4C-NC	-3.09	1.34	1.37
21	34	415	CL7	O2D-CGD	3.09	1.40	1.33
23	1K	101	8CT	C07-C02	-3.09	1.44	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	13	511	CL7	C4C-C3C	-3.09	1.39	1.45
21	43	412	CL7	C4C-C3C	-3.09	1.39	1.45
21	22	518	CL7	C2A-C1A	3.09	1.55	1.50
21	1B	602	CL7	O2D-CGD	3.09	1.40	1.33
21	3B	602	CL7	O2D-CGD	3.09	1.40	1.33
21	12	510	CL7	C4C-C3C	-3.09	1.39	1.45
21	13	512	CL7	C4C-C3C	-3.09	1.39	1.45
21	1C	501	CL7	O2D-CGD	3.09	1.40	1.33
21	3C	509	CL7	C4C-C3C	-3.09	1.39	1.45
21	3B	603	CL7	O2A-CGA	3.08	1.42	1.33
21	23	412	CL7	O2D-CGD	3.08	1.40	1.33
32	34	419	ZEX	C21-C26	-3.08	1.49	1.53
21	2B	611	CL7	C4C-NC	-3.08	1.34	1.37
21	23	403	CL7	O2D-CGD	3.08	1.40	1.33
21	12	516	CL7	C4C-C3C	-3.08	1.39	1.45
21	42	516	CL7	C4C-C3C	-3.08	1.39	1.45
21	13	503	CL7	O2A-CGA	3.08	1.42	1.33
21	1D	404	CL7	C4C-C3C	-3.08	1.39	1.45
21	4D	404	CL7	C4C-C3C	-3.08	1.39	1.45
21	1C	506	CL7	C4C-C3C	-3.08	1.39	1.45
21	4C	506	CL7	C4C-C3C	-3.08	1.39	1.45
21	14	415	CL7	O2D-CGD	3.08	1.40	1.33
21	4B	612	CL7	C4C-NC	-3.08	1.34	1.37
21	33	511	CL7	C4C-C3C	-3.08	1.39	1.45
21	13	509	CL7	O2A-CGA	3.08	1.42	1.33
21	3B	609	CL7	O2A-CGA	3.08	1.42	1.33
21	43	410	CL7	O2A-CGA	3.08	1.42	1.33
21	33	511	CL7	O2A-CGA	3.08	1.42	1.33
21	1B	609	CL7	O2A-CGA	3.08	1.42	1.33
21	33	509	CL7	O2A-CGA	3.08	1.42	1.33
23	3K	101	8CT	C07-C02	-3.08	1.44	1.51
21	1C	512	CL7	O2D-CGD	3.08	1.40	1.33
21	2B	603	CL7	O2D-CGD	3.08	1.40	1.33
21	33	502	CL7	O2D-CGD	3.08	1.40	1.33
21	4C	512	CL7	O2D-CGD	3.08	1.40	1.33
21	2C	511	CL7	C4C-C3C	-3.08	1.39	1.45
21	2C	508	CL7	C4C-NC	-3.07	1.34	1.37
21	3C	508	CL7	C4C-NC	-3.07	1.34	1.37
21	14	410	CL7	C4C-C3C	-3.07	1.39	1.45
21	1B	604	CL7	O2A-CGA	3.07	1.42	1.33
21	4B	605	CL7	O2A-CGA	3.07	1.42	1.33
21	2C	501	CL7	O2D-CGD	3.07	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3C	501	CL7	O2D-CGD	3.07	1.40	1.33
21	32	506	CL7	C2A-C1A	3.07	1.55	1.50
21	43	412	CL7	O2A-CGA	3.07	1.42	1.33
21	22	517	CL7	O2D-CGD	3.07	1.40	1.33
21	3C	512	CL7	O2D-CGD	3.07	1.40	1.33
21	44	415	CL7	O2D-CGD	3.07	1.40	1.33
21	14	406	CL7	C4C-C3C	-3.07	1.39	1.45
21	44	406	CL7	C4C-C3C	-3.07	1.39	1.45
21	23	410	CL7	O2A-CGA	3.07	1.42	1.33
21	2B	607	CL7	O2A-CGA	3.07	1.42	1.33
21	23	413	CL7	C4C-C3C	-3.06	1.39	1.45
21	34	411	CL7	C4C-C3C	-3.06	1.39	1.45
21	22	516	CL7	C4C-C3C	-3.06	1.39	1.45
21	3C	508	CL7	C4C-C3C	-3.06	1.39	1.45
21	2B	614	CL7	O2A-CGA	3.06	1.42	1.33
21	32	515	CL7	C2A-C1A	3.06	1.55	1.50
21	41	409	CL7	C2A-C1A	3.06	1.55	1.50
21	4C	501	CL7	O2D-CGD	3.06	1.40	1.33
21	1B	606	CL7	O2A-CGA	3.06	1.42	1.33
21	1C	508	CL7	C4C-C3C	-3.06	1.39	1.45
21	1C	509	CL7	O2A-CGA	3.06	1.42	1.33
21	42	510	CL7	C4C-C3C	-3.06	1.39	1.45
21	2B	605	CL7	O2A-CGA	3.06	1.42	1.33
21	12	514	CL7	C2A-C1A	3.06	1.55	1.50
21	3C	506	CL7	O2A-CGA	3.06	1.42	1.33
21	1B	610	CL7	O2D-CGD	3.06	1.40	1.33
21	4B	614	CL7	O2A-CGA	3.06	1.42	1.33
21	24	412	CL7	O2D-CGD	3.06	1.40	1.33
21	34	412	CL7	O2D-CGD	3.06	1.40	1.33
21	4C	510	CL7	C4C-C3C	-3.06	1.39	1.45
21	4C	511	CL7	C4C-C3C	-3.06	1.39	1.45
21	2C	513	CL7	C2A-C1A	3.06	1.55	1.50
21	1C	513	CL7	C2A-C1A	3.06	1.55	1.50
21	24	415	CL7	O2D-CGD	3.06	1.40	1.33
23	44	402	8CT	C07-C02	-3.06	1.45	1.51
21	1C	508	CL7	C4C-NC	-3.06	1.34	1.37
21	1C	506	CL7	O2A-CGA	3.06	1.42	1.33
21	4C	506	CL7	O2A-CGA	3.06	1.42	1.33
23	2C	515	8CT	C07-C02	-3.06	1.45	1.51
23	3C	515	8CT	C07-C02	-3.06	1.45	1.51
21	1B	603	CL7	O2A-CGA	3.05	1.42	1.33
21	4B	604	CL7	O2A-CGA	3.05	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	606	CL7	O2A-CGA	3.05	1.42	1.33
21	34	406	CL7	C4C-C3C	-3.05	1.39	1.45
21	43	408	CL7	C4C-C3C	-3.05	1.39	1.45
21	3C	506	CL7	C4C-C3C	-3.05	1.39	1.45
32	22	519	ZEX	C1-C6	-3.05	1.49	1.53
21	1B	605	CL7	O2A-CGA	3.05	1.42	1.33
21	2C	508	CL7	C4C-C3C	-3.05	1.39	1.45
21	21	409	CL7	C2A-C1A	3.05	1.55	1.50
32	12	519	ZEX	C1-C6	-3.05	1.49	1.53
32	42	519	ZEX	C1-C6	-3.05	1.49	1.53
22	1A	402	PHO	C3A-C2A	-3.05	1.51	1.54
21	2B	604	CL7	O2A-CGA	3.05	1.42	1.33
21	1B	606	CL7	O2D-CGD	3.05	1.40	1.33
21	4B	607	CL7	O2D-CGD	3.05	1.40	1.33
21	22	510	CL7	C4C-C3C	-3.05	1.39	1.45
21	24	411	CL7	C4C-C3C	-3.05	1.39	1.45
21	44	410	CL7	C4C-C3C	-3.05	1.39	1.45
21	14	408	CL7	O2D-CGD	3.05	1.40	1.33
21	4C	509	CL7	O2A-CGA	3.05	1.42	1.33
21	31	409	CL7	C2A-C1A	3.05	1.55	1.50
21	24	408	CL7	O2D-CGD	3.05	1.40	1.33
21	22	515	CL7	C2A-C1A	3.05	1.55	1.50
23	2K	101	8CT	C07-C02	-3.05	1.45	1.51
21	14	411	CL7	C4C-C3C	-3.05	1.39	1.45
21	32	510	CL7	C4C-C3C	-3.05	1.39	1.45
21	44	411	CL7	C4C-C3C	-3.05	1.39	1.45
21	3B	612	CL7	O2A-CGA	3.05	1.42	1.33
23	1B	618	8CT	C07-C02	-3.05	1.45	1.51
21	22	509	CL7	C4C-C3C	-3.05	1.39	1.45
21	43	413	CL7	C4C-C3C	-3.05	1.39	1.45
21	2C	512	CL7	O2D-CGD	3.05	1.40	1.33
21	32	516	CL7	C4C-C3C	-3.05	1.39	1.45
23	2C	515	8CT	C19-C20	3.05	1.52	1.43
21	1B	612	CL7	O2A-CGA	3.05	1.42	1.33
21	24	406	CL7	C4C-C3C	-3.05	1.39	1.45
32	32	519	ZEX	C1-C6	-3.04	1.49	1.53
21	3B	613	CL7	O2A-CGA	3.04	1.42	1.33
21	43	405	CL7	O2A-CGA	3.04	1.42	1.33
21	22	509	CL7	O2A-CGA	3.04	1.42	1.33
21	42	515	CL7	C2A-C1A	3.04	1.55	1.50
21	2B	606	CL7	O2A-CGA	3.04	1.42	1.33
21	3B	605	CL7	O2A-CGA	3.04	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2B	607	CL7	O2D-CGD	3.04	1.40	1.33
21	3B	606	CL7	O2D-CGD	3.04	1.40	1.33
21	34	408	CL7	O2D-CGD	3.04	1.40	1.33
21	1B	613	CL7	O2A-CGA	3.04	1.42	1.33
21	3C	506	CL7	O2D-CGD	3.04	1.40	1.33
21	13	503	CL7	C2A-C1A	3.04	1.55	1.50
21	43	404	CL7	C2A-C1A	3.04	1.55	1.50
21	13	505	CL7	C4C-C3C	-3.04	1.39	1.45
21	43	406	CL7	C4C-C3C	-3.04	1.39	1.45
21	3C	511	CL7	C4C-C3C	-3.04	1.39	1.45
21	1A	403	CL7	O2D-CGD	3.04	1.40	1.33
21	4A	403	CL7	O2D-CGD	3.04	1.40	1.33
21	12	507	CL7	C2A-C1A	3.04	1.55	1.50
21	22	510	CL7	O2A-CGA	3.04	1.42	1.33
21	32	510	CL7	O2A-CGA	3.04	1.42	1.33
21	1C	506	CL7	O2D-CGD	3.04	1.40	1.33
21	4C	506	CL7	O2D-CGD	3.04	1.40	1.33
21	3C	509	CL7	O2A-CGA	3.04	1.42	1.33
21	33	508	CL7	O2D-CGD	3.04	1.40	1.33
21	3B	604	CL7	O2A-CGA	3.04	1.42	1.33
21	2C	506	CL7	O2A-CGA	3.04	1.42	1.33
21	12	501	CL7	O2A-CGA	3.04	1.42	1.33
21	41	406	CL7	C2A-C1A	3.04	1.55	1.50
21	14	412	CL7	O2D-CGD	3.04	1.40	1.33
21	44	412	CL7	O2D-CGD	3.04	1.40	1.33
21	22	505	CL7	O2A-CGA	3.04	1.42	1.33
21	2C	509	CL7	O2A-CGA	3.04	1.42	1.33
21	44	408	CL7	O2D-CGD	3.03	1.40	1.33
21	4C	508	CL7	C4C-NC	-3.03	1.34	1.37
21	1C	510	CL7	C4C-C3C	-3.03	1.39	1.45
21	23	408	CL7	C4C-C3C	-3.03	1.39	1.45
21	12	509	CL7	O2A-CGA	3.03	1.42	1.33
21	12	515	CL7	C2A-C1A	3.03	1.55	1.50
21	11	408	CL7	C2A-C1A	3.03	1.55	1.50
21	12	505	CL7	O2A-CGA	3.03	1.42	1.33
21	32	505	CL7	O2A-CGA	3.03	1.42	1.33
21	12	510	CL7	O2A-CGA	3.03	1.42	1.33
21	42	510	CL7	O2A-CGA	3.03	1.42	1.33
23	3B	618	8CT	C19-C20	3.03	1.52	1.43
21	32	501	CL7	C4C-C3C	-3.03	1.39	1.45
21	3A	403	CL7	O2D-CGD	3.03	1.40	1.33
21	24	410	CL7	C4C-C3C	-3.03	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	410	CL7	C4C-C3C	-3.03	1.39	1.45
21	1C	511	CL7	C2A-C1A	3.03	1.55	1.50
21	13	516	CL7	O2D-CGD	3.03	1.40	1.33
21	2B	605	CL7	O2D-CGD	3.03	1.40	1.33
21	3B	604	CL7	O2D-CGD	3.03	1.40	1.33
21	43	417	CL7	O2D-CGD	3.03	1.40	1.33
21	23	405	CL7	O2A-CGA	3.02	1.42	1.33
21	33	504	CL7	O2A-CGA	3.02	1.42	1.33
21	1B	611	CL7	C4C-NC	-3.02	1.34	1.37
21	2A	403	CL7	O2D-CGD	3.02	1.40	1.33
21	42	501	CL7	C4C-C3C	-3.02	1.39	1.45
21	2B	613	CL7	O2A-CGA	3.02	1.42	1.33
21	13	504	CL7	O2A-CGA	3.02	1.42	1.33
21	11	406	CL7	C4C-C3C	-3.02	1.39	1.45
21	2C	510	CL7	C4C-C3C	-3.02	1.39	1.45
21	24	413	CL7	C4C-C3C	-3.02	1.39	1.45
21	3C	510	CL7	C4C-C3C	-3.02	1.39	1.45
21	3D	404	CL7	C4C-C3C	-3.02	1.39	1.45
21	42	509	CL7	O2A-CGA	3.02	1.42	1.33
21	13	516	CL7	C4C-C3C	-3.02	1.39	1.45
21	12	506	CL7	C2A-C1A	3.02	1.55	1.50
23	1C	515	8CT	C19-C20	3.02	1.52	1.43
23	4C	515	8CT	C19-C20	3.02	1.52	1.43
21	32	508	CL7	C4C-C3C	-3.02	1.39	1.45
21	3B	613	CL7	O2D-CGD	3.02	1.40	1.33
21	23	406	CL7	O2A-CGA	3.02	1.42	1.33
21	32	509	CL7	O2A-CGA	3.02	1.42	1.33
21	33	505	CL7	O2A-CGA	3.02	1.42	1.33
23	2B	619	8CT	C19-C20	3.02	1.52	1.43
21	3C	513	CL7	C2A-C1A	3.02	1.55	1.50
21	2C	506	CL7	O2D-CGD	3.02	1.40	1.33
21	2B	614	CL7	O2D-CGD	3.02	1.40	1.33
21	14	409	CL7	O2D-CGD	3.02	1.40	1.33
21	12	508	CL7	C4C-C3C	-3.01	1.39	1.45
23	1B	618	8CT	C19-C20	3.01	1.52	1.43
23	4B	619	8CT	C19-C20	3.01	1.52	1.43
21	31	406	CL7	C2A-C1A	3.01	1.55	1.50
21	4B	613	CL7	O2A-CGA	3.01	1.42	1.33
21	23	402	CL7	O2A-CGA	3.01	1.42	1.33
23	3D	406	8CT	C07-C02	-3.01	1.45	1.51
21	14	413	CL7	C4C-C3C	-3.01	1.39	1.45
21	33	512	CL7	C4C-C3C	-3.01	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	413	CL7	C4C-C3C	-3.01	1.39	1.45
21	14	411	CL7	O2A-CGA	3.01	1.42	1.33
21	14	406	CL7	O2D-CGD	3.01	1.40	1.33
21	22	508	CL7	C4C-C3C	-3.01	1.39	1.45
21	3D	404	CL7	O2A-CGA	3.01	1.42	1.33
21	34	411	CL7	O2A-CGA	3.01	1.42	1.33
21	43	402	CL7	O2A-CGA	3.01	1.42	1.33
21	3B	604	CL7	C4C-NC	-3.01	1.34	1.37
21	42	501	CL7	O2A-CGA	3.01	1.42	1.33
21	42	507	CL7	C2A-C1A	3.01	1.55	1.50
23	4B	619	8CT	C07-C02	-3.01	1.45	1.51
21	42	508	CL7	C4C-C3C	-3.01	1.39	1.45
21	21	404	CL7	C2A-C1A	3.01	1.55	1.50
21	21	406	CL7	C2A-C1A	3.01	1.55	1.50
21	2B	613	CL7	O2D-CGD	3.01	1.40	1.33
21	3B	612	CL7	O2D-CGD	3.01	1.40	1.33
21	2B	617	CL7	C4C-C3C	-3.01	1.39	1.45
21	3B	616	CL7	C4C-C3C	-3.01	1.39	1.45
21	23	404	CL7	C2A-C1A	3.01	1.55	1.50
21	13	508	CL7	O2D-CGD	3.01	1.40	1.33
21	43	409	CL7	O2D-CGD	3.01	1.40	1.33
21	23	417	CL7	O2D-CGD	3.01	1.40	1.33
21	31	404	CL7	C2A-C1A	3.01	1.55	1.50
23	3C	515	8CT	C19-C20	3.01	1.52	1.43
21	13	507	CL7	C2A-C1A	3.00	1.55	1.50
21	43	408	CL7	C2A-C1A	3.00	1.55	1.50
21	33	505	CL7	O2D-CGD	3.00	1.40	1.33
21	1D	404	CL7	O2A-CGA	3.00	1.42	1.33
21	2D	404	CL7	O2A-CGA	3.00	1.42	1.33
21	4D	404	CL7	O2A-CGA	3.00	1.42	1.33
21	1B	612	CL7	O2D-CGD	3.00	1.40	1.33
21	4B	613	CL7	O2D-CGD	3.00	1.40	1.33
21	24	409	CL7	O2D-CGD	3.00	1.40	1.33
23	1D	406	8CT	C19-C20	3.00	1.52	1.43
21	1D	404	CL7	O2D-CGD	3.00	1.40	1.33
21	43	413	CL7	O2D-CGD	3.00	1.40	1.33
21	34	409	CL7	O2D-CGD	3.00	1.40	1.33
21	23	408	CL7	C2A-C1A	3.00	1.55	1.50
21	33	507	CL7	C2A-C1A	3.00	1.55	1.50
21	31	418	CL7	O2D-CGD	3.00	1.40	1.33
21	32	512	CL7	C4C-NC	-3.00	1.34	1.37
21	12	502	CL7	C4C-C3C	-3.00	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	502	CL7	C4C-C3C	-3.00	1.39	1.45
21	4B	617	CL7	C4C-C3C	-3.00	1.39	1.45
21	23	406	CL7	O2D-CGD	3.00	1.40	1.33
21	1B	604	CL7	O2D-CGD	3.00	1.40	1.33
21	4B	605	CL7	O2D-CGD	3.00	1.40	1.33
21	4B	608	CL7	O2D-CGD	3.00	1.40	1.33
21	13	505	CL7	O2A-CGA	3.00	1.42	1.33
21	43	406	CL7	O2A-CGA	3.00	1.42	1.33
21	42	505	CL7	O2A-CGA	3.00	1.42	1.33
21	44	406	CL7	O2D-CGD	3.00	1.40	1.33
21	12	501	CL7	C4C-C3C	-2.99	1.39	1.45
21	13	507	CL7	C4C-C3C	-2.99	1.39	1.45
21	22	501	CL7	C4C-C3C	-2.99	1.39	1.45
21	33	501	CL7	O2A-CGA	2.99	1.42	1.33
21	21	418	CL7	O2D-CGD	2.99	1.40	1.33
21	22	506	CL7	C4C-C3C	-2.99	1.39	1.45
21	34	407	CL7	C4C-C3C	-2.99	1.39	1.45
21	33	512	CL7	O2D-CGD	2.99	1.40	1.33
21	23	409	CL7	O2D-CGD	2.99	1.40	1.33
21	23	417	CL7	C4C-C3C	-2.99	1.39	1.45
21	22	512	CL7	O2D-CGD	2.99	1.40	1.33
21	32	512	CL7	O2D-CGD	2.99	1.40	1.33
21	43	406	CL7	O2D-CGD	2.99	1.40	1.33
21	24	411	CL7	O2A-CGA	2.99	1.42	1.33
21	31	406	CL7	C4C-C3C	-2.99	1.39	1.45
21	33	516	CL7	O2D-CGD	2.99	1.40	1.33
22	2A	402	PHO	C3A-C2A	-2.99	1.52	1.54
22	3A	402	PHO	C3A-C2A	-2.99	1.52	1.54
21	43	417	CL7	C4C-C3C	-2.99	1.39	1.45
21	23	406	CL7	C4C-C3C	-2.99	1.39	1.45
21	32	501	CL7	O2A-CGA	2.99	1.42	1.33
21	1B	607	CL7	O2D-CGD	2.99	1.40	1.33
21	12	507	CL7	O2D-CGD	2.99	1.40	1.33
23	3D	406	8CT	C19-C20	2.99	1.52	1.43
21	3C	511	CL7	C2A-C1A	2.99	1.55	1.50
21	23	413	CL7	O2D-CGD	2.99	1.40	1.33
21	33	507	CL7	C4C-C3C	-2.99	1.39	1.45
21	33	505	CL7	C4C-C3C	-2.99	1.39	1.45
21	1B	613	CL7	O2D-CGD	2.99	1.40	1.33
21	4B	614	CL7	O2D-CGD	2.99	1.40	1.33
21	13	501	CL7	O2A-CGA	2.99	1.42	1.33
21	2B	608	CL7	O2D-CGD	2.99	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	406	CL7	O2D-CGD	2.99	1.40	1.33
21	3B	607	CL7	O2D-CGD	2.99	1.40	1.33
21	34	413	CL7	C4C-C3C	-2.99	1.39	1.45
21	13	505	CL7	O2D-CGD	2.99	1.40	1.33
21	2D	404	CL7	O2D-CGD	2.99	1.40	1.33
21	3D	404	CL7	O2D-CGD	2.99	1.40	1.33
21	21	405	CL7	C4C-C3C	-2.98	1.39	1.45
21	31	405	CL7	C4C-C3C	-2.98	1.39	1.45
21	41	406	CL7	C4C-C3C	-2.98	1.39	1.45
21	4B	604	CL7	C4C-C3C	-2.98	1.39	1.45
21	42	512	CL7	O2D-CGD	2.98	1.40	1.33
21	13	508	CL7	C2A-C1A	2.98	1.55	1.50
21	11	418	CL7	O2D-CGD	2.98	1.40	1.33
21	4B	607	CL7	C2A-C1A	2.98	1.55	1.50
22	4A	402	PHO	C3A-C2A	-2.98	1.52	1.54
21	32	502	CL7	C4C-C3C	-2.98	1.39	1.45
21	32	509	CL7	C4C-C3C	-2.98	1.39	1.45
21	2C	511	CL7	C2A-C1A	2.98	1.55	1.50
21	22	502	CL7	C4C-C3C	-2.98	1.39	1.45
21	22	507	CL7	C2A-C1A	2.98	1.55	1.50
21	32	507	CL7	C2A-C1A	2.98	1.55	1.50
21	22	507	CL7	O2D-CGD	2.98	1.40	1.33
21	32	507	CL7	O2D-CGD	2.98	1.40	1.33
23	4D	406	8CT	C19-C20	2.98	1.52	1.43
21	22	501	CL7	O2A-CGA	2.98	1.42	1.33
21	2B	612	CL7	O2A-CGA	2.98	1.42	1.33
21	12	512	CL7	O2D-CGD	2.98	1.40	1.33
22	2A	402	PHO	CBD-CGD	-2.98	1.48	1.52
21	14	407	CL7	C4C-C3C	-2.98	1.39	1.45
21	2B	616	CL7	C4C-NC	-2.97	1.34	1.37
23	1D	406	8CT	C07-C02	-2.97	1.45	1.51
23	4D	406	8CT	C07-C02	-2.97	1.45	1.51
21	22	512	CL7	C4C-NC	-2.97	1.34	1.37
21	2D	405	CL7	O2D-CGD	2.97	1.40	1.33
21	3D	405	CL7	O2D-CGD	2.97	1.40	1.33
21	2B	612	CL7	O2D-CGD	2.97	1.40	1.33
23	2B	619	8CT	C07-C02	-2.97	1.45	1.51
23	3B	618	8CT	C07-C02	-2.97	1.45	1.51
21	21	408	CL7	C2A-C1A	2.97	1.55	1.50
21	31	408	CL7	C2A-C1A	2.97	1.55	1.50
21	4C	502	CL7	C2A-C1A	2.97	1.55	1.50
21	2B	605	CL7	C4C-NC	-2.97	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4D	404	CL7	O2D-CGD	2.97	1.40	1.33
21	34	406	CL7	O2D-CGD	2.97	1.40	1.33
21	41	418	CL7	O2D-CGD	2.97	1.40	1.33
21	1C	504	CL7	C4C-C3C	-2.97	1.39	1.45
21	2A	403	CL7	C4C-C3C	-2.97	1.39	1.45
21	3A	403	CL7	C4C-C3C	-2.97	1.39	1.45
21	13	510	CL7	C2A-C1A	2.97	1.55	1.50
21	43	411	CL7	C2A-C1A	2.97	1.55	1.50
21	44	411	CL7	O2A-CGA	2.97	1.42	1.33
21	41	408	CL7	C2A-C1A	2.97	1.55	1.50
23	2D	406	8CT	C07-C02	-2.97	1.45	1.51
32	12	524	ZEX	C21-C26	-2.97	1.49	1.53
32	42	524	ZEX	C21-C26	-2.97	1.49	1.53
21	44	409	CL7	O2D-CGD	2.97	1.40	1.33
21	1D	405	CL7	O2D-CGD	2.96	1.40	1.33
21	4D	405	CL7	O2D-CGD	2.96	1.40	1.33
21	1B	606	CL7	C2A-C1A	2.96	1.55	1.50
21	4B	605	CL7	C4C-NC	-2.96	1.34	1.37
21	3B	615	CL7	C4C-C3C	-2.96	1.39	1.45
21	1C	503	CL7	C4C-C3C	-2.96	1.39	1.45
21	1B	611	CL7	O2A-CGA	2.96	1.42	1.33
21	4B	612	CL7	O2D-CGD	2.96	1.40	1.33
21	1A	403	CL7	C4C-C3C	-2.96	1.39	1.45
21	4A	403	CL7	C4C-C3C	-2.96	1.39	1.45
21	12	509	CL7	C4C-C3C	-2.96	1.39	1.45
21	42	509	CL7	C4C-C3C	-2.96	1.39	1.45
21	21	413	CL7	C4C-C3C	-2.96	1.39	1.45
21	2C	502	CL7	C2A-C1A	2.96	1.55	1.50
21	3C	502	CL7	C2A-C1A	2.96	1.55	1.50
21	12	506	CL7	C4C-C3C	-2.96	1.39	1.45
21	4C	503	CL7	C4C-C3C	-2.96	1.39	1.45
21	42	506	CL7	C4C-C3C	-2.96	1.39	1.45
21	23	411	CL7	C2A-C1A	2.96	1.55	1.50
21	34	417	CL7	C2A-C1A	2.96	1.55	1.50
21	1B	616	CL7	C4C-C3C	-2.96	1.39	1.45
21	42	512	CL7	C4C-NC	-2.96	1.34	1.37
21	13	515	CL7	C4C-C3C	-2.96	1.40	1.45
23	2D	406	8CT	C19-C20	2.96	1.52	1.43
21	13	512	CL7	O2D-CGD	2.96	1.40	1.33
21	2C	508	CL7	O2D-CGD	2.96	1.40	1.33
21	13	508	CL7	C4C-C3C	-2.95	1.40	1.45
21	44	407	CL7	C4C-C3C	-2.95	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	21	417	CL7	C4C-C3C	-2.95	1.40	1.45
21	1B	615	CL7	C4C-NC	-2.95	1.34	1.37
21	4B	616	CL7	C4C-NC	-2.95	1.34	1.37
21	11	403	CL7	C4C-C3C	-2.95	1.40	1.45
21	41	403	CL7	C4C-C3C	-2.95	1.40	1.45
21	24	405	CL7	C2A-C1A	2.95	1.55	1.50
21	34	405	CL7	C2A-C1A	2.95	1.55	1.50
21	4B	612	CL7	O2A-CGA	2.95	1.41	1.33
21	1C	508	CL7	O2D-CGD	2.95	1.40	1.33
23	2A	404	8CT	C19-C20	2.95	1.52	1.43
21	2B	604	CL7	C4C-C3C	-2.95	1.40	1.45
21	1B	611	CL7	O2D-CGD	2.95	1.40	1.33
21	33	516	CL7	C4C-C3C	-2.95	1.40	1.45
21	3B	603	CL7	C4C-C3C	-2.95	1.40	1.45
21	3C	512	CL7	C4C-C3C	-2.95	1.40	1.45
21	31	417	CL7	C4C-C3C	-2.95	1.40	1.45
21	4B	603	CL7	C4C-C3C	-2.95	1.40	1.45
21	22	517	CL7	C4C-C3C	-2.94	1.40	1.45
21	24	407	CL7	C4C-C3C	-2.94	1.40	1.45
21	32	506	CL7	C4C-C3C	-2.94	1.40	1.45
21	1C	512	CL7	C4C-C3C	-2.94	1.40	1.45
21	2A	403	CL7	C2A-C1A	2.94	1.55	1.50
21	3A	403	CL7	C2A-C1A	2.94	1.55	1.50
21	32	502	CL7	O2D-CGD	2.94	1.40	1.33
21	31	403	CL7	C4C-C3C	-2.94	1.40	1.45
21	4C	512	CL7	C4C-C3C	-2.94	1.40	1.45
23	2B	601	8CT	C07-C02	-2.94	1.45	1.51
21	11	404	CL7	C2A-C1A	2.94	1.55	1.50
21	14	417	CL7	C2A-C1A	2.94	1.55	1.50
21	41	404	CL7	C2A-C1A	2.94	1.55	1.50
21	1C	502	CL7	C2A-C1A	2.94	1.55	1.50
21	4C	511	CL7	C2A-C1A	2.94	1.55	1.50
21	33	508	CL7	C4C-C3C	-2.94	1.40	1.45
32	22	524	ZEX	C21-C26	-2.94	1.49	1.53
21	4C	508	CL7	O2D-CGD	2.94	1.40	1.33
21	14	404	CL7	C4C-C3C	-2.94	1.40	1.45
21	44	404	CL7	C4C-C3C	-2.94	1.40	1.45
21	44	405	CL7	C2A-C1A	2.94	1.55	1.50
21	43	416	CL7	C4C-C3C	-2.94	1.40	1.45
21	1A	403	CL7	C2A-C1A	2.94	1.55	1.50
21	4A	403	CL7	C2A-C1A	2.94	1.55	1.50
21	21	406	CL7	C4C-C3C	-2.94	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	13	510	CL7	C4C-NC	-2.94	1.34	1.37
21	42	505	CL7	C4C-NC	-2.94	1.34	1.37
21	12	502	CL7	O2D-CGD	2.94	1.40	1.33
21	42	502	CL7	O2D-CGD	2.94	1.40	1.33
21	11	405	CL7	C4C-C3C	-2.93	1.40	1.45
21	41	405	CL7	C4C-C3C	-2.93	1.40	1.45
23	1B	626	8CT	C07-C02	-2.93	1.45	1.51
21	42	507	CL7	O2D-CGD	2.93	1.40	1.33
21	1B	603	CL7	C4C-C3C	-2.93	1.40	1.45
21	23	416	CL7	C4C-C3C	-2.93	1.40	1.45
21	11	413	CL7	C4C-C3C	-2.93	1.40	1.45
21	2C	504	CL7	C4C-C3C	-2.93	1.40	1.45
21	3C	504	CL7	C4C-C3C	-2.93	1.40	1.45
21	41	413	CL7	C4C-C3C	-2.93	1.40	1.45
21	23	404	CL7	O2D-CGD	2.93	1.40	1.33
21	1B	613	CL7	C4C-NC	-2.93	1.34	1.37
21	33	515	CL7	C4C-C3C	-2.93	1.40	1.45
21	2B	614	CL7	C4C-NC	-2.93	1.34	1.37
21	3B	613	CL7	C4C-NC	-2.93	1.34	1.37
21	24	414	CL7	C4C-NC	-2.93	1.34	1.37
21	3B	611	CL7	O2A-CGA	2.93	1.41	1.33
21	23	411	CL7	C4C-NC	-2.93	1.34	1.37
21	32	516	CL7	C4C-NC	-2.93	1.34	1.37
21	33	510	CL7	C4C-NC	-2.93	1.34	1.37
21	24	417	CL7	C2A-C1A	2.93	1.55	1.50
23	1A	404	8CT	C19-C20	2.93	1.52	1.43
21	2B	603	CL7	C4C-C3C	-2.93	1.40	1.45
21	2C	512	CL7	C4C-C3C	-2.93	1.40	1.45
23	4B	601	8CT	C07-C02	-2.93	1.45	1.51
21	3B	611	CL7	O2D-CGD	2.93	1.40	1.33
21	4C	517	CL7	C4C-C3C	-2.93	1.40	1.45
21	3B	606	CL7	C2A-C1A	2.93	1.55	1.50
21	12	505	CL7	C4C-NC	-2.92	1.34	1.37
21	3C	503	CL7	C4C-C3C	-2.92	1.40	1.45
21	14	405	CL7	C2A-C1A	2.92	1.55	1.50
23	3A	404	8CT	C19-C20	2.92	1.52	1.43
21	22	502	CL7	O2D-CGD	2.92	1.40	1.33
21	1B	604	CL7	C4C-NC	-2.92	1.34	1.37
21	13	513	CL7	C4C-C3C	-2.92	1.40	1.45
21	31	402	CL7	C4C-C3C	-2.92	1.40	1.45
21	2C	503	CL7	C4C-C3C	-2.92	1.40	1.45
21	11	402	CL7	C4C-C3C	-2.92	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	402	CL7	C4C-C3C	-2.92	1.40	1.45
21	3C	508	CL7	O2D-CGD	2.92	1.40	1.33
21	12	517	CL7	C4C-C3C	-2.92	1.40	1.45
23	4A	404	8CT	C19-C20	2.92	1.52	1.43
21	21	418	CL7	C4C-NC	-2.92	1.34	1.37
21	3B	615	CL7	C4C-NC	-2.92	1.34	1.37
21	1B	613	CL7	C1B-C2B	-2.92	1.36	1.43
21	1C	517	CL7	C4C-C3C	-2.92	1.40	1.45
21	43	409	CL7	C4C-C3C	-2.92	1.40	1.45
21	1D	404	CL7	C4C-NC	-2.92	1.34	1.37
21	4D	404	CL7	C4C-NC	-2.92	1.34	1.37
21	12	512	CL7	C4C-NC	-2.92	1.34	1.37
21	24	404	CL7	C4C-C3C	-2.91	1.40	1.45
32	13	525	ZEX	C21-C26	-2.91	1.49	1.53
32	43	401	ZEX	C21-C26	-2.91	1.49	1.53
23	3B	626	8CT	C07-C02	-2.91	1.45	1.51
21	3D	404	CL7	C4C-NC	-2.91	1.34	1.37
21	42	510	CL7	C4C-NC	-2.91	1.34	1.37
21	23	409	CL7	C2A-C1A	2.91	1.55	1.50
21	33	508	CL7	C2A-C1A	2.91	1.55	1.50
21	12	516	CL7	C4C-NC	-2.91	1.34	1.37
21	33	513	CL7	C4C-C3C	-2.91	1.40	1.45
21	32	505	CL7	C4C-NC	-2.91	1.34	1.37
21	34	405	CL7	C4C-C3C	-2.91	1.40	1.45
21	43	414	CL7	C4C-C3C	-2.91	1.40	1.45
21	44	417	CL7	C2A-C1A	2.91	1.55	1.50
21	2B	607	CL7	C2A-C1A	2.91	1.55	1.50
21	4C	501	CL7	C4C-NC	-2.91	1.34	1.37
21	2D	405	CL7	C4C-C3C	-2.91	1.40	1.45
21	43	411	CL7	C4C-NC	-2.91	1.34	1.37
21	33	503	CL7	O2D-CGD	2.91	1.40	1.33
32	23	401	ZEX	C21-C26	-2.91	1.49	1.53
21	4C	504	CL7	C4C-C3C	-2.90	1.40	1.45
21	13	503	CL7	O2D-CGD	2.90	1.40	1.33
21	43	404	CL7	O2D-CGD	2.90	1.40	1.33
22	1A	402	PHO	CBD-CGD	-2.90	1.48	1.52
22	4A	402	PHO	CBD-CGD	-2.90	1.48	1.52
21	23	409	CL7	C4C-C3C	-2.90	1.40	1.45
21	42	517	CL7	C4C-C3C	-2.90	1.40	1.45
21	14	414	CL7	C4C-NC	-2.90	1.34	1.37
21	44	414	CL7	C4C-NC	-2.90	1.34	1.37
22	3A	402	PHO	CBD-CGD	-2.90	1.48	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	414	CL7	C4C-NC	-2.90	1.34	1.37
21	21	403	CL7	C4C-C3C	-2.90	1.40	1.45
21	34	408	CL7	C4C-C3C	-2.90	1.40	1.45
21	21	402	CL7	C4C-C3C	-2.90	1.40	1.45
21	2C	517	CL7	C4C-C3C	-2.90	1.40	1.45
21	3C	517	CL7	C4C-C3C	-2.90	1.40	1.45
21	22	502	CL7	C4C-NC	-2.90	1.34	1.37
21	3B	602	CL7	C4C-C3C	-2.90	1.40	1.45
21	34	404	CL7	C4C-C3C	-2.90	1.40	1.45
21	11	418	CL7	C4C-NC	-2.90	1.34	1.37
21	22	505	CL7	C4C-NC	-2.90	1.34	1.37
21	2B	614	CL7	C1B-C2B	-2.90	1.36	1.43
21	3B	613	CL7	C1B-C2B	-2.90	1.36	1.43
21	1B	615	CL7	C4C-C3C	-2.90	1.40	1.45
21	33	516	CL7	C4C-NC	-2.90	1.34	1.37
21	33	510	CL7	C2A-C1A	2.90	1.55	1.50
21	2A	407	CL7	C4C-NC	-2.89	1.34	1.37
21	2B	603	CL7	C4C-NC	-2.89	1.34	1.37
21	4B	616	CL7	C2A-C1A	2.89	1.55	1.50
21	2C	509	CL7	C4C-NC	-2.89	1.34	1.37
21	1C	501	CL7	C4C-NC	-2.89	1.34	1.37
21	21	405	CL7	C2A-C1A	2.89	1.55	1.50
21	3C	509	CL7	C4C-NC	-2.89	1.34	1.37
21	31	413	CL7	C4C-C3C	-2.89	1.40	1.45
21	23	414	CL7	C4C-C3C	-2.89	1.40	1.45
21	32	502	CL7	C4C-NC	-2.89	1.34	1.37
23	4C	518	8CT	C19-C20	2.89	1.52	1.43
21	1D	405	CL7	C4C-C3C	-2.89	1.40	1.45
21	4D	405	CL7	C4C-C3C	-2.89	1.40	1.45
21	3C	507	CL7	O2A-CGA	2.89	1.41	1.33
23	1C	518	8CT	C19-C20	2.89	1.52	1.43
21	1A	407	CL7	C4C-NC	-2.89	1.34	1.37
21	43	418	CL7	C2A-C1A	2.88	1.55	1.50
21	32	517	CL7	C4C-C3C	-2.88	1.40	1.45
23	2C	518	8CT	C19-C20	2.88	1.52	1.43
23	3C	518	8CT	C19-C20	2.88	1.52	1.43
21	2C	507	CL7	C4C-NC	-2.88	1.34	1.37
21	43	418	CL7	C4C-C3C	-2.88	1.40	1.45
21	42	503	CL7	O2A-CGA	2.88	1.41	1.33
21	24	408	CL7	C4C-C3C	-2.88	1.40	1.45
23	34	402	8CT	C19-C20	2.88	1.52	1.43
21	1D	405	CL7	C2A-C1A	2.88	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	603	CL7	C4C-NC	-2.88	1.34	1.37
32	32	524	ZEX	C21-C26	-2.88	1.49	1.53
21	4C	501	CL7	C2A-C1A	2.88	1.55	1.50
21	43	409	CL7	C2A-C1A	2.88	1.55	1.50
23	44	402	8CT	C19-C20	2.88	1.52	1.43
21	1B	602	CL7	C4C-C3C	-2.88	1.40	1.45
21	23	418	CL7	C2A-C1A	2.88	1.55	1.50
21	14	408	CL7	C4C-C3C	-2.88	1.40	1.45
23	3B	617	8CT	C19-C20	2.88	1.52	1.43
21	24	405	CL7	C4C-C3C	-2.87	1.40	1.45
21	4B	614	CL7	C1B-C2B	-2.87	1.36	1.43
21	1C	507	CL7	O2A-CGA	2.87	1.41	1.33
21	4C	507	CL7	O2A-CGA	2.87	1.41	1.33
21	11	417	CL7	C4C-C3C	-2.87	1.40	1.45
21	41	417	CL7	C4C-C3C	-2.87	1.40	1.45
21	13	517	CL7	C4C-C3C	-2.87	1.40	1.45
21	3D	405	CL7	C4C-C3C	-2.87	1.40	1.45
21	2B	616	CL7	C4C-C3C	-2.87	1.40	1.45
21	3B	602	CL7	C4C-NC	-2.87	1.34	1.37
21	43	419	CL7	C4C-C3C	-2.87	1.40	1.45
23	1A	404	8CT	C07-C02	-2.87	1.45	1.51
23	1C	514	8CT	C19-C20	2.87	1.52	1.43
23	4C	514	8CT	C19-C20	2.87	1.52	1.43
21	13	507	CL7	O2D-CGD	2.87	1.40	1.33
21	4B	614	CL7	C4C-NC	-2.87	1.34	1.37
21	1C	509	CL7	C4C-NC	-2.87	1.34	1.37
21	4C	509	CL7	C4C-NC	-2.87	1.34	1.37
23	3C	514	8CT	C19-C20	2.86	1.52	1.43
21	31	418	CL7	C4C-NC	-2.86	1.34	1.37
21	43	417	CL7	C4C-NC	-2.86	1.34	1.37
21	23	408	CL7	O2D-CGD	2.86	1.40	1.33
21	42	516	CL7	C4C-NC	-2.86	1.34	1.37
21	1C	507	CL7	O2D-CGD	2.86	1.40	1.33
32	33	525	ZEX	C21-C26	-2.86	1.49	1.53
21	41	405	CL7	C2A-C1A	2.86	1.55	1.50
21	23	418	CL7	C4C-C3C	-2.86	1.40	1.45
23	24	402	8CT	C19-C20	2.86	1.52	1.43
21	1B	602	CL7	C4C-NC	-2.86	1.34	1.37
21	1C	507	CL7	C4C-NC	-2.86	1.34	1.37
21	2D	404	CL7	C4C-NC	-2.86	1.34	1.37
21	4C	507	CL7	C4C-NC	-2.86	1.34	1.37
21	33	507	CL7	O2D-CGD	2.86	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4C	507	CL7	O2D-CGD	2.86	1.40	1.33
21	13	517	CL7	C2A-C1A	2.86	1.55	1.50
23	1B	617	8CT	C19-C20	2.86	1.52	1.43
21	22	503	CL7	O2A-CGA	2.86	1.41	1.33
21	3C	507	CL7	C4C-NC	-2.86	1.34	1.37
23	14	402	8CT	C19-C20	2.86	1.52	1.43
21	33	505	CL7	C2A-C1A	2.86	1.55	1.50
21	43	412	CL7	C2A-C1A	2.86	1.55	1.50
23	4A	404	8CT	C07-C02	-2.86	1.45	1.51
21	44	408	CL7	C4C-C3C	-2.86	1.40	1.45
21	12	517	CL7	C2A-C1A	2.86	1.55	1.50
21	22	517	CL7	C2A-C1A	2.86	1.55	1.50
21	2C	502	CL7	C4C-C3C	-2.85	1.40	1.45
21	1C	509	CL7	C2A-C1A	2.85	1.55	1.50
21	4B	616	CL7	C4C-C3C	-2.85	1.40	1.45
21	2C	507	CL7	O2A-CGA	2.85	1.41	1.33
21	3A	407	CL7	O2A-CGA	2.85	1.41	1.33
21	34	404	CL7	C4C-NC	-2.85	1.34	1.37
21	2A	407	CL7	O2A-CGA	2.85	1.41	1.33
23	2B	618	8CT	C19-C20	2.85	1.52	1.43
21	3C	509	CL7	C2A-C1A	2.85	1.55	1.50
21	12	503	CL7	O2A-CGA	2.85	1.41	1.33
23	2C	514	8CT	C19-C20	2.84	1.52	1.43
21	14	405	CL7	C4C-C3C	-2.84	1.40	1.45
21	43	408	CL7	O2D-CGD	2.84	1.40	1.33
21	41	418	CL7	C4C-NC	-2.84	1.34	1.37
21	1A	407	CL7	O2A-CGA	2.84	1.41	1.33
21	4A	407	CL7	O2A-CGA	2.84	1.41	1.33
21	12	502	CL7	C4C-NC	-2.84	1.34	1.37
21	4A	407	CL7	C4C-NC	-2.84	1.34	1.37
21	42	502	CL7	C4C-NC	-2.84	1.34	1.37
21	2C	507	CL7	O2D-CGD	2.84	1.40	1.33
21	3C	507	CL7	O2D-CGD	2.84	1.40	1.33
21	3D	405	CL7	C2A-C1A	2.84	1.55	1.50
21	4C	509	CL7	C2A-C1A	2.84	1.55	1.50
21	32	503	CL7	O2A-CGA	2.84	1.41	1.33
21	3C	501	CL7	C4C-NC	-2.84	1.34	1.37
21	23	412	CL7	C2A-C1A	2.84	1.55	1.50
21	33	517	CL7	C2A-C1A	2.84	1.55	1.50
21	4D	405	CL7	C2A-C1A	2.84	1.55	1.50
21	43	402	CL7	C4C-NC	-2.84	1.34	1.37
21	44	415	CL7	C2A-C1A	2.84	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2B	613	CL7	C4C-NC	-2.84	1.34	1.37
21	11	405	CL7	C2A-C1A	2.83	1.55	1.50
21	43	410	CL7	C4C-C3C	-2.83	1.40	1.45
23	1B	619	8CT	C19-C20	2.83	1.52	1.43
23	4B	618	8CT	C19-C20	2.83	1.52	1.43
21	2B	604	CL7	C4C-NC	-2.83	1.34	1.37
21	22	510	CL7	C4C-NC	-2.83	1.34	1.37
21	32	510	CL7	C4C-NC	-2.83	1.34	1.37
23	2A	404	8CT	C07-C02	-2.83	1.45	1.51
23	3A	404	8CT	C07-C02	-2.83	1.45	1.51
21	23	406	CL7	C2A-C1A	2.83	1.55	1.50
21	31	405	CL7	C2A-C1A	2.83	1.55	1.50
21	2B	616	CL7	C2A-C1A	2.83	1.55	1.50
21	3B	615	CL7	C2A-C1A	2.83	1.55	1.50
21	32	517	CL7	C2A-C1A	2.83	1.55	1.50
21	24	406	CL7	C4C-NC	-2.83	1.34	1.37
21	23	409	CL7	C4C-NC	-2.83	1.34	1.37
21	14	410	CL7	C4C-NC	-2.83	1.34	1.37
21	44	410	CL7	C4C-NC	-2.83	1.34	1.37
21	1B	606	CL7	C4C-C3C	-2.83	1.40	1.45
21	2D	405	CL7	C2A-C1A	2.83	1.55	1.50
21	22	516	CL7	C4C-NC	-2.83	1.34	1.37
21	1B	608	CL7	C4C-C3C	-2.83	1.40	1.45
21	13	518	CL7	C4C-C3C	-2.83	1.40	1.45
21	23	417	CL7	C4C-NC	-2.83	1.34	1.37
21	31	411	CL7	C2A-C1A	2.82	1.55	1.50
21	3A	407	CL7	C4C-NC	-2.82	1.34	1.37
21	4C	502	CL7	C4C-C3C	-2.82	1.40	1.45
21	33	518	CL7	C4C-C3C	-2.82	1.40	1.45
21	21	407	CL7	C4C-C3C	-2.82	1.40	1.45
21	14	406	CL7	C4C-NC	-2.82	1.34	1.37
31	4F	101	HEM	C1C-C2C	-2.82	1.39	1.45
21	33	509	CL7	C4C-C3C	-2.82	1.40	1.45
21	33	501	CL7	C4C-NC	-2.82	1.34	1.37
21	2C	509	CL7	C2A-C1A	2.82	1.55	1.50
21	1C	502	CL7	C4C-C3C	-2.82	1.40	1.45
21	1C	501	CL7	C2A-C1A	2.82	1.55	1.50
21	13	517	CL7	C4C-NC	-2.82	1.34	1.37
21	23	419	CL7	C4C-C3C	-2.82	1.40	1.45
21	2C	501	CL7	C4C-NC	-2.82	1.34	1.37
21	33	511	CL7	C2A-C1A	2.81	1.55	1.50
21	44	405	CL7	C4C-C3C	-2.81	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	510	CL7	C4C-NC	-2.81	1.34	1.37
23	2B	620	8CT	C19-C20	2.81	1.52	1.43
21	14	404	CL7	C4C-NC	-2.81	1.34	1.37
21	43	409	CL7	C4C-NC	-2.81	1.34	1.37
21	24	415	CL7	C2A-C1A	2.81	1.55	1.50
21	34	415	CL7	C2A-C1A	2.81	1.55	1.50
21	3C	513	CL7	C4C-C3C	-2.81	1.40	1.45
21	42	517	CL7	C2A-C1A	2.81	1.55	1.50
21	13	505	CL7	C2A-C1A	2.81	1.55	1.50
21	43	406	CL7	C2A-C1A	2.81	1.55	1.50
21	4B	604	CL7	C4C-NC	-2.81	1.34	1.37
21	2C	501	CL7	C2A-C1A	2.81	1.55	1.50
21	3C	501	CL7	C2A-C1A	2.81	1.55	1.50
21	14	415	CL7	C4C-C3C	-2.81	1.40	1.45
21	44	415	CL7	C4C-C3C	-2.81	1.40	1.45
21	13	502	CL7	C4C-C3C	-2.81	1.40	1.45
21	3C	502	CL7	C4C-C3C	-2.81	1.40	1.45
23	4B	620	8CT	C19-C20	2.81	1.52	1.43
21	33	508	CL7	C4C-NC	-2.80	1.34	1.37
23	3B	619	8CT	C19-C20	2.80	1.52	1.43
31	1F	101	HEM	C1C-C2C	-2.80	1.39	1.45
32	22	522	ZEX	C21-C26	-2.80	1.49	1.53
32	32	522	ZEX	C21-C26	-2.80	1.49	1.53
21	11	409	CL7	C4C-C3C	-2.80	1.40	1.45
21	41	409	CL7	C4C-C3C	-2.80	1.40	1.45
21	1B	615	CL7	C2A-C1A	2.80	1.55	1.50
21	33	517	CL7	C4C-C3C	-2.80	1.40	1.45
21	13	511	CL7	C2A-C1A	2.80	1.55	1.50
21	24	404	CL7	C4C-NC	-2.80	1.34	1.37
21	1D	405	CL7	C4C-NC	-2.80	1.34	1.37
21	4D	405	CL7	C4C-NC	-2.80	1.34	1.37
21	11	407	CL7	C4C-C3C	-2.80	1.40	1.45
21	13	516	CL7	C4C-NC	-2.80	1.34	1.37
31	3F	101	HEM	FE-ND	-2.79	1.86	1.94
21	2B	609	CL7	C4C-C3C	-2.79	1.40	1.45
21	3B	608	CL7	C4C-C3C	-2.79	1.40	1.45
21	2C	503	CL7	C2A-C1A	2.79	1.55	1.50
21	3C	503	CL7	C2A-C1A	2.79	1.55	1.50
21	22	504	CL7	C4C-C3C	-2.79	1.40	1.45
21	14	411	CL7	C1B-C2B	-2.79	1.36	1.43
21	2C	513	CL7	C4C-C3C	-2.79	1.40	1.45
21	4B	607	CL7	C4C-C3C	-2.79	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	404	CL7	C2A-C1A	2.79	1.55	1.50
31	4F	101	HEM	FE-ND	-2.79	1.86	1.94
21	12	517	CL7	C4C-NC	-2.79	1.34	1.37
21	12	504	CL7	C4C-C3C	-2.79	1.40	1.45
21	14	415	CL7	C2A-C1A	2.79	1.55	1.50
21	4B	613	CL7	MG-ND	-2.79	2.00	2.05
21	1C	513	CL7	C4C-C3C	-2.79	1.40	1.45
32	12	522	ZEX	C21-C26	-2.79	1.49	1.53
32	42	522	ZEX	C21-C26	-2.79	1.49	1.53
21	1C	503	CL7	C4C-NC	-2.79	1.34	1.37
21	11	403	CL7	C4C-NC	-2.79	1.34	1.37
21	11	411	CL7	C2A-C1A	2.79	1.55	1.50
21	13	508	CL7	C4C-NC	-2.79	1.34	1.37
21	23	412	CL7	C4C-NC	-2.79	1.34	1.37
21	2B	608	CL7	C1B-C2B	-2.79	1.36	1.43
21	2B	607	CL7	C4C-C3C	-2.79	1.40	1.45
21	3B	606	CL7	C4C-C3C	-2.79	1.40	1.45
21	31	407	CL7	C4C-C3C	-2.79	1.40	1.45
21	13	509	CL7	C4C-C3C	-2.79	1.40	1.45
21	23	418	CL7	C4C-NC	-2.79	1.34	1.37
21	33	517	CL7	C4C-NC	-2.78	1.34	1.37
21	42	517	CL7	C4C-NC	-2.78	1.34	1.37
21	3B	622	CL7	C4C-C3C	-2.78	1.40	1.45
21	34	406	CL7	C4C-NC	-2.78	1.34	1.37
21	21	411	CL7	C2A-C1A	2.78	1.55	1.50
21	34	412	CL7	C2A-C1A	2.78	1.55	1.50
21	22	501	CL7	C4C-NC	-2.78	1.34	1.37
21	32	501	CL7	C4C-NC	-2.78	1.34	1.37
21	4B	623	CL7	C4C-C3C	-2.78	1.40	1.45
31	2F	101	HEM	C1C-C2C	-2.78	1.39	1.45
31	3F	101	HEM	C1C-C2C	-2.78	1.39	1.45
21	22	516	CL7	C2A-C1A	2.78	1.55	1.50
21	3B	603	CL7	C4C-NC	-2.78	1.34	1.37
21	3B	612	CL7	C4C-NC	-2.78	1.34	1.37
21	44	406	CL7	C4C-NC	-2.78	1.34	1.37
21	24	410	CL7	C4C-NC	-2.78	1.34	1.37
21	34	410	CL7	C4C-NC	-2.78	1.34	1.37
21	1B	612	CL7	C4C-NC	-2.78	1.34	1.37
21	41	407	CL7	C4C-C3C	-2.78	1.40	1.45
21	44	411	CL7	C1B-C2B	-2.78	1.36	1.43
21	42	504	CL7	C4C-C3C	-2.78	1.40	1.45
21	24	415	CL7	C4C-NC	-2.77	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	415	CL7	C4C-NC	-2.77	1.34	1.37
21	12	501	CL7	C4C-NC	-2.77	1.34	1.37
21	33	511	CL7	C4C-NC	-2.77	1.34	1.37
21	13	511	CL7	C4C-NC	-2.77	1.34	1.37
21	44	411	CL7	C2A-C1A	2.77	1.55	1.50
21	3B	612	CL7	MG-ND	-2.77	2.00	2.05
21	1C	502	CL7	C4C-NC	-2.77	1.34	1.37
21	2B	613	CL7	MG-ND	-2.77	2.00	2.05
21	21	420	CL7	C4C-C3C	-2.77	1.40	1.45
21	23	410	CL7	C4C-C3C	-2.77	1.40	1.45
21	24	415	CL7	C4C-C3C	-2.77	1.40	1.45
21	34	415	CL7	C4C-C3C	-2.77	1.40	1.45
21	4C	513	CL7	C4C-C3C	-2.77	1.40	1.45
31	1F	101	HEM	FE-ND	-2.77	1.86	1.94
21	14	412	CL7	C2A-C1A	2.77	1.55	1.50
21	44	412	CL7	C2A-C1A	2.77	1.55	1.50
21	31	403	CL7	C4C-NC	-2.77	1.34	1.37
21	21	409	CL7	C4C-C3C	-2.77	1.40	1.45
21	31	409	CL7	C4C-C3C	-2.77	1.40	1.45
21	4B	609	CL7	C4C-C3C	-2.77	1.40	1.45
21	4B	608	CL7	C1B-C2B	-2.77	1.36	1.43
21	4B	605	CL7	C2A-C1A	2.77	1.55	1.50
21	3B	603	CL7	C2A-C1A	2.77	1.55	1.50
21	41	420	CL7	C4C-C3C	-2.77	1.40	1.45
21	1C	503	CL7	C2A-C1A	2.76	1.55	1.50
21	4C	503	CL7	C2A-C1A	2.76	1.55	1.50
32	22	519	ZEX	C21-C26	-2.76	1.50	1.53
21	41	411	CL7	C4C-C3C	-2.76	1.40	1.45
21	4C	503	CL7	C4C-NC	-2.76	1.34	1.37
21	4B	613	CL7	C4C-NC	-2.76	1.34	1.37
21	3B	607	CL7	C1B-C2B	-2.76	1.36	1.43
21	3C	503	CL7	C4C-NC	-2.76	1.34	1.37
21	1C	509	CL7	MG-ND	-2.76	2.00	2.05
21	1B	622	CL7	C4C-C3C	-2.76	1.40	1.45
21	3C	506	CL7	C4C-NC	-2.76	1.34	1.37
23	2C	518	8CT	C07-C02	-2.76	1.45	1.51
21	12	509	CL7	C4C-NC	-2.76	1.34	1.37
21	2B	607	CL7	C4C-NC	-2.76	1.34	1.37
21	42	509	CL7	C4C-NC	-2.76	1.34	1.37
21	1B	607	CL7	C1B-C2B	-2.76	1.36	1.43
21	43	412	CL7	C4C-NC	-2.76	1.34	1.37
21	11	420	CL7	C4C-C3C	-2.76	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	411	CL7	C1B-C2B	-2.75	1.36	1.43
21	34	411	CL7	C1B-C2B	-2.75	1.36	1.43
21	4C	509	CL7	MG-ND	-2.75	2.00	2.05
21	23	403	CL7	C4C-C3C	-2.75	1.40	1.45
21	1B	603	CL7	C4C-NC	-2.75	1.34	1.37
21	32	507	CL7	C3B-C4B	-2.75	1.36	1.42
21	42	507	CL7	C4C-C3C	-2.75	1.40	1.45
21	12	507	CL7	C3B-C4B	-2.75	1.36	1.42
21	42	507	CL7	C3B-C4B	-2.75	1.36	1.42
21	43	403	CL7	C1B-C2B	-2.75	1.36	1.43
23	3C	518	8CT	C07-C02	-2.75	1.45	1.51
21	1B	622	CL7	CHC-C4B	2.75	1.45	1.39
21	2B	623	CL7	C4C-C3C	-2.75	1.40	1.45
21	3B	608	CL7	C2A-C1A	2.75	1.55	1.50
21	23	402	CL7	C4C-NC	-2.75	1.34	1.37
21	32	517	CL7	C4C-NC	-2.75	1.34	1.37
21	31	420	CL7	C4C-C3C	-2.75	1.40	1.45
21	1B	603	CL7	C2A-C1A	2.75	1.55	1.50
21	4B	604	CL7	C2A-C1A	2.75	1.55	1.50
31	2F	101	HEM	FE-ND	-2.75	1.86	1.94
23	1C	518	8CT	C07-C02	-2.75	1.45	1.51
21	4B	617	CL7	C4C-NC	-2.75	1.34	1.37
21	34	404	CL7	C2A-C1A	2.75	1.55	1.50
21	11	411	CL7	C4C-C3C	-2.75	1.40	1.45
21	3B	609	CL7	C4C-C3C	-2.75	1.40	1.45
21	43	404	CL7	C4C-NC	-2.75	1.34	1.37
32	32	519	ZEX	C21-C26	-2.75	1.50	1.53
21	41	411	CL7	C2A-C1A	2.74	1.55	1.50
21	2B	606	CL7	C4C-NC	-2.74	1.34	1.37
21	2B	617	CL7	C1B-C2B	-2.74	1.36	1.43
23	4C	518	8CT	C07-C02	-2.74	1.45	1.51
21	23	409	CL7	C1B-C2B	-2.74	1.36	1.43
21	3C	502	CL7	C4C-NC	-2.74	1.34	1.37
21	4B	610	CL7	C4C-C3C	-2.74	1.40	1.45
21	21	410	CL7	C4C-C3C	-2.74	1.40	1.45
21	31	410	CL7	C4C-C3C	-2.74	1.40	1.45
21	44	416	CL7	C4C-C3C	-2.74	1.40	1.45
21	44	404	CL7	C2A-C1A	2.74	1.55	1.50
21	43	405	CL7	C4C-NC	-2.74	1.34	1.37
21	14	416	CL7	C4C-C3C	-2.74	1.40	1.45
21	32	504	CL7	C4C-C3C	-2.74	1.40	1.45
21	41	410	CL7	C4C-C3C	-2.74	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	404	CL7	C4C-NC	-2.74	1.34	1.37
21	2C	509	CL7	MG-ND	-2.74	2.00	2.05
21	2C	505	CL7	C2A-C1A	2.74	1.54	1.50
21	3C	505	CL7	C2A-C1A	2.74	1.54	1.50
21	2B	617	CL7	C4C-NC	-2.73	1.34	1.37
21	4C	505	CL7	C2A-C1A	2.73	1.54	1.50
21	3B	622	CL7	CHC-C4B	2.73	1.45	1.39
21	21	411	CL7	C4C-C3C	-2.73	1.40	1.45
21	11	410	CL7	C4C-C3C	-2.73	1.40	1.45
21	3A	401	CL7	CHC-C4B	2.73	1.45	1.39
21	1C	505	CL7	C2A-C1A	2.73	1.54	1.50
21	22	507	CL7	C3B-C4B	-2.73	1.36	1.42
21	43	403	CL7	C4C-C3C	-2.73	1.40	1.45
21	23	405	CL7	C4C-NC	-2.73	1.34	1.37
21	43	413	CL7	C4C-NC	-2.73	1.34	1.37
21	22	507	CL7	MG-ND	-2.73	2.00	2.05
21	4B	616	CL7	MG-ND	-2.73	2.00	2.05
21	24	412	CL7	C2A-C1A	2.73	1.54	1.50
21	23	403	CL7	C1B-C2B	-2.73	1.36	1.43
21	1B	612	CL7	MG-ND	-2.73	2.00	2.05
21	13	501	CL7	C4C-NC	-2.73	1.34	1.37
21	14	415	CL7	C4C-NC	-2.73	1.34	1.37
21	2C	510	CL7	C4C-NC	-2.73	1.34	1.37
21	44	415	CL7	C4C-NC	-2.73	1.34	1.37
21	3C	509	CL7	MG-ND	-2.73	2.00	2.05
21	32	503	CL7	C4C-NC	-2.73	1.34	1.37
21	1C	506	CL7	C4C-NC	-2.73	1.34	1.37
21	4C	506	CL7	C4C-NC	-2.73	1.34	1.37
21	3D	405	CL7	C4C-NC	-2.73	1.34	1.37
21	22	508	CL7	C2A-C1A	2.72	1.54	1.50
21	2B	604	CL7	C2A-C1A	2.72	1.54	1.50
21	33	502	CL7	C4C-C3C	-2.72	1.40	1.45
21	33	508	CL7	C1B-C2B	-2.72	1.36	1.43
21	1B	608	CL7	C2A-C1A	2.72	1.54	1.50
21	4B	609	CL7	C2A-C1A	2.72	1.54	1.50
21	42	501	CL7	C4C-NC	-2.72	1.34	1.37
21	24	411	CL7	C2A-C1A	2.72	1.54	1.50
21	43	418	CL7	C4C-NC	-2.72	1.34	1.37
21	2B	605	CL7	C2A-C1A	2.72	1.54	1.50
21	42	503	CL7	C4C-NC	-2.72	1.34	1.37
21	42	516	CL7	C2A-C1A	2.72	1.54	1.50
21	1B	616	CL7	C1B-C2B	-2.72	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	617	CL7	C1B-C2B	-2.72	1.36	1.43
21	2B	610	CL7	C4C-C3C	-2.71	1.40	1.45
21	1B	604	CL7	C2A-C1A	2.71	1.54	1.50
21	33	502	CL7	C1B-C2B	-2.71	1.36	1.43
21	13	508	CL7	C1B-C2B	-2.71	1.36	1.43
21	22	508	CL7	C4C-NC	-2.71	1.34	1.37
21	4B	623	CL7	CHC-C4B	2.71	1.45	1.39
21	2B	623	CL7	CHC-C4B	2.71	1.45	1.39
21	23	406	CL7	MG-ND	-2.71	2.00	2.05
21	41	406	CL7	C4C-NC	-2.71	1.34	1.37
21	22	507	CL7	C4C-C3C	-2.71	1.40	1.45
21	32	507	CL7	C4C-C3C	-2.71	1.40	1.45
21	42	508	CL7	C2A-C1A	2.71	1.54	1.50
21	4A	401	CL7	CHC-C4B	2.71	1.45	1.39
21	2B	612	CL7	C2A-C1A	2.71	1.54	1.50
21	13	502	CL7	C1B-C2B	-2.71	1.36	1.43
21	43	409	CL7	C1B-C2B	-2.71	1.36	1.43
21	3B	616	CL7	C1B-C2B	-2.71	1.36	1.43
21	1B	609	CL7	C4C-C3C	-2.71	1.40	1.45
21	14	411	CL7	C2A-C1A	2.71	1.54	1.50
21	11	407	CL7	C4C-NC	-2.71	1.34	1.37
21	3C	510	CL7	C4C-NC	-2.71	1.34	1.37
21	11	405	CL7	C4C-NC	-2.71	1.34	1.37
21	41	405	CL7	C4C-NC	-2.71	1.34	1.37
21	2D	405	CL7	C4C-NC	-2.71	1.34	1.37
21	34	411	CL7	C2A-C1A	2.70	1.54	1.50
21	3A	403	CL7	C4C-NC	-2.70	1.34	1.37
21	12	507	CL7	C4C-C3C	-2.70	1.40	1.45
21	22	517	CL7	C4C-NC	-2.70	1.34	1.37
21	3B	605	CL7	C4C-NC	-2.70	1.34	1.37
21	3B	615	CL7	MG-ND	-2.70	2.00	2.05
21	32	516	CL7	C2A-C1A	2.70	1.54	1.50
21	14	417	CL7	C4C-C3C	-2.70	1.40	1.45
21	2C	506	CL7	C4C-NC	-2.70	1.34	1.37
21	3B	604	CL7	C2A-C1A	2.70	1.54	1.50
21	32	507	CL7	MG-ND	-2.70	2.00	2.05
21	2C	505	CL7	C4C-NC	-2.70	1.34	1.37
21	33	512	CL7	C4C-NC	-2.70	1.34	1.37
21	42	518	CL7	C4C-C3C	-2.70	1.40	1.45
21	12	507	CL7	MG-ND	-2.70	2.00	2.05
21	32	508	CL7	C2A-C1A	2.70	1.54	1.50
21	1C	510	CL7	C4C-NC	-2.70	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	616	CL7	C4C-NC	-2.70	1.34	1.37
21	24	416	CL7	C4C-C3C	-2.70	1.40	1.45
21	34	416	CL7	C4C-C3C	-2.70	1.40	1.45
21	21	403	CL7	C4C-NC	-2.70	1.34	1.37
21	3B	606	CL7	C4C-NC	-2.70	1.34	1.37
21	31	407	CL7	C4C-NC	-2.70	1.34	1.37
32	12	519	ZEX	C21-C26	-2.70	1.50	1.53
32	42	519	ZEX	C21-C26	-2.70	1.50	1.53
21	3C	505	CL7	C4C-NC	-2.69	1.34	1.37
21	4C	502	CL7	C4C-NC	-2.69	1.34	1.37
21	13	503	CL7	C4C-NC	-2.69	1.34	1.37
21	2C	503	CL7	C4C-NC	-2.69	1.34	1.37
21	14	404	CL7	C2A-C1A	2.69	1.54	1.50
21	1B	615	CL7	MG-ND	-2.69	2.00	2.05
21	2C	502	CL7	C4C-NC	-2.69	1.34	1.37
21	2B	609	CL7	C2A-C1A	2.69	1.54	1.50
21	1B	605	CL7	C4C-NC	-2.69	1.34	1.37
21	4B	606	CL7	C4C-NC	-2.69	1.34	1.37
32	33	525	ZEX	C30-C29	-2.69	1.32	1.35
21	13	512	CL7	C4C-NC	-2.69	1.34	1.37
21	2A	401	CL7	CHC-C4B	2.69	1.45	1.39
21	22	518	CL7	C4C-C3C	-2.69	1.40	1.45
21	32	518	CL7	C4C-C3C	-2.69	1.40	1.45
21	22	509	CL7	C4C-NC	-2.69	1.34	1.37
21	12	518	CL7	C4C-C3C	-2.69	1.40	1.45
21	12	516	CL7	C2A-C1A	2.69	1.54	1.50
21	12	503	CL7	C4C-NC	-2.69	1.34	1.37
21	23	413	CL7	C4C-NC	-2.69	1.34	1.37
21	44	417	CL7	C4C-C3C	-2.69	1.40	1.45
21	31	411	CL7	C4C-C3C	-2.68	1.40	1.45
21	41	403	CL7	C4C-NC	-2.68	1.34	1.37
21	2B	617	CL7	C2A-C1A	2.68	1.54	1.50
21	24	417	CL7	C4C-C3C	-2.68	1.40	1.45
21	42	509	CL7	MG-ND	-2.68	2.00	2.05
21	14	412	CL7	C4C-NC	-2.68	1.34	1.37
21	14	414	CL7	C2A-C1A	2.68	1.54	1.50
21	44	414	CL7	C2A-C1A	2.68	1.54	1.50
21	31	415	CL7	CHC-C4B	2.68	1.45	1.39
21	1C	505	CL7	C4C-C3C	-2.68	1.40	1.45
21	33	504	CL7	C4C-NC	-2.68	1.34	1.37
21	1B	611	CL7	C2A-C1A	2.68	1.54	1.50
21	4B	612	CL7	C2A-C1A	2.68	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	518	CL7	C4C-NC	-2.68	1.34	1.37
21	13	504	CL7	C4C-NC	-2.68	1.34	1.37
21	22	503	CL7	C4C-NC	-2.68	1.34	1.37
21	21	407	CL7	C4C-NC	-2.68	1.34	1.37
21	2C	505	CL7	MG-ND	-2.68	2.00	2.05
21	3C	505	CL7	MG-ND	-2.68	2.00	2.05
21	42	507	CL7	MG-ND	-2.68	2.00	2.05
21	4C	506	CL7	C1B-C2B	-2.68	1.36	1.43
21	12	510	CL7	MG-ND	-2.68	2.00	2.05
21	41	407	CL7	C4C-NC	-2.68	1.34	1.37
21	3C	506	CL7	C1B-C2B	-2.68	1.36	1.43
21	3C	506	CL7	C2A-C1A	2.68	1.54	1.50
21	23	404	CL7	C4C-NC	-2.68	1.34	1.37
21	33	503	CL7	C4C-NC	-2.68	1.34	1.37
21	4C	505	CL7	C4C-NC	-2.68	1.34	1.37
21	1A	401	CL7	CHC-C4B	2.67	1.45	1.39
21	1B	616	CL7	C4C-NC	-2.67	1.34	1.37
21	21	405	CL7	C4C-NC	-2.67	1.34	1.37
21	31	405	CL7	C4C-NC	-2.67	1.34	1.37
21	2C	506	CL7	C1B-C2B	-2.67	1.37	1.43
21	1C	505	CL7	C4C-NC	-2.67	1.34	1.37
21	13	506	CL7	C4C-C3C	-2.67	1.40	1.45
21	12	508	CL7	C4C-NC	-2.67	1.34	1.37
21	3B	606	CL7	C1B-C2B	-2.67	1.37	1.43
21	23	408	CL7	MG-ND	-2.67	2.00	2.05
21	2B	610	CL7	C4C-NC	-2.67	1.34	1.37
21	22	510	CL7	MG-ND	-2.67	2.00	2.05
21	34	412	CL7	C4C-NC	-2.67	1.34	1.37
21	21	415	CL7	CHC-C4B	2.67	1.45	1.39
21	1A	403	CL7	MG-ND	-2.67	2.00	2.05
21	33	509	CL7	C2A-C1A	2.67	1.54	1.50
21	3C	510	CL7	C1B-C2B	-2.66	1.37	1.43
21	13	514	CL7	C4C-C3C	-2.66	1.40	1.45
21	33	517	CL7	MG-ND	-2.66	2.00	2.05
21	1C	506	CL7	C1B-C2B	-2.66	1.37	1.43
21	3B	611	CL7	C2A-C1A	2.66	1.54	1.50
21	12	508	CL7	C2A-C1A	2.66	1.54	1.50
21	1B	616	CL7	C2A-C1A	2.66	1.54	1.50
21	4B	617	CL7	C2A-C1A	2.66	1.54	1.50
21	1A	403	CL7	C4C-NC	-2.66	1.34	1.37
21	1B	606	CL7	C4C-NC	-2.66	1.34	1.37
21	4B	607	CL7	C4C-NC	-2.66	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	609	CL7	C4C-NC	-2.66	1.34	1.37
32	23	401	ZEX	C30-C29	-2.66	1.32	1.35
21	11	415	CL7	CHC-C4B	2.66	1.45	1.39
21	41	415	CL7	CHC-C4B	2.66	1.45	1.39
21	42	515	CL7	C4C-C3C	-2.66	1.40	1.45
21	22	515	CL7	C4C-C3C	-2.66	1.40	1.45
21	1C	505	CL7	MG-ND	-2.66	2.00	2.05
21	4C	505	CL7	MG-ND	-2.66	2.00	2.05
21	32	518	CL7	C4C-NC	-2.66	1.34	1.37
32	13	525	ZEX	C30-C29	-2.66	1.32	1.35
21	21	404	CL7	C4C-C3C	-2.66	1.40	1.45
21	1C	506	CL7	C2A-C1A	2.66	1.54	1.50
21	24	414	CL7	C2A-C1A	2.66	1.54	1.50
21	34	414	CL7	C2A-C1A	2.66	1.54	1.50
21	4C	506	CL7	C2A-C1A	2.66	1.54	1.50
21	31	404	CL7	C4C-C3C	-2.65	1.40	1.45
23	1C	518	8CT	C01-C02	2.65	1.55	1.50
21	21	406	CL7	C4C-NC	-2.65	1.34	1.37
21	3C	517	CL7	MG-ND	-2.65	2.00	2.05
21	1C	506	CL7	MG-ND	-2.65	2.00	2.05
21	2B	616	CL7	MG-ND	-2.65	2.00	2.05
21	2A	403	CL7	C4C-NC	-2.65	1.34	1.37
21	22	504	CL7	MG-ND	-2.65	2.00	2.05
21	33	507	CL7	MG-ND	-2.65	2.00	2.05
21	3B	612	CL7	C3B-C4B	-2.65	1.36	1.42
21	4C	517	CL7	MG-ND	-2.65	2.00	2.05
21	31	413	CL7	C4C-NC	-2.65	1.34	1.37
21	33	505	CL7	MG-ND	-2.65	2.00	2.05
21	43	406	CL7	MG-ND	-2.65	2.00	2.05
21	13	507	CL7	MG-ND	-2.65	2.00	2.05
21	43	408	CL7	MG-ND	-2.65	2.00	2.05
21	24	412	CL7	C4C-NC	-2.65	1.34	1.37
21	3C	507	CL7	C1B-C2B	-2.65	1.37	1.43
21	32	509	CL7	MG-ND	-2.65	2.00	2.05
21	11	404	CL7	C4C-C3C	-2.65	1.40	1.45
21	1B	606	CL7	C1B-C2B	-2.65	1.37	1.43
21	4B	607	CL7	C1B-C2B	-2.65	1.37	1.43
21	42	508	CL7	C4C-NC	-2.65	1.34	1.37
21	21	414	CL7	CHC-C4B	2.65	1.45	1.39
21	13	505	CL7	MG-NB	-2.64	2.00	2.05
21	3B	604	CL7	C3B-C4B	-2.64	1.36	1.42
21	1B	607	CL7	C2A-C1A	2.64	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	404	CL7	C4C-C3C	-2.64	1.40	1.45
21	1B	610	CL7	C1B-C2B	-2.64	1.37	1.43
32	24	420	ZEX	C1-C6	-2.64	1.50	1.53
21	4C	510	CL7	C4C-NC	-2.64	1.34	1.37
21	1B	611	CL7	C1B-C2B	-2.64	1.37	1.43
21	1C	510	CL7	C1B-C2B	-2.64	1.37	1.43
21	4C	510	CL7	C1B-C2B	-2.64	1.37	1.43
21	4A	403	CL7	MG-ND	-2.64	2.00	2.05
21	11	406	CL7	C4C-NC	-2.64	1.34	1.37
21	2A	403	CL7	MG-ND	-2.64	2.00	2.05
21	21	418	CL7	C2A-C1A	2.64	1.54	1.50
21	42	510	CL7	MG-ND	-2.64	2.00	2.05
21	2B	607	CL7	C1B-C2B	-2.64	1.37	1.43
21	13	505	CL7	C4C-NC	-2.64	1.34	1.37
21	43	406	CL7	C4C-NC	-2.64	1.34	1.37
21	1B	607	CL7	C4C-NC	-2.64	1.34	1.37
32	34	420	ZEX	C1-C6	-2.64	1.50	1.53
21	32	508	CL7	C4C-NC	-2.64	1.34	1.37
21	23	407	CL7	C4C-C3C	-2.64	1.40	1.45
21	31	406	CL7	C4C-NC	-2.64	1.34	1.37
21	3B	609	CL7	C2A-C1A	2.63	1.54	1.50
21	4B	612	CL7	C1B-C2B	-2.63	1.37	1.43
21	12	509	CL7	MG-ND	-2.63	2.00	2.05
21	2C	506	CL7	MG-ND	-2.63	2.00	2.05
21	3C	506	CL7	MG-ND	-2.63	2.00	2.05
21	1B	612	CL7	C1B-C2B	-2.63	1.37	1.43
21	32	509	CL7	C4C-NC	-2.63	1.34	1.37
21	2C	505	CL7	C4C-C3C	-2.63	1.40	1.45
21	2B	623	CL7	C1B-C2B	-2.63	1.37	1.43
21	3B	622	CL7	C1B-C2B	-2.63	1.37	1.43
21	44	412	CL7	C4C-NC	-2.63	1.34	1.37
21	1B	609	CL7	C4C-NC	-2.63	1.34	1.37
21	1C	512	CL7	C4C-NC	-2.63	1.34	1.37
23	2B	601	8CT	C01-C02	2.63	1.55	1.50
21	4C	505	CL7	C4C-C3C	-2.63	1.40	1.45
21	2B	612	CL7	C1B-C2B	-2.63	1.37	1.43
21	3B	611	CL7	C1B-C2B	-2.63	1.37	1.43
21	13	505	CL7	MG-ND	-2.63	2.00	2.05
21	4B	613	CL7	C3B-C4B	-2.63	1.36	1.42
21	3C	505	CL7	C4C-C3C	-2.63	1.40	1.45
21	32	510	CL7	MG-ND	-2.63	2.00	2.05
21	32	505	CL7	C2A-C1A	2.63	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	601	CL7	C4C-C3C	-2.63	1.40	1.45
21	2C	506	CL7	C2A-C1A	2.63	1.54	1.50
21	23	410	CL7	C1B-C2B	-2.63	1.37	1.43
21	4A	403	CL7	C4C-NC	-2.63	1.34	1.37
21	22	517	CL7	MG-ND	-2.63	2.00	2.05
21	13	507	CL7	C4C-NC	-2.63	1.34	1.37
21	2B	608	CL7	C4C-NC	-2.62	1.34	1.37
21	3B	607	CL7	C4C-NC	-2.62	1.34	1.37
21	22	509	CL7	MG-ND	-2.62	2.00	2.05
21	43	418	CL7	MG-ND	-2.62	2.00	2.05
21	1B	601	CL7	C4C-C3C	-2.62	1.40	1.45
21	32	511	CL7	C4C-NC	-2.62	1.34	1.37
21	41	413	CL7	C4C-NC	-2.62	1.34	1.37
21	13	509	CL7	C2A-C1A	2.62	1.54	1.50
21	43	410	CL7	C2A-C1A	2.62	1.54	1.50
21	4C	507	CL7	C1B-C2B	-2.62	1.37	1.43
21	4B	602	CL7	C4C-C3C	-2.62	1.40	1.45
21	3C	512	CL7	C4C-NC	-2.62	1.34	1.37
21	34	417	CL7	C4C-C3C	-2.62	1.40	1.45
21	43	407	CL7	C4C-C3C	-2.62	1.40	1.45
21	11	413	CL7	C4C-NC	-2.62	1.34	1.37
21	2B	613	CL7	C1B-C2B	-2.62	1.37	1.43
21	3B	612	CL7	C1B-C2B	-2.62	1.37	1.43
32	14	420	ZEX	C1-C6	-2.62	1.50	1.53
32	44	420	ZEX	C1-C6	-2.62	1.50	1.53
21	2C	507	CL7	C1B-C2B	-2.62	1.37	1.43
23	4C	518	8CT	C01-C02	2.62	1.55	1.50
21	32	515	CL7	C4C-C3C	-2.62	1.40	1.45
21	14	409	CL7	MG-ND	-2.62	2.00	2.05
21	42	504	CL7	MG-ND	-2.62	2.00	2.05
21	44	409	CL7	MG-ND	-2.62	2.00	2.05
21	21	417	CL7	CHC-C4B	2.62	1.45	1.39
21	31	417	CL7	CHC-C4B	2.62	1.45	1.39
21	2B	603	CL7	C2A-C1A	2.62	1.54	1.50
21	22	505	CL7	C2A-C1A	2.62	1.54	1.50
21	41	414	CL7	CHC-C4B	2.62	1.45	1.39
21	12	504	CL7	MG-ND	-2.62	2.00	2.05
21	33	505	CL7	C4C-NC	-2.62	1.34	1.37
21	4B	605	CL7	C3B-C4B	-2.62	1.36	1.42
21	24	413	CL7	C4C-NC	-2.62	1.34	1.37
21	24	409	CL7	MG-ND	-2.62	2.00	2.05
21	12	503	CL7	CBD-CGD	-2.61	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	503	CL7	CBD-CGD	-2.61	1.44	1.52
23	2C	518	8CT	C01-C02	2.61	1.55	1.50
21	13	512	CL7	C1B-C2B	-2.61	1.37	1.43
21	31	414	CL7	CHC-C4B	2.61	1.45	1.39
21	42	518	CL7	C4C-NC	-2.61	1.34	1.37
21	1B	612	CL7	C3B-C4B	-2.61	1.36	1.42
21	1C	507	CL7	C1B-C2B	-2.61	1.37	1.43
21	4B	611	CL7	C1B-C2B	-2.61	1.37	1.43
21	33	506	CL7	C4C-C3C	-2.61	1.40	1.45
21	33	505	CL7	MG-NB	-2.61	2.00	2.05
21	23	412	CL7	C1B-C2B	-2.61	1.37	1.43
21	42	513	CL7	C4C-C3C	-2.61	1.40	1.45
21	41	415	CL7	C4C-C3C	-2.61	1.40	1.45
21	23	413	CL7	MG-ND	-2.61	2.00	2.05
21	33	512	CL7	MG-ND	-2.61	2.00	2.05
21	3B	602	CL7	C2A-C1A	2.61	1.54	1.50
21	23	408	CL7	C4C-NC	-2.61	1.34	1.37
21	12	505	CL7	C2A-C1A	2.61	1.54	1.50
21	42	505	CL7	C2A-C1A	2.61	1.54	1.50
21	14	413	CL7	MG-ND	-2.61	2.00	2.05
21	33	514	CL7	C4C-C3C	-2.61	1.40	1.45
21	43	412	CL7	C1B-C2B	-2.61	1.37	1.43
21	14	413	CL7	C4C-NC	-2.61	1.34	1.37
21	44	413	CL7	C4C-NC	-2.61	1.34	1.37
21	2B	611	CL7	C1B-C2B	-2.61	1.37	1.43
21	3B	610	CL7	C1B-C2B	-2.61	1.37	1.43
21	43	415	CL7	C4C-C3C	-2.61	1.40	1.45
21	13	512	CL7	MG-ND	-2.61	2.00	2.05
21	22	518	CL7	C4C-NC	-2.61	1.34	1.37
21	11	417	CL7	CHC-C4B	2.61	1.45	1.39
21	11	419	CL7	CHC-C4B	2.61	1.45	1.39
21	41	417	CL7	CHC-C4B	2.61	1.45	1.39
21	2C	510	CL7	C1B-C2B	-2.61	1.37	1.43
21	23	415	CL7	C4C-C3C	-2.61	1.40	1.45
21	43	413	CL7	MG-ND	-2.61	2.00	2.05
21	42	511	CL7	C4C-NC	-2.61	1.34	1.37
21	3B	615	CL7	C3B-C4B	-2.61	1.36	1.42
21	34	411	CL7	C4C-NC	-2.61	1.34	1.37
21	3C	507	CL7	C3B-C4B	-2.61	1.36	1.42
21	4C	506	CL7	MG-ND	-2.61	2.00	2.05
21	22	503	CL7	CBD-CGD	-2.60	1.44	1.52
21	32	503	CL7	CBD-CGD	-2.60	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	32	504	CL7	C4C-NC	-2.60	1.34	1.37
21	1C	517	CL7	MG-ND	-2.60	2.00	2.05
21	2C	517	CL7	MG-ND	-2.60	2.00	2.05
21	33	511	CL7	C1B-C2B	-2.60	1.37	1.43
21	2B	605	CL7	C3B-C4B	-2.60	1.36	1.42
21	32	504	CL7	MG-ND	-2.60	2.00	2.05
21	23	410	CL7	C2A-C1A	2.60	1.54	1.50
21	3B	616	CL7	C2A-C1A	2.60	1.54	1.50
21	31	419	CL7	CHC-C4B	2.60	1.45	1.39
21	1C	507	CL7	C3B-C4B	-2.60	1.36	1.42
21	21	413	CL7	C4C-NC	-2.60	1.34	1.37
21	2B	613	CL7	C3B-C4B	-2.60	1.36	1.42
21	23	419	CL7	CHC-C4B	2.60	1.45	1.39
21	23	411	CL7	C1B-C2B	-2.60	1.37	1.43
21	11	414	CL7	CHC-C4B	2.60	1.45	1.39
21	3A	403	CL7	MG-ND	-2.60	2.00	2.05
21	11	415	CL7	C4C-C3C	-2.60	1.40	1.45
21	13	510	CL7	MG-ND	-2.60	2.00	2.05
21	13	509	CL7	MG-ND	-2.60	2.00	2.05
21	34	413	CL7	MG-ND	-2.60	2.00	2.05
21	2B	616	CL7	C3B-C4B	-2.60	1.36	1.42
21	41	417	CL7	C4C-NC	-2.60	1.34	1.37
21	32	513	CL7	C4C-C3C	-2.60	1.40	1.45
21	33	509	CL7	MG-ND	-2.59	2.00	2.05
21	1C	517	CL7	C4C-NC	-2.59	1.34	1.37
21	23	406	CL7	C4C-NC	-2.59	1.34	1.37
21	13	509	CL7	C1B-C2B	-2.59	1.37	1.43
21	33	512	CL7	C1B-C2B	-2.59	1.37	1.43
21	43	410	CL7	C1B-C2B	-2.59	1.37	1.43
21	13	517	CL7	MG-ND	-2.59	2.00	2.05
21	43	411	CL7	MG-ND	-2.59	2.00	2.05
21	4B	610	CL7	C4C-NC	-2.59	1.34	1.37
21	2B	602	CL7	C4C-C3C	-2.59	1.40	1.45
21	2B	615	CL7	C4C-NC	-2.59	1.34	1.37
23	1B	626	8CT	C01-C02	2.59	1.55	1.50
21	13	511	CL7	C1B-C2B	-2.59	1.37	1.43
21	11	419	CL7	C4C-C3C	-2.59	1.40	1.45
21	41	419	CL7	C4C-C3C	-2.59	1.40	1.45
21	12	517	CL7	MG-ND	-2.59	2.00	2.05
21	3C	512	CL7	MG-ND	-2.59	2.00	2.05
21	12	515	CL7	C4C-C3C	-2.59	1.40	1.45
21	2B	608	CL7	C2A-C1A	2.59	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	613	CL7	C1B-C2B	-2.59	1.37	1.43
21	1B	602	CL7	C2A-C1A	2.59	1.54	1.50
21	4B	603	CL7	C2A-C1A	2.59	1.54	1.50
21	1A	401	CL7	C4C-C3C	-2.59	1.40	1.45
23	4B	601	8CT	C01-C02	2.59	1.55	1.50
21	2D	404	CL7	C1B-C2B	-2.59	1.37	1.43
21	3D	404	CL7	C1B-C2B	-2.59	1.37	1.43
21	2B	611	CL7	MG-ND	-2.59	2.00	2.05
21	21	419	CL7	C4C-C3C	-2.59	1.40	1.45
21	3D	404	CL7	MG-ND	-2.59	2.00	2.05
21	3C	504	CL7	C4C-NC	-2.59	1.34	1.37
21	42	504	CL7	C4C-NC	-2.59	1.34	1.37
21	4B	608	CL7	C4C-NC	-2.59	1.34	1.37
21	4C	517	CL7	C4C-NC	-2.59	1.34	1.37
21	2B	610	CL7	C2A-C1A	2.59	1.54	1.50
21	2C	507	CL7	C2A-C1A	2.59	1.54	1.50
21	1B	604	CL7	C3B-C4B	-2.59	1.36	1.42
21	44	411	CL7	C4C-NC	-2.59	1.34	1.37
21	43	406	CL7	MG-NB	-2.59	2.00	2.05
21	12	511	CL7	C4C-NC	-2.59	1.34	1.37
21	23	410	CL7	MG-ND	-2.59	2.00	2.05
21	23	418	CL7	MG-ND	-2.59	2.00	2.05
21	33	502	CL7	C4C-NC	-2.58	1.34	1.37
21	21	415	CL7	C4C-C3C	-2.58	1.40	1.45
21	31	415	CL7	C4C-C3C	-2.58	1.40	1.45
21	33	509	CL7	C1B-C2B	-2.58	1.37	1.43
23	4K	101	8CT	C22-C21	2.58	1.56	1.50
21	2D	402	CL7	C4C-C3C	-2.58	1.40	1.45
21	34	413	CL7	C4C-NC	-2.58	1.34	1.37
21	14	405	CL7	C4C-NC	-2.58	1.34	1.37
21	23	419	CL7	C4C-NC	-2.58	1.34	1.37
21	33	518	CL7	C4C-NC	-2.58	1.34	1.37
21	23	413	CL7	C1B-C2B	-2.58	1.37	1.43
21	2C	505	CL7	C3B-C4B	-2.58	1.36	1.42
21	3C	505	CL7	C3B-C4B	-2.58	1.36	1.42
21	1C	505	CL7	C3B-C4B	-2.58	1.36	1.42
21	4C	505	CL7	C3B-C4B	-2.58	1.36	1.42
21	2A	401	CL7	C4C-C3C	-2.58	1.40	1.45
23	1K	101	8CT	C22-C21	2.58	1.56	1.50
21	4D	404	CL7	C2A-C1A	2.58	1.54	1.50
21	31	419	CL7	C4C-C3C	-2.58	1.40	1.45
21	14	412	CL7	MG-ND	-2.58	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3C	518	8CT	C01-C02	2.58	1.55	1.50
21	1B	622	CL7	C1B-C2B	-2.58	1.37	1.43
21	4B	623	CL7	C1B-C2B	-2.58	1.37	1.43
21	22	510	CL7	C2A-C1A	2.58	1.54	1.50
21	31	418	CL7	C2A-C1A	2.58	1.54	1.50
21	14	411	CL7	MG-ND	-2.58	2.00	2.05
21	42	517	CL7	MG-ND	-2.58	2.00	2.05
21	44	411	CL7	MG-ND	-2.58	2.00	2.05
21	2C	507	CL7	C3B-C4B	-2.58	1.36	1.42
21	11	418	CL7	C2A-C1A	2.58	1.54	1.50
21	22	513	CL7	C4C-C3C	-2.58	1.40	1.45
21	13	518	CL7	CHC-C4B	2.58	1.45	1.39
21	2B	610	CL7	C1B-C2B	-2.58	1.37	1.43
32	43	401	ZEX	C30-C29	-2.58	1.32	1.35
21	24	413	CL7	MG-ND	-2.58	2.00	2.05
21	33	510	CL7	C1B-C2B	-2.57	1.37	1.43
21	23	406	CL7	MG-NB	-2.57	2.00	2.05
23	1B	619	8CT	C01-C02	2.57	1.55	1.50
23	4B	620	8CT	C01-C02	2.57	1.55	1.50
21	21	412	CL7	C4C-C3C	-2.57	1.40	1.45
21	31	412	CL7	C4C-C3C	-2.57	1.40	1.45
21	41	418	CL7	C2A-C1A	2.57	1.54	1.50
23	2K	101	8CT	C22-C21	2.57	1.56	1.50
21	11	420	CL7	CHC-C4B	2.57	1.45	1.39
21	24	411	CL7	MG-ND	-2.57	2.00	2.05
32	13	520	ZEX	C21-C26	-2.57	1.50	1.53
21	22	504	CL7	C4C-NC	-2.57	1.34	1.37
21	4D	404	CL7	C1B-C2B	-2.57	1.37	1.43
21	33	518	CL7	CHC-C4B	2.57	1.45	1.39
23	3K	101	8CT	C22-C21	2.57	1.56	1.50
21	4C	512	CL7	C4C-NC	-2.57	1.34	1.37
21	23	411	CL7	MG-ND	-2.57	2.00	2.05
21	33	510	CL7	MG-ND	-2.57	2.00	2.05
21	1C	507	CL7	C2A-C1A	2.57	1.54	1.50
21	4C	507	CL7	C2A-C1A	2.57	1.54	1.50
21	4B	603	CL7	C1B-C2B	-2.57	1.37	1.43
23	3B	626	8CT	C01-C02	2.57	1.55	1.50
21	43	419	CL7	CHC-C4B	2.57	1.45	1.39
21	4C	507	CL7	C3B-C4B	-2.57	1.36	1.42
21	43	413	CL7	C1B-C2B	-2.57	1.37	1.43
21	3D	402	CL7	C4C-C3C	-2.57	1.40	1.45
21	1B	615	CL7	C3B-C4B	-2.57	1.36	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	616	CL7	C3B-C4B	-2.57	1.36	1.42
21	43	419	CL7	C4C-NC	-2.57	1.34	1.37
21	32	510	CL7	C2A-C1A	2.57	1.54	1.50
21	34	409	CL7	MG-ND	-2.57	2.00	2.05
21	41	419	CL7	CHC-C4B	2.57	1.45	1.39
21	43	410	CL7	MG-ND	-2.57	2.00	2.05
21	32	517	CL7	MG-ND	-2.57	2.00	2.05
21	1C	509	CL7	C1B-C2B	-2.57	1.37	1.43
23	1B	626	8CT	C22-C21	2.56	1.56	1.50
21	21	416	CL7	CHC-C4B	2.56	1.45	1.39
21	11	411	CL7	C4C-NC	-2.56	1.34	1.37
21	2C	504	CL7	C4C-NC	-2.56	1.34	1.37
21	1D	404	CL7	C1B-C2B	-2.56	1.37	1.43
23	4B	601	8CT	C22-C21	2.56	1.56	1.50
21	2B	604	CL7	CHC-C4B	2.56	1.45	1.39
21	21	417	CL7	C4C-NC	-2.56	1.34	1.37
21	3B	602	CL7	C1B-C2B	-2.56	1.37	1.43
21	11	412	CL7	C4C-NC	-2.56	1.34	1.37
21	13	518	CL7	C4C-NC	-2.56	1.34	1.37
21	41	412	CL7	C4C-NC	-2.56	1.34	1.37
21	43	403	CL7	C4C-NC	-2.56	1.34	1.37
21	12	513	CL7	C4C-C3C	-2.56	1.40	1.45
21	4B	604	CL7	C1B-C2B	-2.56	1.37	1.43
21	33	507	CL7	C4C-NC	-2.56	1.34	1.37
21	4B	608	CL7	C2A-C1A	2.56	1.54	1.50
21	41	420	CL7	CHC-C4B	2.56	1.45	1.39
21	22	502	CL7	C2A-C1A	2.56	1.54	1.50
21	43	408	CL7	C3B-C4B	-2.56	1.36	1.42
21	2C	511	CL7	C4C-NC	-2.56	1.34	1.37
21	3C	511	CL7	C4C-NC	-2.56	1.34	1.37
21	21	412	CL7	C4C-NC	-2.56	1.34	1.37
21	31	412	CL7	C4C-NC	-2.56	1.34	1.37
21	4B	613	CL7	C1C-NC	-2.56	1.34	1.37
21	13	502	CL7	MG-ND	-2.56	2.00	2.05
21	1D	402	CL7	C4C-C3C	-2.56	1.40	1.45
21	1C	504	CL7	C4C-NC	-2.56	1.34	1.37
21	4C	504	CL7	C4C-NC	-2.56	1.34	1.37
21	2C	510	CL7	MG-ND	-2.56	2.00	2.05
21	2D	404	CL7	C2A-C1A	2.56	1.54	1.50
21	3D	404	CL7	C2A-C1A	2.56	1.54	1.50
21	34	411	CL7	MG-ND	-2.55	2.00	2.05
21	43	403	CL7	MG-ND	-2.55	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	413	CL7	MG-ND	-2.55	2.00	2.05
21	13	510	CL7	C1B-C2B	-2.55	1.37	1.43
32	23	420	ZEX	C21-C26	-2.55	1.50	1.53
21	12	504	CL7	C4C-NC	-2.55	1.34	1.37
21	11	416	CL7	CHC-C4B	2.55	1.45	1.39
21	41	416	CL7	CHC-C4B	2.55	1.45	1.39
21	2C	517	CL7	C4C-NC	-2.55	1.34	1.37
21	3C	517	CL7	C4C-NC	-2.55	1.34	1.37
21	1C	508	CL7	MG-ND	-2.55	2.00	2.05
21	22	502	CL7	MG-ND	-2.55	2.00	2.05
21	2B	603	CL7	C1B-C2B	-2.55	1.37	1.43
21	1C	512	CL7	MG-ND	-2.55	2.00	2.05
21	4C	512	CL7	MG-ND	-2.55	2.00	2.05
21	24	411	CL7	C4C-NC	-2.55	1.34	1.37
21	33	509	CL7	C4C-NC	-2.55	1.34	1.37
21	43	411	CL7	C1B-C2B	-2.55	1.37	1.43
21	13	502	CL7	C4C-NC	-2.55	1.34	1.37
21	2B	615	CL7	C1B-C2B	-2.55	1.37	1.43
21	3B	614	CL7	C1B-C2B	-2.55	1.37	1.43
21	14	413	CL7	C1B-C2B	-2.55	1.37	1.43
21	44	410	CL7	C1B-C2B	-2.55	1.37	1.43
21	41	414	CL7	C4C-C3C	-2.55	1.40	1.45
21	3B	608	CL7	MG-ND	-2.55	2.00	2.05
21	12	502	CL7	C2A-C1A	2.55	1.54	1.50
21	42	502	CL7	C2A-C1A	2.55	1.54	1.50
21	44	413	CL7	C1B-C2B	-2.55	1.37	1.43
21	2C	512	CL7	MG-ND	-2.55	2.00	2.05
21	1B	603	CL7	C1B-C2B	-2.55	1.37	1.43
21	4A	401	CL7	C4C-C3C	-2.55	1.40	1.45
21	41	420	CL7	C4C-NC	-2.55	1.34	1.37
21	23	408	CL7	C3B-C4B	-2.55	1.36	1.42
21	2C	509	CL7	MG-NB	-2.55	2.00	2.05
21	3C	509	CL7	MG-NB	-2.55	2.00	2.05
21	21	420	CL7	CHC-C4B	2.55	1.45	1.39
21	31	420	CL7	CHC-C4B	2.55	1.45	1.39
21	33	502	CL7	MG-ND	-2.55	2.00	2.05
21	24	408	CL7	C4C-NC	-2.55	1.34	1.37
21	24	409	CL7	C4C-NC	-2.55	1.34	1.37
21	34	408	CL7	C4C-NC	-2.55	1.34	1.37
21	2C	507	CL7	MG-ND	-2.54	2.00	2.05
21	3C	507	CL7	MG-ND	-2.54	2.00	2.05
21	2B	609	CL7	C1B-C2B	-2.54	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	404	CL7	C1B-C2B	-2.54	1.37	1.43
21	31	416	CL7	CHC-C4B	2.54	1.45	1.39
21	34	410	CL7	C1B-C2B	-2.54	1.37	1.43
21	1B	610	CL7	MG-ND	-2.54	2.00	2.05
21	4B	611	CL7	MG-ND	-2.54	2.00	2.05
21	12	502	CL7	MG-ND	-2.54	2.00	2.05
21	42	502	CL7	MG-ND	-2.54	2.00	2.05
21	4B	610	CL7	C2A-C1A	2.54	1.54	1.50
21	1B	603	CL7	CHC-C4B	2.54	1.45	1.39
21	4B	604	CL7	CHC-C4B	2.54	1.45	1.39
21	3B	609	CL7	C1B-C2B	-2.54	1.37	1.43
21	33	501	CL7	C2A-C1A	2.54	1.54	1.50
21	1B	614	CL7	C4C-NC	-2.54	1.34	1.37
21	31	417	CL7	C4C-NC	-2.54	1.34	1.37
21	14	407	CL7	CHC-C4B	2.54	1.45	1.39
21	11	416	CL7	C4C-C3C	-2.54	1.40	1.45
21	42	514	CL7	C4C-NC	-2.54	1.34	1.37
21	21	419	CL7	CHC-C4B	2.54	1.45	1.39
21	43	402	CL7	C2A-C1A	2.54	1.54	1.50
21	1D	404	CL7	MG-ND	-2.54	2.00	2.05
21	12	506	CL7	C4C-NC	-2.54	1.34	1.37
21	1B	602	CL7	C1B-C2B	-2.54	1.37	1.43
21	13	509	CL7	C4C-NC	-2.54	1.34	1.37
21	14	404	CL7	C1B-C2B	-2.54	1.37	1.43
21	44	404	CL7	C1B-C2B	-2.54	1.37	1.43
21	33	502	CL7	CHC-C4B	2.54	1.45	1.39
21	2B	609	CL7	MG-ND	-2.54	2.00	2.05
21	3A	401	CL7	C4C-C3C	-2.54	1.40	1.45
21	1B	614	CL7	C1B-C2B	-2.54	1.37	1.43
21	4B	615	CL7	C1B-C2B	-2.54	1.37	1.43
21	32	506	CL7	C4C-NC	-2.54	1.34	1.37
21	12	509	CL7	C1B-C2B	-2.54	1.37	1.43
21	42	509	CL7	C1B-C2B	-2.54	1.37	1.43
21	4C	507	CL7	MG-ND	-2.54	2.00	2.05
21	23	402	CL7	C2A-C1A	2.54	1.54	1.50
21	3B	607	CL7	C2A-C1A	2.54	1.54	1.50
21	1C	507	CL7	MG-ND	-2.54	2.00	2.05
21	23	403	CL7	MG-ND	-2.54	2.00	2.05
21	13	507	CL7	C3B-C4B	-2.54	1.36	1.42
21	2C	512	CL7	C4C-NC	-2.54	1.34	1.37
21	44	405	CL7	C4C-NC	-2.54	1.34	1.37
21	1C	510	CL7	MG-ND	-2.54	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1B	626	8CT	C30-C29	2.54	1.54	1.50
21	3B	612	CL7	C1C-NC	-2.54	1.34	1.37
21	4C	511	CL7	C4C-NC	-2.54	1.34	1.37
21	11	404	CL7	CHC-C4B	2.54	1.45	1.39
21	41	404	CL7	CHC-C4B	2.54	1.45	1.39
21	4C	510	CL7	MG-ND	-2.54	2.00	2.05
21	4D	404	CL7	MG-ND	-2.54	2.00	2.05
21	2B	604	CL7	C1B-C2B	-2.54	1.37	1.43
21	44	407	CL7	CHC-C4B	2.54	1.45	1.39
21	1B	609	CL7	C1B-C2B	-2.53	1.37	1.43
21	24	412	CL7	MG-ND	-2.53	2.00	2.05
21	31	404	CL7	CHC-C4B	2.53	1.45	1.39
21	44	408	CL7	C4C-NC	-2.53	1.34	1.37
21	32	502	CL7	C2A-C1A	2.53	1.54	1.50
32	43	421	ZEX	C21-C26	-2.53	1.50	1.53
21	1C	511	CL7	C4C-NC	-2.53	1.34	1.37
21	21	418	CL7	MG-ND	-2.53	2.00	2.05
21	31	418	CL7	MG-ND	-2.53	2.00	2.05
21	1C	510	CL7	CHC-C4B	2.53	1.45	1.39
21	4C	501	CL7	C1B-C2B	-2.53	1.37	1.43
21	24	414	CL7	MG-ND	-2.53	2.00	2.05
21	3B	610	CL7	MG-ND	-2.53	2.00	2.05
21	11	412	CL7	C4C-C3C	-2.53	1.40	1.45
21	41	412	CL7	C4C-C3C	-2.53	1.40	1.45
21	24	407	CL7	CHC-C4B	2.53	1.45	1.39
21	34	407	CL7	CHC-C4B	2.53	1.45	1.39
21	43	410	CL7	C4C-NC	-2.53	1.34	1.37
21	3B	603	CL7	C1B-C2B	-2.53	1.37	1.43
21	31	416	CL7	C4C-C3C	-2.53	1.40	1.45
21	2D	404	CL7	MG-ND	-2.53	2.00	2.05
21	2C	509	CL7	C1B-C2B	-2.53	1.37	1.43
21	3C	509	CL7	C1B-C2B	-2.53	1.37	1.43
21	32	511	CL7	MG-ND	-2.53	2.00	2.05
32	13	519	ZEX	C21-C26	-2.53	1.50	1.53
32	23	421	ZEX	C21-C26	-2.53	1.50	1.53
21	13	517	CL7	C1B-C2B	-2.53	1.37	1.43
23	2B	620	8CT	C01-C02	2.53	1.55	1.50
23	3B	619	8CT	C01-C02	2.53	1.55	1.50
21	31	414	CL7	C4C-C3C	-2.53	1.40	1.45
23	4C	514	8CT	C22-C21	2.53	1.56	1.50
21	32	516	CL7	MG-ND	-2.53	2.00	2.05
32	24	419	ZEX	C1-C6	-2.53	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	34	419	ZEX	C1-C6	-2.53	1.50	1.53
21	12	510	CL7	C2A-C1A	2.53	1.54	1.50
21	4C	509	CL7	C1B-C2B	-2.53	1.37	1.43
21	3B	614	CL7	C4C-NC	-2.53	1.34	1.37
21	3C	507	CL7	C2A-C1A	2.53	1.54	1.50
23	1C	514	8CT	C22-C21	2.52	1.56	1.50
21	32	518	CL7	CHC-C4B	2.52	1.45	1.39
21	24	410	CL7	C1B-C2B	-2.52	1.37	1.43
21	11	418	CL7	MG-ND	-2.52	2.00	2.05
21	41	418	CL7	MG-ND	-2.52	2.00	2.05
32	33	519	ZEX	C21-C26	-2.52	1.50	1.53
21	11	417	CL7	C4C-NC	-2.52	1.34	1.37
21	4B	609	CL7	MG-ND	-2.52	2.00	2.05
23	2B	601	8CT	C22-C21	2.52	1.56	1.50
23	3B	626	8CT	C22-C21	2.52	1.56	1.50
21	24	413	CL7	C1B-C2B	-2.52	1.37	1.43
21	34	413	CL7	C1B-C2B	-2.52	1.37	1.43
21	22	511	CL7	C4C-NC	-2.52	1.34	1.37
21	1D	404	CL7	C2A-C1A	2.52	1.54	1.50
21	21	411	CL7	C4C-NC	-2.52	1.34	1.37
21	31	411	CL7	C4C-NC	-2.52	1.34	1.37
21	4B	614	CL7	MG-ND	-2.52	2.00	2.05
21	42	506	CL7	C4C-NC	-2.52	1.34	1.37
21	14	410	CL7	C1B-C2B	-2.52	1.37	1.43
21	34	412	CL7	MG-ND	-2.52	2.00	2.05
21	31	410	CL7	C4C-NC	-2.52	1.34	1.37
21	1C	510	CL7	C2A-C1A	2.52	1.54	1.50
21	4D	402	CL7	C4C-C3C	-2.52	1.40	1.45
21	1B	613	CL7	MG-ND	-2.52	2.00	2.05
21	44	414	CL7	MG-ND	-2.52	2.00	2.05
32	14	419	ZEX	C1-C6	-2.52	1.50	1.53
32	44	419	ZEX	C1-C6	-2.52	1.50	1.53
21	22	509	CL7	C1B-C2B	-2.52	1.37	1.43
21	32	509	CL7	C1B-C2B	-2.52	1.37	1.43
21	2B	607	CL7	C1C-NC	-2.52	1.34	1.37
21	14	414	CL7	MG-ND	-2.52	2.00	2.05
21	34	405	CL7	C4C-NC	-2.52	1.34	1.37
21	43	418	CL7	C1B-C2B	-2.52	1.37	1.43
21	13	505	CL7	C1C-NC	-2.52	1.34	1.37
21	43	406	CL7	C1C-NC	-2.52	1.34	1.37
21	14	409	CL7	C4C-C3C	-2.52	1.40	1.45
21	44	409	CL7	C4C-C3C	-2.52	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	23	403	CL7	C4C-NC	-2.52	1.34	1.37
21	23	414	CL7	C4C-NC	-2.52	1.34	1.37
21	34	404	CL7	C1B-C2B	-2.52	1.37	1.43
21	1B	608	CL7	MG-ND	-2.51	2.00	2.05
21	4B	609	CL7	C4C-NC	-2.51	1.34	1.37
21	21	404	CL7	CHC-C4B	2.51	1.45	1.39
21	22	514	CL7	C4C-NC	-2.51	1.34	1.37
21	4B	610	CL7	C1B-C2B	-2.51	1.37	1.43
21	1A	407	CL7	C2A-C1A	2.51	1.54	1.50
21	44	412	CL7	MG-ND	-2.51	2.00	2.05
21	1C	509	CL7	MG-NB	-2.51	2.00	2.05
21	4C	509	CL7	MG-NB	-2.51	2.00	2.05
21	24	405	CL7	C4C-NC	-2.51	1.34	1.37
21	2B	613	CL7	C1C-NC	-2.51	1.34	1.37
21	43	408	CL7	C4C-NC	-2.51	1.34	1.37
32	11	421	ZEX	C21-C26	-2.51	1.50	1.53
21	33	507	CL7	C3B-C4B	-2.51	1.37	1.42
21	2C	501	CL7	C1B-C2B	-2.51	1.37	1.43
21	3C	501	CL7	C1B-C2B	-2.51	1.37	1.43
21	43	405	CL7	C1B-C2B	-2.51	1.37	1.43
21	34	414	CL7	MG-ND	-2.51	2.00	2.05
23	3C	514	8CT	C22-C21	2.51	1.56	1.50
21	22	506	CL7	C4C-NC	-2.51	1.34	1.37
23	2B	601	8CT	C30-C29	2.51	1.54	1.50
23	3B	626	8CT	C30-C29	2.51	1.54	1.50
21	24	409	CL7	C4C-C3C	-2.51	1.40	1.45
21	3B	607	CL7	MG-ND	-2.51	2.00	2.05
21	1B	609	CL7	C2A-C1A	2.51	1.54	1.50
21	21	414	CL7	C4C-C3C	-2.51	1.40	1.45
21	2B	614	CL7	MG-ND	-2.51	2.00	2.05
21	12	508	CL7	C1B-C2B	-2.51	1.37	1.43
21	42	508	CL7	C1B-C2B	-2.51	1.37	1.43
21	14	409	CL7	C4C-NC	-2.51	1.34	1.37
21	44	409	CL7	C4C-NC	-2.51	1.34	1.37
21	13	502	CL7	CHC-C4B	2.51	1.45	1.39
21	43	403	CL7	CHC-C4B	2.51	1.45	1.39
21	3B	608	CL7	C1B-C2B	-2.51	1.37	1.43
21	23	403	CL7	CHC-C4B	2.51	1.45	1.39
21	22	507	CL7	C4C-NC	-2.51	1.34	1.37
21	32	507	CL7	C4C-NC	-2.51	1.34	1.37
23	2C	514	8CT	C22-C21	2.51	1.56	1.50
21	21	420	CL7	C4C-NC	-2.51	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	420	CL7	C4C-NC	-2.51	1.34	1.37
21	22	514	CL7	MG-ND	-2.51	2.00	2.05
21	3B	613	CL7	MG-ND	-2.51	2.00	2.05
21	32	514	CL7	MG-ND	-2.51	2.00	2.05
21	21	416	CL7	C4C-C3C	-2.51	1.40	1.45
23	4B	601	8CT	C30-C29	2.50	1.54	1.50
21	3B	603	CL7	CHC-C4B	2.50	1.45	1.39
21	4C	510	CL7	CHC-C4B	2.50	1.45	1.39
21	12	516	CL7	MG-ND	-2.50	2.00	2.05
21	13	506	CL7	MG-ND	-2.50	2.00	2.05
21	4C	513	CL7	CHC-C4B	2.50	1.45	1.39
21	41	410	CL7	C4C-NC	-2.50	1.34	1.37
21	42	514	CL7	C4C-C3C	-2.50	1.40	1.45
21	32	502	CL7	MG-ND	-2.50	2.00	2.05
21	1B	606	CL7	C1C-NC	-2.50	1.34	1.37
21	22	518	CL7	CHC-C4B	2.50	1.45	1.39
32	43	420	ZEX	C21-C26	-2.50	1.50	1.53
21	14	411	CL7	C4C-NC	-2.50	1.34	1.37
21	2A	403	CL7	C1C-NC	-2.50	1.34	1.37
21	3D	404	CL7	C1C-C2C	-2.50	1.40	1.45
21	33	504	CL7	C1B-C2B	-2.50	1.37	1.43
21	41	416	CL7	C4C-C3C	-2.50	1.40	1.45
21	2A	407	CL7	C2A-C1A	2.50	1.54	1.50
21	23	418	CL7	C1B-C2B	-2.50	1.37	1.43
21	33	517	CL7	C1B-C2B	-2.50	1.37	1.43
32	41	421	ZEX	C21-C26	-2.50	1.50	1.53
21	1C	501	CL7	C1B-C2B	-2.50	1.37	1.43
23	3K	101	8CT	C30-C29	2.50	1.54	1.50
21	1B	604	CL7	MG-ND	-2.50	2.00	2.05
21	4B	605	CL7	MG-ND	-2.50	2.00	2.05
21	23	410	CL7	C4C-NC	-2.50	1.34	1.37
21	4B	615	CL7	C4C-NC	-2.50	1.34	1.37
21	11	414	CL7	C4C-C3C	-2.50	1.40	1.45
21	4C	508	CL7	MG-ND	-2.50	2.00	2.05
21	13	503	CL7	MG-ND	-2.50	2.00	2.05
21	34	409	CL7	C4C-NC	-2.50	1.34	1.37
21	22	517	CL7	C1B-C2B	-2.50	1.37	1.43
21	32	517	CL7	C1B-C2B	-2.50	1.37	1.43
21	42	510	CL7	C2A-C1A	2.50	1.54	1.50
21	2C	508	CL7	C1B-C2B	-2.49	1.37	1.43
21	3C	508	CL7	C1B-C2B	-2.49	1.37	1.43
21	13	514	CL7	CHC-C4B	2.49	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	13	515	CL7	C4C-NC	-2.49	1.34	1.37
21	13	507	CL7	MG-NB	-2.49	2.00	2.05
21	43	408	CL7	MG-NB	-2.49	2.00	2.05
21	3C	510	CL7	MG-ND	-2.49	2.00	2.05
32	14	403	ZEX	C21-C26	-2.49	1.50	1.53
32	21	421	ZEX	C21-C26	-2.49	1.50	1.53
32	31	421	ZEX	C21-C26	-2.49	1.50	1.53
32	44	403	ZEX	C21-C26	-2.49	1.50	1.53
21	12	501	CL7	MG-ND	-2.49	2.00	2.05
21	42	501	CL7	MG-ND	-2.49	2.00	2.05
21	1D	402	CL7	CHD-C1D	2.49	1.45	1.39
21	4D	402	CL7	CHD-C1D	2.49	1.45	1.39
21	12	517	CL7	C1B-C2B	-2.49	1.37	1.43
21	42	517	CL7	C1B-C2B	-2.49	1.37	1.43
21	4B	609	CL7	C1B-C2B	-2.49	1.37	1.43
21	34	409	CL7	C4C-C3C	-2.49	1.40	1.45
21	12	518	CL7	CHC-C4B	2.49	1.45	1.39
21	42	518	CL7	CHC-C4B	2.49	1.45	1.39
21	2C	508	CL7	MG-ND	-2.49	2.00	2.05
21	3C	508	CL7	MG-ND	-2.49	2.00	2.05
21	13	501	CL7	C2A-C1A	2.49	1.54	1.50
21	24	406	CL7	MG-ND	-2.49	2.00	2.05
21	33	507	CL7	MG-NB	-2.49	2.00	2.05
21	34	406	CL7	MG-ND	-2.49	2.00	2.05
21	12	514	CL7	MG-ND	-2.49	2.00	2.05
21	42	514	CL7	MG-ND	-2.49	2.00	2.05
21	12	511	CL7	MG-ND	-2.49	2.00	2.05
21	42	511	CL7	MG-ND	-2.49	2.00	2.05
21	3C	510	CL7	C2A-C1A	2.49	1.54	1.50
21	4A	407	CL7	C2A-C1A	2.49	1.54	1.50
21	4D	404	CL7	C1C-C2C	-2.49	1.40	1.45
21	1B	601	CL7	C4C-NC	-2.49	1.34	1.37
21	13	513	CL7	C4C-NC	-2.49	1.34	1.37
21	4B	614	CL7	C1B-NB	-2.49	1.34	1.37
21	43	414	CL7	C4C-NC	-2.49	1.34	1.37
21	31	409	CL7	CHC-C4B	2.49	1.45	1.39
21	44	417	CL7	CHC-C4B	2.49	1.45	1.39
21	32	508	CL7	C1B-C2B	-2.49	1.37	1.43
32	33	520	ZEX	C21-C26	-2.49	1.50	1.53
21	1B	612	CL7	C1C-NC	-2.49	1.34	1.37
21	2D	404	CL7	C1C-C2C	-2.49	1.40	1.45
21	4C	510	CL7	C2A-C1A	2.49	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2D	402	CL7	CHD-C1D	2.49	1.45	1.39
21	1B	608	CL7	C1B-C2B	-2.49	1.37	1.43
21	23	408	CL7	C1B-C2B	-2.49	1.37	1.43
21	11	402	CL7	C4C-NC	-2.49	1.34	1.37
21	41	402	CL7	C4C-NC	-2.49	1.34	1.37
21	44	406	CL7	MG-ND	-2.49	2.00	2.05
21	1B	607	CL7	MG-ND	-2.49	2.00	2.05
21	4B	608	CL7	MG-ND	-2.49	2.00	2.05
21	42	516	CL7	MG-ND	-2.49	2.00	2.05
21	2C	510	CL7	CHC-C4B	2.49	1.45	1.39
21	22	511	CL7	MG-ND	-2.48	2.00	2.05
21	3B	606	CL7	C1C-NC	-2.48	1.34	1.37
21	41	411	CL7	C4C-NC	-2.48	1.34	1.37
21	1D	404	CL7	C1C-C2C	-2.48	1.40	1.45
21	3D	402	CL7	CHD-C1D	2.48	1.45	1.39
21	32	501	CL7	MG-ND	-2.48	2.00	2.05
21	4B	607	CL7	C1C-NC	-2.48	1.34	1.37
21	14	406	CL7	MG-ND	-2.48	2.00	2.05
21	33	503	CL7	MG-ND	-2.48	2.00	2.05
21	23	415	CL7	CHC-C4B	2.48	1.45	1.39
21	33	514	CL7	CHC-C4B	2.48	1.45	1.39
21	23	406	CL7	C1C-NC	-2.48	1.34	1.37
21	22	516	CL7	MG-ND	-2.48	2.00	2.05
21	41	415	CL7	CAB-C3B	2.48	1.50	1.45
21	32	514	CL7	C4C-NC	-2.48	1.34	1.37
21	23	405	CL7	C1B-C2B	-2.48	1.37	1.43
21	1B	608	CL7	C4C-NC	-2.48	1.34	1.37
21	31	415	CL7	CAB-C3B	2.48	1.50	1.45
21	14	416	CL7	MG-ND	-2.48	2.00	2.05
21	42	506	CL7	MG-ND	-2.48	2.00	2.05
21	44	416	CL7	MG-ND	-2.48	2.00	2.05
21	14	408	CL7	C4C-NC	-2.48	1.34	1.37
21	4A	403	CL7	C1C-NC	-2.48	1.34	1.37
21	44	416	CL7	CHC-C4B	2.48	1.45	1.39
21	22	508	CL7	C1B-C2B	-2.48	1.37	1.43
21	32	504	CL7	C1B-C2B	-2.48	1.37	1.43
21	2B	605	CL7	MG-ND	-2.48	2.00	2.05
21	3B	604	CL7	MG-ND	-2.48	2.00	2.05
21	13	507	CL7	C1B-C2B	-2.48	1.37	1.43
21	43	408	CL7	C1B-C2B	-2.48	1.37	1.43
32	23	421	ZEX	C1-C6	-2.48	1.50	1.53
32	33	520	ZEX	C1-C6	-2.48	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	415	CL7	MG-ND	-2.48	2.00	2.05
21	33	515	CL7	CHC-C4B	2.48	1.45	1.39
21	14	417	CL7	MG-ND	-2.48	2.00	2.05
21	13	504	CL7	C1B-C2B	-2.48	1.37	1.43
21	11	409	CL7	CHC-C4B	2.48	1.45	1.39
21	41	409	CL7	CHC-C4B	2.48	1.45	1.39
21	12	513	CL7	C4C-NC	-2.48	1.34	1.37
21	1C	513	CL7	CHC-C4B	2.47	1.45	1.39
21	23	416	CL7	CHC-C4B	2.47	1.45	1.39
21	22	503	CL7	MG-ND	-2.47	2.00	2.05
21	32	503	CL7	MG-ND	-2.47	2.00	2.05
21	2C	503	CL7	MG-ND	-2.47	2.00	2.05
21	3C	503	CL7	MG-ND	-2.47	2.00	2.05
32	34	403	ZEX	C21-C26	-2.47	1.50	1.53
21	21	413	CL7	CAB-C3B	2.47	1.50	1.45
21	21	415	CL7	CAB-C3B	2.47	1.50	1.45
21	2C	502	CL7	C1B-C2B	-2.47	1.37	1.43
21	3C	502	CL7	C1B-C2B	-2.47	1.37	1.43
21	2B	602	CL7	C4C-NC	-2.47	1.34	1.37
21	33	516	CL7	MG-ND	-2.47	2.00	2.05
32	13	520	ZEX	C1-C6	-2.47	1.50	1.53
21	31	407	CL7	C1B-C2B	-2.47	1.37	1.43
21	21	402	CL7	C4C-NC	-2.47	1.34	1.37
21	31	402	CL7	C4C-NC	-2.47	1.34	1.37
23	2K	101	8CT	C30-C29	2.47	1.53	1.50
21	42	510	CL7	C1B-C2B	-2.47	1.37	1.43
21	23	408	CL7	MG-NB	-2.47	2.00	2.05
21	24	416	CL7	CHC-C4B	2.47	1.44	1.39
21	23	406	CL7	C1B-C2B	-2.47	1.37	1.43
21	41	407	CL7	C1B-C2B	-2.47	1.37	1.43
21	22	501	CL7	MG-ND	-2.47	2.00	2.05
21	23	404	CL7	MG-ND	-2.47	2.00	2.05
21	1D	404	CL7	C1B-NB	-2.47	1.34	1.37
21	13	506	CL7	C4C-NC	-2.47	1.34	1.37
21	43	407	CL7	C4C-NC	-2.47	1.34	1.37
21	3C	507	CL7	MG-NB	-2.47	2.00	2.05
21	12	505	CL7	C3B-C4B	-2.47	1.37	1.42
21	42	516	CL7	C1C-NC	-2.47	1.34	1.37
21	1B	613	CL7	C1B-NB	-2.47	1.34	1.37
21	24	411	CL7	CHC-C4B	2.47	1.44	1.39
21	4C	511	CL7	CHC-C4B	2.47	1.44	1.39
21	12	504	CL7	C1B-C2B	-2.47	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	22	504	CL7	C1B-C2B	-2.47	1.37	1.43
21	2B	608	CL7	MG-ND	-2.47	2.00	2.05
23	3C	514	8CT	C01-C02	2.46	1.55	1.50
21	1C	508	CL7	C1B-C2B	-2.46	1.37	1.43
21	32	503	CL7	C1B-C2B	-2.46	1.37	1.43
21	4C	508	CL7	C1B-C2B	-2.46	1.37	1.43
21	3B	614	CL7	MG-ND	-2.46	2.00	2.05
21	44	407	CL7	MG-ND	-2.46	2.00	2.05
21	12	514	CL7	C4C-NC	-2.46	1.34	1.37
21	43	406	CL7	C1B-C2B	-2.46	1.37	1.43
21	22	514	CL7	C3B-C4B	-2.46	1.37	1.42
21	11	415	CL7	CAB-C3B	2.46	1.50	1.45
21	4C	513	CL7	CHD-C1D	2.46	1.44	1.39
21	1A	407	CL7	C1B-C2B	-2.46	1.37	1.43
21	4A	403	CL7	C1B-C2B	-2.46	1.37	1.43
32	24	403	ZEX	C21-C26	-2.46	1.50	1.53
32	43	423	ZEX	C21-C26	-2.46	1.50	1.53
21	11	403	CL7	MG-ND	-2.46	2.00	2.05
21	41	403	CL7	MG-ND	-2.46	2.00	2.05
21	33	505	CL7	C1C-NC	-2.46	1.34	1.37
21	34	416	CL7	CHC-C4B	2.46	1.44	1.39
21	3A	407	CL7	C2A-C1A	2.46	1.54	1.50
21	2B	615	CL7	MG-ND	-2.46	2.00	2.05
21	31	406	CL7	MG-ND	-2.46	2.00	2.05
21	4B	607	CL7	MG-ND	-2.46	2.00	2.05
21	42	503	CL7	MG-ND	-2.46	2.00	2.05
21	33	501	CL7	MG-ND	-2.46	2.00	2.05
21	22	516	CL7	C1C-NC	-2.46	1.34	1.37
21	31	417	CL7	C1B-C2B	-2.46	1.37	1.43
21	12	512	CL7	MG-ND	-2.46	2.00	2.05
21	1A	403	CL7	C1B-C2B	-2.46	1.37	1.43
21	13	505	CL7	C1B-C2B	-2.46	1.37	1.43
21	21	409	CL7	CHC-C4B	2.46	1.44	1.39
32	23	423	ZEX	C21-C26	-2.46	1.50	1.53
21	44	407	CL7	C4C-NC	-2.46	1.34	1.37
21	12	503	CL7	C1B-C2B	-2.46	1.37	1.43
21	42	503	CL7	C1B-C2B	-2.46	1.37	1.43
21	3C	510	CL7	CHC-C4B	2.46	1.44	1.39
32	11	422	ZEX	C21-C26	-2.46	1.50	1.53
32	21	422	ZEX	C21-C26	-2.46	1.50	1.53
32	31	422	ZEX	C21-C26	-2.46	1.50	1.53
21	12	507	CL7	C4C-NC	-2.46	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	507	CL7	C4C-NC	-2.46	1.34	1.37
21	3D	402	CL7	CHC-C4B	2.46	1.44	1.39
21	4C	502	CL7	MG-ND	-2.46	2.00	2.05
21	11	408	CL7	C4C-C3C	-2.46	1.40	1.45
21	41	408	CL7	C4C-C3C	-2.46	1.40	1.45
21	11	417	CL7	C1B-C2B	-2.46	1.37	1.43
21	2C	510	CL7	C2A-C1A	2.46	1.54	1.50
21	43	415	CL7	CHC-C4B	2.46	1.44	1.39
21	1C	502	CL7	C1B-C2B	-2.46	1.37	1.43
21	4C	502	CL7	C1B-C2B	-2.46	1.37	1.43
21	11	411	CL7	CHC-C4B	2.46	1.44	1.39
21	24	417	CL7	CHC-C4B	2.46	1.44	1.39
23	2C	514	8CT	C01-C02	2.46	1.55	1.50
21	24	415	CL7	MG-ND	-2.45	2.00	2.05
21	43	407	CL7	MG-ND	-2.45	2.00	2.05
23	4C	514	8CT	C01-C02	2.45	1.55	1.50
21	13	515	CL7	CHC-C4B	2.45	1.44	1.39
21	43	416	CL7	CHC-C4B	2.45	1.44	1.39
21	42	508	CL7	C3B-C4B	-2.45	1.37	1.42
21	13	508	CL7	MG-ND	-2.45	2.00	2.05
21	33	505	CL7	C1B-C2B	-2.45	1.37	1.43
21	2B	613	CL7	C2A-C1A	2.45	1.54	1.50
21	4C	507	CL7	MG-NB	-2.45	2.00	2.05
21	23	407	CL7	MG-ND	-2.45	2.00	2.05
21	33	506	CL7	MG-ND	-2.45	2.00	2.05
21	43	406	CL7	C3B-C4B	-2.45	1.37	1.42
21	22	503	CL7	O2D-CGD	2.45	1.39	1.33
21	22	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	32	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	24	416	CL7	MG-ND	-2.45	2.00	2.05
21	2B	609	CL7	C4C-NC	-2.45	1.34	1.37
21	3B	608	CL7	C4C-NC	-2.45	1.34	1.37
21	33	513	CL7	C4C-NC	-2.45	1.34	1.37
21	24	412	CL7	CHC-C4B	2.45	1.44	1.39
21	21	407	CL7	C1B-C2B	-2.45	1.37	1.43
21	1B	612	CL7	C2A-C1A	2.45	1.54	1.50
21	3B	615	CL7	C1C-C2C	-2.45	1.40	1.45
21	22	506	CL7	MG-ND	-2.45	2.00	2.05
21	32	506	CL7	MG-ND	-2.45	2.00	2.05
21	13	516	CL7	C1C-NC	-2.45	1.34	1.37
21	21	403	CL7	MG-ND	-2.45	2.00	2.05
21	31	403	CL7	MG-ND	-2.45	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	606	CL7	C1C-NC	-2.45	1.34	1.37
21	2A	403	CL7	MG-NB	-2.45	2.00	2.05
21	23	409	CL7	MG-ND	-2.45	2.00	2.05
21	33	508	CL7	MG-ND	-2.45	2.00	2.05
21	3A	407	CL7	C1B-C2B	-2.45	1.37	1.43
21	13	508	CL7	C3B-C4B	-2.45	1.37	1.42
21	4A	407	CL7	C1B-C2B	-2.45	1.37	1.43
21	2B	614	CL7	C1B-NB	-2.45	1.34	1.37
21	42	516	CL7	C1B-C2B	-2.45	1.37	1.43
23	1K	101	8CT	C30-C29	2.45	1.53	1.50
21	41	406	CL7	MG-ND	-2.45	2.00	2.05
21	1C	509	CL7	C3B-C4B	-2.45	1.37	1.42
21	24	410	CL7	MG-ND	-2.45	2.00	2.05
21	34	410	CL7	MG-ND	-2.45	2.00	2.05
32	13	522	ZEX	C21-C26	-2.45	1.50	1.53
21	33	507	CL7	C1B-C2B	-2.45	1.37	1.43
21	22	513	CL7	C4C-NC	-2.45	1.34	1.37
21	32	513	CL7	C4C-NC	-2.45	1.34	1.37
21	3B	606	CL7	MG-ND	-2.45	2.00	2.05
21	1C	503	CL7	MG-ND	-2.45	2.00	2.05
21	4C	503	CL7	MG-ND	-2.45	2.00	2.05
21	21	410	CL7	C4C-NC	-2.45	1.34	1.37
21	2C	513	CL7	CHC-C4B	2.45	1.44	1.39
21	3C	513	CL7	CHC-C4B	2.45	1.44	1.39
21	12	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	12	503	CL7	MG-ND	-2.45	2.00	2.05
21	44	411	CL7	CHC-C4B	2.45	1.44	1.39
32	33	522	ZEX	C21-C26	-2.45	1.50	1.53
23	1C	514	8CT	C01-C02	2.45	1.54	1.50
21	3C	509	CL7	C3B-C4B	-2.45	1.37	1.42
21	13	516	CL7	MG-ND	-2.45	2.00	2.05
21	2B	607	CL7	MG-ND	-2.45	2.00	2.05
21	43	417	CL7	MG-ND	-2.45	2.00	2.05
21	14	409	CL7	C3B-C4B	-2.45	1.37	1.42
21	2C	509	CL7	C3B-C4B	-2.45	1.37	1.42
21	44	409	CL7	C3B-C4B	-2.45	1.37	1.42
21	23	417	CL7	C1C-NC	-2.45	1.34	1.37
21	3C	511	CL7	CHC-C4B	2.44	1.44	1.39
21	2A	407	CL7	C1B-C2B	-2.44	1.37	1.43
21	21	411	CL7	MG-ND	-2.44	2.00	2.05
21	3C	502	CL7	MG-ND	-2.44	2.00	2.05
21	31	411	CL7	MG-ND	-2.44	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	503	CL7	O2D-CGD	2.44	1.39	1.33
21	42	503	CL7	O2D-CGD	2.44	1.39	1.33
21	23	418	CL7	C3B-C4B	-2.44	1.37	1.42
21	33	517	CL7	C3B-C4B	-2.44	1.37	1.42
21	34	416	CL7	MG-ND	-2.44	2.00	2.05
21	11	410	CL7	C4C-NC	-2.44	1.34	1.37
21	3B	601	CL7	C4C-NC	-2.44	1.34	1.37
21	34	417	CL7	CHC-C4B	2.44	1.44	1.39
21	4D	402	CL7	CHC-C4B	2.44	1.44	1.39
21	43	407	CL7	C3B-C4B	-2.44	1.37	1.42
21	13	501	CL7	MG-ND	-2.44	2.00	2.05
21	2A	403	CL7	C1B-C2B	-2.44	1.37	1.43
21	22	503	CL7	C1B-C2B	-2.44	1.37	1.43
21	3A	403	CL7	C1B-C2B	-2.44	1.37	1.43
21	1B	612	CL7	MG-NB	-2.44	2.00	2.05
21	22	505	CL7	C3B-C4B	-2.44	1.37	1.42
21	3B	613	CL7	C3B-C4B	-2.44	1.37	1.42
21	32	505	CL7	C3B-C4B	-2.44	1.37	1.42
21	42	505	CL7	C3B-C4B	-2.44	1.37	1.42
21	11	406	CL7	MG-ND	-2.44	2.00	2.05
21	33	514	CL7	CAB-C3B	2.44	1.50	1.45
21	4B	609	CL7	C3B-C4B	-2.44	1.37	1.42
21	2B	610	CL7	MG-ND	-2.44	2.00	2.05
21	3B	609	CL7	MG-ND	-2.44	2.00	2.05
21	21	417	CL7	C1B-C2B	-2.44	1.37	1.43
21	1B	608	CL7	C3B-C4B	-2.44	1.37	1.42
21	1D	405	CL7	MG-ND	-2.44	2.00	2.05
21	2D	405	CL7	MG-ND	-2.44	2.00	2.05
21	4D	405	CL7	MG-ND	-2.44	2.00	2.05
21	21	408	CL7	CHC-C4B	2.44	1.44	1.39
21	33	515	CL7	MG-ND	-2.44	2.01	2.05
21	42	504	CL7	C1B-C2B	-2.44	1.37	1.43
21	2C	513	CL7	CHD-C1D	2.44	1.44	1.39
21	21	408	CL7	C4C-C3C	-2.44	1.40	1.45
21	12	512	CL7	CHC-C4B	2.44	1.44	1.39
21	42	516	CL7	CHC-C4B	2.44	1.44	1.39
21	24	409	CL7	C3B-C4B	-2.44	1.37	1.42
21	23	416	CL7	C4C-NC	-2.44	1.34	1.37
21	33	515	CL7	C4C-NC	-2.44	1.34	1.37
21	21	411	CL7	CHC-C4B	2.44	1.44	1.39
21	34	411	CL7	CHC-C4B	2.44	1.44	1.39
21	42	512	CL7	MG-ND	-2.44	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	22	516	CL7	CHC-C4B	2.44	1.44	1.39
21	2B	604	CL7	MG-ND	-2.44	2.01	2.05
21	22	505	CL7	MG-ND	-2.44	2.01	2.05
21	3B	603	CL7	MG-ND	-2.44	2.01	2.05
21	41	418	CL7	C1B-C2B	-2.44	1.37	1.43
21	41	417	CL7	MG-ND	-2.44	2.01	2.05
21	2B	613	CL7	MG-NB	-2.44	2.01	2.05
21	3B	612	CL7	MG-NB	-2.44	2.01	2.05
21	13	505	CL7	C3B-C4B	-2.44	1.37	1.42
21	13	517	CL7	C3B-C4B	-2.44	1.37	1.42
21	1B	614	CL7	MG-ND	-2.44	2.01	2.05
21	2C	507	CL7	MG-NB	-2.44	2.01	2.05
21	4B	615	CL7	MG-ND	-2.44	2.01	2.05
21	33	506	CL7	C3B-C4B	-2.44	1.37	1.42
21	42	512	CL7	CHC-C4B	2.44	1.44	1.39
21	3A	403	CL7	MG-NB	-2.44	2.01	2.05
21	11	420	CL7	C4C-NC	-2.44	1.34	1.37
21	14	415	CL7	C1C-NC	-2.44	1.34	1.37
21	44	415	CL7	C1C-NC	-2.44	1.34	1.37
21	11	407	CL7	C1B-C2B	-2.44	1.37	1.43
21	1B	615	CL7	C1C-C2C	-2.43	1.40	1.45
21	32	516	CL7	CHC-C4B	2.43	1.44	1.39
21	24	407	CL7	C4C-NC	-2.43	1.34	1.37
21	12	508	CL7	MG-ND	-2.43	2.01	2.05
21	4B	613	CL7	MG-NB	-2.43	2.01	2.05
21	21	418	CL7	C1B-C2B	-2.43	1.37	1.43
21	31	418	CL7	C1B-C2B	-2.43	1.37	1.43
21	1C	513	CL7	CHD-C1D	2.43	1.44	1.39
21	13	508	CL7	C1C-C2C	-2.43	1.40	1.45
21	3B	611	CL7	C1C-C2C	-2.43	1.40	1.45
21	3B	604	CL7	C1B-C2B	-2.43	1.37	1.43
21	14	412	CL7	CHC-C4B	2.43	1.44	1.39
21	12	510	CL7	C1B-C2B	-2.43	1.37	1.43
21	44	404	CL7	MG-ND	-2.43	2.01	2.05
21	14	417	CL7	CHC-C4B	2.43	1.44	1.39
21	1D	402	CL7	C4C-NC	-2.43	1.34	1.37
21	22	516	CL7	C1B-C2B	-2.43	1.37	1.43
21	31	408	CL7	C4C-C3C	-2.43	1.40	1.45
21	22	512	CL7	MG-ND	-2.43	2.01	2.05
21	4B	612	CL7	C3B-C4B	-2.43	1.37	1.42
32	43	421	ZEX	C1-C6	-2.43	1.50	1.53
21	2D	402	CL7	C4C-NC	-2.43	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3D	402	CL7	C4C-NC	-2.43	1.34	1.37
21	2B	609	CL7	C3B-C4B	-2.43	1.37	1.42
21	22	510	CL7	C1B-C2B	-2.43	1.37	1.43
21	32	510	CL7	C1B-C2B	-2.43	1.37	1.43
21	23	409	CL7	C3B-C4B	-2.43	1.37	1.42
21	3B	608	CL7	C3B-C4B	-2.43	1.37	1.42
23	4K	101	8CT	C01-C02	2.43	1.54	1.50
21	1C	507	CL7	MG-NB	-2.43	2.01	2.05
21	11	418	CL7	C1B-C2B	-2.43	1.37	1.43
21	2D	402	CL7	CHC-C4B	2.43	1.44	1.39
21	42	514	CL7	MG-NB	-2.43	2.01	2.05
21	12	508	CL7	C1C-C2C	-2.43	1.40	1.45
21	12	516	CL7	CHC-C4B	2.43	1.44	1.39
21	13	514	CL7	MG-ND	-2.43	2.01	2.05
21	11	413	CL7	CAB-C3B	2.43	1.50	1.45
21	41	413	CL7	CAB-C3B	2.43	1.50	1.45
21	22	514	CL7	MG-NB	-2.43	2.01	2.05
21	43	417	CL7	C1B-C2B	-2.43	1.37	1.43
21	33	506	CL7	C4C-NC	-2.43	1.34	1.37
21	11	412	CL7	CAB-C3B	2.43	1.50	1.45
21	23	407	CL7	C4C-NC	-2.43	1.34	1.37
21	43	409	CL7	C1C-C2C	-2.43	1.40	1.45
21	4B	613	CL7	C2A-C1A	2.43	1.54	1.50
21	12	505	CL7	CHC-C4B	2.43	1.44	1.39
21	23	415	CL7	MG-ND	-2.43	2.01	2.05
21	2B	612	CL7	C1C-C2C	-2.43	1.40	1.45
21	31	410	CL7	C1B-C2B	-2.43	1.37	1.43
21	1B	609	CL7	MG-NB	-2.43	2.01	2.05
21	43	404	CL7	MG-ND	-2.43	2.01	2.05
21	4B	612	CL7	C1C-C2C	-2.43	1.40	1.45
21	11	419	CL7	CHD-C1D	2.43	1.44	1.39
21	41	411	CL7	CHC-C4B	2.43	1.44	1.39
21	41	419	CL7	CHD-C1D	2.43	1.44	1.39
21	43	418	CL7	C3B-C4B	-2.43	1.37	1.42
21	13	511	CL7	MG-ND	-2.43	2.01	2.05
21	23	417	CL7	MG-ND	-2.43	2.01	2.05
21	43	412	CL7	MG-ND	-2.43	2.01	2.05
21	2B	605	CL7	C1B-C2B	-2.43	1.37	1.43
22	4A	402	PHO	C4D-CHA	2.43	1.43	1.39
23	1K	101	8CT	C28-C29	2.43	1.38	1.32
21	41	417	CL7	C1B-C2B	-2.42	1.37	1.43
22	2A	402	PHO	C4D-CHA	2.42	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	33	516	CL7	C1C-NC	-2.42	1.34	1.37
21	21	417	CL7	MG-ND	-2.42	2.01	2.05
21	31	417	CL7	MG-ND	-2.42	2.01	2.05
21	32	503	CL7	O2D-CGD	2.42	1.39	1.33
21	22	512	CL7	CHC-C4B	2.42	1.44	1.39
21	32	512	CL7	CHC-C4B	2.42	1.44	1.39
21	23	410	CL7	C3B-C4B	-2.42	1.37	1.42
21	1C	511	CL7	CHC-C4B	2.42	1.44	1.39
21	14	410	CL7	MG-ND	-2.42	2.01	2.05
23	1K	101	8CT	C01-C02	2.42	1.54	1.50
21	4B	606	CL7	CHC-C4B	2.42	1.44	1.39
21	44	412	CL7	CHC-C4B	2.42	1.44	1.39
21	2C	502	CL7	MG-NB	-2.42	2.01	2.05
21	32	514	CL7	C3B-C4B	-2.42	1.37	1.42
21	3A	403	CL7	C1C-NC	-2.42	1.34	1.37
21	43	416	CL7	C4C-NC	-2.42	1.34	1.37
21	1B	608	CL7	MG-NB	-2.42	2.01	2.05
21	4B	604	CL7	MG-ND	-2.42	2.01	2.05
21	4B	609	CL7	MG-NB	-2.42	2.01	2.05
22	3A	402	PHO	C4D-CHA	2.42	1.43	1.39
21	11	408	CL7	CHC-C4B	2.42	1.44	1.39
21	41	408	CL7	CHC-C4B	2.42	1.44	1.39
21	1B	609	CL7	MG-ND	-2.42	2.01	2.05
21	24	407	CL7	MG-ND	-2.42	2.01	2.05
21	31	413	CL7	CAB-C3B	2.42	1.50	1.45
21	11	411	CL7	MG-ND	-2.42	2.01	2.05
21	23	412	CL7	MG-ND	-2.42	2.01	2.05
21	41	411	CL7	MG-ND	-2.42	2.01	2.05
21	42	514	CL7	C3B-C4B	-2.42	1.37	1.42
21	21	410	CL7	C1B-C2B	-2.42	1.37	1.43
21	1B	606	CL7	MG-ND	-2.42	2.01	2.05
21	43	415	CL7	CAB-C3B	2.42	1.50	1.45
21	12	516	CL7	C1B-C2B	-2.42	1.37	1.43
21	32	516	CL7	C1B-C2B	-2.42	1.37	1.43
21	13	506	CL7	C1C-C2C	-2.42	1.40	1.45
21	43	407	CL7	C1C-C2C	-2.42	1.40	1.45
21	1D	404	CL7	C3B-C4B	-2.42	1.37	1.42
21	1D	402	CL7	CHC-C4B	2.42	1.44	1.39
21	14	416	CL7	CHC-C4B	2.42	1.44	1.39
21	41	412	CL7	CAB-C3B	2.42	1.50	1.45
21	11	410	CL7	C1B-C2B	-2.42	1.37	1.43
21	41	410	CL7	C1B-C2B	-2.42	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	411	CL7	CHC-C4B	2.42	1.44	1.39
21	43	408	CL7	CHC-C4B	2.42	1.44	1.39
21	24	416	CL7	C4C-NC	-2.42	1.34	1.37
21	34	416	CL7	C4C-NC	-2.42	1.34	1.37
21	1A	403	CL7	MG-NB	-2.42	2.01	2.05
21	4A	403	CL7	MG-NB	-2.42	2.01	2.05
21	23	409	CL7	C1C-C2C	-2.42	1.40	1.45
21	33	508	CL7	C1C-C2C	-2.42	1.40	1.45
21	34	409	CL7	C3B-C4B	-2.42	1.37	1.42
21	13	509	CL7	MG-NB	-2.42	2.01	2.05
21	42	505	CL7	MG-ND	-2.42	2.01	2.05
21	3C	501	CL7	MG-ND	-2.42	2.01	2.05
23	4K	101	8CT	C28-C29	2.42	1.38	1.32
21	12	514	CL7	C3B-C4B	-2.42	1.37	1.42
21	21	406	CL7	MG-ND	-2.42	2.01	2.05
23	1A	404	8CT	C01-C02	2.42	1.54	1.50
21	23	406	CL7	C3B-C4B	-2.42	1.37	1.42
21	33	505	CL7	C3B-C4B	-2.42	1.37	1.42
21	1C	501	CL7	MG-ND	-2.42	2.01	2.05
21	34	407	CL7	MG-ND	-2.42	2.01	2.05
21	4C	501	CL7	MG-ND	-2.42	2.01	2.05
21	44	415	CL7	MG-ND	-2.42	2.01	2.05
21	11	417	CL7	MG-ND	-2.41	2.01	2.05
21	4B	612	CL7	MG-ND	-2.41	2.01	2.05
21	2B	612	CL7	C3B-C4B	-2.41	1.37	1.42
21	3B	611	CL7	C3B-C4B	-2.41	1.37	1.42
21	24	408	CL7	C1B-C2B	-2.41	1.37	1.43
21	32	505	CL7	MG-ND	-2.41	2.01	2.05
21	31	402	CL7	CHC-C4B	2.41	1.44	1.39
21	23	417	CL7	C1B-C2B	-2.41	1.37	1.43
21	33	516	CL7	C1B-C2B	-2.41	1.37	1.43
21	2C	511	CL7	CHC-C4B	2.41	1.44	1.39
21	23	407	CL7	C1C-C2C	-2.41	1.40	1.45
21	31	406	CL7	CHC-C4B	2.41	1.44	1.39
21	34	404	CL7	CHC-C4B	2.41	1.44	1.39
21	3B	611	CL7	MG-ND	-2.41	2.01	2.05
21	34	414	CL7	C1B-C2B	-2.41	1.37	1.43
21	12	507	CL7	MG-NB	-2.41	2.01	2.05
21	22	508	CL7	C3B-C4B	-2.41	1.37	1.42
21	32	508	CL7	C3B-C4B	-2.41	1.37	1.42
21	14	414	CL7	C1B-C2B	-2.41	1.37	1.43
21	43	402	CL7	MG-ND	-2.41	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	409	CL7	C4C-NC	-2.41	1.34	1.37
21	1B	604	CL7	C1B-C2B	-2.41	1.37	1.43
21	4B	605	CL7	C1B-C2B	-2.41	1.37	1.43
21	12	511	CL7	CHC-C4B	2.41	1.44	1.39
21	13	513	CL7	CHC-C4B	2.41	1.44	1.39
21	42	511	CL7	CHC-C4B	2.41	1.44	1.39
21	12	508	CL7	C3B-C4B	-2.41	1.37	1.42
21	24	404	CL7	MG-ND	-2.41	2.01	2.05
21	3B	610	CL7	MG-NB	-2.41	2.01	2.05
21	23	415	CL7	CAB-C3B	2.41	1.50	1.45
21	2C	504	CL7	CHC-C4B	2.41	1.44	1.39
21	3C	504	CL7	CHC-C4B	2.41	1.44	1.39
21	43	409	CL7	MG-ND	-2.41	2.01	2.05
21	13	509	CL7	C3B-C4B	-2.41	1.37	1.42
21	43	410	CL7	C3B-C4B	-2.41	1.37	1.42
23	4K	101	8CT	C30-C29	2.41	1.53	1.50
21	32	512	CL7	MG-ND	-2.41	2.01	2.05
21	22	511	CL7	C1B-C2B	-2.41	1.37	1.43
21	32	511	CL7	C1B-C2B	-2.41	1.37	1.43
21	24	415	CL7	C1C-NC	-2.41	1.34	1.37
21	34	415	CL7	C1C-NC	-2.41	1.34	1.37
21	23	402	CL7	CHC-C4B	2.41	1.44	1.39
21	22	508	CL7	MG-ND	-2.41	2.01	2.05
21	32	508	CL7	MG-ND	-2.41	2.01	2.05
21	43	410	CL7	MG-NB	-2.41	2.01	2.05
21	44	417	CL7	MG-ND	-2.41	2.01	2.05
21	12	511	CL7	C1B-C2B	-2.41	1.37	1.43
21	11	411	CL7	C1B-C2B	-2.41	1.37	1.43
21	41	411	CL7	C1B-C2B	-2.41	1.37	1.43
21	22	511	CL7	CHC-C4B	2.41	1.44	1.39
21	34	412	CL7	CHC-C4B	2.41	1.44	1.39
21	34	415	CL7	MG-ND	-2.41	2.01	2.05
21	2B	616	CL7	C1C-C2C	-2.41	1.40	1.45
21	1C	502	CL7	MG-ND	-2.41	2.01	2.05
21	43	415	CL7	MG-ND	-2.41	2.01	2.05
21	4B	616	CL7	C1C-C2C	-2.41	1.40	1.45
21	24	414	CL7	C1B-C2B	-2.41	1.37	1.43
21	33	509	CL7	C3B-C4B	-2.41	1.37	1.42
21	33	513	CL7	CHC-C4B	2.41	1.44	1.39
21	2B	609	CL7	MG-NB	-2.41	2.01	2.05
21	2B	612	CL7	MG-NB	-2.41	2.01	2.05
21	3B	608	CL7	MG-NB	-2.41	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	22	506	CL7	C1B-C2B	-2.41	1.37	1.43
21	32	506	CL7	C1B-C2B	-2.41	1.37	1.43
21	2B	603	CL7	MG-ND	-2.41	2.01	2.05
21	4C	512	CL7	C1B-C2B	-2.41	1.37	1.43
21	11	407	CL7	MG-ND	-2.41	2.01	2.05
21	4C	509	CL7	C3B-C4B	-2.41	1.37	1.42
21	14	415	CL7	C1B-C2B	-2.41	1.37	1.43
21	24	417	CL7	MG-ND	-2.41	2.01	2.05
21	34	417	CL7	MG-ND	-2.41	2.01	2.05
21	43	416	CL7	MG-ND	-2.41	2.01	2.05
21	31	404	CL7	CAB-C3B	2.41	1.50	1.45
21	11	402	CL7	CHC-C4B	2.41	1.44	1.39
21	33	501	CL7	CHC-C4B	2.41	1.44	1.39
21	41	402	CL7	CHC-C4B	2.41	1.44	1.39
21	43	417	CL7	C1C-NC	-2.41	1.34	1.37
21	43	409	CL7	C3B-C4B	-2.41	1.37	1.42
21	21	411	CL7	C1B-C2B	-2.40	1.37	1.43
21	12	506	CL7	MG-ND	-2.40	2.01	2.05
21	2C	501	CL7	MG-ND	-2.40	2.01	2.05
21	21	402	CL7	CHC-C4B	2.40	1.44	1.39
21	11	414	CL7	CHD-C1D	2.40	1.44	1.39
21	14	407	CL7	MG-ND	-2.40	2.01	2.05
21	21	404	CL7	CAB-C3B	2.40	1.50	1.45
21	31	411	CL7	C1B-C2B	-2.40	1.37	1.43
21	4B	611	CL7	MG-NB	-2.40	2.01	2.05
21	42	506	CL7	C1B-C2B	-2.40	1.37	1.43
21	4C	513	CL7	C4C-NC	-2.40	1.34	1.37
21	1C	502	CL7	MG-NB	-2.40	2.01	2.05
21	4C	502	CL7	MG-NB	-2.40	2.01	2.05
21	22	508	CL7	C1C-C2C	-2.40	1.40	1.45
21	32	508	CL7	C1C-C2C	-2.40	1.40	1.45
21	43	414	CL7	CHC-C4B	2.40	1.44	1.39
21	14	404	CL7	CHC-C4B	2.40	1.44	1.39
21	32	511	CL7	CHC-C4B	2.40	1.44	1.39
21	44	404	CL7	CHC-C4B	2.40	1.44	1.39
21	14	408	CL7	C1B-C2B	-2.40	1.37	1.43
21	31	411	CL7	CHC-C4B	2.40	1.44	1.39
21	31	419	CL7	CHD-C1D	2.40	1.44	1.39
23	44	402	8CT	C01-C02	2.40	1.54	1.50
21	13	506	CL7	C3B-C4B	-2.40	1.37	1.42
21	1A	403	CL7	C1C-NC	-2.40	1.34	1.37
21	32	505	CL7	C1B-C2B	-2.40	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1B	611	CL7	MG-NB	-2.40	2.01	2.05
21	4B	612	CL7	MG-NB	-2.40	2.01	2.05
21	41	410	CL7	MG-ND	-2.40	2.01	2.05
32	41	422	ZEX	C21-C26	-2.40	1.50	1.53
21	31	408	CL7	CHC-C4B	2.40	1.44	1.39
21	1B	613	CL7	C3B-C4B	-2.40	1.37	1.42
21	1C	504	CL7	CHC-C4B	2.40	1.44	1.39
23	2K	101	8CT	C28-C29	2.40	1.38	1.32
23	3K	101	8CT	C28-C29	2.40	1.38	1.32
21	44	414	CL7	C1B-C2B	-2.40	1.37	1.43
23	2K	101	8CT	C01-C02	2.40	1.54	1.50
21	23	415	CL7	C4C-NC	-2.40	1.34	1.37
21	33	514	CL7	C4C-NC	-2.40	1.34	1.37
21	3C	513	CL7	CHD-C1D	2.40	1.44	1.39
21	3B	610	CL7	C2A-C1A	2.40	1.54	1.50
21	4B	614	CL7	C3B-C4B	-2.40	1.37	1.42
21	33	506	CL7	C1C-C2C	-2.40	1.40	1.45
21	1B	611	CL7	C3B-C4B	-2.40	1.37	1.42
21	1C	506	CL7	CHC-C4B	2.40	1.44	1.39
21	34	408	CL7	C1B-C2B	-2.40	1.37	1.43
21	3B	613	CL7	C2A-C1A	2.40	1.54	1.50
21	22	507	CL7	MG-NB	-2.40	2.01	2.05
21	32	507	CL7	MG-NB	-2.40	2.01	2.05
21	33	508	CL7	C3B-C4B	-2.40	1.37	1.42
21	33	515	CL7	CAB-C3B	2.40	1.50	1.45
21	12	509	CL7	CHC-C4B	2.40	1.44	1.39
21	2B	610	CL7	MG-NB	-2.40	2.01	2.05
21	3B	609	CL7	MG-NB	-2.40	2.01	2.05
21	21	412	CL7	CAB-C3B	2.40	1.50	1.45
21	32	509	CL7	C3B-C4B	-2.40	1.37	1.42
21	13	501	CL7	CHC-C4B	2.40	1.44	1.39
21	4D	404	CL7	C3B-C4B	-2.40	1.37	1.42
21	1B	603	CL7	MG-ND	-2.40	2.01	2.05
23	1D	406	8CT	C01-C02	2.39	1.54	1.50
23	2A	404	8CT	C01-C02	2.39	1.54	1.50
21	13	515	CL7	MG-ND	-2.39	2.01	2.05
21	2C	502	CL7	MG-ND	-2.39	2.01	2.05
21	23	407	CL7	C3B-C4B	-2.39	1.37	1.42
21	13	515	CL7	CAB-C3B	2.39	1.50	1.45
21	23	402	CL7	MG-ND	-2.39	2.01	2.05
21	34	408	CL7	MG-ND	-2.39	2.01	2.05
21	4B	610	CL7	MG-NB	-2.39	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1C	512	CL7	C1B-C2B	-2.39	1.37	1.43
21	41	414	CL7	CHD-C1D	2.39	1.44	1.39
21	3B	605	CL7	C1C-NC	-2.39	1.34	1.37
21	3B	613	CL7	C1C-NC	-2.39	1.34	1.37
21	12	505	CL7	MG-ND	-2.39	2.01	2.05
21	31	410	CL7	MG-ND	-2.39	2.01	2.05
21	42	507	CL7	MG-NB	-2.39	2.01	2.05
21	2B	614	CL7	C1C-NC	-2.39	1.34	1.37
21	22	505	CL7	CHC-C4B	2.39	1.44	1.39
21	33	511	CL7	MG-NB	-2.39	2.01	2.05
21	21	419	CL7	CHD-C1D	2.39	1.44	1.39
21	32	516	CL7	C1C-NC	-2.39	1.34	1.37
21	1B	613	CL7	C2A-C1A	2.39	1.54	1.50
21	3B	612	CL7	C2A-C1A	2.39	1.54	1.50
21	23	410	CL7	MG-NB	-2.39	2.01	2.05
21	24	412	CL7	C1B-C2B	-2.39	1.37	1.43
21	2B	614	CL7	C3B-C4B	-2.39	1.37	1.42
23	4A	404	8CT	C01-C02	2.39	1.54	1.50
21	3B	601	CL7	CHC-C4B	2.39	1.44	1.39
21	1B	605	CL7	C1C-NC	-2.39	1.34	1.37
21	31	412	CL7	CAB-C3B	2.39	1.50	1.45
21	42	508	CL7	C1C-C2C	-2.39	1.40	1.45
21	21	408	CL7	CHD-C1D	2.39	1.44	1.39
21	44	408	CL7	CHC-C4B	2.39	1.44	1.39
21	1B	613	CL7	C1C-NC	-2.39	1.34	1.37
21	4B	614	CL7	C1C-NC	-2.39	1.34	1.37
21	2C	512	CL7	C1B-C2B	-2.39	1.37	1.43
21	3C	512	CL7	C1B-C2B	-2.39	1.37	1.43
21	21	407	CL7	MG-ND	-2.39	2.01	2.05
21	31	407	CL7	MG-ND	-2.39	2.01	2.05
21	44	410	CL7	MG-ND	-2.39	2.01	2.05
21	13	513	CL7	C1B-C2B	-2.39	1.37	1.43
21	43	414	CL7	C1B-C2B	-2.39	1.37	1.43
21	2C	513	CL7	C4C-NC	-2.39	1.34	1.37
21	3C	513	CL7	C4C-NC	-2.39	1.34	1.37
21	4D	404	CL7	C1B-NB	-2.39	1.34	1.37
21	42	505	CL7	C1B-C2B	-2.39	1.37	1.43
21	22	502	CL7	C3B-C4B	-2.39	1.37	1.42
21	13	514	CL7	CAB-C3B	2.39	1.50	1.45
21	4B	610	CL7	MG-ND	-2.39	2.01	2.05
21	11	402	CL7	MG-ND	-2.39	2.01	2.05
21	14	408	CL7	MG-ND	-2.39	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	33	509	CL7	MG-NB	-2.39	2.01	2.05
21	44	408	CL7	MG-ND	-2.39	2.01	2.05
21	21	409	CL7	C1B-C2B	-2.39	1.37	1.43
21	42	508	CL7	MG-ND	-2.39	2.01	2.05
21	4C	506	CL7	CHC-C4B	2.39	1.44	1.39
23	2D	406	8CT	C22-C21	2.39	1.55	1.50
23	3D	406	8CT	C22-C21	2.39	1.55	1.50
21	22	518	CL7	CAB-C3B	2.39	1.50	1.45
21	1B	605	CL7	CHC-C4B	2.39	1.44	1.39
21	2D	404	CL7	C3B-C4B	-2.39	1.37	1.42
21	3D	404	CL7	C3B-C4B	-2.39	1.37	1.42
21	32	509	CL7	CHC-C4B	2.38	1.44	1.39
21	4D	402	CL7	C4C-NC	-2.38	1.34	1.37
21	44	408	CL7	C1B-C2B	-2.38	1.37	1.43
21	11	406	CL7	CHC-C4B	2.38	1.44	1.39
21	12	514	CL7	MG-NB	-2.38	2.01	2.05
21	22	518	CL7	MG-ND	-2.38	2.01	2.05
21	44	405	CL7	MG-ND	-2.38	2.01	2.05
21	3B	605	CL7	CHC-C4B	2.38	1.44	1.39
21	2D	405	CL7	C1B-C2B	-2.38	1.37	1.43
21	32	515	CL7	C4C-NC	-2.38	1.34	1.37
21	4C	504	CL7	CHC-C4B	2.38	1.44	1.39
21	32	514	CL7	MG-NB	-2.38	2.01	2.05
21	14	408	CL7	CHC-C4B	2.38	1.44	1.39
21	22	503	CL7	CHC-C4B	2.38	1.44	1.39
21	2B	616	CL7	C1B-C2B	-2.38	1.37	1.43
21	33	511	CL7	MG-ND	-2.38	2.01	2.05
21	11	413	CL7	CHC-C4B	2.38	1.44	1.39
21	23	414	CL7	C1B-C2B	-2.38	1.37	1.43
21	4B	602	CL7	C4C-NC	-2.38	1.34	1.37
21	42	513	CL7	C4C-NC	-2.38	1.34	1.37
21	41	402	CL7	MG-ND	-2.38	2.01	2.05
21	2B	608	CL7	CHC-C4B	2.38	1.44	1.39
21	24	408	CL7	CHC-C4B	2.38	1.44	1.39
21	4B	616	CL7	C1B-C2B	-2.38	1.37	1.43
21	2B	606	CL7	C1C-NC	-2.38	1.34	1.37
21	42	503	CL7	C1C-NC	-2.38	1.34	1.37
21	32	502	CL7	C3B-C4B	-2.38	1.37	1.42
21	12	518	CL7	MG-ND	-2.38	2.01	2.05
21	13	508	CL7	MG-NB	-2.38	2.01	2.05
21	24	408	CL7	MG-ND	-2.38	2.01	2.05
21	3D	405	CL7	MG-ND	-2.38	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	43	409	CL7	MG-NB	-2.38	2.01	2.05
21	1A	401	CL7	CHD-C1D	2.38	1.44	1.39
21	4A	401	CL7	CHD-C1D	2.38	1.44	1.39
21	42	511	CL7	C1B-C2B	-2.38	1.37	1.43
21	2B	612	CL7	MG-ND	-2.38	2.01	2.05
21	33	514	CL7	MG-ND	-2.38	2.01	2.05
21	3B	611	CL7	MG-NB	-2.38	2.01	2.05
21	23	414	CL7	CHC-C4B	2.38	1.44	1.39
21	14	416	CL7	C1B-C2B	-2.38	1.37	1.43
21	44	416	CL7	C1B-C2B	-2.38	1.37	1.43
21	12	502	CL7	C3B-C4B	-2.38	1.37	1.42
21	4B	602	CL7	CHC-C4B	2.38	1.44	1.39
21	11	409	CL7	C1B-C2B	-2.38	1.37	1.43
21	41	409	CL7	C1B-C2B	-2.38	1.37	1.43
21	22	509	CL7	C3B-C4B	-2.38	1.37	1.42
21	34	415	CL7	C1B-C2B	-2.38	1.37	1.43
21	12	506	CL7	C1C-NC	-2.38	1.34	1.37
21	11	417	CL7	C2A-C1A	2.38	1.54	1.50
21	41	417	CL7	C2A-C1A	2.38	1.54	1.50
21	31	414	CL7	CHD-C1D	2.38	1.44	1.39
21	13	507	CL7	CHC-C4B	2.38	1.44	1.39
21	12	503	CL7	CHC-C4B	2.38	1.44	1.39
21	11	404	CL7	CHD-C1D	2.38	1.44	1.39
21	41	404	CL7	CHD-C1D	2.38	1.44	1.39
21	32	503	CL7	C1C-NC	-2.38	1.34	1.37
31	4F	101	HEM	C4B-NB	-2.38	1.33	1.38
21	22	515	CL7	MG-ND	-2.37	2.01	2.05
21	31	402	CL7	MG-ND	-2.37	2.01	2.05
21	12	515	CL7	C4C-NC	-2.37	1.34	1.37
21	23	408	CL7	CHC-C4B	2.37	1.44	1.39
21	33	507	CL7	CHC-C4B	2.37	1.44	1.39
21	34	408	CL7	CHC-C4B	2.37	1.44	1.39
23	14	402	8CT	C22-C21	2.37	1.55	1.50
21	12	506	CL7	C1B-C2B	-2.37	1.37	1.43
21	24	416	CL7	C1B-C2B	-2.37	1.37	1.43
21	34	416	CL7	C1B-C2B	-2.37	1.37	1.43
21	12	515	CL7	MG-ND	-2.37	2.01	2.05
21	3C	502	CL7	MG-NB	-2.37	2.01	2.05
21	12	509	CL7	C3B-C4B	-2.37	1.37	1.42
21	42	509	CL7	C3B-C4B	-2.37	1.37	1.42
21	1B	615	CL7	C1B-C2B	-2.37	1.37	1.43
21	11	408	CL7	CHD-C1D	2.37	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	408	CL7	CHD-C1D	2.37	1.44	1.39
21	14	414	CL7	CHC-C4B	2.37	1.44	1.39
21	32	513	CL7	CHC-C4B	2.37	1.44	1.39
21	34	407	CL7	MG-NB	-2.37	2.01	2.05
21	4B	603	CL7	MG-ND	-2.37	2.01	2.05
21	42	518	CL7	CAB-C3B	2.37	1.50	1.45
21	1B	610	CL7	MG-NB	-2.37	2.01	2.05
21	32	506	CL7	C1C-NC	-2.37	1.34	1.37
21	24	415	CL7	C1B-C2B	-2.37	1.37	1.43
21	33	518	CL7	CHD-C1D	2.37	1.44	1.39
21	13	514	CL7	C4C-NC	-2.37	1.34	1.37
21	43	415	CL7	C4C-NC	-2.37	1.34	1.37
21	13	516	CL7	C1B-C2B	-2.37	1.37	1.43
21	14	404	CL7	MG-ND	-2.37	2.01	2.05
21	32	503	CL7	CHC-C4B	2.37	1.44	1.39
21	24	406	CL7	C1B-C2B	-2.37	1.37	1.43
21	34	406	CL7	C1B-C2B	-2.37	1.37	1.43
21	23	415	CL7	C1C-NC	-2.37	1.34	1.37
21	21	414	CL7	CHD-C1D	2.37	1.44	1.39
21	21	410	CL7	MG-ND	-2.37	2.01	2.05
21	23	416	CL7	MG-ND	-2.37	2.01	2.05
21	32	507	CL7	C1C-C2C	-2.37	1.40	1.45
21	31	404	CL7	CHD-C1D	2.37	1.44	1.39
21	2D	404	CL7	C1B-NB	-2.37	1.34	1.37
21	4B	611	CL7	C2A-C1A	2.37	1.54	1.50
21	2B	623	CL7	CHD-C1D	2.37	1.44	1.39
21	21	407	CL7	CHC-C4B	2.37	1.44	1.39
23	3B	618	8CT	C22-C21	2.37	1.55	1.50
21	43	412	CL7	MG-NB	-2.37	2.01	2.05
21	22	505	CL7	C1B-C2B	-2.37	1.37	1.43
21	21	404	CL7	CHD-C1D	2.37	1.44	1.39
21	1B	611	CL7	MG-ND	-2.37	2.01	2.05
21	12	503	CL7	C1C-NC	-2.37	1.34	1.37
21	1B	602	CL7	MG-ND	-2.37	2.01	2.05
21	34	404	CL7	MG-ND	-2.37	2.01	2.05
21	1B	610	CL7	C2A-C1A	2.37	1.54	1.50
21	32	505	CL7	CHC-C4B	2.37	1.44	1.39
21	2B	617	CL7	MG-ND	-2.37	2.01	2.05
21	1C	504	CL7	C1B-C2B	-2.37	1.37	1.43
21	4C	504	CL7	C1B-C2B	-2.37	1.37	1.43
21	42	505	CL7	CHC-C4B	2.37	1.44	1.39
21	43	402	CL7	CHC-C4B	2.37	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	518	CL7	CAB-C3B	2.37	1.50	1.45
21	31	419	CL7	C4C-NC	-2.37	1.34	1.37
21	2C	504	CL7	C1B-C2B	-2.37	1.37	1.43
22	1A	402	PHO	C4D-CHA	2.37	1.43	1.39
21	11	407	CL7	CHC-C4B	2.37	1.44	1.39
21	34	414	CL7	CHC-C4B	2.37	1.44	1.39
21	41	407	CL7	CHC-C4B	2.37	1.44	1.39
21	42	503	CL7	CHC-C4B	2.37	1.44	1.39
21	41	406	CL7	CHC-C4B	2.37	1.44	1.39
23	24	402	8CT	C01-C02	2.36	1.54	1.50
23	34	402	8CT	C01-C02	2.36	1.54	1.50
21	1B	611	CL7	C1C-C2C	-2.36	1.40	1.45
21	11	405	CL7	C1B-C2B	-2.36	1.37	1.43
21	4D	405	CL7	C1B-C2B	-2.36	1.37	1.43
21	12	509	CL7	C2A-C1A	2.36	1.54	1.50
21	42	509	CL7	C2A-C1A	2.36	1.54	1.50
21	34	407	CL7	C4C-NC	-2.36	1.34	1.37
21	14	406	CL7	MG-NB	-2.36	2.01	2.05
21	44	406	CL7	MG-NB	-2.36	2.01	2.05
23	4B	618	8CT	C01-C02	2.36	1.54	1.50
21	1C	513	CL7	C4C-NC	-2.36	1.34	1.37
21	3B	610	CL7	C1C-NC	-2.36	1.34	1.37
21	23	416	CL7	CAB-C3B	2.36	1.50	1.45
21	34	406	CL7	MG-NB	-2.36	2.01	2.05
21	14	406	CL7	C1B-C2B	-2.36	1.37	1.43
23	4D	406	8CT	C01-C02	2.36	1.54	1.50
21	2B	611	CL7	MG-NB	-2.36	2.01	2.05
21	14	404	CL7	MG-NB	-2.36	2.01	2.05
23	34	402	8CT	C22-C21	2.36	1.55	1.50
21	11	404	CL7	CAB-C3B	2.36	1.50	1.45
21	1B	601	CL7	CHC-C4B	2.36	1.44	1.39
21	43	416	CL7	CAB-C3B	2.36	1.50	1.45
21	12	505	CL7	C1B-C2B	-2.36	1.37	1.43
21	14	405	CL7	MG-ND	-2.36	2.01	2.05
21	1C	501	CL7	CHC-C4B	2.36	1.44	1.39
21	24	404	CL7	MG-NB	-2.36	2.01	2.05
21	34	404	CL7	MG-NB	-2.36	2.01	2.05
21	3A	401	CL7	CHD-C1D	2.36	1.44	1.39
21	13	511	CL7	MG-NB	-2.36	2.01	2.05
21	1D	405	CL7	C1B-C2B	-2.36	1.37	1.43
21	42	513	CL7	CHD-C1D	2.36	1.44	1.39
21	34	405	CL7	MG-ND	-2.36	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	407	CL7	MG-ND	-2.36	2.01	2.05
21	44	412	CL7	C1B-C2B	-2.36	1.37	1.43
21	3C	506	CL7	CHC-C4B	2.36	1.44	1.39
21	3D	404	CL7	C1B-NB	-2.36	1.34	1.37
21	41	416	CL7	CHD-C1D	2.36	1.44	1.39
21	23	409	CL7	MG-NB	-2.36	2.01	2.05
21	33	508	CL7	MG-NB	-2.36	2.01	2.05
21	33	518	CL7	MG-ND	-2.36	2.01	2.05
23	3K	101	8CT	C01-C02	2.36	1.54	1.50
23	24	402	8CT	C22-C21	2.36	1.55	1.50
21	34	409	CL7	MG-NB	-2.36	2.01	2.05
21	33	513	CL7	C1B-C2B	-2.36	1.37	1.43
23	3D	406	8CT	C01-C02	2.36	1.54	1.50
21	3B	615	CL7	C1B-C2B	-2.36	1.37	1.43
21	43	405	CL7	MG-ND	-2.36	2.01	2.05
21	12	516	CL7	C1C-NC	-2.36	1.34	1.37
21	11	409	CL7	C4C-NC	-2.36	1.34	1.37
21	11	410	CL7	MG-ND	-2.36	2.01	2.05
21	3B	609	CL7	CHD-C1D	2.36	1.44	1.39
21	31	413	CL7	CHC-C4B	2.36	1.44	1.39
21	21	406	CL7	CHC-C4B	2.35	1.44	1.39
21	24	405	CL7	MG-ND	-2.35	2.01	2.05
21	42	509	CL7	CHC-C4B	2.35	1.44	1.39
21	44	415	CL7	C1B-C2B	-2.35	1.37	1.43
21	22	513	CL7	C1C-C2C	-2.35	1.40	1.45
21	32	513	CL7	C1C-C2C	-2.35	1.40	1.45
21	4B	610	CL7	CHD-C1D	2.35	1.44	1.39
21	13	503	CL7	CHC-C4B	2.35	1.44	1.39
21	13	518	CL7	CHD-C1D	2.35	1.44	1.39
21	4B	608	CL7	CHC-C4B	2.35	1.44	1.39
21	31	409	CL7	C1B-C2B	-2.35	1.37	1.43
21	24	413	CL7	C1B-NB	-2.35	1.34	1.37
21	1C	506	CL7	C3B-C4B	-2.35	1.37	1.42
21	31	408	CL7	CHD-C1D	2.35	1.44	1.39
21	3C	506	CL7	C3B-C4B	-2.35	1.37	1.42
21	2C	501	CL7	CHC-C4B	2.35	1.44	1.39
21	21	416	CL7	CHD-C1D	2.35	1.44	1.39
21	3C	501	CL7	CHC-C4B	2.35	1.44	1.39
21	43	419	CL7	CHD-C1D	2.35	1.44	1.39
21	3B	611	CL7	C1C-NC	-2.35	1.34	1.37
21	3C	502	CL7	C1C-NC	-2.35	1.34	1.37
21	42	513	CL7	CHC-C4B	2.35	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4C	506	CL7	C3B-C4B	-2.35	1.37	1.42
21	42	518	CL7	MG-ND	-2.35	2.01	2.05
21	14	416	CL7	C4C-NC	-2.35	1.34	1.37
21	44	416	CL7	C4C-NC	-2.35	1.34	1.37
21	24	404	CL7	CHC-C4B	2.35	1.44	1.39
21	13	513	CL7	MG-ND	-2.35	2.01	2.05
21	4C	505	CL7	MG-NB	-2.35	2.01	2.05
21	44	406	CL7	C1B-C2B	-2.35	1.37	1.43
21	2B	602	CL7	CHC-C4B	2.35	1.44	1.39
21	11	420	CL7	CAB-C3B	2.35	1.50	1.45
21	41	420	CL7	CAB-C3B	2.35	1.50	1.45
21	3C	504	CL7	C1B-C2B	-2.35	1.37	1.43
21	12	501	CL7	CHC-C4B	2.35	1.44	1.39
21	23	410	CL7	CHC-C4B	2.35	1.44	1.39
23	14	402	8CT	C01-C02	2.35	1.54	1.50
21	1C	503	CL7	CHC-C4B	2.35	1.44	1.39
21	3B	602	CL7	MG-ND	-2.35	2.01	2.05
21	42	508	CL7	MG-NB	-2.35	2.01	2.05
21	2B	614	CL7	MG-NB	-2.35	2.01	2.05
21	3B	613	CL7	MG-NB	-2.35	2.01	2.05
21	21	420	CL7	CAB-C3B	2.35	1.50	1.45
21	31	420	CL7	CAB-C3B	2.35	1.50	1.45
21	3B	607	CL7	CHC-C4B	2.35	1.44	1.39
21	1C	502	CL7	C1C-C2C	-2.35	1.40	1.45
21	2C	505	CL7	MG-NB	-2.35	2.01	2.05
21	3C	505	CL7	MG-NB	-2.35	2.01	2.05
23	44	402	8CT	C22-C21	2.35	1.55	1.50
21	33	517	CL7	CHC-C4B	2.35	1.44	1.39
21	43	411	CL7	C1C-NC	-2.35	1.34	1.37
21	2C	503	CL7	CAB-C3B	2.35	1.50	1.45
21	3C	503	CL7	CAB-C3B	2.35	1.50	1.45
21	23	404	CL7	CHC-C4B	2.35	1.44	1.39
21	32	518	CL7	MG-ND	-2.35	2.01	2.05
21	3B	622	CL7	CHD-C1D	2.35	1.44	1.39
21	42	515	CL7	C4C-NC	-2.35	1.34	1.37
21	12	507	CL7	CHD-C1D	2.35	1.44	1.39
21	22	517	CL7	CHC-C4B	2.35	1.44	1.39
21	42	507	CL7	CHD-C1D	2.35	1.44	1.39
21	22	508	CL7	MG-NB	-2.35	2.01	2.05
21	32	508	CL7	MG-NB	-2.35	2.01	2.05
21	2B	614	CL7	C2A-C1A	2.35	1.54	1.50
21	14	412	CL7	C1B-C2B	-2.35	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	613	CL7	C1B-NB	-2.35	1.34	1.37
21	12	513	CL7	CHD-C1D	2.34	1.44	1.39
21	2C	506	CL7	CHC-C4B	2.34	1.44	1.39
21	21	413	CL7	CHC-C4B	2.34	1.44	1.39
21	34	405	CL7	CHC-C4B	2.34	1.44	1.39
21	44	413	CL7	MG-NB	-2.34	2.01	2.05
23	2B	619	8CT	C22-C21	2.34	1.55	1.50
21	14	407	CL7	C4C-NC	-2.34	1.34	1.37
21	32	504	CL7	C3B-C4B	-2.34	1.37	1.42
21	23	419	CL7	CHD-C1D	2.34	1.44	1.39
21	42	517	CL7	CHC-C4B	2.34	1.44	1.39
21	14	410	CL7	C3B-C4B	-2.34	1.37	1.42
21	44	410	CL7	C3B-C4B	-2.34	1.37	1.42
23	3A	404	8CT	C01-C02	2.34	1.54	1.50
21	2C	511	CL7	C1B-C2B	-2.34	1.37	1.43
21	3C	511	CL7	C1B-C2B	-2.34	1.37	1.43
21	12	501	CL7	C3B-C4B	-2.34	1.37	1.42
21	34	410	CL7	C3B-C4B	-2.34	1.37	1.42
21	42	501	CL7	C3B-C4B	-2.34	1.37	1.42
21	22	507	CL7	CHD-C1D	2.34	1.44	1.39
21	22	509	CL7	CHC-C4B	2.34	1.44	1.39
21	32	507	CL7	CHD-C1D	2.34	1.44	1.39
21	12	508	CL7	MG-NB	-2.34	2.01	2.05
21	4C	512	CL7	CHC-C4B	2.34	1.44	1.39
21	12	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	42	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	3D	405	CL7	C1B-C2B	-2.34	1.37	1.43
21	21	402	CL7	CAB-C3B	2.34	1.50	1.45
21	3C	508	CL7	C3B-C4B	-2.34	1.37	1.42
21	21	405	CL7	CHC-C4B	2.34	1.44	1.39
21	32	514	CL7	CHD-C1D	2.34	1.44	1.39
21	31	405	CL7	CHC-C4B	2.34	1.44	1.39
21	33	509	CL7	CHC-C4B	2.34	1.44	1.39
21	22	506	CL7	C3B-C4B	-2.34	1.37	1.42
21	32	501	CL7	C3B-C4B	-2.34	1.37	1.42
21	32	506	CL7	C3B-C4B	-2.34	1.37	1.42
23	1B	618	8CT	C22-C21	2.34	1.55	1.50
21	2B	610	CL7	CHD-C1D	2.34	1.44	1.39
21	41	413	CL7	CHC-C4B	2.34	1.44	1.39
21	43	417	CL7	CHD-C1D	2.34	1.44	1.39
21	13	518	CL7	MG-ND	-2.34	2.01	2.05
21	23	412	CL7	C1B-NB	-2.34	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	407	CL7	MG-NB	-2.34	2.01	2.05
21	44	407	CL7	MG-NB	-2.34	2.01	2.05
21	22	513	CL7	CHC-C4B	2.34	1.44	1.39
21	2C	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	32	518	CL7	CAB-C3B	2.34	1.50	1.45
21	2C	503	CL7	CHC-C4B	2.34	1.44	1.39
21	44	404	CL7	MG-NB	-2.34	2.01	2.05
21	22	510	CL7	CHC-C4B	2.34	1.44	1.39
21	21	409	CL7	C4C-NC	-2.34	1.34	1.37
21	24	407	CL7	MG-NB	-2.34	2.01	2.05
21	13	516	CL7	CHD-C1D	2.34	1.44	1.39
21	14	405	CL7	CHC-C4B	2.34	1.44	1.39
21	44	405	CL7	CHC-C4B	2.34	1.44	1.39
21	42	502	CL7	C3B-C4B	-2.34	1.37	1.42
21	12	514	CL7	CHD-C1D	2.34	1.44	1.39
21	2C	512	CL7	CHC-C4B	2.34	1.44	1.39
21	31	407	CL7	CHC-C4B	2.34	1.44	1.39
21	1C	508	CL7	C3B-C4B	-2.34	1.37	1.42
21	44	407	CL7	C1B-C2B	-2.34	1.37	1.43
21	32	501	CL7	CHC-C4B	2.34	1.44	1.39
21	33	503	CL7	CHC-C4B	2.34	1.44	1.39
21	4B	614	CL7	C2A-C1A	2.34	1.54	1.50
21	4B	616	CL7	C1C-NC	-2.34	1.34	1.37
21	2A	401	CL7	CHD-C1D	2.34	1.44	1.39
21	22	509	CL7	C2A-C1A	2.34	1.54	1.50
21	32	509	CL7	C2A-C1A	2.34	1.54	1.50
21	31	417	CL7	C2A-C1A	2.34	1.54	1.50
21	1C	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	4C	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	24	413	CL7	MG-NB	-2.34	2.01	2.05
21	13	517	CL7	CHC-C4B	2.34	1.44	1.39
21	4C	501	CL7	CHC-C4B	2.34	1.44	1.39
21	22	513	CL7	CHD-C1D	2.34	1.44	1.39
21	32	513	CL7	CHD-C1D	2.34	1.44	1.39
21	43	412	CL7	CHC-C4B	2.34	1.44	1.39
31	2F	101	HEM	C4B-NB	-2.34	1.34	1.38
21	3C	502	CL7	C1C-C2C	-2.34	1.40	1.45
21	3C	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	21	416	CL7	OBD-CAD	2.34	1.26	1.22
21	31	416	CL7	OBD-CAD	2.34	1.26	1.22
21	1C	512	CL7	CHC-C4B	2.34	1.44	1.39
21	24	414	CL7	CHC-C4B	2.34	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	410	CL7	CHD-C1D	2.34	1.44	1.39
21	1B	603	CL7	MG-NB	-2.34	2.01	2.05
21	4B	604	CL7	MG-NB	-2.34	2.01	2.05
21	22	507	CL7	C1C-C2C	-2.33	1.40	1.45
21	2C	506	CL7	C3B-C4B	-2.33	1.37	1.42
21	34	412	CL7	C1B-C2B	-2.33	1.37	1.43
21	33	506	CL7	CHD-C1D	2.33	1.44	1.39
21	3C	512	CL7	CHC-C4B	2.33	1.44	1.39
21	3C	508	CL7	MG-NB	-2.33	2.01	2.05
21	43	410	CL7	CHC-C4B	2.33	1.44	1.39
23	1D	406	8CT	C22-C21	2.33	1.55	1.50
23	4D	406	8CT	C22-C21	2.33	1.55	1.50
21	22	501	CL7	C1B-C2B	-2.33	1.37	1.43
21	1C	511	CL7	C1B-C2B	-2.33	1.37	1.43
21	11	405	CL7	CHC-C4B	2.33	1.44	1.39
21	41	405	CL7	CHC-C4B	2.33	1.44	1.39
21	2B	611	CL7	C2A-C1A	2.33	1.54	1.50
21	13	501	CL7	C1C-NC	-2.33	1.34	1.37
21	41	409	CL7	C4C-NC	-2.33	1.34	1.37
21	4B	617	CL7	CHC-C4B	2.33	1.44	1.39
21	1B	611	CL7	C1C-NC	-2.33	1.34	1.37
21	31	415	CL7	CHD-C1D	2.33	1.44	1.39
21	4C	503	CL7	CHC-C4B	2.33	1.44	1.39
21	31	413	CL7	MG-ND	-2.33	2.01	2.05
21	41	413	CL7	MG-ND	-2.33	2.01	2.05
21	31	405	CL7	C1B-C2B	-2.33	1.37	1.43
21	1B	609	CL7	CHC-C4B	2.33	1.44	1.39
21	1B	615	CL7	C1C-NC	-2.33	1.34	1.37
21	2B	616	CL7	C1C-NC	-2.33	1.34	1.37
21	2D	404	CL7	MG-NB	-2.33	2.01	2.05
21	3D	404	CL7	MG-NB	-2.33	2.01	2.05
21	41	405	CL7	C1B-C2B	-2.33	1.37	1.43
21	11	415	CL7	CHD-C1D	2.33	1.44	1.39
21	11	402	CL7	CAB-C3B	2.33	1.50	1.45
21	41	402	CL7	CAB-C3B	2.33	1.50	1.45
21	23	417	CL7	C1C-C2C	-2.33	1.40	1.45
21	21	402	CL7	MG-ND	-2.33	2.01	2.05
21	21	408	CL7	MG-ND	-2.33	2.01	2.05
21	41	419	CL7	C4C-NC	-2.33	1.34	1.37
21	22	503	CL7	MG-NB	-2.33	2.01	2.05
21	1B	607	CL7	CHC-C4B	2.33	1.44	1.39
21	12	510	CL7	CHC-C4B	2.33	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	406	CL7	MG-NB	-2.33	2.01	2.05
31	3F	101	HEM	C4B-NB	-2.33	1.34	1.38
23	1B	617	8CT	C01-C02	2.33	1.54	1.50
21	12	501	CL7	C1B-C2B	-2.33	1.37	1.43
21	1B	613	CL7	MG-NB	-2.33	2.01	2.05
21	23	412	CL7	MG-NB	-2.33	2.01	2.05
21	4B	614	CL7	MG-NB	-2.33	2.01	2.05
21	41	406	CL7	C3B-C4B	-2.33	1.37	1.42
21	41	404	CL7	CAB-C3B	2.33	1.50	1.45
21	12	517	CL7	CHC-C4B	2.33	1.44	1.39
21	2B	606	CL7	CHC-C4B	2.33	1.44	1.39
21	14	409	CL7	MG-NB	-2.33	2.01	2.05
21	44	409	CL7	MG-NB	-2.33	2.01	2.05
21	4C	511	CL7	C1B-C2B	-2.33	1.37	1.43
21	2C	502	CL7	CHC-C4B	2.33	1.44	1.39
21	23	418	CL7	CHC-C4B	2.33	1.44	1.39
21	4B	608	CL7	CHD-C1D	2.33	1.44	1.39
21	33	513	CL7	MG-ND	-2.33	2.01	2.05
21	2B	610	CL7	CHC-C4B	2.33	1.44	1.39
21	3B	609	CL7	CHC-C4B	2.33	1.44	1.39
21	3C	503	CL7	CHC-C4B	2.33	1.44	1.39
21	43	404	CL7	CHC-C4B	2.33	1.44	1.39
21	34	412	CL7	C1C-NC	-2.33	1.34	1.37
21	44	411	CL7	CHD-C1D	2.33	1.44	1.39
21	4B	605	CL7	C1C-C2C	-2.32	1.40	1.45
21	2B	617	CL7	CHC-C4B	2.32	1.44	1.39
21	42	510	CL7	CHC-C4B	2.32	1.44	1.39
21	13	509	CL7	CHC-C4B	2.32	1.44	1.39
21	11	418	CL7	MG-NB	-2.32	2.01	2.05
21	12	513	CL7	C1C-C2C	-2.32	1.40	1.45
21	1B	607	CL7	CHD-C1D	2.32	1.44	1.39
21	12	513	CL7	CHC-C4B	2.32	1.44	1.39
21	11	419	CL7	C4C-NC	-2.32	1.34	1.37
21	41	408	CL7	C3B-C4B	-2.32	1.37	1.42
21	31	402	CL7	CAB-C3B	2.32	1.50	1.45
21	12	514	CL7	C1C-C2C	-2.32	1.40	1.45
21	3B	606	CL7	CHC-C4B	2.32	1.44	1.39
23	2D	406	8CT	C01-C02	2.32	1.54	1.50
21	13	514	CL7	C1C-NC	-2.32	1.34	1.37
21	33	506	CL7	C1C-NC	-2.32	1.34	1.37
21	43	415	CL7	C1C-NC	-2.32	1.34	1.37
21	11	416	CL7	OBD-CAD	2.32	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	416	CL7	OBD-CAD	2.32	1.26	1.22
21	3A	401	CL7	CAA-C2A	-2.32	1.49	1.54
21	32	506	CL7	CHC-C4B	2.32	1.44	1.39
23	1C	515	8CT	C22-C21	2.32	1.55	1.50
21	4C	502	CL7	C1C-C2C	-2.32	1.40	1.45
21	23	403	CL7	CHD-C1D	2.32	1.44	1.39
21	33	502	CL7	CHD-C1D	2.32	1.44	1.39
21	41	415	CL7	CHD-C1D	2.32	1.44	1.39
32	23	423	ZEX	C1-C6	-2.32	1.50	1.53
21	1B	609	CL7	CHD-C1D	2.32	1.44	1.39
21	3B	602	CL7	MG-NB	-2.32	2.01	2.05
21	3D	405	CL7	MG-NB	-2.32	2.01	2.05
21	43	403	CL7	CHD-C1D	2.32	1.44	1.39
21	3B	605	CL7	C2A-C1A	2.32	1.54	1.50
31	1F	101	HEM	C4B-NB	-2.32	1.34	1.38
21	1C	505	CL7	MG-NB	-2.32	2.01	2.05
21	12	505	CL7	MG-NB	-2.32	2.01	2.05
21	12	516	CL7	MG-NB	-2.32	2.01	2.05
21	42	505	CL7	MG-NB	-2.32	2.01	2.05
21	43	414	CL7	MG-ND	-2.32	2.01	2.05
21	42	513	CL7	C1C-C2C	-2.32	1.40	1.45
21	42	507	CL7	C1B-C2B	-2.32	1.37	1.43
21	1B	622	CL7	CHD-C1D	2.32	1.44	1.39
21	4B	623	CL7	CHD-C1D	2.32	1.44	1.39
21	43	407	CL7	CHD-C1D	2.32	1.44	1.39
21	34	407	CL7	C1B-C2B	-2.32	1.37	1.43
23	4B	619	8CT	C22-C21	2.32	1.55	1.50
21	1C	508	CL7	CHC-C4B	2.32	1.44	1.39
21	12	506	CL7	CHC-C4B	2.32	1.44	1.39
21	43	412	CL7	C1B-NB	-2.32	1.34	1.37
21	24	409	CL7	MG-NB	-2.32	2.01	2.05
21	21	408	CL7	C1B-C2B	-2.32	1.37	1.43
32	13	522	ZEX	C1-C6	-2.32	1.50	1.53
32	43	423	ZEX	C1-C6	-2.32	1.50	1.53
21	31	406	CL7	C3B-C4B	-2.32	1.37	1.42
21	22	501	CL7	CHC-C4B	2.32	1.44	1.39
21	42	501	CL7	CHC-C4B	2.32	1.44	1.39
21	2A	401	CL7	CAA-C2A	-2.32	1.49	1.54
21	23	411	CL7	MG-NB	-2.32	2.01	2.05
21	33	510	CL7	MG-NB	-2.32	2.01	2.05
21	1A	403	CL7	CAB-C3B	2.32	1.50	1.45
21	22	501	CL7	C3B-C4B	-2.32	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4C	506	CL7	C1C-NC	-2.32	1.34	1.37
21	21	412	CL7	CHC-C4B	2.32	1.44	1.39
21	23	417	CL7	CHD-C1D	2.32	1.44	1.39
21	31	412	CL7	CHC-C4B	2.32	1.44	1.39
21	33	516	CL7	CHD-C1D	2.32	1.44	1.39
21	4B	610	CL7	CHC-C4B	2.32	1.44	1.39
21	34	416	CL7	CHD-C1D	2.32	1.44	1.39
21	22	507	CL7	C1B-C2B	-2.32	1.37	1.43
21	32	507	CL7	C1B-C2B	-2.32	1.37	1.43
21	3B	604	CL7	C1C-C2C	-2.32	1.40	1.45
21	42	507	CL7	C1C-NC	-2.32	1.34	1.37
21	22	515	CL7	CHC-C4B	2.32	1.44	1.39
21	44	414	CL7	CHC-C4B	2.32	1.44	1.39
21	12	518	CL7	C1B-C2B	-2.32	1.37	1.43
21	42	518	CL7	C1B-C2B	-2.32	1.37	1.43
21	3B	603	CL7	MG-NB	-2.32	2.01	2.05
21	23	412	CL7	CHC-C4B	2.32	1.44	1.39
21	32	510	CL7	CHC-C4B	2.32	1.44	1.39
21	44	406	CL7	CHC-C4B	2.32	1.44	1.39
21	1C	503	CL7	CAB-C3B	2.31	1.50	1.45
21	4C	503	CL7	CAB-C3B	2.31	1.50	1.45
21	11	408	CL7	MG-ND	-2.31	2.01	2.05
21	3B	616	CL7	CHC-C4B	2.31	1.44	1.39
21	4B	607	CL7	CHD-C1D	2.31	1.44	1.39
21	23	413	CL7	CHC-C4B	2.31	1.44	1.39
21	33	511	CL7	CHC-C4B	2.31	1.44	1.39
21	4A	403	CL7	CHC-C4B	2.31	1.44	1.39
21	32	514	CL7	C1C-C2C	-2.31	1.40	1.45
21	24	405	CL7	CHC-C4B	2.31	1.44	1.39
21	42	516	CL7	MG-NB	-2.31	2.01	2.05
21	21	419	CL7	C4C-NC	-2.31	1.34	1.37
21	2B	607	CL7	CHC-C4B	2.31	1.44	1.39
21	31	418	CL7	C1C-NC	-2.31	1.34	1.37
21	21	405	CL7	C1B-C2B	-2.31	1.37	1.43
21	32	501	CL7	C1B-C2B	-2.31	1.37	1.43
21	13	511	CL7	CHC-C4B	2.31	1.44	1.39
21	42	515	CL7	CHC-C4B	2.31	1.44	1.39
21	12	503	CL7	MG-NB	-2.31	2.01	2.05
21	42	503	CL7	MG-NB	-2.31	2.01	2.05
21	12	506	CL7	C3B-C4B	-2.31	1.37	1.42
21	1D	404	CL7	MG-NB	-2.31	2.01	2.05
21	4D	404	CL7	MG-NB	-2.31	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2C	502	CL7	C1C-C2C	-2.31	1.40	1.45
21	22	503	CL7	C1C-NC	-2.31	1.34	1.37
21	1B	616	CL7	MG-ND	-2.31	2.01	2.05
21	4B	617	CL7	MG-ND	-2.31	2.01	2.05
21	21	417	CL7	C2A-C1A	2.31	1.54	1.50
21	24	410	CL7	C3B-C4B	-2.31	1.37	1.42
21	32	515	CL7	MG-ND	-2.31	2.01	2.05
21	22	506	CL7	C1C-NC	-2.31	1.34	1.37
21	21	405	CL7	MG-ND	-2.31	2.01	2.05
21	31	408	CL7	MG-ND	-2.31	2.01	2.05
23	2C	515	8CT	C22-C21	2.31	1.55	1.50
21	3C	517	CL7	C3B-C4B	-2.31	1.37	1.42
32	43	423	ZEX	C10-C9	-2.31	1.32	1.35
21	12	504	CL7	CHC-C4B	2.31	1.44	1.39
21	34	405	CL7	C1B-C2B	-2.31	1.37	1.43
21	22	512	CL7	MG-NB	-2.31	2.01	2.05
21	44	413	CL7	C1B-NB	-2.31	1.34	1.37
21	1C	517	CL7	C3B-C4B	-2.31	1.37	1.42
21	4C	517	CL7	C3B-C4B	-2.31	1.37	1.42
21	13	502	CL7	CHD-C1D	2.31	1.44	1.39
21	34	416	CL7	MG-NB	-2.31	2.01	2.05
21	12	504	CL7	C3B-C4B	-2.31	1.37	1.42
21	21	408	CL7	C3B-C4B	-2.31	1.37	1.42
21	23	417	CL7	C3B-C4B	-2.31	1.37	1.42
21	31	408	CL7	C3B-C4B	-2.31	1.37	1.42
21	43	417	CL7	C3B-C4B	-2.31	1.37	1.42
21	13	516	CL7	CHC-C4B	2.31	1.44	1.39
21	2B	611	CL7	CHC-C4B	2.31	1.44	1.39
21	43	413	CL7	CHC-C4B	2.31	1.44	1.39
21	13	511	CL7	C1B-NB	-2.31	1.34	1.37
21	42	506	CL7	CHC-C4B	2.31	1.44	1.39
21	2C	517	CL7	C3B-C4B	-2.30	1.37	1.42
21	41	412	CL7	CHC-C4B	2.30	1.44	1.39
21	4B	606	CL7	C2A-C1A	2.30	1.54	1.50
21	11	412	CL7	CHC-C4B	2.30	1.44	1.39
21	12	502	CL7	CHC-C4B	2.30	1.44	1.39
21	23	412	CL7	C1C-C2C	-2.30	1.40	1.45
21	33	511	CL7	C1C-C2C	-2.30	1.40	1.45
21	4B	612	CL7	C1C-NC	-2.30	1.35	1.37
21	24	407	CL7	C1B-C2B	-2.30	1.37	1.43
23	3B	617	8CT	C01-C02	2.30	1.54	1.50
21	21	410	CL7	CHD-C1D	2.30	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	14	418	ZEX	C21-C26	-2.30	1.50	1.53
21	42	515	CL7	MG-ND	-2.30	2.01	2.05
21	42	504	CL7	C3B-C4B	-2.30	1.37	1.42
21	2B	604	CL7	MG-NB	-2.30	2.01	2.05
21	32	502	CL7	MG-NB	-2.30	2.01	2.05
21	32	512	CL7	MG-NB	-2.30	2.01	2.05
21	4B	615	CL7	C3B-C4B	-2.30	1.37	1.42
21	21	406	CL7	MG-NB	-2.30	2.01	2.05
21	3B	616	CL7	MG-ND	-2.30	2.01	2.05
21	1C	502	CL7	C1C-NC	-2.30	1.35	1.37
21	33	514	CL7	C1C-NC	-2.30	1.35	1.37
21	4C	502	CL7	C1C-NC	-2.30	1.35	1.37
21	21	414	CL7	CAB-C3B	2.30	1.50	1.45
21	4C	508	CL7	C3B-C4B	-2.30	1.37	1.42
21	22	502	CL7	CHC-C4B	2.30	1.44	1.39
21	24	406	CL7	CHC-C4B	2.30	1.44	1.39
21	14	413	CL7	C1B-NB	-2.30	1.35	1.37
21	42	505	CL7	C1B-NB	-2.30	1.35	1.37
21	22	504	CL7	C3B-C4B	-2.30	1.37	1.42
21	23	419	CL7	MG-ND	-2.30	2.01	2.05
21	34	413	CL7	MG-NB	-2.30	2.01	2.05
21	13	506	CL7	CHD-C1D	2.30	1.44	1.39
21	3C	502	CL7	CHC-C4B	2.30	1.44	1.39
21	4C	502	CL7	CHC-C4B	2.30	1.44	1.39
21	1B	605	CL7	C1C-C2C	-2.30	1.40	1.45
21	32	504	CL7	CHC-C4B	2.30	1.44	1.39
21	3B	605	CL7	C1C-C2C	-2.30	1.40	1.45
21	11	416	CL7	CHD-C1D	2.30	1.44	1.39
21	3B	606	CL7	CHD-C1D	2.30	1.44	1.39
21	1B	602	CL7	MG-NB	-2.30	2.01	2.05
21	1D	405	CL7	MG-NB	-2.30	2.01	2.05
21	34	411	CL7	CHD-C1D	2.30	1.44	1.39
21	31	414	CL7	CAB-C3B	2.30	1.50	1.45
21	2C	505	CL7	C1B-C2B	-2.30	1.37	1.43
21	11	406	CL7	C3B-C4B	-2.30	1.37	1.42
21	14	416	CL7	MG-NB	-2.30	2.01	2.05
21	44	416	CL7	MG-NB	-2.30	2.01	2.05
21	11	408	CL7	C3B-C4B	-2.30	1.37	1.42
21	1B	606	CL7	CHC-C4B	2.30	1.44	1.39
21	12	504	CL7	CHD-C1D	2.30	1.44	1.39
21	33	514	CL7	C1B-C2B	-2.30	1.37	1.43
21	42	514	CL7	C1C-C2C	-2.30	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	514	CL7	CHD-C1D	2.30	1.44	1.39
21	13	506	CL7	C1C-NC	-2.30	1.35	1.37
23	1B	618	8CT	C01-C02	2.30	1.54	1.50
21	11	406	CL7	MG-NB	-2.30	2.01	2.05
21	41	406	CL7	MG-NB	-2.30	2.01	2.05
23	1D	406	8CT	C38-C31	2.30	1.54	1.50
21	3C	508	CL7	CHC-C4B	2.30	1.44	1.39
21	1D	405	CL7	C3B-C4B	-2.30	1.37	1.42
21	13	510	CL7	MG-NB	-2.30	2.01	2.05
21	23	414	CL7	MG-ND	-2.30	2.01	2.05
21	23	402	CL7	C1C-NC	-2.30	1.35	1.37
21	33	501	CL7	C1C-NC	-2.30	1.35	1.37
21	14	406	CL7	CHC-C4B	2.30	1.44	1.39
21	31	416	CL7	CHD-C1D	2.30	1.44	1.39
21	24	411	CL7	CHD-C1D	2.30	1.44	1.39
21	41	410	CL7	CHD-C1D	2.30	1.44	1.39
21	11	418	CL7	C1C-NC	-2.30	1.35	1.37
21	41	418	CL7	C1C-NC	-2.30	1.35	1.37
21	3B	614	CL7	C3B-C4B	-2.30	1.37	1.42
21	34	413	CL7	C1B-NB	-2.29	1.35	1.37
21	23	407	CL7	CHD-C1D	2.29	1.44	1.39
21	13	504	CL7	MG-ND	-2.29	2.01	2.05
21	21	404	CL7	C1B-C2B	-2.29	1.37	1.43
21	31	404	CL7	C1B-C2B	-2.29	1.37	1.43
21	2C	508	CL7	C3B-C4B	-2.29	1.37	1.42
21	14	416	CL7	CHD-C1D	2.29	1.44	1.39
21	22	506	CL7	CHC-C4B	2.29	1.44	1.39
21	22	514	CL7	CHD-C1D	2.29	1.44	1.39
21	44	416	CL7	CHD-C1D	2.29	1.44	1.39
21	2B	605	CL7	C1C-C2C	-2.29	1.40	1.45
21	4A	401	CL7	OBD-CAD	2.29	1.26	1.22
21	22	505	CL7	MG-NB	-2.29	2.01	2.05
21	32	505	CL7	MG-NB	-2.29	2.01	2.05
21	34	415	CL7	CHC-C4B	2.29	1.44	1.39
21	24	416	CL7	MG-NB	-2.29	2.01	2.05
21	33	504	CL7	MG-ND	-2.29	2.01	2.05
21	43	415	CL7	C1B-C2B	-2.29	1.37	1.43
21	43	411	CL7	MG-NB	-2.29	2.01	2.05
21	1C	505	CL7	C1B-C2B	-2.29	1.37	1.43
21	4C	505	CL7	C1B-C2B	-2.29	1.37	1.43
23	3C	515	8CT	C22-C21	2.29	1.55	1.50
21	24	405	CL7	C1B-C2B	-2.29	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1A	403	CL7	C3B-C4B	-2.29	1.37	1.42
21	43	417	CL7	C2A-C1A	2.29	1.54	1.50
21	33	510	CL7	C1C-NC	-2.29	1.35	1.37
21	43	418	CL7	CHC-C4B	2.29	1.44	1.39
21	42	501	CL7	C1B-C2B	-2.29	1.37	1.43
21	2B	615	CL7	C3B-C4B	-2.29	1.37	1.42
21	33	516	CL7	C2A-C1A	2.29	1.54	1.50
21	32	517	CL7	CHC-C4B	2.29	1.44	1.39
32	33	522	ZEX	C1-C6	-2.29	1.50	1.53
21	13	506	CL7	C1B-C2B	-2.29	1.37	1.43
21	2B	612	CL7	C1C-NC	-2.29	1.35	1.37
21	1A	407	CL7	CHC-C4B	2.29	1.44	1.39
21	4A	407	CL7	CHC-C4B	2.29	1.44	1.39
21	2C	508	CL7	MG-NB	-2.29	2.01	2.05
21	42	506	CL7	C3B-C4B	-2.29	1.37	1.42
21	22	515	CL7	C4C-NC	-2.29	1.35	1.37
21	41	409	CL7	C1C-C2C	-2.29	1.40	1.45
21	14	415	CL7	CHC-C4B	2.29	1.44	1.39
21	22	514	CL7	C1C-C2C	-2.29	1.40	1.45
21	41	408	CL7	C1B-C2B	-2.29	1.37	1.43
21	3B	615	CL7	C1C-NC	-2.29	1.35	1.37
21	22	516	CL7	MG-NB	-2.29	2.01	2.05
21	32	516	CL7	MG-NB	-2.29	2.01	2.05
21	1B	610	CL7	CHC-C4B	2.29	1.44	1.39
21	13	516	CL7	C3B-C4B	-2.29	1.37	1.42
21	4C	508	CL7	MG-NB	-2.29	2.01	2.05
21	42	512	CL7	C1B-C2B	-2.29	1.37	1.43
21	13	512	CL7	CHC-C4B	2.29	1.44	1.39
21	2B	608	CL7	CHD-C1D	2.29	1.44	1.39
21	3B	607	CL7	CHD-C1D	2.29	1.44	1.39
21	1B	610	CL7	C1C-NC	-2.29	1.35	1.37
21	4B	611	CL7	C1C-NC	-2.29	1.35	1.37
21	1B	604	CL7	C1C-C2C	-2.29	1.40	1.45
21	43	404	CL7	MG-NB	-2.29	2.01	2.05
21	3A	403	CL7	CAB-C3B	2.29	1.50	1.45
21	1B	606	CL7	CHD-C1D	2.29	1.44	1.39
21	11	403	CL7	CHC-C4B	2.29	1.44	1.39
21	23	417	CL7	CHC-C4B	2.29	1.44	1.39
21	33	516	CL7	CHC-C4B	2.29	1.44	1.39
21	41	403	CL7	CHC-C4B	2.29	1.44	1.39
21	43	407	CL7	C1B-C2B	-2.29	1.37	1.43
21	13	516	CL7	C2A-C1A	2.29	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	507	CL7	C1B-C2B	-2.29	1.37	1.43
21	1B	616	CL7	CHC-C4B	2.29	1.44	1.39
21	4D	405	CL7	MG-NB	-2.29	2.01	2.05
32	13	522	ZEX	C10-C9	-2.28	1.32	1.35
21	24	405	CL7	CAB-C3B	2.28	1.50	1.45
21	14	405	CL7	C1B-C2B	-2.28	1.37	1.43
21	44	405	CL7	C1B-C2B	-2.28	1.37	1.43
21	2A	403	CL7	CHC-C4B	2.28	1.44	1.39
21	3A	403	CL7	CHC-C4B	2.28	1.44	1.39
21	41	404	CL7	C1B-C2B	-2.28	1.37	1.43
21	12	515	CL7	CHC-C4B	2.28	1.44	1.39
21	14	411	CL7	CHD-C1D	2.28	1.44	1.39
21	31	403	CL7	CHC-C4B	2.28	1.44	1.39
21	14	407	CL7	C1B-C2B	-2.28	1.37	1.43
21	21	415	CL7	CHD-C1D	2.28	1.44	1.39
21	1B	622	CL7	CAB-C3B	2.28	1.50	1.45
21	4B	623	CL7	CAB-C3B	2.28	1.50	1.45
21	1B	606	CL7	C1C-C2C	-2.28	1.40	1.45
21	31	402	CL7	C1B-C2B	-2.28	1.37	1.43
21	43	402	CL7	C1B-C2B	-2.28	1.37	1.43
21	21	413	CL7	MG-ND	-2.28	2.01	2.05
21	42	504	CL7	CHD-C1D	2.28	1.44	1.39
21	43	402	CL7	C3B-C4B	-2.28	1.37	1.42
21	2A	403	CL7	C1B-NB	-2.28	1.35	1.37
21	3A	403	CL7	C1B-NB	-2.28	1.35	1.37
21	2B	606	CL7	C1C-C2C	-2.28	1.40	1.45
23	1D	406	8CT	C30-C29	2.28	1.53	1.50
21	13	510	CL7	C1C-NC	-2.28	1.35	1.37
21	2A	401	CL7	OBD-CAD	2.28	1.26	1.22
21	3A	401	CL7	OBD-CAD	2.28	1.26	1.22
21	34	406	CL7	CHC-C4B	2.28	1.44	1.39
21	3C	505	CL7	C1B-C2B	-2.28	1.37	1.43
21	23	404	CL7	MG-NB	-2.28	2.01	2.05
21	2B	607	CL7	CHD-C1D	2.28	1.44	1.39
21	2A	403	CL7	CAB-C3B	2.28	1.50	1.45
21	32	515	CL7	CHC-C4B	2.28	1.44	1.39
21	4C	508	CL7	CHC-C4B	2.28	1.44	1.39
21	21	402	CL7	C1B-C2B	-2.28	1.37	1.43
21	1A	403	CL7	CHC-C4B	2.28	1.44	1.39
21	42	502	CL7	CHC-C4B	2.28	1.44	1.39
21	23	405	CL7	MG-ND	-2.28	2.01	2.05
21	21	406	CL7	C3B-C4B	-2.28	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	414	CL7	CAB-C3B	2.28	1.50	1.45
21	11	405	CL7	CHD-C1D	2.28	1.44	1.39
21	44	404	CL7	C1C-C2C	-2.28	1.40	1.45
21	1A	401	CL7	CAA-C2A	-2.28	1.49	1.54
21	44	405	CL7	CAB-C3B	2.28	1.50	1.45
23	2B	619	8CT	C01-C02	2.28	1.54	1.50
23	3B	618	8CT	C01-C02	2.28	1.54	1.50
21	11	402	CL7	C1B-C2B	-2.28	1.37	1.43
21	33	511	CL7	C1C-NC	-2.28	1.35	1.37
21	11	419	CL7	MG-ND	-2.28	2.01	2.05
21	31	418	CL7	MG-NB	-2.28	2.01	2.05
21	33	511	CL7	C1B-NB	-2.28	1.35	1.37
21	13	518	CL7	C1B-C2B	-2.28	1.37	1.43
21	14	413	CL7	MG-NB	-2.28	2.01	2.05
21	43	419	CL7	MG-ND	-2.28	2.01	2.05
23	4C	515	8CT	C22-C21	2.28	1.55	1.50
21	2D	405	CL7	C3B-C4B	-2.28	1.37	1.42
21	3D	405	CL7	C3B-C4B	-2.28	1.37	1.42
21	43	404	CL7	C1B-C2B	-2.28	1.37	1.43
21	3C	504	CL7	CHD-C1D	2.28	1.44	1.39
23	2D	406	8CT	C38-C31	2.28	1.54	1.50
21	2D	405	CL7	MG-NB	-2.28	2.01	2.05
21	1B	614	CL7	C3B-C4B	-2.28	1.37	1.42
21	4A	403	CL7	C3B-C4B	-2.28	1.37	1.42
21	14	410	CL7	CHC-C4B	2.28	1.44	1.39
21	22	504	CL7	CHC-C4B	2.28	1.44	1.39
21	21	409	CL7	C1C-C2C	-2.28	1.40	1.45
21	1C	508	CL7	MG-NB	-2.28	2.01	2.05
21	1C	503	CL7	C1B-C2B	-2.28	1.37	1.43
21	22	518	CL7	C1B-C2B	-2.28	1.37	1.43
21	23	415	CL7	C1B-C2B	-2.28	1.37	1.43
21	32	518	CL7	C1B-C2B	-2.28	1.37	1.43
21	4C	503	CL7	C1B-C2B	-2.28	1.37	1.43
21	2C	508	CL7	CHC-C4B	2.28	1.44	1.39
21	13	516	CL7	C1C-C2C	-2.28	1.40	1.45
21	43	417	CL7	C1C-C2C	-2.28	1.40	1.45
21	13	504	CL7	C1C-NC	-2.28	1.35	1.37
21	43	416	CL7	C1B-C2B	-2.27	1.37	1.43
21	32	503	CL7	MG-NB	-2.27	2.01	2.05
21	41	408	CL7	MG-ND	-2.27	2.01	2.05
21	41	418	CL7	MG-NB	-2.27	2.01	2.05
21	31	409	CL7	CHD-C1D	2.27	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	13	511	CL7	C1C-C2C	-2.27	1.40	1.45
21	13	501	CL7	C1B-C2B	-2.27	1.37	1.43
21	31	411	CL7	CAB-C3B	2.27	1.50	1.45
21	21	403	CL7	CHC-C4B	2.27	1.44	1.39
21	33	512	CL7	CHC-C4B	2.27	1.44	1.39
21	1C	505	CL7	C1C-C2C	-2.27	1.40	1.45
21	24	404	CL7	C1C-C2C	-2.27	1.40	1.45
21	34	404	CL7	C1C-C2C	-2.27	1.40	1.45
21	4C	505	CL7	C1C-C2C	-2.27	1.40	1.45
21	1C	502	CL7	CHC-C4B	2.27	1.44	1.39
21	3C	510	CL7	CHD-C1D	2.27	1.44	1.39
21	43	417	CL7	CHC-C4B	2.27	1.44	1.39
21	14	405	CL7	CAB-C3B	2.27	1.50	1.45
21	21	418	CL7	MG-NB	-2.27	2.01	2.05
21	4C	504	CL7	CHD-C1D	2.27	1.44	1.39
21	1A	403	CL7	C1B-NB	-2.27	1.35	1.37
21	31	408	CL7	C4C-NC	-2.27	1.35	1.37
21	23	404	CL7	C3B-C4B	-2.27	1.37	1.42
21	2C	510	CL7	CHD-C1D	2.27	1.44	1.39
21	23	402	CL7	C3B-C4B	-2.27	1.37	1.42
21	33	501	CL7	C3B-C4B	-2.27	1.37	1.42
21	23	402	CL7	C1B-C2B	-2.27	1.37	1.43
21	33	501	CL7	C1B-C2B	-2.27	1.37	1.43
21	2B	623	CL7	CAB-C3B	2.27	1.50	1.45
21	3B	622	CL7	CAB-C3B	2.27	1.50	1.45
21	43	405	CL7	C1C-NC	-2.27	1.35	1.37
21	2C	503	CL7	C1B-C2B	-2.27	1.37	1.43
21	3C	503	CL7	C1B-C2B	-2.27	1.37	1.43
21	22	514	CL7	CHC-C4B	2.27	1.44	1.39
21	4D	405	CL7	C3B-C4B	-2.27	1.37	1.42
21	23	404	CL7	C1B-C2B	-2.27	1.37	1.43
21	14	404	CL7	C1C-NC	-2.27	1.35	1.37
21	44	404	CL7	C1C-NC	-2.27	1.35	1.37
21	4C	511	CL7	CHD-C1D	2.27	1.44	1.39
21	14	404	CL7	C1C-C2C	-2.27	1.40	1.45
21	12	512	CL7	MG-NB	-2.27	2.01	2.05
21	2A	407	CL7	CHC-C4B	2.27	1.44	1.39
21	3A	407	CL7	CHC-C4B	2.27	1.44	1.39
21	42	504	CL7	CHC-C4B	2.27	1.44	1.39
21	44	416	CL7	CAB-C3B	2.27	1.50	1.45
21	2C	502	CL7	C1C-NC	-2.27	1.35	1.37
21	11	417	CL7	CHD-C1D	2.27	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	415	CL7	CHC-C4B	2.27	1.44	1.39
21	11	407	CL7	CHD-C1D	2.27	1.44	1.39
21	1B	622	CL7	MG-ND	-2.27	2.01	2.05
21	11	413	CL7	MG-ND	-2.27	2.01	2.05
21	2C	512	CL7	CAB-C3B	2.27	1.50	1.45
21	13	512	CL7	C1C-NC	-2.27	1.35	1.37
21	3C	505	CL7	C1C-C2C	-2.27	1.40	1.45
21	32	502	CL7	CHC-C4B	2.27	1.44	1.39
21	13	510	CL7	C3B-C4B	-2.27	1.37	1.42
21	33	516	CL7	C3B-C4B	-2.27	1.37	1.42
21	4C	512	CL7	CAB-C3B	2.27	1.50	1.45
21	2B	608	CL7	MG-NB	-2.27	2.01	2.05
32	23	423	ZEX	C10-C9	-2.27	1.32	1.35
32	33	522	ZEX	C10-C9	-2.27	1.32	1.35
21	22	505	CL7	C1B-NB	-2.27	1.35	1.37
21	32	505	CL7	C1B-NB	-2.27	1.35	1.37
21	43	412	CL7	C1C-NC	-2.27	1.35	1.37
21	11	405	CL7	MG-ND	-2.27	2.01	2.05
21	41	405	CL7	MG-ND	-2.27	2.01	2.05
21	23	407	CL7	C1B-C2B	-2.27	1.37	1.43
21	41	406	CL7	C1B-C2B	-2.27	1.37	1.43
23	2B	618	8CT	C01-C02	2.27	1.54	1.50
21	24	410	CL7	MG-NB	-2.27	2.01	2.05
21	34	410	CL7	MG-NB	-2.27	2.01	2.05
21	12	505	CL7	C1B-NB	-2.27	1.35	1.37
21	12	514	CL7	CHC-C4B	2.27	1.44	1.39
21	31	410	CL7	CHC-C4B	2.27	1.44	1.39
21	42	514	CL7	CHC-C4B	2.27	1.44	1.39
21	1B	607	CL7	MG-NB	-2.27	2.01	2.05
21	14	413	CL7	CHC-C4B	2.27	1.44	1.39
21	2C	504	CL7	CHD-C1D	2.27	1.44	1.39
21	31	418	CL7	CHC-C4B	2.27	1.44	1.39
21	4B	607	CL7	CHC-C4B	2.27	1.44	1.39
21	11	409	CL7	C1C-C2C	-2.27	1.40	1.45
21	11	404	CL7	C1B-C2B	-2.27	1.37	1.43
21	4B	603	CL7	MG-NB	-2.27	2.01	2.05
21	24	416	CL7	CHD-C1D	2.27	1.44	1.39
21	2C	505	CL7	C1C-C2C	-2.27	1.40	1.45
21	14	412	CL7	C1C-NC	-2.27	1.35	1.37
21	44	412	CL7	C1C-NC	-2.27	1.35	1.37
21	11	418	CL7	C3B-C4B	-2.27	1.37	1.42
21	4C	501	CL7	C3B-C4B	-2.27	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	413	CL7	CHC-C4B	2.27	1.44	1.39
21	4A	403	CL7	CAB-C3B	2.27	1.50	1.45
21	1C	506	CL7	C1C-NC	-2.27	1.35	1.37
21	33	512	CL7	C1B-NB	-2.27	1.35	1.37
21	1C	510	CL7	CHD-C1D	2.27	1.44	1.39
21	14	410	CL7	MG-NB	-2.26	2.01	2.05
21	2B	603	CL7	MG-NB	-2.26	2.01	2.05
21	44	410	CL7	MG-NB	-2.26	2.01	2.05
21	32	507	CL7	CHC-C4B	2.26	1.44	1.39
21	21	419	CL7	MG-ND	-2.26	2.01	2.05
21	31	419	CL7	MG-ND	-2.26	2.01	2.05
21	33	503	CL7	MG-NB	-2.26	2.01	2.05
21	4B	623	CL7	MG-ND	-2.26	2.01	2.05
21	13	510	CL7	CHC-C4B	2.26	1.44	1.39
21	23	416	CL7	C1B-C2B	-2.26	1.37	1.43
21	33	515	CL7	C1B-C2B	-2.26	1.37	1.43
21	22	506	CL7	C1C-C2C	-2.26	1.40	1.45
21	2B	614	CL7	CHC-C4B	2.26	1.44	1.39
21	33	508	CL7	CHD-C1D	2.26	1.44	1.39
21	31	405	CL7	MG-ND	-2.26	2.01	2.05
21	3B	602	CL7	C3B-C4B	-2.26	1.37	1.42
21	31	409	CL7	C1C-C2C	-2.26	1.40	1.45
21	2C	506	CL7	C1C-NC	-2.26	1.35	1.37
21	3C	506	CL7	C1C-NC	-2.26	1.35	1.37
32	34	418	ZEX	C21-C26	-2.26	1.50	1.53
21	4B	614	CL7	CHC-C4B	2.26	1.44	1.39
21	12	514	CL7	C1B-C2B	-2.26	1.37	1.43
21	31	408	CL7	C1B-C2B	-2.26	1.37	1.43
21	12	512	CL7	CAB-C3B	2.26	1.49	1.45
21	42	512	CL7	CAB-C3B	2.26	1.49	1.45
21	31	414	CL7	C4C-NC	-2.26	1.35	1.37
21	24	410	CL7	CHC-C4B	2.26	1.44	1.39
21	34	410	CL7	CHC-C4B	2.26	1.44	1.39
21	41	417	CL7	CHD-C1D	2.26	1.44	1.39
21	2A	407	CL7	MG-NB	-2.26	2.01	2.05
23	4D	406	8CT	C38-C31	2.26	1.54	1.50
21	1C	504	CL7	CHD-C1D	2.26	1.44	1.39
21	24	413	CL7	CHC-C4B	2.26	1.44	1.39
21	12	502	CL7	MG-NB	-2.26	2.01	2.05
21	42	502	CL7	MG-NB	-2.26	2.01	2.05
21	22	512	CL7	CAB-C3B	2.26	1.49	1.45
21	3B	610	CL7	CHC-C4B	2.26	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	21	414	CL7	C4C-NC	-2.26	1.35	1.37
21	2B	606	CL7	C2A-C1A	2.26	1.54	1.50
21	21	403	CL7	CAB-C3B	2.26	1.49	1.45
21	33	517	CL7	CHD-C1D	2.26	1.44	1.39
21	21	411	CL7	CAB-C3B	2.26	1.49	1.45
21	41	414	CL7	CAB-C3B	2.26	1.49	1.45
21	31	406	CL7	MG-NB	-2.26	2.01	2.05
21	31	418	CL7	C3B-C4B	-2.26	1.37	1.42
21	1B	608	CL7	CHC-C4B	2.26	1.44	1.39
21	21	415	CL7	OBD-CAD	2.26	1.26	1.22
21	21	404	CL7	MG-ND	-2.26	2.01	2.05
21	31	404	CL7	MG-ND	-2.26	2.01	2.05
21	11	415	CL7	OBD-CAD	2.26	1.26	1.22
21	3B	605	CL7	C1B-C2B	-2.26	1.37	1.43
21	43	419	CL7	C1B-C2B	-2.26	1.37	1.43
21	3C	517	CL7	CHC-C4B	2.26	1.44	1.39
21	13	501	CL7	C3B-C4B	-2.26	1.37	1.42
21	33	510	CL7	C3B-C4B	-2.26	1.37	1.42
21	21	407	CL7	CHD-C1D	2.26	1.44	1.39
21	31	407	CL7	CHD-C1D	2.26	1.44	1.39
21	44	415	CL7	CHC-C4B	2.26	1.44	1.39
21	24	410	CL7	C1C-C2C	-2.26	1.40	1.45
21	13	514	CL7	C1B-C2B	-2.26	1.37	1.43
21	11	410	CL7	CHC-C4B	2.26	1.44	1.39
21	21	419	CL7	CAB-C3B	2.26	1.49	1.45
21	31	419	CL7	CAB-C3B	2.26	1.49	1.45
21	2A	403	CL7	C3B-C4B	-2.26	1.37	1.42
21	3A	403	CL7	C3B-C4B	-2.26	1.37	1.42
21	42	506	CL7	C1C-C2C	-2.26	1.40	1.45
21	22	503	CL7	C3B-C4B	-2.26	1.37	1.42
21	44	415	CL7	C3B-C4B	-2.26	1.37	1.42
21	11	411	CL7	CAB-C3B	2.26	1.49	1.45
21	41	407	CL7	CAB-C3B	2.26	1.49	1.45
21	41	411	CL7	CAB-C3B	2.26	1.49	1.45
21	42	506	CL7	C1C-NC	-2.26	1.35	1.37
32	22	520	ZEX	C21-C26	-2.26	1.50	1.53
21	31	410	CL7	CHD-C1D	2.26	1.44	1.39
21	34	405	CL7	CAB-C3B	2.26	1.49	1.45
21	13	503	CL7	C3B-C4B	-2.25	1.37	1.42
21	22	510	CL7	C1C-NC	-2.25	1.35	1.37
21	3C	509	CL7	C1C-NC	-2.25	1.35	1.37
21	3B	614	CL7	C1C-C2C	-2.25	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	507	CL7	CHC-C4B	2.25	1.44	1.39
21	1D	402	CL7	MG-ND	-2.25	2.01	2.05
21	22	510	CL7	MG-NB	-2.25	2.01	2.05
21	4D	402	CL7	MG-ND	-2.25	2.01	2.05
21	34	409	CL7	CHD-C1D	2.25	1.44	1.39
21	22	514	CL7	C1B-C2B	-2.25	1.37	1.43
21	1A	401	CL7	OBD-CAD	2.25	1.26	1.22
21	1A	407	CL7	C3B-C4B	-2.25	1.37	1.42
21	4A	407	CL7	C3B-C4B	-2.25	1.37	1.42
21	4C	509	CL7	C1C-NC	-2.25	1.35	1.37
21	24	404	CL7	CAB-C3B	2.25	1.49	1.45
21	34	404	CL7	CAB-C3B	2.25	1.49	1.45
21	42	512	CL7	MG-NB	-2.25	2.01	2.05
21	41	415	CL7	OBD-CAD	2.25	1.26	1.22
21	1C	513	CL7	C1B-C2B	-2.25	1.38	1.43
21	11	408	CL7	C1B-C2B	-2.25	1.38	1.43
21	11	403	CL7	CAB-C3B	2.25	1.49	1.45
21	41	403	CL7	CAB-C3B	2.25	1.49	1.45
21	12	507	CL7	C1C-NC	-2.25	1.35	1.37
21	11	402	CL7	C1C-NC	-2.25	1.35	1.37
21	2B	611	CL7	C1C-NC	-2.25	1.35	1.37
21	41	402	CL7	C1C-NC	-2.25	1.35	1.37
21	12	512	CL7	C1B-C2B	-2.25	1.38	1.43
21	32	512	CL7	CAB-C3B	2.25	1.49	1.45
21	1D	405	CL7	CHC-C4B	2.25	1.44	1.39
21	4B	609	CL7	CHC-C4B	2.25	1.44	1.39
21	4D	405	CL7	CHC-C4B	2.25	1.44	1.39
21	21	402	CL7	C1C-NC	-2.25	1.35	1.37
21	21	409	CL7	CAB-C3B	2.25	1.49	1.45
21	2C	513	CL7	C1B-C2B	-2.25	1.38	1.43
21	3C	513	CL7	C1B-C2B	-2.25	1.38	1.43
21	33	506	CL7	C1B-C2B	-2.25	1.38	1.43
21	3D	405	CL7	C1C-NC	-2.25	1.35	1.37
21	3A	407	CL7	MG-NB	-2.25	2.01	2.05
21	14	415	CL7	C3B-C4B	-2.25	1.37	1.42
21	2C	509	CL7	CHC-C4B	2.25	1.44	1.39
21	24	404	CL7	C1C-NC	-2.25	1.35	1.37
23	2B	620	8CT	C22-C21	2.25	1.55	1.50
21	4A	401	CL7	C1B-C2B	-2.25	1.38	1.43
21	32	515	CL7	CHD-C1D	2.25	1.44	1.39
21	4B	612	CL7	CHC-C4B	2.25	1.44	1.39
21	44	410	CL7	CHC-C4B	2.25	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	607	CL7	C1C-C2C	-2.25	1.40	1.45
21	2D	405	CL7	CHC-C4B	2.25	1.44	1.39
21	3D	405	CL7	CHC-C4B	2.25	1.44	1.39
21	3C	506	CL7	CHD-C1D	2.25	1.44	1.39
23	4B	619	8CT	C01-C02	2.25	1.54	1.50
21	22	504	CL7	CHD-C1D	2.25	1.44	1.39
21	33	503	CL7	C3B-C4B	-2.25	1.37	1.42
32	23	420	ZEX	C10-C9	-2.25	1.32	1.35
21	3B	606	CL7	C1C-C2C	-2.25	1.40	1.45
21	2B	615	CL7	C1C-NC	-2.25	1.35	1.37
21	3A	407	CL7	C1C-NC	-2.25	1.35	1.37
21	3B	614	CL7	C1C-NC	-2.25	1.35	1.37
21	3B	613	CL7	CHC-C4B	2.25	1.44	1.39
21	13	504	CL7	CHC-C4B	2.25	1.44	1.39
21	21	406	CL7	C1B-C2B	-2.25	1.38	1.43
21	23	419	CL7	C1B-C2B	-2.25	1.38	1.43
21	31	406	CL7	C1B-C2B	-2.25	1.38	1.43
21	32	514	CL7	CHC-C4B	2.25	1.44	1.39
21	4B	611	CL7	CHC-C4B	2.25	1.44	1.39
21	1D	405	CL7	C1C-NC	-2.24	1.35	1.37
21	24	411	CL7	C1C-NC	-2.24	1.35	1.37
21	33	504	CL7	C1C-NC	-2.24	1.35	1.37
21	34	411	CL7	C1C-NC	-2.24	1.35	1.37
21	4D	405	CL7	C1C-NC	-2.24	1.35	1.37
21	1A	407	CL7	MG-NB	-2.24	2.01	2.05
23	2D	406	8CT	C30-C29	2.24	1.53	1.50
23	3D	406	8CT	C30-C29	2.24	1.53	1.50
21	23	417	CL7	C2A-C1A	2.24	1.54	1.50
21	1A	407	CL7	C1C-C2C	-2.24	1.40	1.45
21	4A	407	CL7	C1C-C2C	-2.24	1.40	1.45
21	42	502	CL7	C1B-C2B	-2.24	1.38	1.43
23	1C	518	8CT	C38-C31	2.24	1.54	1.50
21	32	516	CL7	C1C-C2C	-2.24	1.40	1.45
21	21	418	CL7	C1C-NC	-2.24	1.35	1.37
21	24	414	CL7	C3B-C4B	-2.24	1.37	1.42
32	13	519	ZEX	C10-C9	-2.24	1.32	1.35
32	43	420	ZEX	C10-C9	-2.24	1.32	1.35
21	41	402	CL7	C1B-C2B	-2.24	1.38	1.43
21	24	415	CL7	CAB-C3B	2.24	1.49	1.45
21	1C	509	CL7	CHC-C4B	2.24	1.44	1.39
21	1C	517	CL7	CHC-C4B	2.24	1.44	1.39
21	4C	517	CL7	CHC-C4B	2.24	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	13	503	CL7	MG-NB	-2.24	2.01	2.05
21	24	416	CL7	CAB-C3B	2.24	1.49	1.45
21	34	416	CL7	CAB-C3B	2.24	1.49	1.45
23	3D	406	8CT	C38-C31	2.24	1.54	1.50
21	1C	510	CL7	C3B-C4B	-2.24	1.37	1.42
21	22	517	CL7	C3B-C4B	-2.24	1.37	1.42
21	42	517	CL7	C3B-C4B	-2.24	1.37	1.42
21	13	508	CL7	CHD-C1D	2.24	1.44	1.39
21	21	405	CL7	CHD-C1D	2.24	1.44	1.39
21	31	405	CL7	CHD-C1D	2.24	1.44	1.39
21	33	516	CL7	C1C-C2C	-2.24	1.40	1.45
21	32	514	CL7	C1B-C2B	-2.24	1.38	1.43
21	33	518	CL7	C1B-C2B	-2.24	1.38	1.43
21	1C	504	CL7	MG-ND	-2.24	2.01	2.05
21	2B	602	CL7	MG-ND	-2.24	2.01	2.05
21	3B	601	CL7	MG-ND	-2.24	2.01	2.05
21	13	503	CL7	C1B-C2B	-2.24	1.38	1.43
21	33	504	CL7	CHC-C4B	2.24	1.44	1.39
21	2B	602	CL7	C3B-C4B	-2.24	1.37	1.42
21	3B	601	CL7	C3B-C4B	-2.24	1.37	1.42
21	41	409	CL7	CAB-C3B	2.24	1.49	1.45
21	23	411	CL7	C1C-NC	-2.24	1.35	1.37
21	3B	612	CL7	CHC-C4B	2.24	1.44	1.39
21	22	502	CL7	MG-NB	-2.24	2.01	2.05
21	41	419	CL7	MG-ND	-2.24	2.01	2.05
21	43	406	CL7	C1B-NB	-2.24	1.35	1.37
21	4B	615	CL7	C1C-C2C	-2.24	1.40	1.45
21	32	510	CL7	MG-NB	-2.24	2.01	2.05
21	12	506	CL7	C1C-C2C	-2.24	1.40	1.45
21	2A	407	CL7	C1C-C2C	-2.24	1.40	1.45
21	2C	511	CL7	CHD-C1D	2.24	1.44	1.39
21	21	410	CL7	CHC-C4B	2.24	1.44	1.39
21	3C	511	CL7	CHD-C1D	2.24	1.44	1.39
21	3B	602	CL7	CHC-C4B	2.24	1.44	1.39
21	3B	608	CL7	CHC-C4B	2.24	1.44	1.39
32	13	525	ZEX	C14-C13	-2.24	1.32	1.35
32	43	401	ZEX	C14-C13	-2.24	1.32	1.35
21	3B	601	CL7	CAB-C3B	2.24	1.49	1.45
21	44	404	CL7	CAB-C3B	2.24	1.49	1.45
21	11	406	CL7	C1B-C2B	-2.24	1.38	1.43
21	14	413	CL7	C3B-C4B	-2.24	1.37	1.42
21	14	414	CL7	C3B-C4B	-2.24	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	402	CL7	C1C-NC	-2.24	1.35	1.37
21	33	512	CL7	C1C-NC	-2.24	1.35	1.37
21	24	415	CL7	C3B-C4B	-2.24	1.37	1.42
21	34	415	CL7	C3B-C4B	-2.24	1.37	1.42
21	2D	405	CL7	CAB-C3B	2.24	1.49	1.45
21	3D	405	CL7	CAB-C3B	2.24	1.49	1.45
21	12	513	CL7	C3B-C4B	-2.24	1.37	1.42
21	2C	501	CL7	C3B-C4B	-2.24	1.37	1.42
21	3C	501	CL7	C3B-C4B	-2.24	1.37	1.42
21	11	418	CL7	CHC-C4B	2.24	1.44	1.39
21	3C	509	CL7	CHC-C4B	2.24	1.44	1.39
21	41	418	CL7	CHC-C4B	2.24	1.44	1.39
21	33	503	CL7	C1B-C2B	-2.24	1.38	1.43
21	1B	601	CL7	CAB-C3B	2.24	1.49	1.45
21	14	404	CL7	CAB-C3B	2.24	1.49	1.45
21	4B	606	CL7	C3B-C4B	-2.24	1.37	1.42
21	12	507	CL7	CBD-CGD	-2.24	1.45	1.52
21	34	409	CL7	CHC-C4B	2.24	1.44	1.39
21	1B	605	CL7	C1B-C2B	-2.24	1.38	1.43
21	32	512	CL7	C1B-C2B	-2.24	1.38	1.43
21	4B	606	CL7	C1B-C2B	-2.24	1.38	1.43
21	13	512	CL7	C1B-NB	-2.24	1.35	1.37
21	43	413	CL7	C1B-NB	-2.24	1.35	1.37
21	2B	616	CL7	CHD-C1D	2.24	1.44	1.39
21	3B	615	CL7	CHD-C1D	2.24	1.44	1.39
32	24	418	ZEX	C21-C26	-2.24	1.50	1.53
21	12	510	CL7	MG-NB	-2.24	2.01	2.05
21	2A	407	CL7	C3B-C4B	-2.24	1.37	1.42
21	3A	407	CL7	C3B-C4B	-2.24	1.37	1.42
21	4B	606	CL7	C1C-C2C	-2.24	1.40	1.45
21	2D	402	CL7	MG-ND	-2.24	2.01	2.05
21	22	507	CL7	CBD-CGD	-2.24	1.45	1.52
21	32	507	CL7	CBD-CGD	-2.24	1.45	1.52
21	1D	405	CL7	CAB-C3B	2.24	1.49	1.45
21	14	416	CL7	CAB-C3B	2.24	1.49	1.45
21	41	410	CL7	CHC-C4B	2.24	1.44	1.39
21	43	412	CL7	C1C-C2C	-2.24	1.40	1.45
21	1B	601	CL7	MG-ND	-2.24	2.01	2.05
21	4B	602	CL7	MG-ND	-2.24	2.01	2.05
32	44	418	ZEX	C21-C26	-2.23	1.50	1.53
21	11	409	CL7	CAB-C3B	2.23	1.49	1.45
21	11	409	CL7	CHD-C1D	2.23	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	403	CL7	C1B-C2B	-2.23	1.38	1.43
21	11	404	CL7	MG-ND	-2.23	2.01	2.05
21	41	404	CL7	MG-ND	-2.23	2.01	2.05
21	4A	403	CL7	C1B-NB	-2.23	1.35	1.37
21	43	413	CL7	CAB-C3B	2.23	1.49	1.45
21	3B	622	CL7	MG-ND	-2.23	2.01	2.05
21	1C	517	CL7	CHD-C1D	2.23	1.44	1.39
21	43	407	CL7	C1C-NC	-2.23	1.35	1.37
21	21	409	CL7	CHD-C1D	2.23	1.44	1.39
21	11	419	CL7	CAB-C3B	2.23	1.49	1.45
21	41	419	CL7	CAB-C3B	2.23	1.49	1.45
21	43	409	CL7	CHD-C1D	2.23	1.44	1.39
21	1C	517	CL7	C1B-C2B	-2.23	1.38	1.43
23	1B	619	8CT	C22-C21	2.23	1.55	1.50
21	23	407	CL7	C1C-NC	-2.23	1.35	1.37
21	2D	405	CL7	C1C-C2C	-2.23	1.40	1.45
32	23	401	ZEX	C14-C13	-2.23	1.32	1.35
21	32	502	CL7	C1B-C2B	-2.23	1.38	1.43
21	43	418	CL7	CHD-C1D	2.23	1.44	1.39
21	1C	501	CL7	C3B-C4B	-2.23	1.37	1.42
21	14	416	CL7	OBD-CAD	2.23	1.26	1.22
21	44	413	CL7	CHC-C4B	2.23	1.44	1.39
21	1B	602	CL7	C3B-C4B	-2.23	1.37	1.42
21	4B	603	CL7	C3B-C4B	-2.23	1.37	1.42
21	1A	407	CL7	C1C-NC	-2.23	1.35	1.37
21	42	514	CL7	C1B-C2B	-2.23	1.38	1.43
23	2C	518	8CT	C38-C31	2.23	1.54	1.50
21	24	406	CL7	CAB-C3B	2.23	1.49	1.45
21	1B	615	CL7	CHD-C1D	2.23	1.44	1.39
21	4B	615	CL7	CHC-C4B	2.23	1.44	1.39
21	4B	616	CL7	CHD-C1D	2.23	1.44	1.39
21	34	414	CL7	C3B-C4B	-2.23	1.37	1.42
21	21	409	CL7	MG-ND	-2.23	2.01	2.05
21	14	409	CL7	CHD-C1D	2.23	1.44	1.39
21	44	409	CL7	CHD-C1D	2.23	1.44	1.39
21	4B	602	CL7	C3B-C4B	-2.23	1.37	1.42
21	41	407	CL7	CHD-C1D	2.23	1.44	1.39
21	2B	607	CL7	C1C-C2C	-2.23	1.40	1.45
21	4A	401	CL7	CAA-C2A	-2.23	1.50	1.54
21	31	415	CL7	OBD-CAD	2.23	1.26	1.22
21	1A	401	CL7	C1B-C2B	-2.23	1.38	1.43
21	1B	603	CL7	C3B-C4B	-2.23	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	413	CL7	C3B-C4B	-2.23	1.37	1.42
21	4B	604	CL7	C3B-C4B	-2.23	1.37	1.42
21	2A	401	CL7	C1B-C2B	-2.23	1.38	1.43
21	12	503	CL7	C3B-C4B	-2.23	1.37	1.42
21	42	503	CL7	C3B-C4B	-2.23	1.37	1.42
21	33	510	CL7	C1C-C2C	-2.23	1.40	1.45
21	21	407	CL7	CAB-C3B	2.23	1.49	1.45
21	31	407	CL7	CAB-C3B	2.23	1.49	1.45
21	4D	405	CL7	CAB-C3B	2.23	1.49	1.45
23	1A	404	8CT	C22-C21	2.23	1.55	1.50
21	22	509	CL7	MG-NB	-2.23	2.01	2.05
21	32	509	CL7	MG-NB	-2.23	2.01	2.05
21	32	504	CL7	CHD-C1D	2.23	1.44	1.39
21	12	502	CL7	C1B-C2B	-2.23	1.38	1.43
21	22	513	CL7	C1B-C2B	-2.23	1.38	1.43
21	43	404	CL7	C3B-C4B	-2.23	1.37	1.42
21	1B	613	CL7	CHC-C4B	2.23	1.44	1.39
21	4C	513	CL7	C1B-C2B	-2.23	1.38	1.43
21	23	405	CL7	C1C-C2C	-2.23	1.40	1.45
21	32	504	CL7	C1C-C2C	-2.23	1.40	1.45
21	33	504	CL7	C1C-C2C	-2.23	1.40	1.45
21	22	515	CL7	CHD-C1D	2.23	1.44	1.39
21	4C	517	CL7	CHD-C1D	2.23	1.44	1.39
21	34	406	CL7	CAB-C3B	2.23	1.49	1.45
21	12	506	CL7	CHD-C1D	2.23	1.44	1.39
21	31	417	CL7	CHD-C1D	2.23	1.44	1.39
21	2B	623	CL7	MG-ND	-2.23	2.01	2.05
21	41	418	CL7	C3B-C4B	-2.23	1.37	1.42
21	21	417	CL7	CHD-C1D	2.23	1.44	1.39
21	23	405	CL7	CHC-C4B	2.23	1.44	1.39
21	1B	614	CL7	C1C-C2C	-2.23	1.40	1.45
21	4B	604	CL7	C1C-C2C	-2.23	1.40	1.45
21	43	416	CL7	CHD-C1D	2.23	1.44	1.39
21	3D	402	CL7	CAB-C3B	2.23	1.49	1.45
21	4A	407	CL7	C1C-NC	-2.23	1.35	1.37
21	3B	607	CL7	MG-NB	-2.23	2.01	2.05
21	24	412	CL7	C3B-C4B	-2.23	1.37	1.42
21	2B	615	CL7	CHC-C4B	2.23	1.44	1.39
21	31	403	CL7	CAB-C3B	2.23	1.49	1.45
21	44	415	CL7	CAB-C3B	2.23	1.49	1.45
21	12	510	CL7	C1C-C2C	-2.23	1.40	1.45
21	33	509	CL7	C1B-NB	-2.23	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2B	604	CL7	C3B-C4B	-2.23	1.37	1.42
21	4B	608	CL7	MG-NB	-2.23	2.01	2.05
21	2C	517	CL7	CHC-C4B	2.23	1.44	1.39
23	2B	618	8CT	C22-C21	2.22	1.55	1.50
21	13	504	CL7	MG-NB	-2.22	2.01	2.05
21	43	405	CL7	CHC-C4B	2.22	1.44	1.39
21	13	515	CL7	C1B-C2B	-2.22	1.38	1.43
21	22	512	CL7	C1B-C2B	-2.22	1.38	1.43
23	4A	404	8CT	C22-C21	2.22	1.55	1.50
21	41	405	CL7	CHD-C1D	2.22	1.44	1.39
21	21	403	CL7	C1B-C2B	-2.22	1.38	1.43
21	32	506	CL7	C1C-C2C	-2.22	1.40	1.45
21	13	511	CL7	C3B-C4B	-2.22	1.37	1.42
21	43	412	CL7	C3B-C4B	-2.22	1.37	1.42
21	22	507	CL7	CHC-C4B	2.22	1.44	1.39
21	34	404	CL7	C1C-NC	-2.22	1.35	1.37
23	3A	404	8CT	C22-C21	2.22	1.55	1.50
21	34	416	CL7	OBD-CAD	2.22	1.26	1.22
21	23	416	CL7	CHD-C1D	2.22	1.44	1.39
21	33	515	CL7	CHD-C1D	2.22	1.44	1.39
21	3A	407	CL7	C1C-C2C	-2.22	1.40	1.45
21	11	409	CL7	MG-ND	-2.22	2.01	2.05
21	33	514	CL7	MG-NB	-2.22	2.01	2.05
21	3A	401	CL7	C1B-C2B	-2.22	1.38	1.43
21	23	409	CL7	CHD-C1D	2.22	1.44	1.39
21	2A	407	CL7	C1C-NC	-2.22	1.35	1.37
21	1B	605	CL7	C2A-C1A	2.22	1.54	1.50
21	11	407	CL7	CAB-C3B	2.22	1.49	1.45
21	2B	615	CL7	C1C-C2C	-2.22	1.40	1.45
21	44	413	CL7	C3B-C4B	-2.22	1.37	1.42
21	11	414	CL7	C4C-NC	-2.22	1.35	1.37
21	41	414	CL7	C4C-NC	-2.22	1.35	1.37
21	43	410	CL7	C1B-NB	-2.22	1.35	1.37
21	24	409	CL7	CHC-C4B	2.22	1.44	1.39
21	42	515	CL7	CHD-C1D	2.22	1.44	1.39
21	1B	601	CL7	C3B-C4B	-2.22	1.37	1.42
21	21	418	CL7	C3B-C4B	-2.22	1.37	1.42
21	1B	613	CL7	CHD-C1D	2.22	1.44	1.39
21	4B	603	CL7	CHC-C4B	2.22	1.44	1.39
21	41	409	CL7	CHD-C1D	2.22	1.44	1.39
32	33	525	ZEX	C14-C13	-2.22	1.32	1.35
21	42	510	CL7	MG-NB	-2.22	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1B	614	CL7	CHC-C4B	2.22	1.44	1.39
21	33	512	CL7	CAB-C3B	2.22	1.49	1.45
21	3B	614	CL7	CHC-C4B	2.22	1.44	1.39
21	3B	616	CL7	CAB-C3B	2.22	1.49	1.45
21	22	502	CL7	C1B-C2B	-2.22	1.38	1.43
21	32	517	CL7	MG-NB	-2.22	2.01	2.05
21	24	409	CL7	CHD-C1D	2.22	1.44	1.39
21	34	415	CL7	CAB-C3B	2.22	1.49	1.45
21	44	406	CL7	CAB-C3B	2.22	1.49	1.45
23	3B	619	8CT	C22-C21	2.22	1.55	1.50
21	23	411	CL7	CHC-C4B	2.22	1.44	1.39
21	44	414	CL7	C3B-C4B	-2.22	1.37	1.42
21	11	408	CL7	C4C-NC	-2.22	1.35	1.37
21	41	408	CL7	C4C-NC	-2.22	1.35	1.37
21	1B	616	CL7	CAB-C3B	2.22	1.49	1.45
21	4B	617	CL7	CAB-C3B	2.22	1.49	1.45
21	12	517	CL7	C3B-C4B	-2.22	1.37	1.42
21	32	503	CL7	C3B-C4B	-2.22	1.37	1.42
21	2C	506	CL7	CHD-C1D	2.22	1.44	1.39
21	31	402	CL7	CHD-C1D	2.22	1.44	1.39
32	33	519	ZEX	C10-C9	-2.22	1.32	1.35
21	42	513	CL7	MG-ND	-2.22	2.01	2.05
21	4C	511	CL7	MG-ND	-2.22	2.01	2.05
21	33	518	CL7	CAB-C3B	2.22	1.49	1.45
23	4D	406	8CT	C30-C29	2.22	1.53	1.50
32	42	520	ZEX	C21-C26	-2.22	1.50	1.53
21	2B	611	CL7	C3B-C4B	-2.22	1.37	1.42
21	3B	610	CL7	C3B-C4B	-2.22	1.37	1.42
21	43	411	CL7	C3B-C4B	-2.22	1.37	1.42
21	3C	505	CL7	C1B-NB	-2.21	1.35	1.37
21	12	515	CL7	CHD-C1D	2.21	1.44	1.39
23	4B	620	8CT	C22-C21	2.21	1.55	1.50
21	21	416	CL7	C4C-NC	-2.21	1.35	1.37
21	1C	512	CL7	CAB-C3B	2.21	1.49	1.45
21	23	419	CL7	CAB-C3B	2.21	1.49	1.45
21	4B	602	CL7	CAB-C3B	2.21	1.49	1.45
21	1C	501	CL7	MG-NB	-2.21	2.01	2.05
21	4C	501	CL7	MG-NB	-2.21	2.01	2.05
21	1C	507	CL7	CHC-C4B	2.21	1.44	1.39
21	4C	507	CL7	CHC-C4B	2.21	1.44	1.39
21	2B	603	CL7	C3B-C4B	-2.21	1.37	1.42
21	33	511	CL7	C3B-C4B	-2.21	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1C	512	CL7	MG-NB	-2.21	2.01	2.05
21	4C	512	CL7	MG-NB	-2.21	2.01	2.05
21	43	415	CL7	MG-NB	-2.21	2.01	2.05
21	24	405	CL7	CHD-C1D	2.21	1.44	1.39
21	44	405	CL7	CHD-C1D	2.21	1.44	1.39
21	14	409	CL7	C1C-NC	-2.21	1.35	1.37
21	43	402	CL7	C1C-NC	-2.21	1.35	1.37
21	31	409	CL7	CAB-C3B	2.21	1.49	1.45
21	3D	402	CL7	MG-ND	-2.21	2.01	2.05
21	23	411	CL7	C3B-C4B	-2.21	1.37	1.42
21	3C	512	CL7	CAB-C3B	2.21	1.49	1.45
21	22	506	CL7	CHD-C1D	2.21	1.44	1.39
21	24	413	CL7	C3B-C4B	-2.21	1.37	1.42
21	1B	612	CL7	CHC-C4B	2.21	1.44	1.39
21	3B	603	CL7	C3B-C4B	-2.21	1.37	1.42
21	12	509	CL7	MG-NB	-2.21	2.01	2.05
21	11	419	CL7	C1B-C2B	-2.21	1.38	1.43
21	41	419	CL7	C1B-C2B	-2.21	1.38	1.43
21	21	418	CL7	CHC-C4B	2.21	1.44	1.39
21	32	513	CL7	C3B-C4B	-2.21	1.37	1.42
21	2B	602	CL7	CAB-C3B	2.21	1.49	1.45
21	3B	605	CL7	MG-ND	-2.21	2.01	2.05
21	1B	603	CL7	C1C-C2C	-2.21	1.41	1.45
21	1B	602	CL7	CHC-C4B	2.21	1.44	1.39
21	3B	613	CL7	CHD-C1D	2.21	1.44	1.39
21	3A	407	CL7	MG-ND	-2.21	2.01	2.05
21	22	502	CL7	C1C-C2C	-2.21	1.41	1.45
21	44	416	CL7	OBD-CAD	2.21	1.26	1.22
21	1B	605	CL7	MG-ND	-2.21	2.01	2.05
21	2C	501	CL7	MG-NB	-2.21	2.01	2.05
21	3C	501	CL7	MG-NB	-2.21	2.01	2.05
21	2C	517	CL7	CHD-C1D	2.21	1.44	1.39
21	23	418	CL7	CHD-C1D	2.21	1.44	1.39
21	3C	517	CL7	CHD-C1D	2.21	1.44	1.39
21	2B	612	CL7	CHC-C4B	2.21	1.44	1.39
21	3B	611	CL7	CHC-C4B	2.21	1.44	1.39
21	4B	614	CL7	CHD-C1D	2.21	1.44	1.39
32	32	524	ZEX	C1-C6	-2.21	1.50	1.53
21	13	517	CL7	CHD-C1D	2.21	1.44	1.39
21	14	408	CL7	CHD-C1D	2.21	1.44	1.39
21	2C	504	CL7	MG-ND	-2.21	2.01	2.05
21	3C	504	CL7	MG-ND	-2.21	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	409	CL7	MG-ND	-2.21	2.01	2.05
21	23	411	CL7	C1C-C2C	-2.21	1.41	1.45
21	3B	608	CL7	C1C-C2C	-2.21	1.41	1.45
21	2C	517	CL7	C1B-C2B	-2.21	1.38	1.43
21	3C	517	CL7	C1B-C2B	-2.21	1.38	1.43
21	12	510	CL7	C1C-NC	-2.21	1.35	1.37
21	1C	511	CL7	CHD-C1D	2.21	1.44	1.39
21	31	411	CL7	CHD-C1D	2.21	1.44	1.39
21	2B	616	CL7	MG-NB	-2.21	2.01	2.05
21	13	506	CL7	CAB-C3B	2.21	1.49	1.45
32	14	403	ZEX	C14-C13	-2.21	1.32	1.35
21	23	413	CL7	C1B-NB	-2.21	1.35	1.37
21	24	412	CL7	C1C-NC	-2.21	1.35	1.37
21	11	411	CL7	CHD-C1D	2.21	1.44	1.39
21	33	504	CL7	CHD-C1D	2.21	1.44	1.39
21	41	402	CL7	CHD-C1D	2.21	1.44	1.39
21	41	411	CL7	CHD-C1D	2.21	1.44	1.39
21	21	408	CL7	C4C-NC	-2.21	1.35	1.37
21	4C	505	CL7	C1B-NB	-2.21	1.35	1.37
21	41	409	CL7	MG-ND	-2.21	2.01	2.05
21	13	512	CL7	CAB-C3B	2.21	1.49	1.45
21	3C	507	CL7	CHC-C4B	2.21	1.44	1.39
21	41	414	CL7	OBD-CAD	2.21	1.26	1.22
21	12	503	CL7	CAB-C3B	2.21	1.49	1.45
21	42	503	CL7	CAB-C3B	2.21	1.49	1.45
21	1C	506	CL7	CHD-C1D	2.21	1.44	1.39
21	4C	506	CL7	CHD-C1D	2.21	1.44	1.39
21	11	403	CL7	C3B-C4B	-2.21	1.37	1.42
21	41	403	CL7	C3B-C4B	-2.21	1.37	1.42
21	2C	509	CL7	C1C-NC	-2.21	1.35	1.37
32	12	520	ZEX	C21-C26	-2.21	1.50	1.53
32	12	524	ZEX	C1-C6	-2.21	1.50	1.53
32	42	524	ZEX	C1-C6	-2.21	1.50	1.53
21	11	403	CL7	C1B-C2B	-2.20	1.38	1.43
21	3C	511	CL7	MG-ND	-2.20	2.01	2.05
21	31	420	CL7	C1B-C2B	-2.20	1.38	1.43
21	43	411	CL7	CHC-C4B	2.20	1.44	1.39
21	12	504	CL7	C1C-C2C	-2.20	1.41	1.45
21	2B	613	CL7	C1B-NB	-2.20	1.35	1.37
21	44	411	CL7	C1C-NC	-2.20	1.35	1.37
21	4C	517	CL7	C1B-C2B	-2.20	1.38	1.43
21	14	409	CL7	CHC-C4B	2.20	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4C	509	CL7	CHC-C4B	2.20	1.44	1.39
21	4C	510	CL7	CHD-C1D	2.20	1.44	1.39
21	44	409	CL7	CHC-C4B	2.20	1.44	1.39
21	12	513	CL7	C1B-C2B	-2.20	1.38	1.43
21	2B	606	CL7	C1B-C2B	-2.20	1.38	1.43
21	1B	611	CL7	CHC-C4B	2.20	1.44	1.39
21	4D	404	CL7	CHC-C4B	2.20	1.44	1.39
21	2C	510	CL7	C3B-C4B	-2.20	1.37	1.42
32	32	520	ZEX	C21-C26	-2.20	1.50	1.53
21	1B	603	CL7	C1B-NB	-2.20	1.35	1.37
21	1A	407	CL7	MG-ND	-2.20	2.01	2.05
21	3C	512	CL7	MG-NB	-2.20	2.01	2.05
21	4A	407	CL7	MG-ND	-2.20	2.01	2.05
21	32	513	CL7	C1B-C2B	-2.20	1.38	1.43
21	1B	608	CL7	C1C-C2C	-2.20	1.41	1.45
21	31	416	CL7	CAB-C3B	2.20	1.49	1.45
21	1D	402	CL7	C1B-C2B	-2.20	1.38	1.43
21	42	513	CL7	C1B-C2B	-2.20	1.38	1.43
21	22	513	CL7	MG-ND	-2.20	2.01	2.05
21	12	505	CL7	C1C-C2C	-2.20	1.41	1.45
21	2B	614	CL7	CHD-C1D	2.20	1.44	1.39
21	3C	510	CL7	C3B-C4B	-2.20	1.37	1.42
21	2B	605	CL7	C1C-NC	-2.20	1.35	1.37
21	2B	609	CL7	CHC-C4B	2.20	1.44	1.39
21	23	406	CL7	CHC-C4B	2.20	1.44	1.39
21	33	505	CL7	CHC-C4B	2.20	1.44	1.39
21	1C	508	CL7	C2A-C1A	2.20	1.54	1.50
21	4C	508	CL7	C2A-C1A	2.20	1.54	1.50
21	2C	512	CL7	MG-NB	-2.20	2.01	2.05
21	2B	604	CL7	C1C-C2C	-2.20	1.41	1.45
21	3B	603	CL7	C1C-C2C	-2.20	1.41	1.45
21	3C	508	CL7	C1C-C2C	-2.20	1.41	1.45
21	4D	402	CL7	CAB-C3B	2.20	1.49	1.45
21	1B	605	CL7	C3B-C4B	-2.20	1.37	1.42
21	22	513	CL7	C3B-C4B	-2.20	1.37	1.42
21	12	517	CL7	MG-NB	-2.20	2.01	2.05
21	1D	404	CL7	CHC-C4B	2.20	1.44	1.39
21	42	507	CL7	CHC-C4B	2.20	1.44	1.39
21	2B	606	CL7	C3D-C4D	-2.20	1.33	1.39
21	3B	605	CL7	C3D-C4D	-2.20	1.33	1.39
21	4C	510	CL7	C3B-C4B	-2.20	1.37	1.42
21	13	514	CL7	MG-NB	-2.20	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	516	CL7	C1C-C2C	-2.20	1.41	1.45
21	42	516	CL7	C1C-C2C	-2.20	1.41	1.45
21	2B	603	CL7	CHC-C4B	2.20	1.44	1.39
21	21	403	CL7	C3B-C4B	-2.20	1.37	1.42
21	31	403	CL7	C3B-C4B	-2.20	1.37	1.42
21	42	504	CL7	C1C-C2C	-2.20	1.41	1.45
32	32	524	ZEX	C30-C29	-2.20	1.32	1.35
21	3D	402	CL7	C1B-C2B	-2.20	1.38	1.43
21	42	507	CL7	CBD-CGD	-2.20	1.45	1.52
23	2C	515	8CT	C01-C02	2.20	1.54	1.50
21	11	408	CL7	MG-NB	-2.20	2.01	2.05
21	2B	605	CL7	MG-NB	-2.20	2.01	2.05
21	3B	604	CL7	MG-NB	-2.20	2.01	2.05
21	4B	613	CL7	CHC-C4B	2.20	1.44	1.39
21	2D	404	CL7	CHC-C4B	2.20	1.44	1.39
21	3D	404	CL7	CHC-C4B	2.20	1.44	1.39
23	3C	518	8CT	C38-C31	2.20	1.54	1.50
21	24	416	CL7	OBD-CAD	2.20	1.26	1.22
21	1B	610	CL7	C3B-C4B	-2.20	1.37	1.42
21	14	409	CL7	C1C-C2C	-2.20	1.41	1.45
21	1C	509	CL7	C1C-NC	-2.20	1.35	1.37
21	43	407	CL7	CAB-C3B	2.20	1.49	1.45
21	32	505	CL7	C1C-NC	-2.20	1.35	1.37
21	1C	511	CL7	MG-ND	-2.19	2.01	2.05
21	32	510	CL7	C1C-NC	-2.19	1.35	1.37
21	3B	613	CL7	CBD-CGD	-2.19	1.45	1.52
21	2B	604	CL7	CHD-C1D	2.19	1.44	1.39
21	14	410	CL7	C1C-C2C	-2.19	1.41	1.45
21	32	503	CL7	CAB-C3B	2.19	1.49	1.45
21	43	405	CL7	CHD-C1D	2.19	1.44	1.39
21	2C	505	CL7	CHC-C4B	2.19	1.44	1.39
21	12	509	CL7	C1C-NC	-2.19	1.35	1.37
21	11	417	CL7	C1C-NC	-2.19	1.35	1.37
21	24	414	CL7	C1C-NC	-2.19	1.35	1.37
21	42	509	CL7	C1C-NC	-2.19	1.35	1.37
21	31	408	CL7	MG-NB	-2.19	2.01	2.05
21	22	505	CL7	C1C-C2C	-2.19	1.41	1.45
21	31	403	CL7	C1B-C2B	-2.19	1.38	1.43
21	3B	606	CL7	CAB-C3B	2.19	1.49	1.45
21	2B	617	CL7	CHD-C1D	2.19	1.44	1.39
21	42	517	CL7	MG-NB	-2.19	2.01	2.05
21	31	419	CL7	C1B-C2B	-2.19	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1C	505	CL7	C1B-NB	-2.19	1.35	1.37
21	23	412	CL7	C1C-NC	-2.19	1.35	1.37
21	41	416	CL7	C4C-NC	-2.19	1.35	1.37
21	13	518	CL7	CAB-C3B	2.19	1.49	1.45
21	12	502	CL7	C1C-C2C	-2.19	1.41	1.45
21	44	409	CL7	C1C-C2C	-2.19	1.41	1.45
21	44	410	CL7	C1C-C2C	-2.19	1.41	1.45
21	43	415	CL7	CHD-C1D	2.19	1.44	1.39
21	13	504	CL7	C1C-C2C	-2.19	1.41	1.45
21	43	405	CL7	C1C-C2C	-2.19	1.41	1.45
21	41	420	CL7	C1B-C2B	-2.19	1.38	1.43
21	3B	616	CL7	C1C-NC	-2.19	1.35	1.37
23	4B	618	8CT	C22-C21	2.19	1.55	1.50
21	2B	613	CL7	CHC-C4B	2.19	1.44	1.39
21	42	502	CL7	C1C-C2C	-2.19	1.41	1.45
21	42	508	CL7	CHD-C1D	2.19	1.44	1.39
21	22	507	CL7	C1C-NC	-2.19	1.35	1.37
21	23	405	CL7	C1C-NC	-2.19	1.35	1.37
21	32	507	CL7	C1C-NC	-2.19	1.35	1.37
21	14	412	CL7	C3B-C4B	-2.19	1.37	1.42
21	23	412	CL7	C3B-C4B	-2.19	1.37	1.42
21	3B	605	CL7	C3B-C4B	-2.19	1.37	1.42
21	13	514	CL7	CHD-C1D	2.19	1.44	1.39
21	23	415	CL7	MG-NB	-2.19	2.01	2.05
21	43	406	CL7	CHC-C4B	2.19	1.44	1.39
21	14	406	CL7	CAB-C3B	2.19	1.49	1.45
21	2B	617	CL7	CAB-C3B	2.19	1.49	1.45
21	31	416	CL7	C4C-NC	-2.19	1.35	1.37
21	4B	615	CL7	C1C-NC	-2.19	1.35	1.37
21	4A	407	CL7	MG-NB	-2.19	2.01	2.05
21	13	515	CL7	CHD-C1D	2.19	1.44	1.39
21	21	411	CL7	CHD-C1D	2.19	1.44	1.39
21	33	510	CL7	CHC-C4B	2.19	1.44	1.39
21	34	405	CL7	CHD-C1D	2.19	1.44	1.39
21	1B	604	CL7	MG-NB	-2.19	2.01	2.05
21	4B	605	CL7	MG-NB	-2.19	2.01	2.05
31	2F	101	HEM	C1D-ND	-2.19	1.34	1.38
31	4F	101	HEM	C1D-ND	-2.19	1.34	1.38
21	32	502	CL7	C1C-C2C	-2.19	1.41	1.45
21	42	506	CL7	CHD-C1D	2.19	1.44	1.39
21	1C	501	CL7	C1B-NB	-2.19	1.35	1.37
21	2A	401	CL7	CAB-C3B	2.19	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	22	503	CL7	CAB-C3B	2.19	1.49	1.45
21	3A	401	CL7	CAB-C3B	2.19	1.49	1.45
21	1B	616	CL7	MG-NB	-2.19	2.01	2.05
21	4B	617	CL7	MG-NB	-2.19	2.01	2.05
21	22	510	CL7	C1C-C2C	-2.19	1.41	1.45
21	4B	616	CL7	MG-NB	-2.19	2.01	2.05
21	22	511	CL7	C1B-NB	-2.19	1.35	1.37
21	14	415	CL7	CAB-C3B	2.19	1.49	1.45
21	2B	603	CL7	CAB-C3B	2.19	1.49	1.45
21	2B	606	CL7	MG-ND	-2.19	2.01	2.05
21	23	405	CL7	MG-NB	-2.19	2.01	2.05
21	33	504	CL7	MG-NB	-2.19	2.01	2.05
23	3K	101	8CT	C10-C03	2.19	1.52	1.45
23	1B	617	8CT	C22-C21	2.19	1.55	1.50
21	21	412	CL7	C1B-C2B	-2.19	1.38	1.43
21	31	412	CL7	C1B-C2B	-2.19	1.38	1.43
21	11	402	CL7	CHD-C1D	2.19	1.44	1.39
21	23	415	CL7	CHD-C1D	2.19	1.44	1.39
21	22	504	CL7	C1C-C2C	-2.19	1.41	1.45
21	34	410	CL7	C1C-C2C	-2.19	1.41	1.45
21	2B	606	CL7	C3B-C4B	-2.19	1.37	1.42
21	2B	617	CL7	MG-NB	-2.19	2.01	2.05
21	3B	616	CL7	MG-NB	-2.19	2.01	2.05
21	2B	617	CL7	C1C-NC	-2.19	1.35	1.37
21	23	407	CL7	CAB-C3B	2.19	1.49	1.45
21	23	413	CL7	CAB-C3B	2.19	1.49	1.45
21	33	506	CL7	CAB-C3B	2.19	1.49	1.45
21	4B	608	CL7	C3B-C4B	-2.19	1.37	1.42
21	14	405	CL7	CHD-C1D	2.19	1.44	1.39
21	33	514	CL7	CHD-C1D	2.19	1.44	1.39
21	1B	606	CL7	CAB-C3B	2.19	1.49	1.45
21	4B	607	CL7	CAB-C3B	2.19	1.49	1.45
23	2K	101	8CT	C10-C03	2.18	1.52	1.45
21	2C	508	CL7	C2A-C1A	2.18	1.54	1.50
21	3C	508	CL7	C2A-C1A	2.18	1.54	1.50
21	43	413	CL7	C1C-NC	-2.18	1.35	1.37
21	44	417	CL7	C4C-NC	-2.18	1.35	1.37
21	21	410	CL7	CAB-C3B	2.18	1.49	1.45
21	34	409	CL7	C1C-C2C	-2.18	1.41	1.45
21	23	404	CL7	C1C-NC	-2.18	1.35	1.37
21	33	503	CL7	C1C-NC	-2.18	1.35	1.37
21	4B	623	CL7	C4C-NC	-2.18	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	602	CL7	CAB-C3B	2.18	1.49	1.45
21	1B	616	CL7	CHD-C1D	2.18	1.44	1.39
21	32	517	CL7	C3B-C4B	-2.18	1.37	1.42
21	1B	616	CL7	C1C-NC	-2.18	1.35	1.37
21	14	413	CL7	C1C-NC	-2.18	1.35	1.37
21	23	413	CL7	C1C-NC	-2.18	1.35	1.37
21	4B	617	CL7	C1C-NC	-2.18	1.35	1.37
21	4B	617	CL7	CHD-C1D	2.18	1.44	1.39
21	2B	610	CL7	C1C-C2C	-2.18	1.41	1.45
21	3B	609	CL7	C1C-C2C	-2.18	1.41	1.45
21	1C	508	CL7	C1C-C2C	-2.18	1.41	1.45
21	4C	508	CL7	C1C-C2C	-2.18	1.41	1.45
21	44	412	CL7	C3B-C4B	-2.18	1.37	1.42
21	23	410	CL7	C1B-NB	-2.18	1.35	1.37
21	24	412	CL7	CHD-C1D	2.18	1.44	1.39
21	34	412	CL7	CHD-C1D	2.18	1.44	1.39
21	4B	605	CL7	CHD-C1D	2.18	1.44	1.39
21	2D	402	CL7	CAB-C3B	2.18	1.49	1.45
21	4B	605	CL7	CAB-C3B	2.18	1.49	1.45
21	11	414	CL7	MG-ND	-2.18	2.01	2.05
21	2B	613	CL7	C1C-C2C	-2.18	1.41	1.45
21	3B	612	CL7	C1C-C2C	-2.18	1.41	1.45
21	11	407	CL7	C3B-C4B	-2.18	1.37	1.42
21	3C	503	CL7	MG-NB	-2.18	2.01	2.05
21	4B	613	CL7	C1C-C2C	-2.18	1.41	1.45
21	32	506	CL7	CHD-C1D	2.18	1.44	1.39
21	21	416	CL7	CAB-C3B	2.18	1.49	1.45
23	1B	617	8CT	C39-C16	2.18	1.55	1.50
23	2A	404	8CT	C22-C21	2.18	1.55	1.50
23	4B	618	8CT	C39-C16	2.18	1.55	1.50
21	13	509	CL7	C1B-NB	-2.18	1.35	1.37
21	33	508	CL7	C1B-NB	-2.18	1.35	1.37
21	2B	605	CL7	CAB-C3B	2.18	1.49	1.45
21	32	504	CL7	MG-NB	-2.18	2.01	2.05
21	41	408	CL7	MG-NB	-2.18	2.01	2.05
21	3B	608	CL7	C1B-NB	-2.18	1.35	1.37
21	4C	504	CL7	MG-ND	-2.18	2.01	2.05
21	22	508	CL7	CHD-C1D	2.18	1.44	1.39
21	32	508	CL7	CHD-C1D	2.18	1.44	1.39
21	21	419	CL7	C1B-C2B	-2.18	1.38	1.43
21	13	513	CL7	CHD-C1D	2.18	1.44	1.39
21	14	412	CL7	CHD-C1D	2.18	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	412	CL7	CHD-C1D	2.18	1.44	1.39
23	3B	617	8CT	C22-C21	2.18	1.55	1.50
21	4B	608	CL7	C1C-NC	-2.18	1.35	1.37
21	21	407	CL7	C3B-C4B	-2.18	1.37	1.42
21	31	414	CL7	MG-ND	-2.18	2.01	2.05
21	12	506	CL7	MG-NB	-2.18	2.01	2.05
21	42	506	CL7	MG-NB	-2.18	2.01	2.05
21	4D	402	CL7	C1B-C2B	-2.18	1.38	1.43
21	4B	602	CL7	CHD-C1D	2.18	1.44	1.39
21	1C	504	CL7	CAB-C3B	2.18	1.49	1.45
21	4C	504	CL7	CAB-C3B	2.18	1.49	1.45
21	1B	609	CL7	C1C-C2C	-2.18	1.41	1.45
21	42	510	CL7	C1C-C2C	-2.18	1.41	1.45
21	2C	502	CL7	C3B-C4B	-2.18	1.37	1.42
21	3B	607	CL7	C3B-C4B	-2.18	1.37	1.42
21	21	402	CL7	CHD-C1D	2.18	1.44	1.39
32	22	524	ZEX	C1-C6	-2.18	1.50	1.53
21	1B	602	CL7	CAB-C3B	2.18	1.49	1.45
21	1B	612	CL7	C1C-C2C	-2.18	1.41	1.45
21	12	508	CL7	CHD-C1D	2.18	1.44	1.39
21	1A	401	CL7	CAB-C3B	2.18	1.49	1.45
21	4A	401	CL7	CAB-C3B	2.18	1.49	1.45
21	41	420	CL7	CHD-C1D	2.18	1.44	1.39
21	2C	511	CL7	MG-ND	-2.18	2.01	2.05
21	24	404	CL7	CHD-C1D	2.18	1.44	1.39
23	4C	518	8CT	C38-C31	2.18	1.54	1.50
21	43	410	CL7	C3D-C4D	-2.18	1.34	1.39
21	22	502	CL7	CAB-C3B	2.18	1.49	1.45
21	2C	501	CL7	C1C-NC	-2.18	1.35	1.37
23	3C	515	8CT	C01-C02	2.17	1.54	1.50
21	13	511	CL7	C1C-NC	-2.17	1.35	1.37
21	22	515	CL7	C3B-C4B	-2.17	1.37	1.42
21	23	414	CL7	CHD-C1D	2.17	1.44	1.39
21	33	513	CL7	CHD-C1D	2.17	1.44	1.39
21	4B	603	CL7	CAB-C3B	2.17	1.49	1.45
21	4B	606	CL7	C3D-C4D	-2.17	1.34	1.39
21	2D	402	CL7	C1B-C2B	-2.17	1.38	1.43
21	42	513	CL7	C3B-C4B	-2.17	1.37	1.42
21	32	511	CL7	CHD-C1D	2.17	1.44	1.39
21	4B	609	CL7	C1C-C2C	-2.17	1.41	1.45
21	11	412	CL7	C1B-C2B	-2.17	1.38	1.43
21	41	412	CL7	C1B-C2B	-2.17	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	32	506	CL7	MG-NB	-2.17	2.01	2.05
21	1B	605	CL7	C3D-C4D	-2.17	1.34	1.39
21	12	505	CL7	C3D-C4D	-2.17	1.34	1.39
21	11	420	CL7	C1B-C2B	-2.17	1.38	1.43
21	3C	504	CL7	C3B-C4B	-2.17	1.37	1.42
21	2C	503	CL7	MG-NB	-2.17	2.01	2.05
21	12	518	CL7	CHD-C1D	2.17	1.44	1.39
21	4B	614	CL7	CBD-CGD	-2.17	1.45	1.52
21	11	416	CL7	C4C-NC	-2.17	1.35	1.37
21	13	503	CL7	C1C-NC	-2.17	1.35	1.37
21	24	409	CL7	C1C-C2C	-2.17	1.41	1.45
21	34	414	CL7	MG-NB	-2.17	2.01	2.05
21	4B	611	CL7	C3B-C4B	-2.17	1.37	1.42
21	2B	602	CL7	CHD-C1D	2.17	1.44	1.39
21	3B	603	CL7	C1B-NB	-2.17	1.35	1.37
21	43	409	CL7	C1B-NB	-2.17	1.35	1.37
21	21	413	CL7	CHD-C1D	2.17	1.44	1.39
21	21	408	CL7	MG-NB	-2.17	2.01	2.05
21	13	510	CL7	C1C-C2C	-2.17	1.41	1.45
21	43	411	CL7	C1C-C2C	-2.17	1.41	1.45
21	43	414	CL7	CHD-C1D	2.17	1.44	1.39
21	3C	504	CL7	CAB-C3B	2.17	1.49	1.45
21	42	515	CL7	C3B-C4B	-2.17	1.37	1.42
21	23	413	CL7	MG-NB	-2.17	2.01	2.05
21	41	410	CL7	CAB-C3B	2.17	1.49	1.45
21	14	411	CL7	C1C-NC	-2.17	1.35	1.37
21	14	414	CL7	C1B-NB	-2.17	1.35	1.37
21	3C	501	CL7	C1C-NC	-2.17	1.35	1.37
21	2B	607	CL7	CAB-C3B	2.17	1.49	1.45
21	24	408	CL7	CHD-C1D	2.17	1.44	1.39
21	2B	623	CL7	C4C-NC	-2.17	1.35	1.37
21	12	515	CL7	C3B-C4B	-2.17	1.37	1.42
21	34	412	CL7	C3B-C4B	-2.17	1.37	1.42
21	42	510	CL7	C3B-C4B	-2.17	1.37	1.42
21	42	509	CL7	MG-NB	-2.17	2.01	2.05
21	21	420	CL7	C1B-C2B	-2.17	1.38	1.43
21	3B	601	CL7	CHD-C1D	2.17	1.44	1.39
21	41	413	CL7	CHD-C1D	2.17	1.44	1.39
21	32	510	CL7	C1C-C2C	-2.17	1.41	1.45
21	22	510	CL7	C3B-C4B	-2.17	1.37	1.42
21	2C	504	CL7	CAB-C3B	2.17	1.49	1.45
21	11	414	CL7	OBD-CAD	2.17	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	606	CL7	MG-ND	-2.17	2.01	2.05
21	43	405	CL7	MG-NB	-2.17	2.01	2.05
21	1C	505	CL7	CHD-C1D	2.16	1.44	1.39
21	21	420	CL7	CHD-C1D	2.16	1.44	1.39
21	2C	501	CL7	C1B-NB	-2.16	1.35	1.37
21	22	509	CL7	C1C-NC	-2.16	1.35	1.37
21	3C	501	CL7	C1B-NB	-2.16	1.35	1.37
21	32	509	CL7	C1C-NC	-2.16	1.35	1.37
21	42	510	CL7	C1C-NC	-2.16	1.35	1.37
21	41	415	CL7	C3A-C2A	2.16	1.56	1.54
21	2B	609	CL7	C1C-C2C	-2.16	1.41	1.45
21	3D	405	CL7	C1C-C2C	-2.16	1.41	1.45
21	11	416	CL7	C1B-C2B	-2.16	1.38	1.43
21	41	416	CL7	C1B-C2B	-2.16	1.38	1.43
21	24	417	CL7	MG-NB	-2.16	2.01	2.05
21	2C	507	CL7	CHC-C4B	2.16	1.44	1.39
21	42	518	CL7	CHD-C1D	2.16	1.44	1.39
21	11	416	CL7	CAB-C3B	2.16	1.49	1.45
21	41	416	CL7	CAB-C3B	2.16	1.49	1.45
21	1B	604	CL7	C1C-NC	-2.16	1.35	1.37
21	4B	605	CL7	C1C-NC	-2.16	1.35	1.37
21	32	513	CL7	MG-ND	-2.16	2.01	2.05
21	41	414	CL7	MG-ND	-2.16	2.01	2.05
23	1C	515	8CT	C01-C02	2.16	1.54	1.50
23	4C	515	8CT	C01-C02	2.16	1.54	1.50
21	1B	604	CL7	CAB-C3B	2.16	1.49	1.45
21	1C	505	CL7	CHC-C4B	2.16	1.44	1.39
21	4C	505	CL7	CHC-C4B	2.16	1.44	1.39
21	3B	616	CL7	CHD-C1D	2.16	1.44	1.39
21	24	413	CL7	C1C-NC	-2.16	1.35	1.37
21	34	417	CL7	C4C-NC	-2.16	1.35	1.37
21	22	517	CL7	MG-NB	-2.16	2.01	2.05
21	1D	405	CL7	C1C-C2C	-2.16	1.41	1.45
21	22	516	CL7	C1C-C2C	-2.16	1.41	1.45
21	4D	405	CL7	C1C-C2C	-2.16	1.41	1.45
21	1C	502	CL7	C3B-C4B	-2.16	1.37	1.42
21	4C	502	CL7	C3B-C4B	-2.16	1.37	1.42
21	3C	505	CL7	CHD-C1D	2.16	1.44	1.39
21	43	402	CL7	CHD-C1D	2.16	1.44	1.39
21	1B	613	CL7	CBD-CGD	-2.16	1.45	1.52
21	2C	504	CL7	C3B-C4B	-2.16	1.37	1.42
21	2D	405	CL7	C1C-NC	-2.16	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	404	CL7	C1B-NB	-2.16	1.35	1.37
21	34	413	CL7	C1C-NC	-2.16	1.35	1.37
21	31	413	CL7	CHD-C1D	2.16	1.44	1.39
21	3B	604	CL7	CAB-C3B	2.16	1.49	1.45
21	1B	603	CL7	CHD-C1D	2.16	1.44	1.39
21	1C	504	CL7	C3B-C4B	-2.16	1.37	1.42
21	4C	504	CL7	C3B-C4B	-2.16	1.37	1.42
32	13	525	ZEX	C10-C9	-2.16	1.32	1.35
21	2B	611	CL7	C1B-NB	-2.16	1.35	1.37
23	2K	101	8CT	C39-C16	2.16	1.55	1.50
21	2C	517	CL7	C1C-C2C	-2.16	1.41	1.45
21	2C	509	CL7	CBD-CGD	-2.16	1.45	1.52
32	24	403	ZEX	C14-C13	-2.16	1.32	1.35
32	34	403	ZEX	C14-C13	-2.16	1.32	1.35
21	1B	615	CL7	MG-NB	-2.16	2.01	2.05
21	1C	513	CL7	MG-ND	-2.16	2.01	2.05
21	32	505	CL7	C1C-C2C	-2.16	1.41	1.45
21	23	406	CL7	C1B-NB	-2.16	1.35	1.37
21	22	506	CL7	MG-NB	-2.16	2.01	2.05
21	14	404	CL7	CHD-C1D	2.16	1.44	1.39
21	43	418	CL7	C1C-C2C	-2.16	1.41	1.45
21	44	405	CL7	C3B-C4B	-2.16	1.37	1.42
21	1D	402	CL7	CAB-C3B	2.16	1.49	1.45
21	13	505	CL7	CHC-C4B	2.16	1.44	1.39
21	1B	614	CL7	C1C-NC	-2.16	1.35	1.37
21	22	502	CL7	C1C-NC	-2.16	1.35	1.37
21	33	505	CL7	C1B-NB	-2.16	1.35	1.37
21	23	414	CL7	MG-NB	-2.16	2.01	2.05
21	33	513	CL7	MG-NB	-2.16	2.01	2.05
21	3C	505	CL7	CHC-C4B	2.16	1.44	1.39
21	21	414	CL7	OBD-CAD	2.16	1.26	1.22
21	31	414	CL7	OBD-CAD	2.16	1.26	1.22
21	33	517	CL7	C1C-C2C	-2.15	1.41	1.45
21	1B	602	CL7	CHD-C1D	2.15	1.44	1.39
21	2B	605	CL7	CHD-C1D	2.15	1.44	1.39
21	3B	604	CL7	CHD-C1D	2.15	1.44	1.39
21	4D	402	CL7	OBD-CAD	2.15	1.26	1.22
21	34	405	CL7	C3B-C4B	-2.15	1.37	1.42
21	11	420	CL7	MG-ND	-2.15	2.01	2.05
21	34	407	CL7	CAB-C3B	2.15	1.49	1.45
21	2B	614	CL7	CBD-CGD	-2.15	1.45	1.52
21	11	419	CL7	OBD-CAD	2.15	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	419	CL7	OBD-CAD	2.15	1.26	1.22
21	13	512	CL7	MG-NB	-2.15	2.01	2.05
21	24	414	CL7	MG-NB	-2.15	2.01	2.05
21	3B	615	CL7	MG-NB	-2.15	2.01	2.05
21	43	413	CL7	MG-NB	-2.15	2.01	2.05
21	31	410	CL7	CAB-C3B	2.15	1.49	1.45
21	21	412	CL7	CHD-C1D	2.15	1.44	1.39
21	23	405	CL7	CHD-C1D	2.15	1.44	1.39
21	42	505	CL7	C1C-NC	-2.15	1.35	1.37
21	11	405	CL7	CAB-C3B	2.15	1.49	1.45
21	33	509	CL7	C3D-C4D	-2.15	1.34	1.39
21	44	407	CL7	CAB-C3B	2.15	1.49	1.45
21	1C	503	CL7	MG-NB	-2.15	2.01	2.05
21	13	513	CL7	MG-NB	-2.15	2.01	2.05
21	4C	503	CL7	MG-NB	-2.15	2.01	2.05
21	1C	501	CL7	C1C-NC	-2.15	1.35	1.37
21	4C	501	CL7	C1C-NC	-2.15	1.35	1.37
21	1B	604	CL7	CHD-C1D	2.15	1.44	1.39
21	22	518	CL7	CHD-C1D	2.15	1.44	1.39
21	3B	603	CL7	CHD-C1D	2.15	1.44	1.39
21	3C	509	CL7	CHD-C1D	2.15	1.44	1.39
21	41	411	CL7	MG-NB	-2.15	2.01	2.05
21	41	407	CL7	C3B-C4B	-2.15	1.37	1.42
21	2A	407	CL7	MG-ND	-2.15	2.01	2.05
21	43	404	CL7	C1C-NC	-2.15	1.35	1.37
21	44	409	CL7	C1C-NC	-2.15	1.35	1.37
32	43	401	ZEX	C10-C9	-2.15	1.32	1.35
21	41	420	CL7	MG-ND	-2.15	2.01	2.05
21	12	511	CL7	CHD-C1D	2.15	1.44	1.39
21	13	504	CL7	CHD-C1D	2.15	1.44	1.39
21	3B	622	CL7	C4C-NC	-2.15	1.35	1.37
21	21	414	CL7	MG-ND	-2.15	2.01	2.05
31	1F	101	HEM	C1D-ND	-2.15	1.34	1.38
21	11	413	CL7	CHD-C1D	2.15	1.44	1.39
21	2B	610	CL7	C3B-C4B	-2.15	1.37	1.42
21	3B	609	CL7	C3B-C4B	-2.15	1.37	1.42
21	12	513	CL7	MG-ND	-2.15	2.01	2.05
21	42	508	CL7	CHC-C4B	2.15	1.44	1.39
23	4K	101	8CT	C39-C16	2.15	1.55	1.50
21	23	409	CL7	C1B-NB	-2.15	1.35	1.37
21	32	515	CL7	C1B-C2B	-2.15	1.38	1.43
21	31	407	CL7	C3B-C4B	-2.15	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2B	618	8CT	C39-C16	2.15	1.55	1.50
23	3B	617	8CT	C39-C16	2.15	1.55	1.50
21	43	402	CL7	CAB-C3B	2.15	1.49	1.45
21	1B	607	CL7	C3B-C4B	-2.15	1.37	1.42
21	42	511	CL7	CHD-C1D	2.15	1.44	1.39
21	21	416	CL7	C1B-C2B	-2.15	1.38	1.43
21	31	416	CL7	C1B-C2B	-2.15	1.38	1.43
21	32	502	CL7	CAB-C3B	2.15	1.49	1.45
21	1C	509	CL7	CHD-C1D	2.15	1.44	1.39
21	4C	509	CL7	CHD-C1D	2.15	1.44	1.39
21	4C	509	CL7	C1B-NB	-2.15	1.35	1.37
21	42	502	CL7	CAB-C3B	2.15	1.49	1.45
21	13	517	CL7	C1C-C2C	-2.15	1.41	1.45
21	12	515	CL7	C1B-C2B	-2.15	1.38	1.43
21	42	515	CL7	C1B-C2B	-2.15	1.38	1.43
21	11	412	CL7	MG-ND	-2.14	2.01	2.05
21	41	412	CL7	MG-ND	-2.14	2.01	2.05
21	12	515	CL7	OBD-CAD	2.14	1.26	1.22
21	21	420	CL7	MG-ND	-2.14	2.01	2.05
21	31	420	CL7	MG-ND	-2.14	2.01	2.05
21	24	411	CL7	C3B-C4B	-2.14	1.37	1.42
21	2A	403	CL7	CHD-C1D	2.14	1.44	1.39
21	22	511	CL7	CHD-C1D	2.14	1.44	1.39
23	1K	101	8CT	C39-C16	2.14	1.55	1.50
21	2C	505	CL7	CHD-C1D	2.14	1.44	1.39
21	3C	508	CL7	CHD-C1D	2.14	1.44	1.39
21	44	408	CL7	CHD-C1D	2.14	1.44	1.39
23	1K	101	8CT	C10-C03	2.14	1.52	1.45
23	4K	101	8CT	C10-C03	2.14	1.52	1.45
21	32	511	CL7	CAB-C3B	2.14	1.49	1.45
21	34	417	CL7	MG-NB	-2.14	2.01	2.05
31	3F	101	HEM	C1D-ND	-2.14	1.34	1.38
21	3B	604	CL7	C1C-NC	-2.14	1.35	1.37
21	32	515	CL7	C3B-C4B	-2.14	1.37	1.42
21	43	409	CL7	CHC-C4B	2.14	1.44	1.39
21	41	414	CL7	C1B-C2B	-2.14	1.38	1.43
21	13	505	CL7	C1B-NB	-2.14	1.35	1.37
21	1B	611	CL7	CHD-C1D	2.14	1.44	1.39
21	1B	614	CL7	CHD-C1D	2.14	1.44	1.39
21	23	406	CL7	C1C-C2C	-2.14	1.41	1.45
21	1B	622	CL7	C4C-NC	-2.14	1.35	1.37
21	14	404	CL7	C1B-NB	-2.14	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	32	504	CL7	C1B-NB	-2.14	1.35	1.37
21	44	404	CL7	C1B-NB	-2.14	1.35	1.37
21	22	509	CL7	C1C-C2C	-2.14	1.41	1.45
21	31	420	CL7	CHD-C1D	2.14	1.44	1.39
21	34	413	CL7	CAB-C3B	2.14	1.49	1.45
21	1C	507	CL7	C1C-NC	-2.14	1.35	1.37
21	23	418	CL7	C1C-C2C	-2.14	1.41	1.45
32	32	522	ZEX	C34-C33	-2.14	1.32	1.35
32	44	403	ZEX	C34-C33	-2.14	1.32	1.35
21	14	414	CL7	MG-NB	-2.14	2.01	2.05
21	44	414	CL7	MG-NB	-2.14	2.01	2.05
23	2B	618	8CT	C30-C29	2.14	1.53	1.50
21	23	410	CL7	C3D-C4D	-2.14	1.34	1.39
21	3B	612	CL7	C1B-NB	-2.14	1.35	1.37
21	42	511	CL7	C1B-NB	-2.14	1.35	1.37
21	2B	602	CL7	C1B-C2B	-2.14	1.38	1.43
21	3B	601	CL7	C1B-C2B	-2.14	1.38	1.43
21	2B	614	CL7	C1C-C2C	-2.14	1.41	1.45
21	3B	613	CL7	C1C-C2C	-2.14	1.41	1.45
21	21	411	CL7	MG-NB	-2.14	2.01	2.05
21	11	410	CL7	CAB-C3B	2.14	1.49	1.45
21	2B	608	CL7	C3B-C4B	-2.14	1.37	1.42
21	22	509	CL7	CHD-C1D	2.14	1.44	1.39
21	32	509	CL7	CHD-C1D	2.14	1.44	1.39
21	2B	604	CL7	C1B-NB	-2.14	1.35	1.37
21	2B	609	CL7	C1C-NC	-2.14	1.35	1.37
21	32	506	CL7	C1B-NB	-2.14	1.35	1.37
21	44	415	CL7	MG-NB	-2.14	2.01	2.05
21	4C	509	CL7	CBD-CGD	-2.14	1.45	1.52
21	4B	604	CL7	CHD-C1D	2.14	1.44	1.39
21	2C	508	CL7	C1C-C2C	-2.14	1.41	1.45
21	33	505	CL7	C1C-C2C	-2.14	1.41	1.45
25	21	423	SQD	O8-S	2.14	1.55	1.47
21	2B	608	CL7	C1C-NC	-2.14	1.35	1.37
21	3B	607	CL7	C1C-NC	-2.14	1.35	1.37
21	24	408	CL7	CAB-C3B	2.14	1.49	1.45
32	22	522	ZEX	C34-C33	-2.14	1.32	1.35
21	1B	614	CL7	MG-NB	-2.14	2.01	2.05
21	4B	615	CL7	MG-NB	-2.14	2.01	2.05
21	1B	601	CL7	CHD-C1D	2.14	1.44	1.39
21	12	514	CL7	C1B-NB	-2.14	1.35	1.37
21	32	514	CL7	C1B-NB	-2.14	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	24	417	CL7	CAB-C3B	2.14	1.49	1.45
21	21	419	CL7	OBD-CAD	2.14	1.26	1.22
21	31	419	CL7	OBD-CAD	2.14	1.26	1.22
21	34	409	CL7	C1C-NC	-2.14	1.35	1.37
21	1C	509	CL7	C3D-C4D	-2.14	1.34	1.39
21	22	505	CL7	C3D-C4D	-2.14	1.34	1.39
21	12	504	CL7	MG-NB	-2.14	2.01	2.05
21	34	411	CL7	C3B-C4B	-2.14	1.37	1.42
21	12	511	CL7	CAB-C3B	2.13	1.49	1.45
21	42	511	CL7	CAB-C3B	2.13	1.49	1.45
21	2C	513	CL7	MG-ND	-2.13	2.01	2.05
21	3C	513	CL7	MG-ND	-2.13	2.01	2.05
21	1A	403	CL7	CHD-C1D	2.13	1.44	1.39
21	34	404	CL7	CHD-C1D	2.13	1.44	1.39
21	21	414	CL7	C1B-C2B	-2.13	1.38	1.43
21	44	404	CL7	CHD-C1D	2.13	1.44	1.39
21	22	515	CL7	C1B-C2B	-2.13	1.38	1.43
21	3C	502	CL7	C3B-C4B	-2.13	1.37	1.42
21	33	504	CL7	C3B-C4B	-2.13	1.37	1.42
21	4B	604	CL7	C1B-NB	-2.13	1.35	1.37
21	2B	615	CL7	CHD-C1D	2.13	1.44	1.39
21	1B	609	CL7	C3B-C4B	-2.13	1.37	1.42
21	4B	610	CL7	C3B-C4B	-2.13	1.37	1.42
21	2B	611	CL7	CAB-C3B	2.13	1.49	1.45
21	21	412	CL7	MG-ND	-2.13	2.01	2.05
21	13	504	CL7	C3B-C4B	-2.13	1.37	1.42
21	22	511	CL7	CAB-C3B	2.13	1.49	1.45
21	4B	602	CL7	C1B-C2B	-2.13	1.38	1.43
21	11	420	CL7	CHD-C1D	2.13	1.44	1.39
21	43	414	CL7	MG-NB	-2.13	2.01	2.05
21	41	409	CL7	OBD-CAD	2.13	1.26	1.22
21	21	405	CL7	CAB-C3B	2.13	1.49	1.45
21	12	511	CL7	C1B-NB	-2.13	1.35	1.37
21	11	415	CL7	C4C-NC	-2.13	1.35	1.37
21	41	415	CL7	C4C-NC	-2.13	1.35	1.37
21	4B	610	CL7	C1C-C2C	-2.13	1.41	1.45
21	2C	505	CL7	CBD-CGD	-2.13	1.45	1.52
21	3C	505	CL7	CBD-CGD	-2.13	1.45	1.52
21	33	512	CL7	MG-NB	-2.13	2.01	2.05
21	44	417	CL7	MG-NB	-2.13	2.01	2.05
21	32	504	CL7	C1C-NC	-2.13	1.35	1.37
21	42	505	CL7	C1C-C2C	-2.13	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	415	CL7	MG-NB	-2.13	2.01	2.05
21	43	419	CL7	CAB-C3B	2.13	1.49	1.45
21	1B	613	CL7	C1C-C2C	-2.13	1.41	1.45
21	4B	614	CL7	C1C-C2C	-2.13	1.41	1.45
21	4C	509	CL7	C3D-C4D	-2.13	1.34	1.39
21	13	501	CL7	CHD-C1D	2.13	1.44	1.39
23	2C	518	8CT	C22-C21	2.13	1.55	1.50
21	44	406	CL7	C3B-C4B	-2.13	1.37	1.42
21	12	502	CL7	C1C-NC	-2.13	1.35	1.37
21	42	502	CL7	C1C-NC	-2.13	1.35	1.37
21	21	409	CL7	OBD-CAD	2.13	1.26	1.22
21	31	409	CL7	OBD-CAD	2.13	1.26	1.22
21	13	505	CL7	C1C-C2C	-2.13	1.41	1.45
21	43	406	CL7	C1C-C2C	-2.13	1.41	1.45
21	1B	611	CL7	CBD-CGD	-2.13	1.45	1.52
21	21	415	CL7	C4C-NC	-2.13	1.35	1.37
21	31	415	CL7	C4C-NC	-2.13	1.35	1.37
23	4B	601	8CT	C39-C16	2.13	1.55	1.50
21	33	501	CL7	C1C-C2C	-2.13	1.41	1.45
21	34	417	CL7	C3B-C4B	-2.13	1.37	1.42
21	1D	402	CL7	OBD-CAD	2.13	1.26	1.22
21	3D	402	CL7	OBD-CAD	2.13	1.26	1.22
21	1B	612	CL7	C1B-NB	-2.13	1.35	1.37
21	4B	613	CL7	C1B-NB	-2.13	1.35	1.37
21	23	414	CL7	C1C-C2C	-2.13	1.41	1.45
21	33	513	CL7	C1C-C2C	-2.13	1.41	1.45
21	14	405	CL7	C3B-C4B	-2.13	1.37	1.42
21	24	417	CL7	C3B-C4B	-2.13	1.37	1.42
25	11	423	SQD	O8-S	2.13	1.55	1.47
21	23	409	CL7	CHC-C4B	2.13	1.44	1.39
21	14	411	CL7	C3B-C4B	-2.13	1.37	1.42
21	13	513	CL7	C1C-C2C	-2.13	1.41	1.45
21	41	417	CL7	C1C-NC	-2.13	1.35	1.37
21	34	408	CL7	CHD-C1D	2.13	1.44	1.39
21	13	509	CL7	C3D-C4D	-2.13	1.34	1.39
23	1B	617	8CT	C38-C31	2.13	1.54	1.50
21	33	506	CL7	CHC-C4B	2.13	1.44	1.39
21	44	415	CL7	CBD-CGD	-2.13	1.45	1.52
32	33	525	ZEX	C10-C9	-2.13	1.33	1.35
21	31	406	CL7	CAB-C3B	2.13	1.49	1.45
21	42	505	CL7	C3D-C4D	-2.13	1.34	1.39
21	12	509	CL7	C1C-C2C	-2.13	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	509	CL7	C1C-C2C	-2.13	1.41	1.45
23	3B	617	8CT	C30-C29	2.13	1.53	1.50
21	14	417	CL7	C3B-C4B	-2.13	1.37	1.42
21	2B	603	CL7	CHD-C1D	2.13	1.44	1.39
21	3B	602	CL7	CHD-C1D	2.13	1.44	1.39
21	3C	517	CL7	C1C-C2C	-2.13	1.41	1.45
21	23	402	CL7	CHD-C1D	2.13	1.44	1.39
21	41	411	CL7	C3B-C4B	-2.12	1.37	1.42
21	2C	509	CL7	CHD-C1D	2.12	1.44	1.39
21	4C	505	CL7	CHD-C1D	2.12	1.44	1.39
21	42	504	CL7	MG-NB	-2.12	2.01	2.05
21	41	408	CL7	C1C-C2C	-2.12	1.41	1.45
23	1B	617	8CT	C30-C29	2.12	1.53	1.50
23	4B	618	8CT	C30-C29	2.12	1.53	1.50
21	32	505	CL7	C3D-C4D	-2.12	1.34	1.39
21	11	405	CL7	C3B-C4B	-2.12	1.37	1.42
21	41	405	CL7	C3B-C4B	-2.12	1.37	1.42
21	31	412	CL7	CHD-C1D	2.12	1.44	1.39
21	4B	603	CL7	CHD-C1D	2.12	1.44	1.39
21	1B	610	CL7	CAB-C3B	2.12	1.49	1.45
21	4B	611	CL7	CAB-C3B	2.12	1.49	1.45
21	12	516	CL7	C3B-C4B	-2.12	1.37	1.42
21	32	510	CL7	C3B-C4B	-2.12	1.37	1.42
21	31	411	CL7	C3B-C4B	-2.12	1.37	1.42
23	1B	619	8CT	C38-C31	2.12	1.54	1.50
23	4B	620	8CT	C38-C31	2.12	1.54	1.50
21	11	406	CL7	C1C-C2C	-2.12	1.41	1.45
21	24	405	CL7	C3B-C4B	-2.12	1.37	1.42
21	31	403	CL7	C1C-NC	-2.12	1.35	1.37
21	31	405	CL7	CAB-C3B	2.12	1.49	1.45
21	24	408	CL7	C3B-C4B	-2.12	1.37	1.42
21	34	408	CL7	C3B-C4B	-2.12	1.37	1.42
21	3B	609	CL7	C3D-C4D	-2.12	1.34	1.39
21	2B	610	CL7	C3D-C4D	-2.12	1.34	1.39
21	42	510	CL7	CHD-C1D	2.12	1.44	1.39
21	31	411	CL7	MG-NB	-2.12	2.01	2.05
25	4B	621	SQD	O8-S	2.12	1.55	1.47
21	21	408	CL7	C1C-C2C	-2.12	1.41	1.45
21	2B	615	CL7	MG-NB	-2.12	2.01	2.05
21	3B	614	CL7	MG-NB	-2.12	2.01	2.05
21	22	515	CL7	OBD-CAD	2.12	1.26	1.22
21	32	515	CL7	OBD-CAD	2.12	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1C	509	CL7	CBD-CGD	-2.12	1.45	1.52
21	13	508	CL7	CHC-C4B	2.12	1.44	1.39
21	43	407	CL7	CHC-C4B	2.12	1.44	1.39
32	34	420	ZEX	C10-C9	-2.12	1.33	1.35
21	2C	509	CL7	C3D-C4D	-2.12	1.34	1.39
21	41	405	CL7	CAB-C3B	2.12	1.49	1.45
21	31	405	CL7	C3B-C4B	-2.12	1.37	1.42
21	12	508	CL7	CHC-C4B	2.12	1.44	1.39
21	13	507	CL7	CBD-CGD	-2.12	1.45	1.52
21	23	408	CL7	CBD-CGD	-2.12	1.45	1.52
21	33	507	CL7	CBD-CGD	-2.12	1.45	1.52
21	2C	505	CL7	C1C-NC	-2.12	1.35	1.37
21	22	505	CL7	C1C-NC	-2.12	1.35	1.37
21	14	413	CL7	CAB-C3B	2.12	1.49	1.45
21	44	413	CL7	CAB-C3B	2.12	1.49	1.45
21	11	411	CL7	C3B-C4B	-2.12	1.37	1.42
32	24	403	ZEX	C34-C33	-2.12	1.33	1.35
21	3A	403	CL7	CBD-CGD	-2.12	1.45	1.52
21	2C	505	CL7	C1B-NB	-2.12	1.35	1.37
21	24	414	CL7	C1B-NB	-2.12	1.35	1.37
21	4C	511	CL7	OBD-CAD	2.12	1.26	1.22
21	34	408	CL7	CBD-CGD	-2.12	1.45	1.52
21	4C	505	CL7	CBD-CGD	-2.12	1.45	1.52
21	34	408	CL7	CAB-C3B	2.12	1.49	1.45
21	4B	606	CL7	CAB-C3B	2.12	1.49	1.45
21	24	405	CL7	C1C-NC	-2.12	1.35	1.37
21	11	412	CL7	C3B-C4B	-2.12	1.37	1.42
21	22	504	CL7	MG-NB	-2.12	2.01	2.05
21	12	510	CL7	C3B-C4B	-2.12	1.37	1.42
21	24	406	CL7	C3B-C4B	-2.12	1.37	1.42
21	23	402	CL7	CAB-C3B	2.12	1.49	1.45
21	33	501	CL7	CAB-C3B	2.12	1.49	1.45
21	1C	508	CL7	CHD-C1D	2.12	1.44	1.39
21	11	412	CL7	CHD-C1D	2.12	1.44	1.39
21	41	412	CL7	CHD-C1D	2.12	1.44	1.39
21	33	514	CL7	C1C-C2C	-2.12	1.41	1.45
21	2B	623	CL7	MG-NB	-2.12	2.01	2.05
21	3B	622	CL7	MG-NB	-2.12	2.01	2.05
32	12	522	ZEX	C34-C33	-2.12	1.33	1.35
32	44	403	ZEX	C14-C13	-2.12	1.33	1.35
21	1C	517	CL7	C1C-C2C	-2.12	1.41	1.45
21	4C	517	CL7	C1C-C2C	-2.12	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2B	612	CL7	CBD-CGD	-2.12	1.45	1.52
21	13	501	CL7	CAB-C3B	2.12	1.49	1.45
21	3B	614	CL7	CHD-C1D	2.12	1.44	1.39
32	22	524	ZEX	C30-C29	-2.12	1.33	1.35
32	23	401	ZEX	C10-C9	-2.12	1.33	1.35
21	32	518	CL7	CHD-C1D	2.12	1.44	1.39
21	14	408	CL7	CAB-C3B	2.12	1.49	1.45
21	1C	511	CL7	CAB-C3B	2.11	1.49	1.45
21	4C	511	CL7	CAB-C3B	2.11	1.49	1.45
21	2B	609	CL7	CAB-C3B	2.11	1.49	1.45
21	3C	509	CL7	C3D-C4D	-2.11	1.34	1.39
21	13	501	CL7	C1C-C2C	-2.11	1.41	1.45
21	14	415	CL7	MG-NB	-2.11	2.01	2.05
21	2B	609	CL7	C1B-NB	-2.11	1.35	1.37
25	41	423	SQD	O8-S	2.11	1.55	1.47
21	3C	509	CL7	CBD-CGD	-2.11	1.45	1.52
21	33	501	CL7	CHD-C1D	2.11	1.44	1.39
21	44	417	CL7	C3B-C4B	-2.11	1.37	1.42
21	34	415	CL7	CHD-C1D	2.11	1.44	1.39
21	21	406	CL7	C1C-C2C	-2.11	1.41	1.45
21	31	412	CL7	MG-ND	-2.11	2.01	2.05
21	34	417	CL7	CAB-C3B	2.11	1.49	1.45
25	31	423	SQD	O8-S	2.11	1.55	1.47
21	3A	403	CL7	CHD-C1D	2.11	1.44	1.39
21	1C	505	CL7	CBD-CGD	-2.11	1.45	1.52
21	2B	616	CL7	CAB-C3B	2.11	1.49	1.45
21	3B	615	CL7	CAB-C3B	2.11	1.49	1.45
21	11	414	CL7	C1B-C2B	-2.11	1.38	1.43
21	3B	603	CL7	C1C-NC	-2.11	1.35	1.37
21	23	403	CL7	C1C-C2C	-2.11	1.41	1.45
21	4A	403	CL7	CHD-C1D	2.11	1.44	1.39
21	11	405	CL7	MG-NB	-2.11	2.01	2.05
21	4C	513	CL7	MG-ND	-2.11	2.01	2.05
21	1C	507	CL7	C1B-NB	-2.11	1.35	1.37
21	21	417	CL7	C1C-NC	-2.11	1.35	1.37
21	32	502	CL7	C1C-NC	-2.11	1.35	1.37
21	42	504	CL7	C1C-NC	-2.11	1.35	1.37
23	3B	617	8CT	C38-C31	2.11	1.54	1.50
21	42	516	CL7	CAB-C3B	2.11	1.49	1.45
32	22	520	ZEX	C1-C6	-2.11	1.50	1.53
21	2A	407	CL7	CHD-C1D	2.11	1.44	1.39
21	1B	608	CL7	C1B-NB	-2.11	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	12	504	CL7	C1C-NC	-2.11	1.35	1.37
21	24	409	CL7	C1C-NC	-2.11	1.35	1.37
23	4B	601	8CT	C10-C03	2.11	1.52	1.45
21	31	408	CL7	C1C-C2C	-2.11	1.41	1.45
21	1A	407	CL7	CHD-C1D	2.11	1.44	1.39
21	12	504	CL7	C1B-NB	-2.11	1.35	1.37
21	4C	501	CL7	C1B-NB	-2.11	1.35	1.37
21	44	414	CL7	C1B-NB	-2.11	1.35	1.37
21	14	415	CL7	CHD-C1D	2.11	1.44	1.39
21	22	508	CL7	CHC-C4B	2.11	1.44	1.39
21	32	508	CL7	CHC-C4B	2.11	1.44	1.39
21	4B	610	CL7	C3D-C4D	-2.11	1.34	1.39
21	14	417	CL7	CAB-C3B	2.11	1.49	1.45
21	44	417	CL7	CAB-C3B	2.11	1.49	1.45
21	32	511	CL7	C1B-NB	-2.11	1.35	1.37
21	1C	511	CL7	OBD-CAD	2.11	1.26	1.22
21	2C	511	CL7	OBD-CAD	2.11	1.26	1.22
21	4A	407	CL7	CHD-C1D	2.11	1.44	1.39
21	11	411	CL7	MG-NB	-2.11	2.01	2.05
21	3C	508	CL7	C1C-NC	-2.11	1.35	1.37
21	3C	509	CL7	C1B-NB	-2.11	1.35	1.37
21	11	409	CL7	OBD-CAD	2.11	1.26	1.22
21	2C	511	CL7	CAB-C3B	2.11	1.49	1.45
21	3C	511	CL7	CAB-C3B	2.11	1.49	1.45
23	1B	626	8CT	C39-C16	2.11	1.55	1.50
21	44	411	CL7	C3B-C4B	-2.11	1.37	1.42
21	22	510	CL7	CHD-C1D	2.11	1.44	1.39
21	32	510	CL7	CHD-C1D	2.11	1.44	1.39
21	31	405	CL7	MG-NB	-2.11	2.01	2.05
21	14	407	CL7	CAB-C3B	2.11	1.49	1.45
21	24	413	CL7	CAB-C3B	2.11	1.49	1.45
32	43	423	ZEX	C30-C29	-2.11	1.33	1.35
21	14	408	CL7	C3B-C4B	-2.11	1.37	1.42
21	21	405	CL7	C3B-C4B	-2.11	1.37	1.42
21	1C	505	CL7	C1C-NC	-2.11	1.35	1.37
21	32	508	CL7	C1C-NC	-2.11	1.35	1.37
21	4C	505	CL7	C1C-NC	-2.11	1.35	1.37
25	1B	620	SQD	O8-S	2.11	1.55	1.47
21	3B	611	CL7	CBD-CGD	-2.11	1.45	1.52
21	44	408	CL7	CBD-CGD	-2.11	1.45	1.52
21	24	407	CL7	CAB-C3B	2.11	1.49	1.45
21	3C	513	CL7	CAB-C3B	2.11	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	22	504	CL7	C1B-NB	-2.11	1.35	1.37
21	4C	506	CL7	C1B-NB	-2.11	1.35	1.37
21	44	413	CL7	C1C-NC	-2.11	1.35	1.37
21	22	516	CL7	C3B-C4B	-2.11	1.37	1.42
21	32	516	CL7	C3B-C4B	-2.11	1.37	1.42
23	2B	618	8CT	C38-C31	2.11	1.54	1.50
23	2B	620	8CT	C38-C31	2.11	1.54	1.50
23	3B	626	8CT	C10-C03	2.11	1.52	1.45
21	14	414	CL7	C1C-NC	-2.11	1.35	1.37
21	3C	505	CL7	C1C-NC	-2.11	1.35	1.37
21	44	414	CL7	C1C-NC	-2.11	1.35	1.37
21	21	411	CL7	C3B-C4B	-2.10	1.37	1.42
21	41	413	CL7	C3B-C4B	-2.10	1.37	1.42
21	23	407	CL7	CHC-C4B	2.10	1.44	1.39
21	21	413	CL7	C3B-C4B	-2.10	1.37	1.42
21	31	413	CL7	C3B-C4B	-2.10	1.37	1.42
32	12	524	ZEX	C30-C29	-2.10	1.33	1.35
32	42	524	ZEX	C30-C29	-2.10	1.33	1.35
21	1C	509	CL7	C1B-NB	-2.10	1.35	1.37
21	14	405	CL7	C1C-C2C	-2.10	1.41	1.45
21	44	405	CL7	C1C-C2C	-2.10	1.41	1.45
21	14	408	CL7	CBD-CGD	-2.10	1.45	1.52
21	1C	513	CL7	OBD-CAD	2.10	1.26	1.22
23	3B	619	8CT	C38-C31	2.10	1.54	1.50
21	41	406	CL7	CAB-C3B	2.10	1.49	1.45
21	24	408	CL7	CBD-CGD	-2.10	1.45	1.52
21	34	417	CL7	CHD-C1D	2.10	1.44	1.39
21	3B	610	CL7	CAB-C3B	2.10	1.49	1.45
21	42	515	CL7	MG-NB	-2.10	2.01	2.05
21	43	415	CL7	C1C-C2C	-2.10	1.41	1.45
25	2B	621	SQD	O8-S	2.10	1.55	1.47
21	2C	507	CL7	C1C-NC	-2.10	1.35	1.37
21	4B	609	CL7	CAB-C3B	2.10	1.49	1.45
21	41	413	CL7	OBD-CAD	2.10	1.26	1.22
21	3A	407	CL7	CHD-C1D	2.10	1.44	1.39
21	44	407	CL7	C3B-C4B	-2.10	1.37	1.42
21	4B	623	CL7	MG-NB	-2.10	2.01	2.05
23	2B	601	8CT	C39-C16	2.10	1.55	1.50
23	3B	626	8CT	C39-C16	2.10	1.55	1.50
21	22	506	CL7	C1B-NB	-2.10	1.35	1.37
32	14	403	ZEX	C1-C6	-2.10	1.50	1.53
21	42	516	CL7	C3B-C4B	-2.10	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	21	407	CL7	C1C-C2C	-2.10	1.41	1.45
21	44	416	CL7	C3B-C4B	-2.10	1.37	1.42
21	1C	511	CL7	MG-NB	-2.10	2.01	2.05
21	43	413	CL7	C1C-C2C	-2.10	1.41	1.45
21	4B	615	CL7	CHD-C1D	2.10	1.44	1.39
32	13	519	ZEX	C30-C29	-2.10	1.33	1.35
21	14	406	CL7	C3B-C4B	-2.10	1.37	1.42
21	12	510	CL7	CHD-C1D	2.10	1.44	1.39
21	44	410	CL7	CAB-C3B	2.10	1.49	1.45
21	2D	402	CL7	OBD-CAD	2.10	1.26	1.22
21	21	413	CL7	OBD-CAD	2.10	1.26	1.22
21	12	505	CL7	C1C-NC	-2.10	1.35	1.37
21	43	414	CL7	C1C-C2C	-2.10	1.41	1.45
21	12	509	CL7	CHD-C1D	2.10	1.44	1.39
21	42	509	CL7	CHD-C1D	2.10	1.44	1.39
21	34	410	CL7	CAB-C3B	2.10	1.49	1.45
21	2C	511	CL7	MG-NB	-2.10	2.01	2.05
21	3C	511	CL7	MG-NB	-2.10	2.01	2.05
21	24	405	CL7	C1C-C2C	-2.10	1.41	1.45
25	1A	406	SQD	O8-S	2.10	1.55	1.47
21	4B	608	CL7	C1B-NB	-2.10	1.35	1.37
21	42	504	CL7	C1B-NB	-2.10	1.35	1.37
23	4B	618	8CT	C38-C31	2.10	1.54	1.50
21	3B	605	CL7	CHD-C1D	2.10	1.44	1.39
21	2B	606	CL7	CAB-C3B	2.10	1.49	1.45
21	12	506	CL7	C1B-NB	-2.10	1.35	1.37
21	2B	603	CL7	C1C-NC	-2.10	1.35	1.37
21	3B	602	CL7	C1C-NC	-2.10	1.35	1.37
25	3B	620	SQD	O8-S	2.10	1.55	1.47
21	12	501	CL7	CHD-C1D	2.10	1.44	1.39
21	4C	513	CL7	CAB-C3B	2.10	1.49	1.45
21	21	405	CL7	MG-NB	-2.10	2.01	2.05
21	42	506	CL7	CAB-C3B	2.10	1.49	1.45
21	34	415	CL7	CBD-CGD	-2.10	1.45	1.52
21	13	506	CL7	CHC-C4B	2.10	1.44	1.39
21	12	510	CL7	C1B-NB	-2.10	1.35	1.37
21	3C	506	CL7	C1B-NB	-2.10	1.35	1.37
21	1B	615	CL7	CAB-C3B	2.10	1.49	1.45
21	43	408	CL7	CBD-CGD	-2.10	1.45	1.52
21	12	509	CL7	C3D-C4D	-2.10	1.34	1.39
21	11	403	CL7	C1C-NC	-2.10	1.35	1.37
21	13	508	CL7	C1B-NB	-2.10	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4B	609	CL7	C1B-NB	-2.10	1.35	1.37
21	41	403	CL7	C1C-NC	-2.10	1.35	1.37
23	2B	601	8CT	C10-C03	2.10	1.52	1.45
21	11	413	CL7	C3B-C4B	-2.10	1.37	1.42
21	44	408	CL7	C3B-C4B	-2.10	1.37	1.42
32	22	520	ZEX	C30-C29	-2.10	1.33	1.35
32	24	420	ZEX	C10-C9	-2.10	1.33	1.35
23	4B	601	8CT	C28-C29	2.10	1.37	1.32
21	2B	607	CL7	C3B-C4B	-2.10	1.37	1.42
21	24	416	CL7	C3B-C4B	-2.10	1.37	1.42
21	34	416	CL7	C3B-C4B	-2.10	1.37	1.42
21	3C	511	CL7	OBD-CAD	2.09	1.26	1.22
21	1B	622	CL7	MG-NB	-2.09	2.01	2.05
21	32	515	CL7	MG-NB	-2.09	2.01	2.05
21	1A	403	CL7	CBD-CGD	-2.09	1.45	1.52
21	4A	403	CL7	CBD-CGD	-2.09	1.45	1.52
23	3K	101	8CT	C39-C16	2.09	1.55	1.50
21	1B	603	CL7	C1C-NC	-2.09	1.35	1.37
21	44	415	CL7	CHD-C1D	2.09	1.44	1.39
21	44	408	CL7	CAB-C3B	2.09	1.49	1.45
32	42	522	ZEX	C34-C33	-2.09	1.33	1.35
21	31	417	CL7	C1C-NC	-2.09	1.35	1.37
21	12	502	CL7	CAB-C3B	2.09	1.49	1.45
21	4C	507	CL7	CBD-CGD	-2.09	1.45	1.52
21	41	419	CL7	MG-NB	-2.09	2.01	2.05
21	13	514	CL7	C1C-C2C	-2.09	1.41	1.45
21	2C	509	CL7	C1C-C2C	-2.09	1.41	1.45
21	34	406	CL7	C3B-C4B	-2.09	1.38	1.42
21	31	405	CL7	C1B-NB	-2.09	1.35	1.37
21	43	414	CL7	C1C-NC	-2.09	1.35	1.37
21	42	515	CL7	OBD-CAD	2.09	1.26	1.22
21	4B	616	CL7	CAB-C3B	2.09	1.49	1.45
21	22	501	CL7	C1C-C2C	-2.09	1.41	1.45
21	23	402	CL7	C1C-C2C	-2.09	1.41	1.45
21	2B	612	CL7	CHD-C1D	2.09	1.44	1.39
21	3B	611	CL7	CHD-C1D	2.09	1.44	1.39
21	24	410	CL7	CAB-C3B	2.09	1.49	1.45
21	43	405	CL7	C3B-C4B	-2.09	1.38	1.42
21	1B	601	CL7	C1B-C2B	-2.09	1.38	1.43
23	4C	518	8CT	C22-C21	2.09	1.55	1.50
21	1B	605	CL7	CHD-C1D	2.09	1.44	1.39
21	4B	606	CL7	CHD-C1D	2.09	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4A	406	SQD	O8-S	2.09	1.55	1.47
21	41	405	CL7	MG-NB	-2.09	2.01	2.05
21	42	509	CL7	C3D-C4D	-2.09	1.34	1.39
21	12	502	CL7	CHD-C1D	2.09	1.44	1.39
21	14	407	CL7	CHD-C1D	2.09	1.44	1.39
21	43	409	CL7	C1C-NC	-2.09	1.35	1.37
21	43	403	CL7	C1C-C2C	-2.09	1.41	1.45
21	41	406	CL7	C1C-C2C	-2.09	1.41	1.45
21	12	516	CL7	CAB-C3B	2.09	1.49	1.45
21	32	516	CL7	CAB-C3B	2.09	1.49	1.45
21	2A	403	CL7	CBD-CGD	-2.09	1.45	1.52
21	1B	609	CL7	C3D-C4D	-2.09	1.34	1.39
21	4C	513	CL7	OBD-CAD	2.09	1.26	1.22
21	32	508	CL7	C1B-NB	-2.09	1.35	1.37
21	4C	507	CL7	C1C-NC	-2.09	1.35	1.37
21	24	410	CL7	CHD-C1D	2.09	1.44	1.39
21	14	417	CL7	MG-NB	-2.09	2.01	2.05
21	4B	612	CL7	CBD-CGD	-2.09	1.45	1.52
32	24	403	ZEX	C1-C6	-2.09	1.50	1.53
32	34	403	ZEX	C1-C6	-2.09	1.50	1.53
21	33	508	CL7	CHC-C4B	2.09	1.44	1.39
21	11	407	CL7	C1C-C2C	-2.09	1.41	1.45
21	22	517	CL7	C1B-NB	-2.09	1.35	1.37
32	33	519	ZEX	C30-C29	-2.09	1.33	1.35
21	3A	407	CL7	C3D-C4D	-2.09	1.34	1.39
25	2A	406	SQD	O8-S	2.09	1.55	1.47
25	3A	406	SQD	O8-S	2.09	1.55	1.47
21	32	503	CL7	C1C-C2C	-2.09	1.41	1.45
21	41	412	CL7	C3B-C4B	-2.09	1.38	1.42
21	1A	407	CL7	C3D-C4D	-2.09	1.34	1.39
21	31	404	CL7	MG-NB	-2.09	2.01	2.05
21	14	407	CL7	C3B-C4B	-2.09	1.38	1.42
21	24	407	CL7	C3B-C4B	-2.09	1.38	1.42
21	34	407	CL7	C3B-C4B	-2.09	1.38	1.42
21	22	501	CL7	MG-NB	-2.09	2.01	2.05
21	32	501	CL7	MG-NB	-2.09	2.01	2.05
23	3C	518	8CT	C22-C21	2.09	1.55	1.50
21	2C	508	CL7	CHD-C1D	2.09	1.44	1.39
23	1B	626	8CT	C10-C03	2.09	1.52	1.45
21	24	415	CL7	MG-NB	-2.09	2.01	2.05
21	1C	508	CL7	C1C-NC	-2.09	1.35	1.37
21	2C	504	CL7	C1B-NB	-2.09	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4C	508	CL7	C1C-NC	-2.09	1.35	1.37
31	4F	101	HEM	C3C-C4C	-2.09	1.42	1.46
21	21	403	CL7	CHD-C1D	2.09	1.44	1.39
21	1B	605	CL7	CAB-C3B	2.09	1.49	1.45
21	24	415	CL7	CBD-CGD	-2.09	1.45	1.52
21	41	418	CL7	CHD-C1D	2.09	1.44	1.39
21	32	509	CL7	C1C-C2C	-2.08	1.41	1.45
21	41	407	CL7	C1C-C2C	-2.08	1.41	1.45
21	24	417	CL7	C4C-NC	-2.08	1.35	1.37
21	3C	505	CL7	C3D-C4D	-2.08	1.34	1.39
21	21	419	CL7	MG-NB	-2.08	2.01	2.05
21	31	419	CL7	MG-NB	-2.08	2.01	2.05
21	24	404	CL7	C1B-NB	-2.08	1.35	1.37
21	42	506	CL7	C1B-NB	-2.08	1.35	1.37
21	42	508	CL7	C1B-NB	-2.08	1.35	1.37
21	4C	504	CL7	MG-NB	-2.08	2.01	2.05
21	1B	607	CL7	C1C-C2C	-2.08	1.41	1.45
21	34	414	CL7	C1C-C2C	-2.08	1.41	1.45
21	4B	608	CL7	C1C-C2C	-2.08	1.41	1.45
21	11	406	CL7	CAB-C3B	2.08	1.49	1.45
21	2C	508	CL7	C1C-NC	-2.08	1.35	1.37
21	31	412	CL7	C3B-C4B	-2.08	1.38	1.42
21	11	413	CL7	OBD-CAD	2.08	1.26	1.22
21	2C	502	CL7	CBD-CGD	-2.08	1.45	1.52
23	1C	514	8CT	C39-C16	2.08	1.55	1.50
21	11	403	CL7	CHD-C1D	2.08	1.44	1.39
21	3C	504	CL7	OBD-CAD	2.08	1.26	1.22
21	1C	507	CL7	CHD-C1D	2.08	1.44	1.39
21	14	410	CL7	CHD-C1D	2.08	1.44	1.39
21	4C	507	CL7	CHD-C1D	2.08	1.44	1.39
21	44	410	CL7	CHD-C1D	2.08	1.44	1.39
21	2C	513	CL7	CAB-C3B	2.08	1.49	1.45
21	11	405	CL7	C1C-C2C	-2.08	1.41	1.45
21	22	501	CL7	CHD-C1D	2.08	1.44	1.39
21	32	501	CL7	CHD-C1D	2.08	1.44	1.39
21	22	503	CL7	C1B-NB	-2.08	1.35	1.37
21	21	404	CL7	C4C-NC	-2.08	1.35	1.37
21	31	404	CL7	C4C-NC	-2.08	1.35	1.37
21	1C	502	CL7	CBD-CGD	-2.08	1.45	1.52
21	4C	502	CL7	CBD-CGD	-2.08	1.45	1.52
21	31	416	CL7	MG-ND	-2.08	2.01	2.05
21	12	515	CL7	CAB-C3B	2.08	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	42	515	CL7	CAB-C3B	2.08	1.49	1.45
21	3B	616	CL7	CBD-CGD	-2.08	1.45	1.52
21	24	415	CL7	C1B-NB	-2.08	1.35	1.37
21	4C	503	CL7	C1C-NC	-2.08	1.35	1.37
21	4B	623	CL7	OBD-CAD	2.08	1.26	1.22
21	2C	507	CL7	CHD-C1D	2.08	1.44	1.39
21	3C	507	CL7	CHD-C1D	2.08	1.44	1.39
21	11	415	CL7	C3A-C2A	2.08	1.56	1.54
21	34	414	CL7	C1B-NB	-2.08	1.35	1.37
21	22	515	CL7	CAB-C3B	2.08	1.49	1.45
21	4C	501	CL7	CAB-C3B	2.08	1.49	1.45
21	33	513	CL7	CBD-CGD	-2.08	1.45	1.52
21	2C	513	CL7	OBD-CAD	2.08	1.26	1.22
21	3C	513	CL7	OBD-CAD	2.08	1.26	1.22
21	31	414	CL7	C1B-C2B	-2.08	1.38	1.43
21	3C	509	CL7	C1C-C2C	-2.08	1.41	1.45
21	31	415	CL7	C3A-C2A	2.08	1.56	1.54
21	34	414	CL7	C1C-NC	-2.08	1.35	1.37
21	2C	506	CL7	MG-NB	-2.08	2.01	2.05
21	42	509	CL7	CBD-CGD	-2.08	1.45	1.52
21	42	501	CL7	CHD-C1D	2.08	1.44	1.39
21	23	405	CL7	C3B-C4B	-2.08	1.38	1.42
21	1B	622	CL7	OBD-CAD	2.08	1.26	1.22
32	14	420	ZEX	C10-C9	-2.08	1.33	1.35
32	44	420	ZEX	C10-C9	-2.08	1.33	1.35
21	22	506	CL7	CAB-C3B	2.08	1.49	1.45
21	32	506	CL7	CAB-C3B	2.08	1.49	1.45
21	14	415	CL7	CBD-CGD	-2.08	1.45	1.52
21	13	502	CL7	C1C-C2C	-2.08	1.41	1.45
21	41	405	CL7	C1C-C2C	-2.08	1.41	1.45
21	43	402	CL7	C1C-C2C	-2.08	1.41	1.45
21	1B	607	CL7	C1B-NB	-2.08	1.35	1.37
21	22	510	CL7	C1B-NB	-2.08	1.35	1.37
21	32	510	CL7	C1B-NB	-2.08	1.35	1.37
23	2C	514	8CT	C39-C16	2.08	1.55	1.50
21	3C	510	CL7	MG-NB	-2.08	2.01	2.05
21	11	408	CL7	C1C-C2C	-2.08	1.41	1.45
23	2B	601	8CT	C28-C29	2.08	1.37	1.32
23	1C	518	8CT	C22-C21	2.08	1.55	1.50
21	1B	606	CL7	C3B-C4B	-2.08	1.38	1.42
21	4B	607	CL7	C3B-C4B	-2.08	1.38	1.42
21	2C	507	CL7	CBD-CGD	-2.08	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3B	608	CL7	CAB-C3B	2.08	1.49	1.45
21	2C	517	CL7	MG-NB	-2.08	2.01	2.05
21	31	406	CL7	C1C-C2C	-2.08	1.41	1.45
21	31	407	CL7	C1C-C2C	-2.08	1.41	1.45
32	42	519	ZEX	C10-C9	-2.08	1.33	1.35
21	22	515	CL7	MG-NB	-2.08	2.01	2.05
21	2A	407	CL7	C3D-C4D	-2.08	1.34	1.39
21	21	407	CL7	MG-NB	-2.08	2.01	2.05
21	31	407	CL7	MG-NB	-2.08	2.01	2.05
21	3B	609	CL7	C1C-NC	-2.07	1.35	1.37
21	4B	612	CL7	CHD-C1D	2.07	1.44	1.39
21	4C	508	CL7	CHD-C1D	2.07	1.44	1.39
21	13	516	CL7	MG-NB	-2.07	2.01	2.05
21	21	411	CL7	OBD-CAD	2.07	1.26	1.22
21	12	515	CL7	MG-NB	-2.07	2.01	2.05
21	33	502	CL7	C1C-C2C	-2.07	1.41	1.45
21	24	417	CL7	CHD-C1D	2.07	1.44	1.39
21	14	417	CL7	C4C-NC	-2.07	1.35	1.37
21	2B	604	CL7	C1C-NC	-2.07	1.35	1.37
21	4C	511	CL7	MG-NB	-2.07	2.01	2.05
21	42	501	CL7	MG-NB	-2.07	2.01	2.05
21	14	410	CL7	CAB-C3B	2.07	1.49	1.45
21	23	415	CL7	C1C-C2C	-2.07	1.41	1.45
21	44	407	CL7	CHD-C1D	2.07	1.44	1.39
31	2F	101	HEM	C3C-C4C	-2.07	1.42	1.46
21	14	414	CL7	C1C-C2C	-2.07	1.41	1.45
21	44	414	CL7	C1C-C2C	-2.07	1.41	1.45
21	14	408	CL7	C1C-NC	-2.07	1.35	1.37
21	2C	503	CL7	C1C-NC	-2.07	1.35	1.37
21	22	504	CL7	C1C-NC	-2.07	1.35	1.37
21	11	416	CL7	MG-ND	-2.07	2.01	2.05
21	41	416	CL7	MG-ND	-2.07	2.01	2.05
21	21	406	CL7	CHD-C1D	2.07	1.44	1.39
21	1B	616	CL7	CBD-CGD	-2.07	1.45	1.52
21	4B	617	CL7	CBD-CGD	-2.07	1.45	1.52
32	34	403	ZEX	C34-C33	-2.07	1.33	1.35
21	11	410	CL7	OBD-CAD	2.07	1.26	1.22
21	41	410	CL7	OBD-CAD	2.07	1.26	1.22
21	24	415	CL7	CHD-C1D	2.07	1.44	1.39
21	2D	404	CL7	C1C-NC	-2.07	1.35	1.37
21	3B	608	CL7	C1C-NC	-2.07	1.35	1.37
21	34	409	CL7	C1B-C2B	-2.07	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3C	514	8CT	C39-C16	2.07	1.55	1.50
22	1D	408	PHO	C3A-C2A	-2.07	1.52	1.54
21	44	415	CL7	OBD-CAD	2.07	1.26	1.22
21	1B	607	CL7	C1C-NC	-2.07	1.35	1.37
21	21	418	CL7	CHD-C1D	2.07	1.44	1.39
21	1D	404	CL7	CAB-C3B	2.07	1.49	1.45
21	22	501	CL7	CAB-C3B	2.07	1.49	1.45
21	31	413	CL7	OBD-CAD	2.07	1.26	1.22
21	3B	608	CL7	C3D-C4D	-2.07	1.34	1.39
21	42	505	CL7	CAB-C3B	2.07	1.49	1.45
21	3B	606	CL7	C3B-C4B	-2.07	1.38	1.42
21	11	404	CL7	C4C-NC	-2.07	1.35	1.37
21	22	516	CL7	C1B-NB	-2.07	1.35	1.37
21	32	516	CL7	C1B-NB	-2.07	1.35	1.37
21	41	404	CL7	C4C-NC	-2.07	1.35	1.37
21	32	501	CL7	C1C-C2C	-2.07	1.41	1.45
21	1B	612	CL7	C3D-C4D	-2.07	1.34	1.39
21	13	512	CL7	CHD-C1D	2.07	1.44	1.39
21	13	513	CL7	CBD-CGD	-2.07	1.45	1.52
32	32	520	ZEX	C1-C6	-2.07	1.50	1.53
21	24	414	CL7	CAB-C3B	2.07	1.49	1.45
21	32	517	CL7	C1B-NB	-2.07	1.35	1.37
32	14	403	ZEX	C34-C33	-2.07	1.33	1.35
21	2C	505	CL7	C3D-C4D	-2.07	1.34	1.39
21	13	510	CL7	C1B-NB	-2.07	1.35	1.37
21	22	508	CL7	C1B-NB	-2.07	1.35	1.37
21	22	508	CL7	C1C-NC	-2.07	1.35	1.37
21	22	514	CL7	C1B-NB	-2.07	1.35	1.37
21	42	510	CL7	C1B-NB	-2.07	1.35	1.37
21	43	411	CL7	C1B-NB	-2.07	1.35	1.37
22	4D	408	PHO	C3A-C2A	-2.07	1.52	1.54
21	12	516	CL7	C1B-NB	-2.07	1.35	1.37
21	33	506	CL7	C1B-NB	-2.07	1.35	1.37
21	2B	608	CL7	C1C-C2C	-2.07	1.41	1.45
21	3B	607	CL7	C1C-C2C	-2.07	1.41	1.45
32	12	520	ZEX	C30-C29	-2.07	1.33	1.35
32	42	520	ZEX	C30-C29	-2.07	1.33	1.35
21	43	417	CL7	C3D-C4D	-2.07	1.34	1.39
21	42	514	CL7	C1B-NB	-2.07	1.35	1.37
21	12	503	CL7	C1C-C2C	-2.07	1.41	1.45
21	24	408	CL7	C1C-C2C	-2.07	1.41	1.45
21	34	405	CL7	C1C-C2C	-2.07	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	44	415	CL7	C1C-C2C	-2.07	1.41	1.45
21	4B	614	CL7	C3D-C4D	-2.07	1.34	1.39
21	11	418	CL7	CHD-C1D	2.07	1.44	1.39
21	4B	617	CL7	C1C-C2C	-2.07	1.41	1.45
21	21	409	CL7	C3B-C4B	-2.07	1.38	1.42
21	21	410	CL7	C3B-C4B	-2.07	1.38	1.42
21	22	509	CL7	C3D-C4D	-2.07	1.34	1.39
21	32	509	CL7	C3D-C4D	-2.07	1.34	1.39
21	4B	609	CL7	C3D-C4D	-2.07	1.34	1.39
21	1B	608	CL7	CAB-C3B	2.07	1.49	1.45
23	3B	626	8CT	C28-C29	2.06	1.37	1.32
21	4B	613	CL7	CHD-C1D	2.06	1.44	1.39
21	21	417	CL7	C3B-C4B	-2.06	1.38	1.42
23	1B	617	8CT	C10-C03	2.06	1.52	1.45
21	12	508	CL7	C1B-NB	-2.06	1.35	1.37
21	14	416	CL7	C3B-C4B	-2.06	1.38	1.42
21	31	410	CL7	C3B-C4B	-2.06	1.38	1.42
21	3D	404	CL7	CHD-C1D	2.06	1.44	1.39
21	2C	509	CL7	C1B-NB	-2.06	1.35	1.37
21	23	411	CL7	C1B-NB	-2.06	1.35	1.37
21	3B	610	CL7	C1B-NB	-2.06	1.35	1.37
21	12	506	CL7	CAB-C3B	2.06	1.49	1.45
21	3C	502	CL7	CBD-CGD	-2.06	1.46	1.52
21	1B	614	CL7	C1B-NB	-2.06	1.35	1.37
21	4B	615	CL7	C1B-NB	-2.06	1.35	1.37
21	21	406	CL7	CAB-C3B	2.06	1.49	1.45
21	32	515	CL7	CAB-C3B	2.06	1.49	1.45
21	21	403	CL7	C1C-NC	-2.06	1.35	1.37
21	21	405	CL7	C1C-C2C	-2.06	1.41	1.45
23	3B	617	8CT	C10-C03	2.06	1.52	1.45
21	1C	513	CL7	CAB-C3B	2.06	1.49	1.45
21	24	409	CL7	CBD-CGD	-2.06	1.46	1.52
21	4B	616	CL7	CBD-CGD	-2.06	1.46	1.52
21	43	414	CL7	CBD-CGD	-2.06	1.46	1.52
21	44	413	CL7	C1C-C2C	-2.06	1.41	1.45
21	1C	506	CL7	C1B-NB	-2.06	1.35	1.37
25	32	523	SQD	O8-S	2.06	1.54	1.47
21	11	404	CL7	MG-NB	-2.06	2.01	2.05
21	41	404	CL7	MG-NB	-2.06	2.01	2.05
21	22	502	CL7	CHD-C1D	2.06	1.44	1.39
21	11	411	CL7	OBD-CAD	2.06	1.26	1.22
21	11	420	CL7	OBD-CAD	2.06	1.26	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	411	CL7	OBD-CAD	2.06	1.26	1.22
21	1B	616	CL7	C3B-C4B	-2.06	1.38	1.42
21	31	402	CL7	C1C-C2C	-2.06	1.41	1.45
32	23	420	ZEX	C34-C33	-2.06	1.33	1.35
21	21	406	CL7	OBD-CAD	2.06	1.26	1.22
21	31	406	CL7	OBD-CAD	2.06	1.26	1.22
23	4C	514	8CT	C39-C16	2.06	1.55	1.50
21	23	413	CL7	C1C-C2C	-2.06	1.41	1.45
21	33	512	CL7	C1C-C2C	-2.06	1.41	1.45
21	41	410	CL7	C3B-C4B	-2.06	1.38	1.42
21	1B	608	CL7	C1C-NC	-2.06	1.35	1.37
21	2D	405	CL7	C1B-NB	-2.06	1.35	1.37
21	3D	405	CL7	C1B-NB	-2.06	1.35	1.37
21	4B	609	CL7	C1C-NC	-2.06	1.35	1.37
21	1C	517	CL7	MG-NB	-2.06	2.01	2.05
21	23	417	CL7	C3D-C4D	-2.06	1.34	1.39
21	33	516	CL7	C3D-C4D	-2.06	1.34	1.39
21	34	409	CL7	CBD-CGD	-2.06	1.46	1.52
22	2D	408	PHO	C3A-C2A	-2.06	1.52	1.54
21	31	409	CL7	C3B-C4B	-2.06	1.38	1.42
21	22	505	CL7	CAB-C3B	2.06	1.49	1.45
21	13	516	CL7	C3D-C4D	-2.06	1.34	1.39
21	12	509	CL7	CBD-CGD	-2.06	1.46	1.52
21	2C	512	CL7	CHD-C1D	2.06	1.44	1.39
21	4C	509	CL7	C1C-C2C	-2.06	1.41	1.45
21	4B	603	CL7	C1C-NC	-2.06	1.35	1.37
32	13	522	ZEX	C30-C29	-2.06	1.33	1.35
21	3C	504	CL7	MG-NB	-2.06	2.01	2.05
21	31	412	CL7	OBD-CAD	2.06	1.26	1.22
21	31	403	CL7	MG-NB	-2.06	2.01	2.05
22	3D	408	PHO	C3A-C2A	-2.06	1.52	1.54
21	1B	602	CL7	C1C-NC	-2.06	1.35	1.37
21	1C	512	CL7	C1B-NB	-2.06	1.35	1.37
21	4C	512	CL7	C1B-NB	-2.06	1.35	1.37
21	1C	509	CL7	C1C-C2C	-2.06	1.41	1.45
21	42	506	CL7	OBD-CAD	2.06	1.26	1.22
21	3B	605	CL7	CAB-C3B	2.06	1.49	1.45
21	1C	505	CL7	C3D-C4D	-2.06	1.34	1.39
21	4C	505	CL7	C3D-C4D	-2.06	1.34	1.39
25	22	523	SQD	O8-S	2.06	1.54	1.47
21	14	409	CL7	C1B-C2B	-2.06	1.38	1.43
21	44	409	CL7	C1B-C2B	-2.06	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	34	405	CL7	C1C-NC	-2.06	1.35	1.37
32	43	420	ZEX	C30-C29	-2.06	1.33	1.35
21	2B	606	CL7	CHD-C1D	2.06	1.44	1.39
21	11	418	CL7	CAB-C3B	2.06	1.49	1.45
21	4B	613	CL7	C3D-C4D	-2.06	1.34	1.39
21	42	502	CL7	CHD-C1D	2.06	1.44	1.39
21	12	501	CL7	MG-NB	-2.06	2.01	2.05
32	22	519	ZEX	C10-C9	-2.06	1.33	1.35
32	32	519	ZEX	C10-C9	-2.06	1.33	1.35
21	4A	407	CL7	C3D-C4D	-2.06	1.34	1.39
21	34	408	CL7	C1C-C2C	-2.05	1.41	1.45
21	4B	604	CL7	C1C-NC	-2.05	1.35	1.37
21	4B	605	CL7	C1B-NB	-2.05	1.35	1.37
21	13	508	CL7	CBD-CGD	-2.05	1.46	1.52
21	12	506	CL7	OBD-CAD	2.05	1.26	1.22
21	13	504	CL7	CAB-C3B	2.05	1.49	1.45
21	14	417	CL7	CHD-C1D	2.05	1.44	1.39
21	44	417	CL7	CHD-C1D	2.05	1.44	1.39
21	3C	506	CL7	CBD-CGD	-2.05	1.46	1.52
21	3D	402	CL7	C3B-C4B	-2.05	1.38	1.42
21	11	417	CL7	MG-NB	-2.05	2.01	2.05
21	13	517	CL7	MG-NB	-2.05	2.01	2.05
21	13	512	CL7	C1C-C2C	-2.05	1.41	1.45
21	23	406	CL7	CAB-C3B	2.05	1.49	1.45
21	31	411	CL7	OBD-CAD	2.05	1.26	1.22
21	12	511	CL7	MG-NB	-2.05	2.01	2.05
21	42	511	CL7	MG-NB	-2.05	2.01	2.05
21	21	405	CL7	OBD-CAD	2.05	1.26	1.22
21	31	405	CL7	OBD-CAD	2.05	1.26	1.22
21	23	414	CL7	CBD-CGD	-2.05	1.46	1.52
21	3C	507	CL7	CBD-CGD	-2.05	1.46	1.52
21	32	509	CL7	CBD-CGD	-2.05	1.46	1.52
21	2B	617	CL7	CBD-CGD	-2.05	1.46	1.52
21	4B	617	CL7	C3B-C4B	-2.05	1.38	1.42
21	22	516	CL7	CAB-C3B	2.05	1.49	1.45
21	33	517	CL7	C1C-NC	-2.05	1.35	1.37
21	13	502	CL7	C3D-C4D	-2.05	1.34	1.39
22	4D	408	PHO	C1B-C2B	2.05	1.41	1.39
21	1C	512	CL7	CHD-C1D	2.05	1.44	1.39
21	31	418	CL7	CHD-C1D	2.05	1.44	1.39
21	4C	512	CL7	CHD-C1D	2.05	1.44	1.39
21	41	403	CL7	CHD-C1D	2.05	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1C	504	CL7	C1B-NB	-2.05	1.35	1.37
21	42	517	CL7	C1B-NB	-2.05	1.35	1.37
21	42	517	CL7	C1C-NC	-2.05	1.35	1.37
21	11	419	CL7	MG-NB	-2.05	2.01	2.05
21	33	503	CL7	CBD-CGD	-2.05	1.46	1.52
21	3B	611	CL7	C3D-C4D	-2.05	1.34	1.39
21	4B	603	CL7	C3D-C4D	-2.05	1.34	1.39
21	32	508	CL7	CAB-C3B	2.05	1.49	1.45
32	44	403	ZEX	C1-C6	-2.05	1.50	1.53
21	21	406	CL7	C3D-C4D	-2.05	1.34	1.39
21	31	406	CL7	C3D-C4D	-2.05	1.34	1.39
21	2B	608	CL7	C1B-NB	-2.05	1.35	1.37
21	2C	506	CL7	C1B-NB	-2.05	1.35	1.37
21	3B	607	CL7	C1B-NB	-2.05	1.35	1.37
21	11	409	CL7	C3B-C4B	-2.05	1.38	1.42
32	32	520	ZEX	C30-C29	-2.05	1.33	1.35
21	14	409	CL7	CBD-CGD	-2.05	1.46	1.52
21	44	409	CL7	CBD-CGD	-2.05	1.46	1.52
21	14	413	CL7	C1C-C2C	-2.05	1.41	1.45
21	3B	610	CL7	C1C-C2C	-2.05	1.41	1.45
21	3B	622	CL7	OBD-CAD	2.05	1.26	1.22
21	2B	605	CL7	CHC-C4B	2.05	1.44	1.39
21	3B	604	CL7	CHC-C4B	2.05	1.44	1.39
21	33	508	CL7	CBD-CGD	-2.05	1.46	1.52
21	33	511	CL7	CBD-CGD	-2.05	1.46	1.52
21	4C	504	CL7	OBD-CAD	2.05	1.26	1.22
21	12	501	CL7	C1C-C2C	-2.05	1.41	1.45
21	43	408	CL7	C1C-C2C	-2.05	1.41	1.45
21	3B	615	CL7	CBD-CGD	-2.05	1.46	1.52
21	2B	617	CL7	C3B-C4B	-2.05	1.38	1.42
21	21	412	CL7	C3B-C4B	-2.05	1.38	1.42
21	3B	616	CL7	C3B-C4B	-2.05	1.38	1.42
21	42	511	CL7	C3B-C4B	-2.05	1.38	1.42
31	3F	101	HEM	C3C-C4C	-2.05	1.42	1.46
21	12	508	CL7	CAB-C3B	2.05	1.49	1.45
21	11	406	CL7	OBD-CAD	2.05	1.26	1.22
21	22	506	CL7	OBD-CAD	2.05	1.26	1.22
21	32	506	CL7	OBD-CAD	2.05	1.26	1.22
21	41	406	CL7	OBD-CAD	2.05	1.26	1.22
21	23	418	CL7	C1C-NC	-2.05	1.35	1.37
21	3C	507	CL7	C1B-NB	-2.05	1.35	1.37
21	2D	404	CL7	CAB-C3B	2.05	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3D	404	CL7	CAB-C3B	2.05	1.49	1.45
21	1C	506	CL7	MG-NB	-2.05	2.01	2.05
21	21	417	CL7	MG-NB	-2.05	2.01	2.05
21	31	417	CL7	MG-NB	-2.05	2.01	2.05
21	4C	506	CL7	MG-NB	-2.05	2.01	2.05
21	24	407	CL7	CHD-C1D	2.05	1.44	1.39
21	34	407	CL7	CHD-C1D	2.05	1.44	1.39
21	14	414	CL7	CAB-C3B	2.05	1.49	1.45
21	44	414	CL7	CAB-C3B	2.05	1.49	1.45
21	21	416	CL7	MG-ND	-2.05	2.01	2.05
21	1D	405	CL7	C1B-NB	-2.05	1.35	1.37
21	2C	507	CL7	C1B-NB	-2.05	1.35	1.37
21	4D	405	CL7	C1B-NB	-2.05	1.35	1.37
23	2B	618	8CT	C10-C03	2.05	1.52	1.45
21	4B	611	CL7	C1C-C2C	-2.05	1.41	1.45
21	1C	501	CL7	CAB-C3B	2.05	1.49	1.45
21	11	417	CL7	C3B-C4B	-2.05	1.38	1.42
21	41	417	CL7	C3B-C4B	-2.05	1.38	1.42
21	34	415	CL7	C1C-C2C	-2.05	1.41	1.45
32	12	519	ZEX	C10-C9	-2.05	1.33	1.35
32	12	522	ZEX	C10-C9	-2.05	1.33	1.35
21	43	414	CL7	C3B-C4B	-2.05	1.38	1.42
21	2B	613	CL7	CHD-C1D	2.05	1.44	1.39
21	34	413	CL7	C1C-C2C	-2.05	1.41	1.45
21	4D	404	CL7	CAB-C3B	2.05	1.49	1.45
21	4C	506	CL7	CBD-CGD	-2.05	1.46	1.52
21	21	415	CL7	C3A-C2A	2.05	1.56	1.54
21	23	409	CL7	CBD-CGD	-2.04	1.46	1.52
21	1B	610	CL7	C1C-C2C	-2.04	1.41	1.45
21	31	417	CL7	C3B-C4B	-2.04	1.38	1.42
21	42	511	CL7	OBD-CAD	2.04	1.26	1.22
21	4D	404	CL7	CBD-CGD	-2.04	1.46	1.52
21	41	412	CL7	MG-NB	-2.04	2.01	2.05
21	42	512	CL7	C3B-C4B	-2.04	1.38	1.42
21	23	407	CL7	C1B-NB	-2.04	1.35	1.37
21	42	508	CL7	C1C-NC	-2.04	1.35	1.37
22	1D	408	PHO	C1B-C2B	2.04	1.41	1.39
21	33	516	CL7	MG-NB	-2.04	2.01	2.05
21	13	511	CL7	CBD-CGD	-2.04	1.46	1.52
21	4A	403	CL7	C1C-C2C	-2.04	1.41	1.45
21	2B	604	CL7	C3D-C4D	-2.04	1.34	1.39
21	3B	603	CL7	C3D-C4D	-2.04	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	415	CL7	OBD-CAD	2.04	1.26	1.22
23	1B	626	8CT	C28-C29	2.04	1.37	1.32
21	34	409	CL7	CAB-C3B	2.04	1.49	1.45
21	43	409	CL7	CBD-CGD	-2.04	1.46	1.52
21	14	415	CL7	C1B-NB	-2.04	1.35	1.37
21	1B	604	CL7	CHC-C4B	2.04	1.44	1.39
23	4D	406	8CT	C39-C16	2.04	1.55	1.50
21	23	403	CL7	C3B-C4B	-2.04	1.38	1.42
21	33	502	CL7	C3B-C4B	-2.04	1.38	1.42
21	31	410	CL7	C1C-C2C	-2.04	1.41	1.45
21	34	410	CL7	CHD-C1D	2.04	1.44	1.39
21	2B	623	CL7	OBD-CAD	2.04	1.26	1.22
23	4B	619	8CT	C30-C29	2.04	1.53	1.50
21	21	410	CL7	MG-NB	-2.04	2.01	2.05
21	34	414	CL7	CAB-C3B	2.04	1.49	1.45
21	1D	404	CL7	CHD-C1D	2.04	1.44	1.39
21	14	408	CL7	C1C-C2C	-2.04	1.41	1.45
21	44	408	CL7	C1C-C2C	-2.04	1.41	1.45
21	24	404	CL7	OBD-CAD	2.04	1.26	1.22
21	34	404	CL7	OBD-CAD	2.04	1.26	1.22
21	1B	610	CL7	C1B-NB	-2.04	1.35	1.37
21	13	506	CL7	C1B-NB	-2.04	1.35	1.37
21	4B	611	CL7	C1B-NB	-2.04	1.35	1.37
21	43	418	CL7	C1C-NC	-2.04	1.35	1.37
21	11	406	CL7	CHD-C1D	2.04	1.44	1.39
25	12	523	SQD	O8-S	2.04	1.54	1.47
25	42	523	SQD	O8-S	2.04	1.54	1.47
21	1C	507	CL7	CBD-CGD	-2.04	1.46	1.52
21	4C	503	CL7	CBD-CGD	-2.04	1.46	1.52
23	4B	618	8CT	C10-C03	2.04	1.52	1.45
21	2C	502	CL7	CAB-C3B	2.04	1.49	1.45
21	11	410	CL7	C1C-C2C	-2.04	1.41	1.45
21	41	410	CL7	C1C-C2C	-2.04	1.41	1.45
21	11	410	CL7	C3B-C4B	-2.04	1.38	1.42
21	2D	404	CL7	CHD-C1D	2.04	1.44	1.39
21	4D	402	CL7	C3B-C4B	-2.04	1.38	1.42
21	41	403	CL7	MG-NB	-2.04	2.01	2.05
21	14	405	CL7	C1C-NC	-2.04	1.35	1.37
21	44	405	CL7	C1C-NC	-2.04	1.35	1.37
21	44	410	CL7	C1C-NC	-2.04	1.35	1.37
21	2B	615	CL7	CBD-CGD	-2.04	1.46	1.52
21	23	404	CL7	CBD-CGD	-2.04	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	41	409	CL7	C3B-C4B	-2.04	1.38	1.42
21	2C	504	CL7	OBD-CAD	2.04	1.26	1.22
21	21	410	CL7	OBD-CAD	2.04	1.26	1.22
21	31	410	CL7	OBD-CAD	2.04	1.26	1.22
21	23	405	CL7	CAB-C3B	2.04	1.49	1.45
21	33	504	CL7	CAB-C3B	2.04	1.49	1.45
21	31	405	CL7	C1C-C2C	-2.04	1.41	1.45
21	21	412	CL7	OBD-CAD	2.04	1.26	1.22
21	21	404	CL7	MG-NB	-2.04	2.01	2.05
21	31	412	CL7	MG-NB	-2.04	2.01	2.05
21	23	413	CL7	C3B-C4B	-2.04	1.38	1.42
21	33	512	CL7	C3B-C4B	-2.04	1.38	1.42
21	3C	507	CL7	C1C-NC	-2.04	1.35	1.37
21	24	412	CL7	CAB-C3B	2.04	1.49	1.45
21	41	402	CL7	C1C-C2C	-2.04	1.41	1.45
21	13	512	CL7	C3B-C4B	-2.04	1.38	1.42
31	1F	101	HEM	C3C-C4C	-2.04	1.42	1.46
21	1B	609	CL7	C1C-NC	-2.04	1.35	1.37
21	4B	610	CL7	C1C-NC	-2.04	1.35	1.37
21	4C	507	CL7	C1B-NB	-2.04	1.35	1.37
21	43	414	CL7	C1B-NB	-2.04	1.35	1.37
21	4B	606	CL7	MG-NB	-2.04	2.01	2.05
21	2D	404	CL7	C3D-C4D	-2.04	1.34	1.39
21	41	420	CL7	OBD-CAD	2.04	1.26	1.22
21	13	502	CL7	C3B-C4B	-2.04	1.38	1.42
21	21	402	CL7	C1C-C2C	-2.04	1.41	1.45
21	24	414	CL7	C1C-C2C	-2.04	1.41	1.45
21	3B	614	CL7	CBD-CGD	-2.04	1.46	1.52
21	1D	404	CL7	CBD-CGD	-2.04	1.46	1.52
21	2B	609	CL7	C3D-C4D	-2.04	1.34	1.39
21	22	511	CL7	MG-NB	-2.03	2.01	2.05
21	32	511	CL7	MG-NB	-2.03	2.01	2.05
21	34	412	CL7	CAB-C3B	2.03	1.49	1.45
21	3B	602	CL7	C3D-C4D	-2.03	1.34	1.39
21	32	502	CL7	CHD-C1D	2.03	1.44	1.39
21	2B	617	CL7	C1C-C2C	-2.03	1.41	1.45
21	23	419	CL7	C1C-C2C	-2.03	1.41	1.45
21	3B	616	CL7	C1C-C2C	-2.03	1.41	1.45
21	11	413	CL7	MG-NB	-2.03	2.01	2.05
21	2C	512	CL7	C1B-NB	-2.03	1.35	1.37
21	2B	614	CL7	C3D-C4D	-2.03	1.34	1.39
23	3B	618	8CT	C30-C29	2.03	1.53	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	31	422	ZEX	C30-C29	-2.03	1.33	1.35
21	33	510	CL7	C1B-NB	-2.03	1.35	1.37
21	23	416	CL7	MG-NB	-2.03	2.01	2.05
21	23	418	CL7	MG-NB	-2.03	2.01	2.05
21	44	412	CL7	MG-NB	-2.03	2.01	2.05
21	3D	404	CL7	C3D-C4D	-2.03	1.34	1.39
22	2D	408	PHO	CBD-CGD	-2.03	1.49	1.52
22	3D	408	PHO	CBD-CGD	-2.03	1.49	1.52
21	1B	614	CL7	CBD-CGD	-2.03	1.46	1.52
21	4B	615	CL7	CBD-CGD	-2.03	1.46	1.52
21	11	402	CL7	C1C-C2C	-2.03	1.41	1.45
21	2B	613	CL7	C3D-C4D	-2.03	1.34	1.39
21	44	406	CL7	CHD-C1D	2.03	1.44	1.39
21	13	507	CL7	C1C-C2C	-2.03	1.41	1.45
21	22	503	CL7	C1C-C2C	-2.03	1.41	1.45
21	42	508	CL7	CAB-C3B	2.03	1.49	1.45
21	42	503	CL7	C1B-NB	-2.03	1.35	1.37
21	4B	612	CL7	C3D-C4D	-2.03	1.34	1.39
21	14	404	CL7	C3B-C4B	-2.03	1.38	1.42
21	32	512	CL7	C3B-C4B	-2.03	1.38	1.42
21	43	419	CL7	C1C-C2C	-2.03	1.41	1.45
21	1B	615	CL7	CBD-CGD	-2.03	1.46	1.52
21	13	503	CL7	CBD-CGD	-2.03	1.46	1.52
22	2D	408	PHO	C1B-C2B	2.03	1.41	1.39
21	3C	517	CL7	MG-NB	-2.03	2.01	2.05
21	24	409	CL7	C1B-C2B	-2.03	1.38	1.43
21	2B	605	CL7	C1B-NB	-2.03	1.35	1.37
21	3B	604	CL7	C1B-NB	-2.03	1.35	1.37
21	12	517	CL7	CHD-C1D	2.03	1.44	1.39
21	33	512	CL7	CHD-C1D	2.03	1.44	1.39
21	1D	404	CL7	C3D-C4D	-2.03	1.34	1.39
21	4D	404	CL7	C3D-C4D	-2.03	1.34	1.39
21	1C	510	CL7	MG-NB	-2.03	2.01	2.05
21	4C	510	CL7	MG-NB	-2.03	2.01	2.05
21	1B	608	CL7	C3D-C4D	-2.03	1.34	1.39
21	22	509	CL7	CBD-CGD	-2.03	1.46	1.52
21	43	403	CL7	C3B-C4B	-2.03	1.38	1.42
21	41	406	CL7	CHD-C1D	2.03	1.44	1.39
21	11	407	CL7	MG-NB	-2.03	2.01	2.05
21	41	407	CL7	MG-NB	-2.03	2.01	2.05
21	2B	616	CL7	CBD-CGD	-2.03	1.46	1.52
21	1B	613	CL7	C3D-C4D	-2.03	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	11	412	CL7	OBD-CAD	2.03	1.26	1.22
21	41	412	CL7	OBD-CAD	2.03	1.26	1.22
21	1C	504	CL7	MG-NB	-2.03	2.01	2.05
21	24	406	CL7	C1B-NB	-2.03	1.35	1.37
21	34	406	CL7	C1B-NB	-2.03	1.35	1.37
21	41	405	CL7	C1B-NB	-2.03	1.35	1.37
23	1B	619	8CT	C39-C16	2.03	1.55	1.50
23	4B	620	8CT	C39-C16	2.03	1.55	1.50
21	3B	613	CL7	C3D-C4D	-2.03	1.34	1.39
21	11	407	CL7	OBD-CAD	2.03	1.26	1.22
32	23	420	ZEX	C30-C29	-2.03	1.33	1.35
21	3B	612	CL7	CHD-C1D	2.03	1.44	1.39
21	12	512	CL7	C3B-C4B	-2.03	1.38	1.42
21	21	403	CL7	MG-NB	-2.03	2.01	2.05
21	13	517	CL7	C1C-NC	-2.03	1.35	1.37
21	34	406	CL7	C1C-C2C	-2.03	1.41	1.45
23	1D	406	8CT	C39-C16	2.03	1.55	1.50
21	34	412	CL7	MG-NB	-2.03	2.01	2.05
21	11	417	CL7	CBD-CGD	-2.03	1.46	1.52
21	12	501	CL7	CAB-C3B	2.03	1.49	1.45
21	3C	501	CL7	CAB-C3B	2.03	1.49	1.45
21	1B	612	CL7	CHD-C1D	2.03	1.44	1.39
21	43	413	CL7	C3B-C4B	-2.03	1.38	1.42
21	14	415	CL7	C1C-C2C	-2.03	1.41	1.45
21	13	508	CL7	C1C-NC	-2.03	1.35	1.37
21	31	403	CL7	CHD-C1D	2.03	1.44	1.39
21	1C	502	CL7	CAB-C3B	2.03	1.49	1.45
21	12	505	CL7	CAB-C3B	2.03	1.49	1.45
21	24	409	CL7	CAB-C3B	2.03	1.49	1.45
21	23	408	CL7	C1C-C2C	-2.03	1.41	1.45
21	11	410	CL7	MG-NB	-2.03	2.01	2.05
21	41	410	CL7	MG-NB	-2.03	2.01	2.05
21	42	501	CL7	CAB-C3B	2.03	1.49	1.45
21	1B	602	CL7	C3D-C4D	-2.03	1.34	1.39
21	22	508	CL7	CAB-C3B	2.03	1.49	1.45
21	22	511	CL7	C3B-C4B	-2.03	1.38	1.42
21	32	511	CL7	C3B-C4B	-2.03	1.38	1.42
21	24	404	CL7	C3B-C4B	-2.03	1.38	1.42
21	34	404	CL7	C3B-C4B	-2.03	1.38	1.42
32	21	422	ZEX	C30-C29	-2.03	1.33	1.35
32	41	422	ZEX	C1-C6	-2.03	1.51	1.53
23	3B	619	8CT	C39-C16	2.03	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3A	401	CL7	C4C-NC	-2.02	1.35	1.37
21	23	414	CL7	C3B-C4B	-2.02	1.38	1.42
25	23	422	SQD	O8-S	2.02	1.54	1.47
21	23	412	CL7	CBD-CGD	-2.02	1.46	1.52
21	21	412	CL7	MG-NB	-2.02	2.01	2.05
21	32	513	CL7	MG-NB	-2.02	2.01	2.05
21	43	405	CL7	CAB-C3B	2.02	1.49	1.45
21	11	403	CL7	MG-NB	-2.02	2.01	2.05
21	2B	606	CL7	MG-NB	-2.02	2.01	2.05
21	3B	605	CL7	MG-NB	-2.02	2.01	2.05
21	13	512	CL7	CBD-CGD	-2.02	1.46	1.52
21	13	518	CL7	OBD-CAD	2.02	1.26	1.22
21	4D	405	CL7	CHD-C1D	2.02	1.43	1.39
23	2D	406	8CT	C39-C16	2.02	1.55	1.50
23	3D	406	8CT	C39-C16	2.02	1.55	1.50
23	4K	101	8CT	C38-C31	2.02	1.54	1.50
21	31	417	CL7	CBD-CGD	-2.02	1.46	1.52
21	2C	503	CL7	CBD-CGD	-2.02	1.46	1.52
21	3C	503	CL7	CBD-CGD	-2.02	1.46	1.52
21	4B	605	CL7	CHC-C4B	2.02	1.43	1.39
21	14	409	CL7	CAB-C3B	2.02	1.49	1.45
21	44	409	CL7	CAB-C3B	2.02	1.49	1.45
21	21	420	CL7	OBD-CAD	2.02	1.26	1.22
21	1B	601	CL7	C1C-C2C	-2.02	1.41	1.45
21	4B	602	CL7	C1C-C2C	-2.02	1.41	1.45
21	24	414	CL7	CHD-C1D	2.02	1.43	1.39
21	23	417	CL7	MG-NB	-2.02	2.01	2.05
21	14	410	CL7	C1B-NB	-2.02	1.35	1.37
21	3C	512	CL7	CHD-C1D	2.02	1.43	1.39
21	1B	603	CL7	C3D-C4D	-2.02	1.34	1.39
21	4B	604	CL7	C3D-C4D	-2.02	1.34	1.39
21	24	415	CL7	C1C-C2C	-2.02	1.41	1.45
21	43	412	CL7	CBD-CGD	-2.02	1.46	1.52
21	43	417	CL7	MG-NB	-2.02	2.01	2.05
22	3D	408	PHO	C1B-C2B	2.02	1.41	1.39
21	2C	501	CL7	CAB-C3B	2.02	1.49	1.45
21	2D	404	CL7	CBD-CGD	-2.02	1.46	1.52
21	3D	404	CL7	CBD-CGD	-2.02	1.46	1.52
21	24	406	CL7	C1C-C2C	-2.02	1.41	1.45
21	3B	601	CL7	C1C-C2C	-2.02	1.41	1.45
21	21	416	CL7	MG-NB	-2.02	2.01	2.05
21	23	402	CL7	MG-NB	-2.02	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	31	416	CL7	MG-NB	-2.02	2.01	2.05
21	33	501	CL7	MG-NB	-2.02	2.01	2.05
21	41	417	CL7	MG-NB	-2.02	2.01	2.05
21	1C	503	CL7	CBD-CGD	-2.02	1.46	1.52
21	12	511	CL7	C3B-C4B	-2.02	1.38	1.42
32	11	422	ZEX	C30-C29	-2.02	1.33	1.35
32	42	522	ZEX	C30-C29	-2.02	1.33	1.35
21	12	517	CL7	C1B-NB	-2.02	1.35	1.37
21	3B	612	CL7	C3D-C4D	-2.02	1.34	1.39
32	21	421	ZEX	C1-C6	-2.02	1.51	1.53
21	43	403	CL7	MG-NB	-2.02	2.01	2.05
21	43	418	CL7	MG-NB	-2.02	2.01	2.05
32	14	419	ZEX	C34-C33	-2.02	1.33	1.35
32	44	419	ZEX	C34-C33	-2.02	1.33	1.35
21	31	406	CL7	CHD-C1D	2.02	1.43	1.39
21	44	417	CL7	C1B-C2B	-2.02	1.38	1.43
21	1C	502	CL7	C1B-NB	-2.02	1.35	1.37
21	12	508	CL7	C1C-NC	-2.02	1.35	1.37
21	31	410	CL7	MG-NB	-2.02	2.01	2.05
32	23	423	ZEX	C30-C29	-2.02	1.33	1.35
32	32	522	ZEX	C10-C9	-2.02	1.33	1.35
32	33	522	ZEX	C30-C29	-2.02	1.33	1.35
21	13	501	CL7	OBD-CAD	2.02	1.26	1.22
21	24	411	CL7	MG-NB	-2.02	2.01	2.05
21	11	406	CL7	C3D-C4D	-2.02	1.34	1.39
21	41	406	CL7	C3D-C4D	-2.02	1.34	1.39
32	12	520	ZEX	C1-C6	-2.02	1.51	1.53
32	42	520	ZEX	C1-C6	-2.02	1.51	1.53
21	3C	506	CL7	MG-NB	-2.02	2.01	2.05
21	44	412	CL7	CAB-C3B	2.02	1.49	1.45
21	2B	603	CL7	C3D-C4D	-2.02	1.34	1.39
23	3A	404	8CT	C39-C16	2.02	1.55	1.50
21	24	415	CL7	OBD-CAD	2.02	1.26	1.22
21	34	415	CL7	OBD-CAD	2.02	1.26	1.22
25	22	521	SQD	O8-S	2.02	1.54	1.47
25	32	521	SQD	O8-S	2.02	1.54	1.47
21	33	513	CL7	C3B-C4B	-2.02	1.38	1.42
21	34	413	CL7	CBD-CGD	-2.02	1.46	1.52
23	1A	404	8CT	C39-C16	2.02	1.55	1.50
21	43	412	CL7	CHD-C1D	2.02	1.43	1.39
21	1D	404	CL7	C1C-NC	-2.02	1.35	1.37
21	22	517	CL7	C1C-NC	-2.02	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	32	517	CL7	C1C-NC	-2.02	1.35	1.37
21	4D	404	CL7	C1C-NC	-2.02	1.35	1.37
21	3A	403	CL7	C1C-C2C	-2.02	1.41	1.45
21	1C	506	CL7	CBD-CGD	-2.02	1.46	1.52
21	2C	510	CL7	C3D-C4D	-2.02	1.34	1.39
21	3D	404	CL7	C1C-NC	-2.02	1.35	1.37
21	42	501	CL7	C1C-C2C	-2.02	1.41	1.45
21	34	411	CL7	C3A-C4A	-2.02	1.48	1.52
21	3C	510	CL7	C3D-C4D	-2.02	1.34	1.39
21	2B	612	CL7	C3D-C4D	-2.01	1.34	1.39
23	4A	404	8CT	C39-C16	2.01	1.55	1.50
21	13	513	CL7	C3B-C4B	-2.01	1.38	1.42
21	23	413	CL7	CHD-C1D	2.01	1.43	1.39
21	12	513	CL7	MG-NB	-2.01	2.01	2.05
21	4C	517	CL7	MG-NB	-2.01	2.01	2.05
21	33	512	CL7	CBD-CGD	-2.01	1.46	1.52
21	4C	512	CL7	C3B-C4B	-2.01	1.38	1.42
21	14	412	CL7	CAB-C3B	2.01	1.49	1.45
21	32	505	CL7	CAB-C3B	2.01	1.49	1.45
21	3C	503	CL7	CHD-C1D	2.01	1.43	1.39
21	1C	504	CL7	OBD-CAD	2.01	1.25	1.22
21	43	413	CL7	CHD-C1D	2.01	1.43	1.39
21	11	405	CL7	OBD-CAD	2.01	1.25	1.22
21	43	402	CL7	OBD-CAD	2.01	1.25	1.22
21	11	416	CL7	MG-NB	-2.01	2.01	2.05
21	2C	510	CL7	MG-NB	-2.01	2.01	2.05
21	41	416	CL7	MG-NB	-2.01	2.01	2.05
21	2C	503	CL7	CHD-C1D	2.01	1.43	1.39
21	33	501	CL7	OBD-CAD	2.01	1.25	1.22
21	13	506	CL7	CBD-CGD	-2.01	1.46	1.52
21	2C	506	CL7	CBD-CGD	-2.01	1.46	1.52
21	1B	616	CL7	C1C-C2C	-2.01	1.41	1.45
21	24	412	CL7	MG-NB	-2.01	2.01	2.05
21	3C	502	CL7	CAB-C3B	2.01	1.49	1.45
21	24	410	CL7	C1B-NB	-2.01	1.35	1.37
21	34	410	CL7	C1B-NB	-2.01	1.35	1.37
21	4D	404	CL7	CHD-C1D	2.01	1.43	1.39
21	3C	510	CL7	CAB-C3B	2.01	1.49	1.45
32	24	419	ZEX	C34-C33	-2.01	1.33	1.35
32	34	419	ZEX	C34-C33	-2.01	1.33	1.35
21	42	511	CL7	CBD-CGD	-2.01	1.46	1.52
21	24	413	CL7	C1C-C2C	-2.01	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	12	521	SQD	O8-S	2.01	1.54	1.47
21	14	406	CL7	C1B-NB	-2.01	1.35	1.37
21	23	409	CL7	C1C-NC	-2.01	1.35	1.37
21	33	508	CL7	C1C-NC	-2.01	1.35	1.37
21	34	408	CL7	C1C-NC	-2.01	1.35	1.37
21	13	505	CL7	CAB-C3B	2.01	1.49	1.45
25	13	521	SQD	O8-S	2.01	1.54	1.47
21	43	403	CL7	CAB-C3B	2.01	1.49	1.45
21	3C	503	CL7	C1C-NC	-2.01	1.35	1.37
21	43	407	CL7	C1B-NB	-2.01	1.35	1.37
21	3B	608	CL7	CHD-C1D	2.01	1.43	1.39
21	43	403	CL7	C3D-C4D	-2.01	1.34	1.39
21	2B	616	CL7	CHC-C4B	2.01	1.43	1.39
21	43	404	CL7	CBD-CGD	-2.01	1.46	1.52
21	14	404	CL7	OBD-CAD	2.01	1.25	1.22
21	34	414	CL7	OBD-CAD	2.01	1.25	1.22
21	44	404	CL7	OBD-CAD	2.01	1.25	1.22
21	13	501	CL7	MG-NB	-2.01	2.01	2.05
21	43	402	CL7	MG-NB	-2.01	2.01	2.05
21	44	408	CL7	MG-NB	-2.01	2.01	2.05
21	21	405	CL7	C1C-NC	-2.01	1.35	1.37
21	33	507	CL7	C1C-C2C	-2.01	1.41	1.45
21	2C	504	CL7	MG-NB	-2.01	2.01	2.05
21	21	413	CL7	MG-NB	-2.01	2.01	2.05
21	13	509	CL7	CHD-C1D	2.01	1.43	1.39
21	43	410	CL7	CHD-C1D	2.01	1.43	1.39
21	23	414	CL7	C1B-NB	-2.01	1.35	1.37
21	3B	616	CL7	C1B-NB	-2.01	1.35	1.37
21	44	415	CL7	C1B-NB	-2.01	1.35	1.37
21	13	510	CL7	CHD-C1D	2.01	1.43	1.39
21	34	406	CL7	CHD-C1D	2.01	1.43	1.39
21	31	418	CL7	CAB-C3B	2.01	1.49	1.45
25	33	521	SQD	O8-S	2.01	1.54	1.47
21	1A	403	CL7	C1C-C2C	-2.01	1.41	1.45
23	2K	101	8CT	C38-C31	2.01	1.54	1.50
21	34	411	CL7	C1C-C2C	-2.01	1.41	1.45
21	32	511	CL7	CBD-CGD	-2.01	1.46	1.52
21	43	413	CL7	CBD-CGD	-2.01	1.46	1.52
21	43	406	CL7	CAB-C3B	2.01	1.49	1.45
21	1D	402	CL7	C3B-C4B	-2.01	1.38	1.42
21	2D	402	CL7	C3B-C4B	-2.01	1.38	1.42
21	22	512	CL7	C3B-C4B	-2.01	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	32	501	CL7	CAB-C3B	2.01	1.49	1.45
21	2B	615	CL7	C1B-NB	-2.01	1.35	1.37
21	3B	614	CL7	C1B-NB	-2.01	1.35	1.37
21	1B	609	CL7	CBD-CGD	-2.01	1.46	1.52
21	41	417	CL7	CBD-CGD	-2.01	1.46	1.52
21	21	403	CL7	C1C-C2C	-2.01	1.41	1.45
32	43	420	ZEX	C34-C33	-2.00	1.33	1.35
21	2A	403	CL7	C1C-C2C	-2.00	1.41	1.45
21	14	413	CL7	CBD-CGD	-2.00	1.46	1.52
21	44	413	CL7	CBD-CGD	-2.00	1.46	1.52
21	2B	610	CL7	C1C-NC	-2.00	1.35	1.37
21	24	412	CL7	C1C-C2C	-2.00	1.41	1.45
21	3C	504	CL7	C1C-C2C	-2.00	1.41	1.45
21	13	515	CL7	MG-NB	-2.00	2.01	2.05
21	43	416	CL7	MG-NB	-2.00	2.01	2.05
21	23	412	CL7	CHD-C1D	2.00	1.43	1.39
21	33	511	CL7	CHD-C1D	2.00	1.43	1.39
21	1D	405	CL7	CHD-C1D	2.00	1.43	1.39
21	44	414	CL7	CHD-C1D	2.00	1.43	1.39
21	14	406	CL7	CBD-CGD	-2.00	1.46	1.52
21	21	418	CL7	CAB-C3B	2.00	1.49	1.45
21	42	510	CL7	CAB-C3B	2.00	1.49	1.45
21	1C	503	CL7	C1C-NC	-2.00	1.35	1.37
32	42	522	ZEX	C10-C9	-2.00	1.33	1.35
21	42	503	CL7	C1C-C2C	-2.00	1.41	1.45
22	1D	408	PHO	CBD-CGD	-2.00	1.49	1.52
21	23	411	CL7	CHD-C1D	2.00	1.43	1.39
21	3D	405	CL7	CHD-C1D	2.00	1.43	1.39
21	33	510	CL7	CHD-C1D	2.00	1.43	1.39
21	13	513	CL7	C1B-NB	-2.00	1.35	1.37
25	42	521	SQD	O8-S	2.00	1.54	1.47
21	23	403	CL7	C3D-C4D	-2.00	1.34	1.39
21	33	502	CL7	C3D-C4D	-2.00	1.34	1.39
21	23	410	CL7	CHD-C1D	2.00	1.43	1.39
21	22	501	CL7	C1C-NC	-2.00	1.35	1.37
21	22	518	CL7	C1C-C2C	-2.00	1.41	1.45
21	21	417	CL7	CBD-CGD	-2.00	1.46	1.52
21	11	412	CL7	MG-NB	-2.00	2.01	2.05
21	43	417	CL7	CAB-C3B	2.00	1.49	1.45
21	44	404	CL7	C3B-C4B	-2.00	1.38	1.42
21	1B	604	CL7	C1B-NB	-2.00	1.35	1.37
21	3B	615	CL7	C3D-C4D	-2.00	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	14	411	CL7	MG-NB	-2.00	2.01	2.05
21	23	403	CL7	MG-NB	-2.00	2.01	2.05
21	33	515	CL7	MG-NB	-2.00	2.01	2.05
21	44	411	CL7	MG-NB	-2.00	2.01	2.05

All (11011) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1A	403	CL7	C3C-C4C-NC	10.55	117.82	110.18
21	2A	403	CL7	C3C-C4C-NC	10.52	117.81	110.18
21	3A	403	CL7	C3C-C4C-NC	10.51	117.80	110.18
21	4A	403	CL7	C3C-C4C-NC	10.50	117.78	110.18
21	33	505	CL7	C3C-C4C-NC	10.30	117.64	110.18
21	13	505	CL7	C3C-C4C-NC	10.27	117.62	110.18
21	43	406	CL7	C3C-C4C-NC	10.27	117.62	110.18
21	23	406	CL7	C3C-C4C-NC	10.20	117.57	110.18
23	34	402	8CT	C33-C32-C31	-10.12	115.15	124.85
23	24	402	8CT	C33-C32-C31	-10.10	115.16	124.85
23	14	402	8CT	C33-C32-C31	-10.07	115.19	124.85
23	44	402	8CT	C33-C32-C31	-10.07	115.19	124.85
21	43	415	CL7	C3C-C4C-NC	10.07	117.47	110.18
21	23	415	CL7	C3C-C4C-NC	10.03	117.45	110.18
21	13	514	CL7	C3C-C4C-NC	10.02	117.44	110.18
21	33	514	CL7	C3C-C4C-NC	10.01	117.43	110.18
21	14	415	CL7	C3C-C4C-NC	9.95	117.39	110.18
21	44	415	CL7	C3C-C4C-NC	9.95	117.39	110.18
21	24	415	CL7	C3C-C4C-NC	9.93	117.37	110.18
21	34	415	CL7	C3C-C4C-NC	9.93	117.37	110.18
21	11	415	CL7	C3C-C4C-NC	9.85	117.32	110.18
21	21	415	CL7	C3C-C4C-NC	9.83	117.30	110.18
21	23	412	CL7	C3C-C4C-NC	9.83	117.30	110.18
21	31	415	CL7	C3C-C4C-NC	9.83	117.30	110.18
21	13	511	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	41	415	CL7	C3C-C4C-NC	9.80	117.28	110.18
21	33	511	CL7	C3C-C4C-NC	9.79	117.27	110.18
21	22	512	CL7	C3C-C4C-NC	9.77	117.26	110.18
21	42	512	CL7	C3C-C4C-NC	9.75	117.25	110.18
21	24	416	CL7	C3C-C4C-NC	9.75	117.25	110.18
21	34	416	CL7	C3C-C4C-NC	9.75	117.25	110.18
21	43	412	CL7	C3C-C4C-NC	9.75	117.25	110.18
21	14	416	CL7	C3C-C4C-NC	9.75	117.25	110.18
21	31	414	CL7	C3C-C4C-NC	9.73	117.23	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	512	CL7	C3C-C4C-NC	9.73	117.23	110.18
21	44	417	CL7	C3C-C4C-NC	9.71	117.22	110.18
21	41	414	CL7	C3C-C4C-NC	9.70	117.21	110.18
21	44	416	CL7	C3C-C4C-NC	9.70	117.21	110.18
21	32	512	CL7	C3C-C4C-NC	9.70	117.21	110.18
21	21	414	CL7	C3C-C4C-NC	9.70	117.20	110.18
21	31	420	CL7	C3C-C4C-NC	9.70	117.20	110.18
21	11	414	CL7	C3C-C4C-NC	9.69	117.20	110.18
23	3B	619	8CT	C33-C32-C31	-9.69	115.56	124.85
23	4B	620	8CT	C33-C32-C31	-9.69	115.56	124.85
23	1B	619	8CT	C33-C32-C31	-9.69	115.56	124.85
23	2D	406	8CT	C33-C32-C31	-9.68	115.57	124.85
21	41	420	CL7	C3C-C4C-NC	9.68	117.19	110.18
21	43	404	CL7	C3C-C4C-NC	9.66	117.18	110.18
21	21	420	CL7	C3C-C4C-NC	9.66	117.18	110.18
21	24	417	CL7	C3C-C4C-NC	9.66	117.18	110.18
23	4D	406	8CT	C33-C32-C31	-9.65	115.60	124.85
23	3D	406	8CT	C33-C32-C31	-9.65	115.60	124.85
23	2B	620	8CT	C33-C32-C31	-9.64	115.61	124.85
23	1D	406	8CT	C33-C32-C31	-9.64	115.61	124.85
21	33	503	CL7	C3C-C4C-NC	9.64	117.17	110.18
21	11	420	CL7	C3C-C4C-NC	9.64	117.16	110.18
21	14	417	CL7	C3C-C4C-NC	9.62	117.15	110.18
21	11	413	CL7	C3C-C4C-NC	9.60	117.14	110.18
21	23	404	CL7	C3C-C4C-NC	9.59	117.13	110.18
21	12	503	CL7	C3C-C4C-NC	9.59	117.13	110.18
21	34	417	CL7	C3C-C4C-NC	9.59	117.13	110.18
21	32	503	CL7	C3C-C4C-NC	9.58	117.12	110.18
21	13	503	CL7	C3C-C4C-NC	9.58	117.12	110.18
21	41	413	CL7	C3C-C4C-NC	9.57	117.12	110.18
21	22	503	CL7	C3C-C4C-NC	9.57	117.11	110.18
21	21	413	CL7	C3C-C4C-NC	9.55	117.10	110.18
21	42	503	CL7	C3C-C4C-NC	9.54	117.09	110.18
21	24	409	CL7	C3C-C4C-NC	9.54	117.09	110.18
23	2A	404	8CT	C33-C32-C31	-9.54	115.71	124.85
21	31	413	CL7	C3C-C4C-NC	9.51	117.07	110.18
21	44	407	CL7	C3C-C4C-NC	9.50	117.07	110.18
23	1A	404	8CT	C33-C32-C31	-9.50	115.74	124.85
23	4A	404	8CT	C33-C32-C31	-9.49	115.75	124.85
21	34	409	CL7	C3C-C4C-NC	9.48	117.05	110.18
21	34	407	CL7	C3C-C4C-NC	9.48	117.05	110.18
23	3A	404	8CT	C33-C32-C31	-9.47	115.77	124.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	407	CL7	C3C-C4C-NC	9.46	117.03	110.18
21	4C	501	CL7	C3C-C4C-NC	9.46	117.03	110.18
21	14	409	CL7	C3C-C4C-NC	9.46	117.03	110.18
21	44	409	CL7	C3C-C4C-NC	9.46	117.03	110.18
21	21	417	CL7	C3C-C4C-NC	9.45	117.03	110.18
21	43	413	CL7	C3C-C4C-NC	9.44	117.02	110.18
21	3C	501	CL7	C3C-C4C-NC	9.44	117.02	110.18
21	31	417	CL7	C3C-C4C-NC	9.42	117.00	110.18
21	23	413	CL7	C3C-C4C-NC	9.42	117.00	110.18
21	1C	502	CL7	C3C-C4C-NC	9.40	116.99	110.18
21	24	407	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	41	417	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	11	417	CL7	C3C-C4C-NC	9.37	116.97	110.18
21	33	515	CL7	C3C-C4C-NC	9.37	116.97	110.18
21	3B	610	CL7	C3C-C4C-NC	9.37	116.97	110.18
21	2C	502	CL7	C3C-C4C-NC	9.37	116.97	110.18
21	1B	610	CL7	C3C-C4C-NC	9.36	116.97	110.18
21	4B	611	CL7	C3C-C4C-NC	9.36	116.97	110.18
21	13	512	CL7	C3C-C4C-NC	9.36	116.96	110.18
21	24	413	CL7	C3C-C4C-NC	9.35	116.96	110.18
21	33	512	CL7	C3C-C4C-NC	9.35	116.95	110.18
21	2C	501	CL7	C3C-C4C-NC	9.34	116.95	110.18
21	3C	502	CL7	C3C-C4C-NC	9.34	116.95	110.18
21	2B	611	CL7	C3C-C4C-NC	9.34	116.94	110.18
21	1C	501	CL7	C3C-C4C-NC	9.33	116.94	110.18
21	14	413	CL7	C3C-C4C-NC	9.33	116.94	110.18
21	44	413	CL7	C3C-C4C-NC	9.33	116.94	110.18
21	13	515	CL7	C3C-C4C-NC	9.32	116.93	110.18
21	4C	502	CL7	C3C-C4C-NC	9.32	116.93	110.18
21	1C	512	CL7	C3C-C4C-NC	9.30	116.92	110.18
21	23	414	CL7	C3C-C4C-NC	9.29	116.91	110.18
21	23	416	CL7	C3C-C4C-NC	9.29	116.91	110.18
21	43	414	CL7	C3C-C4C-NC	9.29	116.91	110.18
21	43	416	CL7	C3C-C4C-NC	9.29	116.91	110.18
21	24	414	CL7	C3C-C4C-NC	9.27	116.90	110.18
32	22	519	ZEX	C27-C28-C29	-9.27	112.23	126.23
32	32	519	ZEX	C27-C28-C29	-9.27	112.23	126.23
21	1B	613	CL7	C3C-C4C-NC	9.26	116.89	110.18
21	33	513	CL7	C3C-C4C-NC	9.26	116.89	110.18
21	34	413	CL7	C3C-C4C-NC	9.26	116.89	110.18
32	12	519	ZEX	C27-C28-C29	-9.26	112.25	126.23
32	42	519	ZEX	C27-C28-C29	-9.26	112.25	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	44	408	CL7	C3C-C4C-NC	9.24	116.88	110.18
21	13	507	CL7	C3C-C4C-NC	9.24	116.87	110.18
21	3C	512	CL7	C3C-C4C-NC	9.24	116.87	110.18
21	4C	512	CL7	C3C-C4C-NC	9.23	116.87	110.18
21	2B	614	CL7	C3C-C4C-NC	9.23	116.87	110.18
21	3B	613	CL7	C3C-C4C-NC	9.23	116.87	110.18
21	11	402	CL7	C3C-C4C-NC	9.23	116.87	110.18
21	41	402	CL7	C3C-C4C-NC	9.23	116.87	110.18
21	22	517	CL7	C3C-C4C-NC	9.23	116.86	110.18
21	12	517	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	3C	506	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	31	402	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	11	406	CL7	C3C-C4C-NC	9.21	116.86	110.18
21	14	408	CL7	C3C-C4C-NC	9.21	116.86	110.18
21	44	414	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	13	513	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	34	408	CL7	C3C-C4C-NC	9.20	116.85	110.18
21	14	414	CL7	C3C-C4C-NC	9.20	116.85	110.18
21	34	414	CL7	C3C-C4C-NC	9.20	116.85	110.18
21	2C	509	CL7	C3C-C4C-NC	9.20	116.84	110.18
21	32	517	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	24	408	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	31	406	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	23	408	CL7	C3C-C4C-NC	9.18	116.83	110.18
21	21	402	CL7	C3C-C4C-NC	9.18	116.83	110.18
21	33	507	CL7	C3C-C4C-NC	9.17	116.83	110.18
21	43	408	CL7	C3C-C4C-NC	9.17	116.83	110.18
21	42	517	CL7	C3C-C4C-NC	9.17	116.82	110.18
21	4B	614	CL7	C3C-C4C-NC	9.17	116.82	110.18
21	41	406	CL7	C3C-C4C-NC	9.16	116.82	110.18
21	43	410	CL7	C3C-C4C-NC	9.16	116.81	110.18
21	32	514	CL7	C3C-C4C-NC	9.16	116.81	110.18
21	1C	506	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	4C	506	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	2C	512	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	12	510	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	11	418	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	21	418	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	3B	612	CL7	C3C-C4C-NC	9.15	116.81	110.18
32	13	525	ZEX	C28-C27-C26	-9.15	111.46	127.09
21	1C	509	CL7	C3C-C4C-NC	9.14	116.80	110.18
21	32	510	CL7	C3C-C4C-NC	9.14	116.80	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	509	CL7	C3C-C4C-NC	9.14	116.80	110.18
21	4C	509	CL7	C3C-C4C-NC	9.14	116.80	110.18
21	42	514	CL7	C3C-C4C-NC	9.14	116.80	110.18
21	2C	506	CL7	C3C-C4C-NC	9.13	116.80	110.18
21	42	510	CL7	C3C-C4C-NC	9.13	116.79	110.18
21	21	406	CL7	C3C-C4C-NC	9.12	116.79	110.18
32	23	401	ZEX	C28-C27-C26	-9.12	111.52	127.09
32	33	525	ZEX	C28-C27-C26	-9.12	111.52	127.09
21	12	514	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	23	410	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	31	418	CL7	C3C-C4C-NC	9.10	116.78	110.18
21	41	418	CL7	C3C-C4C-NC	9.10	116.78	110.18
21	22	514	CL7	C3C-C4C-NC	9.10	116.78	110.18
21	3A	401	CL7	C3C-C4C-NC	9.10	116.78	110.18
21	4B	613	CL7	C3C-C4C-NC	9.10	116.77	110.18
21	13	509	CL7	C3C-C4C-NC	9.10	116.77	110.18
32	43	401	ZEX	C28-C27-C26	-9.09	111.56	127.09
21	2A	401	CL7	C3C-C4C-NC	9.09	116.77	110.18
21	41	403	CL7	C3C-C4C-NC	9.09	116.77	110.18
21	22	510	CL7	C3C-C4C-NC	9.08	116.76	110.18
21	4A	401	CL7	C3C-C4C-NC	9.08	116.76	110.18
21	4B	603	CL7	C3C-C4C-NC	9.08	116.76	110.18
21	31	403	CL7	C3C-C4C-NC	9.06	116.75	110.18
21	1B	612	CL7	C3C-C4C-NC	9.06	116.74	110.18
21	41	404	CL7	C3C-C4C-NC	9.06	116.74	110.18
21	2B	613	CL7	C3C-C4C-NC	9.06	116.74	110.18
21	24	406	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	3C	509	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	11	403	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	11	404	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	2B	603	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	1B	602	CL7	C3C-C4C-NC	9.04	116.73	110.18
21	1A	401	CL7	C3C-C4C-NC	9.04	116.73	110.18
23	2B	601	8CT	C33-C32-C31	-9.03	116.19	124.85
21	34	406	CL7	C3C-C4C-NC	9.03	116.72	110.18
23	4B	601	8CT	C33-C32-C31	-9.03	116.19	124.85
21	11	411	CL7	C3C-C4C-NC	9.03	116.72	110.18
21	13	518	CL7	C3C-C4C-NC	9.02	116.72	110.18
21	21	404	CL7	C3C-C4C-NC	9.02	116.72	110.18
21	12	505	CL7	C3C-C4C-NC	9.02	116.71	110.18
21	31	404	CL7	C3C-C4C-NC	9.01	116.71	110.18
21	21	411	CL7	C3C-C4C-NC	9.01	116.71	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	505	CL7	C3C-C4C-NC	9.01	116.70	110.18
21	23	405	CL7	C3C-C4C-NC	9.01	116.70	110.18
21	31	411	CL7	C3C-C4C-NC	9.00	116.70	110.18
21	21	403	CL7	C3C-C4C-NC	9.00	116.70	110.18
21	14	406	CL7	C3C-C4C-NC	8.99	116.69	110.18
21	3B	602	CL7	C3C-C4C-NC	8.98	116.69	110.18
21	32	502	CL7	C3C-C4C-NC	8.98	116.69	110.18
21	33	518	CL7	C3C-C4C-NC	8.98	116.68	110.18
21	13	504	CL7	C3C-C4C-NC	8.98	116.68	110.18
23	2C	518	8CT	C33-C32-C31	-8.97	116.25	124.85
21	43	419	CL7	C3C-C4C-NC	8.97	116.68	110.18
21	41	411	CL7	C3C-C4C-NC	8.96	116.67	110.18
23	3B	626	8CT	C33-C32-C31	-8.96	116.26	124.85
21	44	406	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	1B	614	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	2D	405	CL7	C3C-C4C-NC	8.96	116.67	110.18
23	1B	626	8CT	C33-C32-C31	-8.96	116.26	124.85
21	32	505	CL7	C3C-C4C-NC	8.95	116.66	110.18
23	3C	518	8CT	C33-C32-C31	-8.94	116.27	124.85
21	1D	405	CL7	C3C-C4C-NC	8.94	116.66	110.18
21	4D	405	CL7	C3C-C4C-NC	8.94	116.66	110.18
21	3B	614	CL7	C3C-C4C-NC	8.94	116.65	110.18
21	2B	615	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	21	412	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	31	412	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	42	505	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	33	504	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	11	412	CL7	C3C-C4C-NC	8.92	116.65	110.18
21	41	412	CL7	C3C-C4C-NC	8.92	116.65	110.18
21	1C	503	CL7	C3C-C4C-NC	8.92	116.64	110.18
21	43	405	CL7	C3C-C4C-NC	8.92	116.64	110.18
21	12	515	CL7	C3C-C4C-NC	8.92	116.64	110.18
23	1C	518	8CT	C33-C32-C31	-8.92	116.30	124.85
21	22	515	CL7	C3C-C4C-NC	8.92	116.64	110.18
21	42	515	CL7	C3C-C4C-NC	8.91	116.64	110.18
23	4C	518	8CT	C33-C32-C31	-8.91	116.31	124.85
21	21	419	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	4B	615	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	23	419	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	44	410	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	12	502	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	42	502	CL7	C3C-C4C-NC	8.90	116.63	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	502	CL7	C3C-C4C-NC	8.89	116.62	110.18
21	2C	513	CL7	C3C-C4C-NC	8.88	116.61	110.18
21	3B	616	CL7	C3C-C4C-NC	8.88	116.61	110.18
21	32	515	CL7	C3C-C4C-NC	8.87	116.61	110.18
21	24	410	CL7	C3C-C4C-NC	8.87	116.61	110.18
21	34	410	CL7	C3C-C4C-NC	8.87	116.61	110.18
21	2B	610	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	13	510	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	14	410	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	3C	503	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	32	511	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	3D	405	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	2B	617	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	2C	503	CL7	C3C-C4C-NC	8.84	116.59	110.18
21	42	511	CL7	C3C-C4C-NC	8.84	116.59	110.18
21	22	511	CL7	C3C-C4C-NC	8.84	116.58	110.18
21	23	418	CL7	C3C-C4C-NC	8.84	116.58	110.18
21	23	411	CL7	C3C-C4C-NC	8.84	116.58	110.18
21	31	408	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	13	517	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	3C	513	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	3B	615	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	11	419	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	4C	513	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	43	418	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	1B	609	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	22	501	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	33	510	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	11	408	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	41	408	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	4B	609	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	4B	617	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	31	419	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	22	507	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	32	507	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	1B	607	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	1C	513	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	3B	609	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	1B	608	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	1B	615	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	11	416	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	2B	616	CL7	C3C-C4C-NC	8.79	116.55	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	610	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	41	412	CL7	C2C-C1C-NC	8.79	116.58	110.10
21	33	517	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	4C	503	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	41	407	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	3C	505	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	34	404	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	1B	616	CL7	C3C-C4C-NC	8.78	116.54	110.18
21	21	407	CL7	C3C-C4C-NC	8.78	116.54	110.18
21	11	412	CL7	C2C-C1C-NC	8.78	116.58	110.10
21	4B	616	CL7	C3C-C4C-NC	8.78	116.54	110.18
21	4B	616	CL7	C2C-C1C-NC	8.78	116.57	110.10
21	31	412	CL7	C2C-C1C-NC	8.77	116.57	110.10
21	3B	615	CL7	C2C-C1C-NC	8.77	116.57	110.10
21	2B	608	CL7	C3C-C4C-NC	8.77	116.53	110.18
21	2B	609	CL7	C3C-C4C-NC	8.77	116.53	110.18
21	3B	607	CL7	C3C-C4C-NC	8.77	116.53	110.18
21	3B	608	CL7	C3C-C4C-NC	8.77	116.53	110.18
21	12	518	CL7	C3C-C4C-NC	8.76	116.53	110.18
21	43	411	CL7	C3C-C4C-NC	8.76	116.53	110.18
21	21	408	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	41	419	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	33	506	CL7	C2C-C1C-NC	8.75	116.55	110.10
21	12	501	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	12	511	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	32	501	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	42	507	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	31	407	CL7	C3C-C4C-NC	8.74	116.52	110.18
21	2C	505	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	12	507	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	43	407	CL7	C2C-C1C-NC	8.74	116.55	110.10
21	3B	622	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	4B	623	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	42	501	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	12	516	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	3A	407	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	21	416	CL7	C3C-C4C-NC	8.72	116.50	110.18
21	32	516	CL7	C3C-C4C-NC	8.72	116.50	110.18
21	21	412	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	1C	507	CL7	C3C-C4C-NC	8.72	116.50	110.18
21	1C	505	CL7	C3C-C4C-NC	8.72	116.50	110.18
21	3C	507	CL7	C3C-C4C-NC	8.72	116.50	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	404	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	32	518	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	43	402	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	13	506	CL7	C2C-C1C-NC	8.71	116.53	110.10
21	2A	407	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	31	416	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	4B	608	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	22	518	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	2B	623	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	11	407	CL7	C3C-C4C-NC	8.70	116.49	110.18
21	44	404	CL7	C3C-C4C-NC	8.70	116.49	110.18
21	13	506	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	23	402	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	42	506	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	22	513	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	12	509	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	22	509	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	42	509	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	43	407	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	2B	616	CL7	C2C-C1C-NC	8.69	116.51	110.10
21	33	506	CL7	C3C-C4C-NC	8.69	116.48	110.18
21	13	501	CL7	C3C-C4C-NC	8.69	116.48	110.18
21	23	407	CL7	C2C-C1C-NC	8.69	116.51	110.10
21	1B	615	CL7	C2C-C1C-NC	8.69	116.50	110.10
21	1A	407	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	41	416	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	1C	504	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	23	407	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	4C	507	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	42	513	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	24	404	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	42	518	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	33	501	CL7	C3C-C4C-NC	8.66	116.46	110.18
21	3C	511	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	32	513	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	42	516	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	1C	511	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	4C	511	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	4B	612	CL7	C2C-C1C-NC	8.65	116.48	110.10
21	31	409	CL7	C3C-C4C-NC	8.65	116.44	110.18
21	4A	407	CL7	C3C-C4C-NC	8.65	116.44	110.18
21	1B	622	CL7	C3C-C4C-NC	8.64	116.44	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	505	CL7	C3C-C4C-NC	8.64	116.44	110.18
21	4C	504	CL7	C3C-C4C-NC	8.64	116.44	110.18
21	2B	602	CL7	C3C-C4C-NC	8.63	116.44	110.18
21	22	516	CL7	C3C-C4C-NC	8.63	116.44	110.18
21	3C	504	CL7	C3C-C4C-NC	8.63	116.44	110.18
21	2C	504	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	12	513	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	32	509	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	21	409	CL7	C3C-C4C-NC	8.62	116.43	110.18
21	24	412	CL7	C3C-C4C-NC	8.62	116.43	110.18
21	2C	511	CL7	C3C-C4C-NC	8.62	116.42	110.18
21	2B	612	CL7	C2C-C1C-NC	8.62	116.45	110.10
21	3B	611	CL7	C2C-C1C-NC	8.62	116.45	110.10
21	41	409	CL7	C3C-C4C-NC	8.62	116.42	110.18
21	3B	605	CL7	C3C-C4C-NC	8.62	116.42	110.18
21	12	506	CL7	C3C-C4C-NC	8.61	116.42	110.18
21	1B	601	CL7	C3C-C4C-NC	8.60	116.41	110.18
21	1B	605	CL7	C3C-C4C-NC	8.60	116.41	110.18
21	4B	606	CL7	C3C-C4C-NC	8.60	116.41	110.18
21	22	506	CL7	C3C-C4C-NC	8.59	116.41	110.18
21	2C	507	CL7	C3C-C4C-NC	8.59	116.41	110.18
21	43	409	CL7	C2C-C1C-NC	8.59	116.44	110.10
21	42	508	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	22	508	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	44	412	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	1B	611	CL7	C2C-C1C-NC	8.58	116.43	110.10
21	4B	602	CL7	C3C-C4C-NC	8.58	116.40	110.18
21	14	412	CL7	C3C-C4C-NC	8.58	116.39	110.18
21	11	405	CL7	C3C-C4C-NC	8.57	116.39	110.18
21	2B	606	CL7	C3C-C4C-NC	8.57	116.39	110.18
21	41	405	CL7	C3C-C4C-NC	8.57	116.39	110.18
21	12	507	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	14	409	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	31	403	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	11	409	CL7	C3C-C4C-NC	8.57	116.39	110.18
21	3B	601	CL7	C3C-C4C-NC	8.56	116.38	110.18
21	31	410	CL7	C3C-C4C-NC	8.55	116.38	110.18
21	13	508	CL7	C2C-C1C-NC	8.55	116.41	110.10
23	2C	515	8CT	C33-C32-C31	-8.55	116.66	124.85
23	3C	515	8CT	C33-C32-C31	-8.55	116.66	124.85
21	42	507	CL7	C2C-C1C-NC	8.54	116.40	110.10
21	32	506	CL7	C3C-C4C-NC	8.54	116.37	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	405	CL7	C3C-C4C-NC	8.54	116.37	110.18
21	31	405	CL7	C3C-C4C-NC	8.54	116.37	110.18
21	11	403	CL7	C2C-C1C-NC	8.54	116.39	110.10
21	21	403	CL7	C2C-C1C-NC	8.54	116.39	110.10
21	4B	602	CL7	C2C-C1C-NC	8.54	116.39	110.10
21	34	409	CL7	C2C-C1C-NC	8.53	116.39	110.10
21	41	403	CL7	C2C-C1C-NC	8.53	116.39	110.10
21	41	410	CL7	C3C-C4C-NC	8.53	116.36	110.18
21	1C	510	CL7	C3C-C4C-NC	8.53	116.36	110.18
23	2B	601	8CT	C19-C20-C21	-8.53	115.14	127.31
23	4B	601	8CT	C19-C20-C21	-8.53	115.14	127.31
21	32	507	CL7	C2C-C1C-NC	8.52	116.39	110.10
21	34	411	CL7	C3C-C4C-NC	8.52	116.36	110.18
21	24	409	CL7	C2C-C1C-NC	8.52	116.39	110.10
21	3C	510	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	3D	402	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	2B	604	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	32	508	CL7	C3C-C4C-NC	8.51	116.35	110.18
23	3B	626	8CT	C19-C20-C21	-8.51	115.17	127.31
23	1B	626	8CT	C19-C20-C21	-8.50	115.17	127.31
23	3B	617	8CT	C33-C32-C31	-8.50	116.70	124.85
21	2C	508	CL7	C3C-C4C-NC	8.50	116.34	110.18
21	4C	508	CL7	C3C-C4C-NC	8.50	116.34	110.18
21	2C	510	CL7	C3C-C4C-NC	8.49	116.33	110.18
21	2D	402	CL7	C3C-C4C-NC	8.49	116.33	110.18
21	21	410	CL7	C3C-C4C-NC	8.49	116.33	110.18
21	1B	601	CL7	C2C-C1C-NC	8.49	116.36	110.10
21	44	409	CL7	C2C-C1C-NC	8.49	116.36	110.10
21	3B	606	CL7	C3C-C4C-NC	8.49	116.33	110.18
21	1D	402	CL7	C3C-C4C-NC	8.49	116.33	110.18
21	4B	604	CL7	C3C-C4C-NC	8.48	116.33	110.18
21	34	412	CL7	C3C-C4C-NC	8.48	116.33	110.18
21	23	409	CL7	C2C-C1C-NC	8.48	116.35	110.10
21	33	508	CL7	C2C-C1C-NC	8.48	116.35	110.10
21	12	508	CL7	C3C-C4C-NC	8.48	116.32	110.18
21	2B	612	CL7	C3C-C4C-NC	8.48	116.32	110.18
21	22	507	CL7	C2C-C1C-NC	8.48	116.35	110.10
23	1C	515	8CT	C33-C32-C31	-8.47	116.73	124.85
21	2B	605	CL7	C3C-C4C-NC	8.47	116.31	110.18
23	4C	515	8CT	C33-C32-C31	-8.46	116.74	124.85
23	1B	617	8CT	C33-C32-C31	-8.46	116.74	124.85
21	4B	612	CL7	C3C-C4C-NC	8.46	116.31	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	410	CL7	C3C-C4C-NC	8.46	116.31	110.18
23	4C	515	8CT	C14-C13-C12	-8.45	115.25	127.31
21	2B	607	CL7	C3C-C4C-NC	8.45	116.30	110.18
21	3B	603	CL7	C3C-C4C-NC	8.45	116.30	110.18
21	1B	606	CL7	C3C-C4C-NC	8.45	116.30	110.18
23	4B	618	8CT	C33-C32-C31	-8.45	116.75	124.85
21	1B	603	CL7	C3C-C4C-NC	8.45	116.30	110.18
23	3C	515	8CT	C14-C13-C12	-8.45	115.26	127.31
21	22	501	CL7	C2C-C1C-NC	8.44	116.33	110.10
21	14	411	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	3C	508	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	4C	510	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	12	514	CL7	C2C-C1C-NC	8.44	116.32	110.10
21	4D	402	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	3B	601	CL7	C2C-C1C-NC	8.44	116.32	110.10
21	13	508	CL7	C3C-C4C-NC	8.44	116.29	110.18
21	24	411	CL7	C3C-C4C-NC	8.44	116.29	110.18
23	2B	618	8CT	C33-C32-C31	-8.44	116.76	124.85
21	2B	602	CL7	C2C-C1C-NC	8.44	116.32	110.10
21	1B	604	CL7	C3C-C4C-NC	8.43	116.29	110.18
21	1C	508	CL7	C3C-C4C-NC	8.43	116.29	110.18
21	4B	607	CL7	C3C-C4C-NC	8.42	116.28	110.18
23	1C	515	8CT	C14-C13-C12	-8.42	115.30	127.31
23	2C	515	8CT	C14-C13-C12	-8.41	115.31	127.31
21	44	411	CL7	C3C-C4C-NC	8.41	116.27	110.18
21	33	508	CL7	C3C-C4C-NC	8.40	116.27	110.18
21	32	514	CL7	C2C-C1C-NC	8.40	116.29	110.10
21	4B	605	CL7	C3C-C4C-NC	8.40	116.26	110.18
21	4C	517	CL7	C3C-C4C-NC	8.39	116.26	110.18
23	3B	626	8CT	C24-C25-C26	-8.39	115.34	127.31
21	1C	517	CL7	C3C-C4C-NC	8.39	116.26	110.18
21	12	501	CL7	C2C-C1C-NC	8.38	116.28	110.10
23	1B	626	8CT	C24-C25-C26	-8.38	115.35	127.31
23	4B	601	8CT	C24-C25-C26	-8.38	115.36	127.31
21	3B	604	CL7	C3C-C4C-NC	8.37	116.25	110.18
21	42	501	CL7	C2C-C1C-NC	8.37	116.28	110.10
21	22	502	CL7	C2C-C1C-NC	8.37	116.27	110.10
21	23	409	CL7	C3C-C4C-NC	8.37	116.24	110.18
23	2B	601	8CT	C24-C25-C26	-8.36	115.38	127.31
21	12	502	CL7	C2C-C1C-NC	8.36	116.26	110.10
23	3D	406	8CT	C19-C20-C21	-8.35	115.39	127.31
21	12	506	CL7	C2C-C1C-NC	8.35	116.26	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	514	CL7	C2C-C1C-NC	8.35	116.25	110.10
21	34	405	CL7	C3C-C4C-NC	8.35	116.23	110.18
21	3B	611	CL7	C3C-C4C-NC	8.34	116.22	110.18
21	42	506	CL7	C2C-C1C-NC	8.34	116.25	110.10
23	4D	406	8CT	C19-C20-C21	-8.34	115.41	127.31
21	32	502	CL7	C2C-C1C-NC	8.33	116.25	110.10
21	14	409	CL7	C4D-C3D-CAD	-8.33	101.81	107.42
21	1B	611	CL7	C3C-C4C-NC	8.33	116.22	110.18
21	43	409	CL7	C3C-C4C-NC	8.33	116.22	110.18
23	1D	406	8CT	C19-C20-C21	-8.33	115.43	127.31
21	32	501	CL7	C2C-C1C-NC	8.33	116.24	110.10
23	2D	406	8CT	C19-C20-C21	-8.32	115.43	127.31
21	22	514	CL7	C2C-C1C-NC	8.32	116.24	110.10
21	12	508	CL7	C2C-C1C-NC	8.32	116.23	110.10
21	3C	506	CL7	C2C-C1C-NC	8.32	116.23	110.10
32	33	522	ZEX	C11-C10-C9	-8.31	115.45	127.31
21	2C	517	CL7	C3C-C4C-NC	8.30	116.20	110.18
21	3C	517	CL7	C3C-C4C-NC	8.30	116.20	110.18
32	13	522	ZEX	C11-C10-C9	-8.30	115.46	127.31
21	4C	506	CL7	C2C-C1C-NC	8.30	116.22	110.10
21	42	513	CL7	C2C-C1C-NC	8.30	116.22	110.10
21	32	508	CL7	C2C-C1C-NC	8.29	116.22	110.10
32	43	423	ZEX	C11-C10-C9	-8.29	115.48	127.31
21	42	502	CL7	C2C-C1C-NC	8.29	116.21	110.10
32	23	423	ZEX	C11-C10-C9	-8.28	115.49	127.31
21	24	405	CL7	C3C-C4C-NC	8.28	116.18	110.18
21	42	508	CL7	C2C-C1C-NC	8.28	116.20	110.10
21	34	409	CL7	C4D-C3D-CAD	-8.28	101.85	107.42
21	2C	505	CL7	C2C-C1C-NC	8.28	116.20	110.10
21	22	506	CL7	C2C-C1C-NC	8.28	116.20	110.10
21	12	504	CL7	C3C-C4C-NC	8.28	116.18	110.18
21	32	506	CL7	C2C-C1C-NC	8.27	116.20	110.10
21	4C	513	CL7	C2C-C1C-NC	8.27	116.19	110.10
21	14	405	CL7	C3C-C4C-NC	8.26	116.17	110.18
21	2C	506	CL7	C2C-C1C-NC	8.26	116.19	110.10
21	2C	513	CL7	C2C-C1C-NC	8.26	116.19	110.10
21	3B	605	CL7	C2C-C1C-NC	8.26	116.19	110.10
21	1B	605	CL7	C2C-C1C-NC	8.26	116.19	110.10
21	1C	506	CL7	C2C-C1C-NC	8.26	116.19	110.10
21	32	504	CL7	C3C-C4C-NC	8.25	116.16	110.18
21	22	504	CL7	C3C-C4C-NC	8.25	116.16	110.18
21	11	413	CL7	C2C-C1C-NC	8.25	116.19	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	44	405	CL7	C3C-C4C-NC	8.25	116.16	110.18
21	2D	404	CL7	C3C-C4C-NC	8.25	116.16	110.18
21	44	410	CL7	C2C-C1C-NC	8.25	116.18	110.10
23	4C	514	8CT	C33-C32-C31	-8.24	116.95	124.85
21	32	513	CL7	C2C-C1C-NC	8.24	116.18	110.10
21	44	409	CL7	C4D-C3D-CAD	-8.24	101.87	107.42
21	22	508	CL7	C2C-C1C-NC	8.24	116.18	110.10
21	34	410	CL7	C2C-C1C-NC	8.24	116.17	110.10
21	1C	513	CL7	C2C-C1C-NC	8.24	116.17	110.10
21	31	402	CL7	C2C-C1C-NC	8.24	116.17	110.10
21	42	504	CL7	C3C-C4C-NC	8.23	116.15	110.18
21	24	409	CL7	C4D-C3D-CAD	-8.23	101.88	107.42
21	3C	505	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	24	410	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	12	513	CL7	C2C-C1C-NC	8.22	116.17	110.10
21	4B	606	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	41	413	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	1C	505	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	31	413	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	4C	505	CL7	C2C-C1C-NC	8.22	116.16	110.10
23	1C	514	8CT	C33-C32-C31	-8.22	116.97	124.85
21	22	513	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	2B	606	CL7	C2C-C1C-NC	8.21	116.16	110.10
21	13	502	CL7	C3C-C4C-NC	8.21	116.13	110.18
23	3C	514	8CT	C33-C32-C31	-8.21	116.98	124.85
21	3C	513	CL7	C2C-C1C-NC	8.21	116.15	110.10
21	1C	517	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	4C	517	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	33	507	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	43	408	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	1D	404	CL7	C3C-C4C-NC	8.20	116.12	110.18
21	4D	404	CL7	C3C-C4C-NC	8.20	116.12	110.18
21	3C	517	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	33	504	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	1C	507	CL7	C4D-C3D-CAD	-8.19	101.91	107.42
21	13	504	CL7	C2C-C1C-NC	8.18	116.13	110.10
21	43	418	CL7	C2C-C1C-NC	8.18	116.13	110.10
21	11	402	CL7	C2C-C1C-NC	8.18	116.13	110.10
21	4C	504	CL7	C2C-C1C-NC	8.18	116.13	110.10
23	2C	514	8CT	C33-C32-C31	-8.18	117.01	124.85
21	41	405	CL7	C2C-C1C-NC	8.18	116.13	110.10
21	31	406	CL7	C2C-C1C-NC	8.17	116.13	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3D	404	CL7	C3C-C4C-NC	8.17	116.10	110.18
21	1C	503	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	12	510	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	23	418	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	14	410	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	2C	511	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	43	405	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	11	406	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	21	413	CL7	C2C-C1C-NC	8.17	116.12	110.10
21	4C	507	CL7	C4D-C3D-CAD	-8.17	101.92	107.42
21	21	409	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	2C	503	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	2C	517	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	23	403	CL7	C3C-C4C-NC	8.16	116.09	110.18
21	21	402	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	4C	511	CL7	C2C-C1C-NC	8.16	116.11	110.10
21	41	409	CL7	C2C-C1C-NC	8.16	116.11	110.10
21	11	409	CL7	C2C-C1C-NC	8.16	116.11	110.10
21	4D	402	CL7	C2C-C1C-NC	8.16	116.11	110.10
21	11	405	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	2B	605	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	3C	511	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	32	510	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	13	507	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	31	409	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	4C	503	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	1C	511	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	1D	402	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	2D	402	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	3C	504	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	23	408	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	41	402	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	21	405	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	21	406	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	23	405	CL7	C2C-C1C-NC	8.13	116.10	110.10
21	1C	504	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	12	504	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	43	403	CL7	C3C-C4C-NC	8.13	116.07	110.18
21	2C	507	CL7	C4D-C3D-CAD	-8.13	101.95	107.42
21	3C	507	CL7	C4D-C3D-CAD	-8.12	101.95	107.42
21	3B	603	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	2C	512	CL7	C2C-C1C-NC	8.12	116.08	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	416	CL7	C2C-C1C-NC	8.12	116.08	110.10
21	1B	603	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	22	510	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	24	405	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	1C	512	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	3D	402	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	1B	604	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	2C	504	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	33	502	CL7	C3C-C4C-NC	8.11	116.05	110.18
21	3C	503	CL7	C2C-C1C-NC	8.10	116.08	110.10
21	33	515	CL7	C2C-C1C-NC	8.10	116.08	110.10
21	33	517	CL7	C2C-C1C-NC	8.10	116.08	110.10
21	44	416	CL7	C2C-C1C-NC	8.10	116.08	110.10
21	4B	604	CL7	C2C-C1C-NC	8.10	116.07	110.10
21	4B	605	CL7	C2C-C1C-NC	8.10	116.07	110.10
21	43	416	CL7	C2C-C1C-NC	8.10	116.07	110.10
21	2D	405	CL7	C2C-C1C-NC	8.10	116.07	110.10
21	14	413	CL7	C2C-C1C-NC	8.09	116.07	110.10
21	42	510	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	34	416	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	2B	604	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	14	415	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	24	416	CL7	C2C-C1C-NC	8.08	116.06	110.10
23	4B	619	8CT	C33-C32-C31	-8.08	117.10	124.85
21	34	413	CL7	C2C-C1C-NC	8.08	116.06	110.10
23	2B	619	8CT	C33-C32-C31	-8.08	117.11	124.85
21	41	406	CL7	C2C-C1C-NC	8.07	116.05	110.10
23	1B	618	8CT	C33-C32-C31	-8.07	117.11	124.85
21	32	516	CL7	C2C-C1C-NC	8.07	116.05	110.10
21	32	515	CL7	C2C-C1C-NC	8.06	116.05	110.10
21	4C	512	CL7	C2C-C1C-NC	8.06	116.05	110.10
21	43	417	CL7	C3C-C4C-NC	8.06	116.02	110.18
21	12	515	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	32	504	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	13	517	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	3D	405	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	31	405	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	22	504	CL7	C2C-C1C-NC	8.05	116.03	110.10
21	44	415	CL7	C2C-C1C-NC	8.05	116.03	110.10
21	14	416	CL7	C2C-C1C-NC	8.05	116.03	110.10
21	3B	604	CL7	C2C-C1C-NC	8.05	116.03	110.10
21	11	407	CL7	C2C-C1C-NC	8.04	116.03	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	404	CL7	C2C-C1C-NC	8.04	116.03	110.10
21	13	501	CL7	C2C-C1C-NC	8.04	116.03	110.10
21	3C	512	CL7	C2C-C1C-NC	8.04	116.03	110.10
23	3B	618	8CT	C33-C32-C31	-8.03	117.15	124.85
21	31	407	CL7	C2C-C1C-NC	8.03	116.02	110.10
21	33	516	CL7	C3C-C4C-NC	8.03	116.00	110.18
21	21	407	CL7	C2C-C1C-NC	8.03	116.02	110.10
21	44	413	CL7	C2C-C1C-NC	8.03	116.02	110.10
21	13	515	CL7	C2C-C1C-NC	8.03	116.02	110.10
21	23	417	CL7	C3C-C4C-NC	8.02	115.99	110.18
21	24	413	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	42	504	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	34	405	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	34	415	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	22	516	CL7	C2C-C1C-NC	8.01	116.01	110.10
21	42	515	CL7	C2C-C1C-NC	8.01	116.01	110.10
21	22	515	CL7	C2C-C1C-NC	8.01	116.00	110.10
21	11	418	CL7	C2C-C1C-NC	8.00	116.00	110.10
21	3C	513	CL7	C4D-C3D-CAD	-8.00	102.03	107.42
21	43	419	CL7	C2C-C1C-NC	8.00	116.00	110.10
21	41	407	CL7	C2C-C1C-NC	8.00	116.00	110.10
21	42	516	CL7	C2C-C1C-NC	8.00	116.00	110.10
21	1D	405	CL7	C2C-C1C-NC	7.99	116.00	110.10
21	3B	612	CL7	C2C-C1C-NC	7.99	116.00	110.10
21	31	418	CL7	C2C-C1C-NC	7.99	116.00	110.10
21	4D	405	CL7	C2C-C1C-NC	7.99	116.00	110.10
21	1B	606	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	14	405	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	44	405	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	13	518	CL7	C2C-C1C-NC	7.98	115.98	110.10
21	24	404	CL7	C2C-C1C-NC	7.98	115.98	110.10
21	33	501	CL7	C2C-C1C-NC	7.98	115.98	110.10
21	12	516	CL7	C2C-C1C-NC	7.98	115.98	110.10
21	23	419	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	32	503	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	4B	607	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	12	503	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	24	415	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	11	410	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	4B	613	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	41	408	CL7	C4D-C3D-CAD	-7.97	102.06	107.42
23	3A	404	8CT	C24-C25-C26	-7.97	115.94	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1A	404	8CT	C24-C25-C26	-7.96	115.95	127.31
23	4A	404	8CT	C24-C25-C26	-7.96	115.95	127.31
21	13	516	CL7	C3C-C4C-NC	7.96	115.95	110.18
21	43	402	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	33	518	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	4C	509	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	23	402	CL7	C2C-C1C-NC	7.95	115.97	110.10
21	41	418	CL7	C2C-C1C-NC	7.95	115.96	110.10
21	1C	513	CL7	C4D-C3D-CAD	-7.95	102.07	107.42
21	4C	513	CL7	C4D-C3D-CAD	-7.95	102.07	107.42
21	2C	509	CL7	C2C-C1C-NC	7.95	115.96	110.10
21	44	404	CL7	C2C-C1C-NC	7.94	115.96	110.10
23	2A	404	8CT	C24-C25-C26	-7.94	115.97	127.31
21	21	408	CL7	C4D-C3D-CAD	-7.94	102.07	107.42
21	41	408	CL7	C2C-C1C-NC	7.94	115.95	110.10
21	2C	513	CL7	C4D-C3D-CAD	-7.94	102.08	107.42
21	31	408	CL7	C4D-C3D-CAD	-7.94	102.08	107.42
21	41	410	CL7	C2C-C1C-NC	7.93	115.95	110.10
21	22	503	CL7	C2C-C1C-NC	7.93	115.95	110.10
21	34	404	CL7	C2C-C1C-NC	7.93	115.95	110.10
21	33	510	CL7	C2C-C1C-NC	7.93	115.94	110.10
21	3B	602	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	21	410	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	34	417	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	14	417	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	2B	613	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	31	410	CL7	C2C-C1C-NC	7.91	115.94	110.10
21	3B	606	CL7	C2C-C1C-NC	7.91	115.93	110.10
32	23	421	ZEX	C11-C10-C9	-7.91	116.02	127.31
21	3A	407	CL7	C2C-C1C-NC	7.91	115.93	110.10
21	21	418	CL7	C2C-C1C-NC	7.91	115.93	110.10
21	31	408	CL7	C2C-C1C-NC	7.91	115.93	110.10
21	11	408	CL7	C4D-C3D-CAD	-7.91	102.10	107.42
21	24	417	CL7	C2C-C1C-NC	7.90	115.93	110.10
32	13	520	ZEX	C11-C10-C9	-7.90	116.04	127.31
21	1B	602	CL7	C2C-C1C-NC	7.90	115.92	110.10
21	2B	607	CL7	C2C-C1C-NC	7.90	115.92	110.10
21	14	408	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	1B	612	CL7	C2C-C1C-NC	7.89	115.92	110.10
32	43	421	ZEX	C11-C10-C9	-7.89	116.06	127.31
21	11	416	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	2B	603	CL7	C2C-C1C-NC	7.89	115.92	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	419	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	1A	407	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	21	408	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	11	408	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	2A	407	CL7	C2C-C1C-NC	7.87	115.91	110.10
21	42	503	CL7	C2C-C1C-NC	7.87	115.91	110.10
32	33	520	ZEX	C11-C10-C9	-7.87	116.08	127.31
21	14	414	CL7	C2C-C1C-NC	7.86	115.90	110.10
21	44	408	CL7	C2C-C1C-NC	7.86	115.90	110.10
21	44	414	CL7	C2C-C1C-NC	7.86	115.90	110.10
21	4B	603	CL7	C2C-C1C-NC	7.86	115.90	110.10
32	11	421	ZEX	C31-C30-C29	-7.86	116.09	127.31
21	43	411	CL7	C2C-C1C-NC	7.86	115.90	110.10
21	4A	407	CL7	C2C-C1C-NC	7.86	115.89	110.10
21	2B	615	CL7	C2C-C1C-NC	7.86	115.89	110.10
21	1C	509	CL7	C2C-C1C-NC	7.85	115.89	110.10
21	3C	509	CL7	C2C-C1C-NC	7.85	115.89	110.10
21	13	510	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	22	509	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	4B	615	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	3C	508	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	31	415	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	34	408	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	23	411	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	3B	608	CL7	C2C-C1C-NC	7.84	115.88	110.10
32	41	421	ZEX	C31-C30-C29	-7.83	116.13	127.31
21	2B	609	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	24	414	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	34	414	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	31	416	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	1C	508	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	4C	508	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	1B	608	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	24	408	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	3B	614	CL7	C2C-C1C-NC	7.82	115.86	110.10
21	2C	508	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	11	415	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	41	415	CL7	C2C-C1C-NC	7.81	115.86	110.10
32	21	421	ZEX	C31-C30-C29	-7.81	116.17	127.31
21	41	416	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	12	509	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	42	509	CL7	C2C-C1C-NC	7.81	115.86	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	415	CL7	C2C-C1C-NC	7.80	115.85	110.10
21	21	415	CL7	C2C-C1C-NC	7.80	115.85	110.10
21	44	406	CL7	C2C-C1C-NC	7.80	115.85	110.10
21	44	417	CL7	C2C-C1C-NC	7.80	115.85	110.10
21	2D	404	CL7	C2C-C1C-NC	7.79	115.85	110.10
21	32	509	CL7	C2C-C1C-NC	7.79	115.85	110.10
21	43	414	CL7	C2C-C1C-NC	7.79	115.85	110.10
32	31	421	ZEX	C31-C30-C29	-7.79	116.19	127.31
21	33	514	CL7	C2C-C1C-NC	7.79	115.84	110.10
21	31	419	CL7	C2C-C1C-NC	7.79	115.84	110.10
21	41	420	CL7	C2C-C1C-NC	7.79	115.84	110.10
21	13	514	CL7	C2C-C1C-NC	7.79	115.84	110.10
21	23	415	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	1B	614	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	44	407	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	41	419	CL7	C2C-C1C-NC	7.78	115.83	110.10
21	1C	507	CL7	C2C-C1C-NC	7.78	115.83	110.10
21	11	420	CL7	C2C-C1C-NC	7.77	115.83	110.10
21	34	406	CL7	C2C-C1C-NC	7.77	115.83	110.10
21	4B	609	CL7	C2C-C1C-NC	7.76	115.83	110.10
21	11	419	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	14	406	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	3D	404	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	21	416	CL7	C2C-C1C-NC	7.75	115.81	110.10
21	24	406	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	21	420	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	34	407	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	23	414	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	33	513	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	14	407	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	4C	507	CL7	C2C-C1C-NC	7.72	115.80	110.10
21	13	513	CL7	C2C-C1C-NC	7.72	115.79	110.10
21	24	407	CL7	C2C-C1C-NC	7.72	115.79	110.10
21	31	420	CL7	C2C-C1C-NC	7.72	115.79	110.10
21	1D	404	CL7	C2C-C1C-NC	7.71	115.79	110.10
21	13	512	CL7	C2C-C1C-NC	7.71	115.78	110.10
21	32	505	CL7	C2C-C1C-NC	7.70	115.78	110.10
21	43	413	CL7	C2C-C1C-NC	7.70	115.78	110.10
21	33	512	CL7	C2C-C1C-NC	7.69	115.77	110.10
21	23	410	CL7	C2C-C1C-NC	7.69	115.77	110.10
21	22	505	CL7	C2C-C1C-NC	7.68	115.77	110.10
32	33	519	ZEX	C31-C30-C29	-7.68	116.35	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	43	420	ZEX	C31-C30-C29	-7.68	116.35	127.31
21	1C	510	CL7	C2C-C1C-NC	7.67	115.76	110.10
32	23	420	ZEX	C31-C30-C29	-7.67	116.36	127.31
21	4D	404	CL7	C2C-C1C-NC	7.67	115.76	110.10
21	23	413	CL7	C2C-C1C-NC	7.67	115.76	110.10
21	12	505	CL7	C2C-C1C-NC	7.67	115.75	110.10
21	13	509	CL7	C2C-C1C-NC	7.66	115.75	110.10
21	2C	507	CL7	C2C-C1C-NC	7.66	115.75	110.10
21	43	410	CL7	C2C-C1C-NC	7.66	115.75	110.10
21	1B	609	CL7	C2C-C1C-NC	7.65	115.75	110.10
21	3C	507	CL7	C2C-C1C-NC	7.65	115.74	110.10
21	13	516	CL7	C2C-C1C-NC	7.65	115.74	110.10
21	3C	510	CL7	C2C-C1C-NC	7.64	115.74	110.10
32	13	519	ZEX	C31-C30-C29	-7.64	116.40	127.31
21	4C	510	CL7	C2C-C1C-NC	7.63	115.73	110.10
21	23	417	CL7	C2C-C1C-NC	7.63	115.73	110.10
21	32	517	CL7	C2C-C1C-NC	7.63	115.72	110.10
21	32	518	CL7	C2C-C1C-NC	7.62	115.72	110.10
21	3B	616	CL7	C2C-C1C-NC	7.62	115.72	110.10
21	33	509	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	13	505	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	43	406	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	22	518	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	33	511	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	2B	610	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	33	505	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	3B	609	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	43	417	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	42	505	CL7	C2C-C1C-NC	7.59	115.70	110.10
21	4B	610	CL7	C2C-C1C-NC	7.59	115.70	110.10
21	33	503	CL7	C2C-C1C-NC	7.58	115.69	110.10
21	42	517	CL7	C2C-C1C-NC	7.58	115.69	110.10
21	1B	606	CL7	C2B-C1B-NB	7.58	115.31	110.23
21	4B	607	CL7	C2B-C1B-NB	7.58	115.31	110.23
21	12	518	CL7	C2C-C1C-NC	7.58	115.69	110.10
21	2C	510	CL7	C2C-C1C-NC	7.57	115.69	110.10
21	22	517	CL7	C2C-C1C-NC	7.57	115.69	110.10
21	3B	606	CL7	C2B-C1B-NB	7.57	115.31	110.23
21	12	517	CL7	C2C-C1C-NC	7.57	115.68	110.10
21	23	404	CL7	C2C-C1C-NC	7.57	115.68	110.10
21	23	412	CL7	C2C-C1C-NC	7.57	115.68	110.10
21	22	511	CL7	C2C-C1C-NC	7.56	115.68	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	403	CL7	C2C-C1C-NC	7.56	115.67	110.10
21	13	511	CL7	C2C-C1C-NC	7.56	115.67	110.10
21	23	406	CL7	C2C-C1C-NC	7.56	115.67	110.10
21	4B	617	CL7	C2C-C1C-NC	7.56	115.67	110.10
21	42	518	CL7	C2C-C1C-NC	7.56	115.67	110.10
21	2B	607	CL7	C2B-C1B-NB	7.56	115.30	110.23
21	4C	501	CL7	C2C-C1C-NC	7.56	115.67	110.10
21	21	411	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	42	511	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	4B	608	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	32	511	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	1B	616	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	33	516	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	13	503	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	2B	617	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	41	411	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	3C	502	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	23	403	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	43	404	CL7	C2C-C1C-NC	7.54	115.66	110.10
21	2C	501	CL7	C2C-C1C-NC	7.53	115.66	110.10
21	1C	502	CL7	C2C-C1C-NC	7.52	115.65	110.10
21	1B	607	CL7	C2C-C1C-NC	7.52	115.65	110.10
21	2B	614	CL7	C2C-C1C-NC	7.52	115.64	110.10
21	3C	501	CL7	C2C-C1C-NC	7.51	115.64	110.10
21	43	412	CL7	C2C-C1C-NC	7.51	115.64	110.10
21	41	414	CL7	C2C-C1C-NC	7.51	115.64	110.10
21	1B	613	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	31	411	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	4B	614	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	1B	610	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	1B	622	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	13	502	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	12	511	CL7	C2C-C1C-NC	7.49	115.63	110.10
21	33	502	CL7	C2C-C1C-NC	7.49	115.62	110.10
21	2B	608	CL7	C2C-C1C-NC	7.49	115.62	110.10
21	3B	607	CL7	C2C-C1C-NC	7.49	115.62	110.10
21	1C	501	CL7	C2C-C1C-NC	7.49	115.62	110.10
21	11	411	CL7	C2C-C1C-NC	7.49	115.62	110.10
21	4C	502	CL7	C2C-C1C-NC	7.48	115.61	110.10
21	3B	610	CL7	C2C-C1C-NC	7.47	115.61	110.10
23	44	402	8CT	C30-C31-C32	-7.47	112.28	121.47
21	14	411	CL7	C2B-C1B-NB	7.47	115.24	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2C	502	CL7	C2C-C1C-NC	7.46	115.60	110.10
21	3B	622	CL7	C2C-C1C-NC	7.46	115.60	110.10
21	4B	611	CL7	C2C-C1C-NC	7.46	115.60	110.10
21	11	414	CL7	C2C-C1C-NC	7.45	115.59	110.10
21	4B	623	CL7	C2C-C1C-NC	7.45	115.59	110.10
23	14	402	8CT	C30-C31-C32	-7.45	112.31	121.47
21	44	411	CL7	C2B-C1B-NB	7.44	115.22	110.23
21	2B	611	CL7	C2C-C1C-NC	7.44	115.59	110.10
21	21	414	CL7	C2C-C1C-NC	7.44	115.59	110.10
21	3B	613	CL7	C2C-C1C-NC	7.44	115.59	110.10
21	2B	623	CL7	C2C-C1C-NC	7.44	115.58	110.10
23	34	402	8CT	C30-C31-C32	-7.44	112.32	121.47
32	14	403	ZEX	C31-C30-C29	-7.43	116.70	127.31
32	44	403	ZEX	C31-C30-C29	-7.43	116.70	127.31
23	24	402	8CT	C30-C31-C32	-7.43	112.32	121.47
32	24	403	ZEX	C31-C30-C29	-7.43	116.71	127.31
32	34	403	ZEX	C31-C30-C29	-7.42	116.72	127.31
21	24	411	CL7	C2B-C1B-NB	7.42	115.21	110.23
21	21	404	CL7	C2C-C1C-NC	7.40	115.56	110.10
21	41	404	CL7	C2C-C1C-NC	7.40	115.56	110.10
21	31	404	CL7	C2C-C1C-NC	7.39	115.55	110.10
21	11	404	CL7	C2C-C1C-NC	7.39	115.55	110.10
21	31	414	CL7	C2C-C1C-NC	7.38	115.54	110.10
21	34	411	CL7	C2B-C1B-NB	7.37	115.18	110.23
21	14	411	CL7	C2C-C1C-NC	7.34	115.52	110.10
32	43	421	ZEX	C31-C30-C29	-7.34	116.84	127.31
21	22	512	CL7	C2C-C1C-NC	7.34	115.51	110.10
32	12	519	ZEX	C31-C30-C29	-7.33	116.84	127.31
32	33	520	ZEX	C31-C30-C29	-7.33	116.84	127.31
32	23	421	ZEX	C31-C30-C29	-7.33	116.85	127.31
21	4A	401	CL7	C2C-C1C-NC	7.32	115.50	110.10
32	32	519	ZEX	C31-C30-C29	-7.32	116.86	127.31
32	13	520	ZEX	C31-C30-C29	-7.32	116.87	127.31
32	22	519	ZEX	C31-C30-C29	-7.32	116.87	127.31
21	14	412	CL7	C2C-C1C-NC	7.31	115.49	110.10
21	44	412	CL7	C2C-C1C-NC	7.31	115.49	110.10
21	42	512	CL7	C2C-C1C-NC	7.30	115.48	110.10
32	42	519	ZEX	C31-C30-C29	-7.30	116.89	127.31
21	24	411	CL7	C2C-C1C-NC	7.30	115.48	110.10
21	1A	401	CL7	C2C-C1C-NC	7.28	115.47	110.10
21	34	411	CL7	C2C-C1C-NC	7.28	115.47	110.10
32	12	524	ZEX	C31-C30-C29	-7.28	116.92	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3A	401	CL7	C2C-C1C-NC	7.28	115.47	110.10
21	44	411	CL7	C2C-C1C-NC	7.28	115.47	110.10
21	34	412	CL7	C2C-C1C-NC	7.28	115.47	110.10
21	24	412	CL7	C2C-C1C-NC	7.27	115.46	110.10
21	32	512	CL7	C2C-C1C-NC	7.27	115.46	110.10
21	2A	403	CL7	C2C-C1C-NC	7.26	115.46	110.10
21	2A	401	CL7	C2C-C1C-NC	7.26	115.45	110.10
21	4A	403	CL7	C2C-C1C-NC	7.26	115.45	110.10
32	22	524	ZEX	C31-C30-C29	-7.25	116.96	127.31
32	42	524	ZEX	C31-C30-C29	-7.25	116.96	127.31
21	12	512	CL7	C2C-C1C-NC	7.25	115.44	110.10
32	32	524	ZEX	C31-C30-C29	-7.25	116.97	127.31
21	1A	403	CL7	C2C-C1C-NC	7.24	115.44	110.10
32	21	422	ZEX	C7-C8-C9	-7.22	115.33	126.23
32	11	422	ZEX	C7-C8-C9	-7.20	115.35	126.23
21	3A	403	CL7	C2C-C1C-NC	7.20	115.41	110.10
32	41	422	ZEX	C7-C8-C9	-7.19	115.37	126.23
32	31	422	ZEX	C7-C8-C9	-7.18	115.39	126.23
32	42	522	ZEX	C35-C34-C33	-7.18	117.06	127.31
32	34	419	ZEX	C28-C27-C26	-7.17	114.84	127.09
32	14	419	ZEX	C28-C27-C26	-7.16	114.85	127.09
32	44	419	ZEX	C28-C27-C26	-7.16	114.85	127.09
32	24	419	ZEX	C28-C27-C26	-7.16	114.86	127.09
23	4C	518	8CT	C24-C25-C26	-7.16	117.10	127.31
32	12	522	ZEX	C35-C34-C33	-7.16	117.10	127.31
23	2C	518	8CT	C24-C25-C26	-7.15	117.10	127.31
32	32	522	ZEX	C35-C34-C33	-7.15	117.11	127.31
23	3C	518	8CT	C24-C25-C26	-7.15	117.11	127.31
32	22	522	ZEX	C35-C34-C33	-7.15	117.11	127.31
23	1C	518	8CT	C24-C25-C26	-7.14	117.12	127.31
32	32	524	ZEX	C28-C27-C26	-7.08	114.99	127.09
32	12	524	ZEX	C28-C27-C26	-7.07	115.01	127.09
32	42	524	ZEX	C28-C27-C26	-7.07	115.01	127.09
32	22	524	ZEX	C28-C27-C26	-7.06	115.02	127.09
32	24	419	ZEX	C15-C14-C13	-7.02	117.29	127.31
32	42	524	ZEX	C7-C8-C9	-7.01	115.64	126.23
32	24	403	ZEX	C28-C27-C26	-7.01	115.11	127.09
32	14	403	ZEX	C28-C27-C26	-7.01	115.11	127.09
32	34	403	ZEX	C28-C27-C26	-7.01	115.11	127.09
21	31	419	CL7	C4D-C3D-CAD	-7.00	102.71	107.42
32	44	403	ZEX	C28-C27-C26	-7.00	115.13	127.09
21	41	419	CL7	C4D-C3D-CAD	-7.00	102.71	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	12	524	ZEX	C7-C8-C9	-6.99	115.67	126.23
32	14	419	ZEX	C15-C14-C13	-6.99	117.34	127.31
32	14	418	ZEX	C31-C30-C29	-6.99	117.34	127.31
32	22	524	ZEX	C7-C8-C9	-6.98	115.68	126.23
32	32	524	ZEX	C7-C8-C9	-6.98	115.68	126.23
32	44	418	ZEX	C31-C30-C29	-6.98	117.34	127.31
32	34	418	ZEX	C31-C30-C29	-6.98	117.35	127.31
21	1B	622	CL7	C2B-C1B-NB	6.98	114.91	110.23
21	4B	623	CL7	C2B-C1B-NB	6.98	114.91	110.23
32	34	419	ZEX	C15-C14-C13	-6.97	117.36	127.31
32	44	419	ZEX	C15-C14-C13	-6.96	117.38	127.31
32	24	418	ZEX	C31-C30-C29	-6.96	117.38	127.31
21	2B	623	CL7	C2B-C1B-NB	6.96	114.89	110.23
21	3B	622	CL7	C2B-C1B-NB	6.96	114.89	110.23
21	12	513	CL7	C4D-C3D-CAD	-6.95	102.74	107.42
21	32	513	CL7	C4D-C3D-CAD	-6.93	102.75	107.42
21	42	513	CL7	C4D-C3D-CAD	-6.93	102.75	107.42
32	14	420	ZEX	C28-C27-C26	-6.92	115.26	127.09
21	21	419	CL7	C4D-C3D-CAD	-6.92	102.76	107.42
21	11	419	CL7	C4D-C3D-CAD	-6.92	102.77	107.42
32	34	420	ZEX	C28-C27-C26	-6.91	115.28	127.09
21	3B	622	CL7	C4D-C3D-CAD	-6.91	102.77	107.42
21	23	403	CL7	C2B-C1B-NB	6.89	114.85	110.23
21	1B	622	CL7	C4D-C3D-CAD	-6.89	102.78	107.42
21	4B	623	CL7	C4D-C3D-CAD	-6.89	102.78	107.42
32	24	420	ZEX	C28-C27-C26	-6.88	115.34	127.09
21	21	402	CL7	C1A-NA-C4A	6.88	110.47	106.30
21	31	402	CL7	C1A-NA-C4A	6.88	110.46	106.30
32	44	420	ZEX	C28-C27-C26	-6.87	115.35	127.09
21	11	402	CL7	C1A-NA-C4A	6.86	110.45	106.30
21	22	513	CL7	C4D-C3D-CAD	-6.86	102.80	107.42
21	43	403	CL7	C2B-C1B-NB	6.86	114.83	110.23
21	41	410	CL7	C2B-C1B-NB	6.84	114.82	110.23
21	31	410	CL7	C2B-C1B-NB	6.84	114.81	110.23
21	4A	401	CL7	C2B-C1B-NB	6.83	114.81	110.23
23	1K	101	8CT	C33-C32-C31	-6.83	118.30	124.85
21	41	402	CL7	C1A-NA-C4A	6.83	110.44	106.30
21	13	518	CL7	C2B-C1B-NB	6.83	114.81	110.23
23	3K	101	8CT	C33-C32-C31	-6.82	118.31	124.85
21	33	512	CL7	C2B-C1B-NB	6.82	114.80	110.23
21	21	410	CL7	C2B-C1B-NB	6.81	114.80	110.23
21	33	502	CL7	C2B-C1B-NB	6.81	114.80	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4K	101	8CT	C33-C32-C31	-6.80	118.33	124.85
21	11	410	CL7	C2B-C1B-NB	6.80	114.79	110.23
21	1B	614	CL7	C2B-C1B-NB	6.80	114.79	110.23
21	4B	615	CL7	C2B-C1B-NB	6.80	114.79	110.23
32	12	522	ZEX	C28-C27-C26	-6.80	115.48	127.09
32	42	522	ZEX	C28-C27-C26	-6.79	115.48	127.09
21	2B	623	CL7	C4D-C3D-CAD	-6.79	102.85	107.42
23	2K	101	8CT	C33-C32-C31	-6.79	118.34	124.85
21	2B	615	CL7	C2B-C1B-NB	6.78	114.78	110.23
21	3B	614	CL7	C2B-C1B-NB	6.78	114.78	110.23
21	13	502	CL7	C2B-C1B-NB	6.77	114.77	110.23
32	22	522	ZEX	C28-C27-C26	-6.77	115.52	127.09
32	32	522	ZEX	C28-C27-C26	-6.77	115.53	127.09
21	11	414	CL7	C2B-C1B-NB	6.77	114.77	110.23
21	41	417	CL7	C2C-C1C-NC	6.77	115.09	110.10
21	43	419	CL7	C2B-C1B-NB	6.76	114.76	110.23
21	3A	401	CL7	C2B-C1B-NB	6.76	114.76	110.23
21	23	419	CL7	C2B-C1B-NB	6.75	114.76	110.23
21	13	517	CL7	C2B-C1B-NB	6.75	114.76	110.23
23	3B	619	8CT	C24-C25-C26	-6.75	117.67	127.31
23	1B	619	8CT	C24-C25-C26	-6.75	117.68	127.31
23	2B	620	8CT	C24-C25-C26	-6.75	117.68	127.31
21	33	516	CL7	C2B-C1B-NB	6.75	114.75	110.23
23	4B	620	8CT	C24-C25-C26	-6.74	117.69	127.31
21	1C	512	CL7	C4D-C3D-CAD	-6.74	102.88	107.42
21	13	512	CL7	C2B-C1B-NB	6.74	114.75	110.23
21	2A	401	CL7	C2B-C1B-NB	6.74	114.75	110.23
21	4C	512	CL7	C4D-C3D-CAD	-6.73	102.89	107.42
21	12	511	CL7	C2B-C1B-NB	6.73	114.75	110.23
21	3C	512	CL7	C4D-C3D-CAD	-6.73	102.89	107.42
21	21	414	CL7	C2B-C1B-NB	6.73	114.74	110.23
21	21	417	CL7	C2C-C1C-NC	6.73	115.06	110.10
21	43	417	CL7	C2B-C1B-NB	6.73	114.74	110.23
21	2C	512	CL7	C4D-C3D-CAD	-6.72	102.89	107.42
21	13	516	CL7	C2B-C1B-NB	6.72	114.74	110.23
21	23	413	CL7	C2B-C1B-NB	6.72	114.74	110.23
21	11	417	CL7	C2C-C1C-NC	6.72	115.05	110.10
21	33	518	CL7	C2B-C1B-NB	6.70	114.73	110.23
21	1A	401	CL7	C2B-C1B-NB	6.70	114.72	110.23
21	41	414	CL7	C2B-C1B-NB	6.70	114.72	110.23
21	23	417	CL7	C2B-C1B-NB	6.69	114.72	110.23
23	4B	601	8CT	C14-C13-C12	-6.69	117.76	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	413	CL7	C2B-C1B-NB	6.69	114.72	110.23
32	22	520	ZEX	C7-C8-C9	-6.69	116.13	126.23
32	32	520	ZEX	C7-C8-C9	-6.69	116.13	126.23
23	1B	626	8CT	C14-C13-C12	-6.68	117.78	127.31
21	31	417	CL7	C2C-C1C-NC	6.67	115.02	110.10
32	12	520	ZEX	C7-C8-C9	-6.67	116.16	126.23
32	42	520	ZEX	C7-C8-C9	-6.67	116.16	126.23
21	4D	402	CL7	C2B-C1B-NB	6.66	114.70	110.23
21	22	511	CL7	C2B-C1B-NB	6.66	114.70	110.23
23	3B	626	8CT	C14-C13-C12	-6.66	117.81	127.31
21	32	511	CL7	C2B-C1B-NB	6.65	114.69	110.23
21	34	417	CL7	C4D-C3D-CAD	-6.65	102.94	107.42
23	2B	601	8CT	C14-C13-C12	-6.65	117.83	127.31
21	42	511	CL7	C2B-C1B-NB	6.64	114.68	110.23
23	2D	406	8CT	C19-C18-C17	-6.64	109.88	123.47
21	23	418	CL7	C2B-C1B-NB	6.64	114.68	110.23
21	33	517	CL7	C2B-C1B-NB	6.64	114.68	110.23
23	1D	406	8CT	C19-C18-C17	-6.63	109.88	123.47
21	1D	402	CL7	C2B-C1B-NB	6.63	114.68	110.23
23	2A	404	8CT	C19-C20-C21	-6.63	117.84	127.31
23	4D	406	8CT	C19-C18-C17	-6.63	109.90	123.47
21	31	414	CL7	C2B-C1B-NB	6.62	114.67	110.23
23	3D	406	8CT	C19-C18-C17	-6.62	109.91	123.47
23	1A	404	8CT	C19-C20-C21	-6.62	117.86	127.31
21	12	518	CL7	C2B-C1B-NB	6.62	114.67	110.23
21	22	518	CL7	C2B-C1B-NB	6.62	114.67	110.23
21	42	518	CL7	C2B-C1B-NB	6.62	114.67	110.23
21	24	417	CL7	C4D-C3D-CAD	-6.62	102.97	107.42
23	4A	404	8CT	C19-C20-C21	-6.61	117.87	127.31
21	3B	615	CL7	C1A-NA-C4A	6.61	110.30	106.30
23	3A	404	8CT	C19-C20-C21	-6.61	117.88	127.31
21	43	418	CL7	C2B-C1B-NB	6.61	114.66	110.23
21	2B	608	CL7	C2B-C1B-NB	6.60	114.66	110.23
21	2D	402	CL7	C2B-C1B-NB	6.60	114.66	110.23
21	4B	616	CL7	C1A-NA-C4A	6.60	110.29	106.30
21	14	417	CL7	C4D-C3D-CAD	-6.59	102.98	107.42
21	44	417	CL7	C4D-C3D-CAD	-6.59	102.98	107.42
21	12	513	CL7	C2B-C1B-NB	6.59	114.65	110.23
21	1B	607	CL7	C2B-C1B-NB	6.58	114.65	110.23
32	22	522	ZEX	C7-C8-C9	-6.58	116.29	126.23
21	44	413	CL7	C2B-C1B-NB	6.58	114.64	110.23
32	42	522	ZEX	C7-C8-C9	-6.57	116.31	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	617	CL7	C2B-C1B-NB	6.57	114.64	110.23
21	3D	402	CL7	C2B-C1B-NB	6.57	114.64	110.23
21	3B	616	CL7	C2B-C1B-NB	6.56	114.63	110.23
23	2C	515	8CT	C10-C11-C12	-6.56	116.32	126.23
21	24	412	CL7	C2B-C1B-NB	6.55	114.63	110.23
21	3B	607	CL7	C2B-C1B-NB	6.55	114.63	110.23
23	4C	515	8CT	C10-C11-C12	-6.55	116.33	126.23
32	32	522	ZEX	C7-C8-C9	-6.55	116.33	126.23
21	14	412	CL7	C2B-C1B-NB	6.55	114.62	110.23
23	3C	515	8CT	C10-C11-C12	-6.55	116.34	126.23
21	2B	616	CL7	C1A-NA-C4A	6.55	110.26	106.30
21	32	518	CL7	C2B-C1B-NB	6.54	114.62	110.23
21	22	513	CL7	C2B-C1B-NB	6.54	114.62	110.23
21	11	417	CL7	C2B-C1B-NB	6.54	114.61	110.23
32	12	522	ZEX	C7-C8-C9	-6.54	116.36	126.23
23	1C	515	8CT	C10-C11-C12	-6.54	116.36	126.23
21	14	404	CL7	C2B-C1B-NB	6.54	114.61	110.23
21	31	417	CL7	C2B-C1B-NB	6.54	114.61	110.23
21	44	404	CL7	C2B-C1B-NB	6.54	114.61	110.23
21	4B	608	CL7	C2B-C1B-NB	6.53	114.61	110.23
21	42	513	CL7	C2B-C1B-NB	6.53	114.61	110.23
21	24	413	CL7	C2B-C1B-NB	6.53	114.61	110.23
21	34	412	CL7	C2B-C1B-NB	6.53	114.61	110.23
21	22	507	CL7	C4D-C3D-CAD	-6.52	103.03	107.42
21	32	507	CL7	C4D-C3D-CAD	-6.52	103.03	107.42
21	32	504	CL7	C2B-C1B-NB	6.52	114.61	110.23
21	1B	603	CL7	C2B-C1B-NB	6.52	114.60	110.23
21	32	513	CL7	C2B-C1B-NB	6.52	114.60	110.23
21	1B	616	CL7	C2B-C1B-NB	6.52	114.60	110.23
21	4B	617	CL7	C2B-C1B-NB	6.52	114.60	110.23
21	34	404	CL7	C2B-C1B-NB	6.51	114.60	110.23
21	34	413	CL7	C2B-C1B-NB	6.51	114.60	110.23
21	44	412	CL7	C2B-C1B-NB	6.51	114.60	110.23
21	14	413	CL7	C2B-C1B-NB	6.51	114.59	110.23
21	42	507	CL7	C4D-C3D-CAD	-6.51	103.04	107.42
21	43	412	CL7	C1A-NA-C4A	6.50	110.24	106.30
21	24	404	CL7	C2B-C1B-NB	6.49	114.58	110.23
21	3C	510	CL7	C2B-C1B-NB	6.49	114.58	110.23
21	41	417	CL7	C2B-C1B-NB	6.49	114.58	110.23
21	42	504	CL7	C2B-C1B-NB	6.48	114.58	110.23
21	12	507	CL7	C4D-C3D-CAD	-6.48	103.06	107.42
23	2B	601	8CT	C10-C11-C12	-6.48	116.44	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3B	626	8CT	C10-C11-C12	-6.48	116.44	126.23
21	2C	504	CL7	C2B-C1B-NB	6.48	114.58	110.23
21	22	503	CL7	C1A-NA-C4A	6.48	110.22	106.30
21	14	405	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	1B	615	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	4B	604	CL7	C2B-C1B-NB	6.47	114.57	110.23
21	24	405	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	2B	604	CL7	C2B-C1B-NB	6.46	114.56	110.23
21	21	417	CL7	C2B-C1B-NB	6.46	114.56	110.23
23	1B	626	8CT	C10-C11-C12	-6.46	116.48	126.23
21	42	503	CL7	C1A-NA-C4A	6.45	110.21	106.30
21	22	504	CL7	C2B-C1B-NB	6.45	114.56	110.23
23	4B	601	8CT	C10-C11-C12	-6.45	116.49	126.23
21	13	511	CL7	C1A-NA-C4A	6.44	110.20	106.30
21	1C	510	CL7	C2B-C1B-NB	6.44	114.55	110.23
21	3B	603	CL7	C2B-C1B-NB	6.44	114.55	110.23
21	4C	510	CL7	C2B-C1B-NB	6.44	114.55	110.23
21	1C	504	CL7	C2B-C1B-NB	6.44	114.55	110.23
21	34	417	CL7	C1A-NA-C4A	6.44	110.20	106.30
21	1B	610	CL7	C1A-NA-C4A	6.44	110.20	106.30
21	3C	513	CL7	C2B-C1B-NB	6.44	114.55	110.23
21	2B	611	CL7	C1A-NA-C4A	6.43	110.20	106.30
21	12	504	CL7	C2B-C1B-NB	6.43	114.54	110.23
21	21	407	CL7	C2B-C1B-NB	6.43	114.54	110.23
21	44	405	CL7	C1A-NA-C4A	6.42	110.19	106.30
21	4B	611	CL7	C1A-NA-C4A	6.42	110.19	106.30
21	3C	504	CL7	C2B-C1B-NB	6.42	114.54	110.23
21	12	503	CL7	C1A-NA-C4A	6.42	110.19	106.30
21	4C	513	CL7	C2B-C1B-NB	6.42	114.53	110.23
21	43	414	CL7	C2B-C1B-NB	6.41	114.53	110.23
21	34	405	CL7	C1A-NA-C4A	6.41	110.18	106.30
21	1B	613	CL7	C2B-C1B-NB	6.40	114.53	110.23
21	2C	513	CL7	C2B-C1B-NB	6.40	114.53	110.23
21	22	505	CL7	C1A-NA-C4A	6.40	110.18	106.30
21	32	505	CL7	C1A-NA-C4A	6.40	110.18	106.30
21	2C	510	CL7	C2B-C1B-NB	6.40	114.52	110.23
21	23	414	CL7	C2B-C1B-NB	6.40	114.52	110.23
21	3B	610	CL7	C1A-NA-C4A	6.40	110.17	106.30
21	23	411	CL7	C2B-C1B-NB	6.39	114.52	110.23
21	4C	504	CL7	C2B-C1B-NB	6.39	114.52	110.23
21	23	412	CL7	C1A-NA-C4A	6.39	110.17	106.30
21	33	511	CL7	C1A-NA-C4A	6.39	110.17	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	503	CL7	C1A-NA-C4A	6.39	110.17	106.30
21	31	407	CL7	C2B-C1B-NB	6.39	114.52	110.23
21	31	405	CL7	C2B-C1B-NB	6.39	114.51	110.23
21	32	517	CL7	C2B-C1B-NB	6.38	114.51	110.23
21	2A	407	CL7	C1A-NA-C4A	6.38	110.17	106.30
21	32	503	CL7	C1A-NA-C4A	6.38	110.17	106.30
21	12	505	CL7	C1A-NA-C4A	6.38	110.16	106.30
21	42	505	CL7	C1A-NA-C4A	6.38	110.16	106.30
32	43	401	ZEX	C31-C30-C29	-6.38	118.21	127.31
21	33	503	CL7	C1A-NA-C4A	6.38	110.16	106.30
21	14	417	CL7	C1A-NA-C4A	6.37	110.16	106.30
21	11	405	CL7	C2B-C1B-NB	6.36	114.50	110.23
21	32	504	CL7	C4D-C3D-CAD	-6.36	103.14	107.42
32	14	418	ZEX	C15-C14-C13	-6.36	118.23	127.31
21	13	513	CL7	C2B-C1B-NB	6.36	114.50	110.23
21	1C	513	CL7	C2B-C1B-NB	6.36	114.50	110.23
21	23	412	CL7	C2B-C1B-NB	6.36	114.49	110.23
21	1A	407	CL7	C1A-NA-C4A	6.35	110.15	106.30
21	21	413	CL7	C1A-NA-C4A	6.35	110.15	106.30
21	22	504	CL7	C4D-C3D-CAD	-6.35	103.14	107.42
21	33	505	CL7	C1A-NA-C4A	6.35	110.15	106.30
32	24	418	ZEX	C15-C14-C13	-6.35	118.25	127.31
32	34	418	ZEX	C15-C14-C13	-6.35	118.25	127.31
32	13	525	ZEX	C31-C30-C29	-6.35	118.25	127.31
32	13	519	ZEX	C15-C14-C13	-6.35	118.25	127.31
21	11	407	CL7	C2B-C1B-NB	6.35	114.49	110.23
32	33	519	ZEX	C15-C14-C13	-6.34	118.25	127.31
21	13	511	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	43	402	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	3B	613	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	2B	614	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	41	407	CL7	C2B-C1B-NB	6.34	114.48	110.23
32	33	525	ZEX	C31-C30-C29	-6.34	118.26	127.31
32	44	418	ZEX	C15-C14-C13	-6.34	118.27	127.31
21	4B	616	CL7	C2B-C1B-NB	6.34	114.48	110.23
21	2B	605	CL7	C1A-NA-C4A	6.33	110.14	106.30
21	43	412	CL7	C2B-C1B-NB	6.33	114.48	110.23
21	1B	604	CL7	C1A-NA-C4A	6.33	110.14	106.30
21	3A	407	CL7	C1A-NA-C4A	6.33	110.13	106.30
21	4B	614	CL7	C2B-C1B-NB	6.33	114.48	110.23
21	41	405	CL7	C2B-C1B-NB	6.33	114.48	110.23
21	43	404	CL7	C1A-NA-C4A	6.33	110.13	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	407	CL7	C1A-NA-C4A	6.33	110.13	106.30
21	33	511	CL7	C2B-C1B-NB	6.33	114.47	110.23
32	23	420	ZEX	C15-C14-C13	-6.33	118.28	127.31
21	23	404	CL7	C1A-NA-C4A	6.33	110.13	106.30
21	33	506	CL7	C1A-NA-C4A	6.33	110.13	106.30
21	22	517	CL7	C2B-C1B-NB	6.32	114.47	110.23
21	3A	407	CL7	C2B-C1B-NB	6.32	114.47	110.23
21	12	504	CL7	C4D-C3D-CAD	-6.32	103.16	107.42
21	21	405	CL7	C2B-C1B-NB	6.32	114.47	110.23
21	42	517	CL7	C2B-C1B-NB	6.32	114.47	110.23
21	13	505	CL7	C1A-NA-C4A	6.32	110.12	106.30
21	43	406	CL7	C1A-NA-C4A	6.32	110.12	106.30
32	23	401	ZEX	C31-C30-C29	-6.31	118.30	127.31
21	12	517	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	14	415	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	1D	405	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	2B	609	CL7	C2B-C1B-NB	6.31	114.46	110.23
32	43	420	ZEX	C15-C14-C13	-6.31	118.30	127.31
21	31	413	CL7	C1A-NA-C4A	6.31	110.12	106.30
21	24	415	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	3B	608	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	33	510	CL7	C2B-C1B-NB	6.31	114.46	110.23
21	33	513	CL7	C2B-C1B-NB	6.30	114.46	110.23
21	4A	407	CL7	C1A-NA-C4A	6.30	110.12	106.30
21	2D	405	CL7	C2B-C1B-NB	6.30	114.45	110.23
21	43	411	CL7	C2B-C1B-NB	6.30	114.45	110.23
21	23	402	CL7	C2B-C1B-NB	6.29	114.45	110.23
21	33	501	CL7	C2B-C1B-NB	6.29	114.45	110.23
21	41	413	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	1C	517	CL7	C2B-C1B-NB	6.29	114.45	110.23
21	3B	604	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	4B	605	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	3B	607	CL7	C4D-C3D-CAD	-6.29	103.19	107.42
21	2B	602	CL7	C2B-C1B-NB	6.29	114.45	110.23
21	2B	616	CL7	C2B-C1B-NB	6.29	114.45	110.23
32	43	420	ZEX	C27-C28-C29	-6.29	116.74	126.23
21	2B	608	CL7	C4D-C3D-CAD	-6.28	103.19	107.42
21	11	413	CL7	C1A-NA-C4A	6.28	110.11	106.30
21	4B	608	CL7	C4D-C3D-CAD	-6.28	103.19	107.42
21	3D	405	CL7	C2B-C1B-NB	6.28	114.44	110.23
21	24	417	CL7	C1A-NA-C4A	6.28	110.10	106.30
21	42	504	CL7	C4D-C3D-CAD	-6.28	103.19	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	13	519	ZEX	C27-C28-C29	-6.27	116.75	126.23
21	4D	405	CL7	C2B-C1B-NB	6.27	114.44	110.23
32	24	403	ZEX	C7-C8-C9	-6.27	116.76	126.23
21	23	406	CL7	C1A-NA-C4A	6.27	110.09	106.30
21	41	418	CL7	C2B-C1B-NB	6.27	114.43	110.23
21	13	506	CL7	C1A-NA-C4A	6.26	110.09	106.30
21	23	407	CL7	C1A-NA-C4A	6.26	110.09	106.30
32	33	519	ZEX	C27-C28-C29	-6.26	116.77	126.23
21	12	510	CL7	C2B-C1B-NB	6.26	114.43	110.23
21	11	418	CL7	C2B-C1B-NB	6.26	114.43	110.23
21	22	516	CL7	C2B-C1B-NB	6.26	114.43	110.23
21	13	501	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	13	510	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	41	420	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	1B	608	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	2B	610	CL7	C2B-C1B-NB	6.25	114.42	110.23
32	23	420	ZEX	C27-C28-C29	-6.25	116.79	126.23
32	44	403	ZEX	C7-C8-C9	-6.25	116.79	126.23
21	11	420	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	1B	615	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	4B	609	CL7	C2B-C1B-NB	6.25	114.42	110.23
21	3C	507	CL7	C2B-C1B-NB	6.25	114.42	110.23
32	14	403	ZEX	C7-C8-C9	-6.24	116.80	126.23
21	12	516	CL7	C2B-C1B-NB	6.24	114.42	110.23
21	4B	602	CL7	C2B-C1B-NB	6.24	114.42	110.23
21	3B	610	CL7	C2B-C1B-NB	6.24	114.42	110.23
21	24	414	CL7	C1A-NA-C4A	6.24	110.08	106.30
21	4C	510	CL7	C4D-C3D-CAD	-6.24	103.22	107.42
21	32	506	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	44	417	CL7	C1A-NA-C4A	6.23	110.07	106.30
21	1C	507	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	3B	609	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	21	420	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	4B	603	CL7	C2B-C1B-NB	6.23	114.41	110.23
21	1B	607	CL7	C4D-C3D-CAD	-6.22	103.23	107.42
21	3D	404	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	1C	503	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	1D	404	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	21	418	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	31	418	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	4C	503	CL7	C2B-C1B-NB	6.22	114.40	110.23
21	4B	610	CL7	C2B-C1B-NB	6.22	114.40	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	611	CL7	C2B-C1B-NB	6.21	114.40	110.23
21	34	415	CL7	C2B-C1B-NB	6.21	114.40	110.23
21	3C	503	CL7	C2B-C1B-NB	6.21	114.40	110.23
21	4C	512	CL7	C2B-C1B-NB	6.21	114.40	110.23
32	34	403	ZEX	C7-C8-C9	-6.21	116.85	126.23
21	31	418	CL7	C4D-C3D-CAD	-6.21	103.24	107.42
21	2C	517	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	22	503	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	3B	601	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	3C	517	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	31	420	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	44	415	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	14	414	CL7	C1A-NA-C4A	6.21	110.06	106.30
21	44	414	CL7	C1A-NA-C4A	6.21	110.06	106.30
21	42	506	CL7	C2B-C1B-NB	6.21	114.39	110.23
21	41	418	CL7	C4D-C3D-CAD	-6.21	103.24	107.42
21	4A	407	CL7	C2B-C1B-NB	6.21	114.39	110.23
23	1B	618	8CT	C30-C31-C32	-6.21	113.83	121.47
21	2A	407	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	42	510	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	1A	403	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	2C	507	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	22	510	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	32	510	CL7	C2B-C1B-NB	6.20	114.39	110.23
21	2B	603	CL7	C2B-C1B-NB	6.20	114.39	110.23
23	3B	618	8CT	C30-C31-C32	-6.19	113.85	121.47
21	24	414	CL7	C2B-C1B-NB	6.19	114.38	110.23
21	2B	606	CL7	C1A-NA-C4A	6.19	110.05	106.30
21	2C	510	CL7	C4D-C3D-CAD	-6.19	103.26	107.42
21	1A	407	CL7	C2B-C1B-NB	6.19	114.38	110.23
21	22	506	CL7	C2B-C1B-NB	6.19	114.38	110.23
21	42	516	CL7	C2B-C1B-NB	6.19	114.38	110.23
23	4B	619	8CT	C30-C31-C32	-6.19	113.86	121.47
23	2B	619	8CT	C30-C31-C32	-6.18	113.86	121.47
21	1B	609	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	41	419	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	2D	404	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	4C	517	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	32	516	CL7	C2B-C1B-NB	6.18	114.38	110.23
21	1C	510	CL7	C4D-C3D-CAD	-6.18	103.26	107.42
21	11	409	CL7	C2B-C1B-NB	6.18	114.37	110.23
21	31	419	CL7	C2B-C1B-NB	6.18	114.37	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	409	CL7	C2B-C1B-NB	6.18	114.37	110.23
21	1B	602	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	2C	503	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	1B	601	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	1B	610	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	3B	602	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	31	404	CL7	C2B-C1B-NB	6.17	114.37	110.23
21	31	416	CL7	C2B-C1B-NB	6.17	114.36	110.23
21	4B	611	CL7	C2B-C1B-NB	6.17	114.36	110.23
21	3B	615	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	4C	507	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	3C	512	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	12	506	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	14	414	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	3C	510	CL7	C4D-C3D-CAD	-6.16	103.28	107.42
21	1C	512	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	21	409	CL7	C2B-C1B-NB	6.16	114.36	110.23
21	24	408	CL7	C2B-C1B-NB	6.15	114.36	110.23
21	12	503	CL7	C2B-C1B-NB	6.15	114.36	110.23
21	4D	404	CL7	C2B-C1B-NB	6.15	114.35	110.23
21	2B	613	CL7	C2B-C1B-NB	6.15	114.35	110.23
21	4B	606	CL7	C1A-NA-C4A	6.15	110.02	106.30
21	31	420	CL7	C1A-NA-C4A	6.14	110.02	106.30
21	11	419	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	31	408	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	34	408	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	41	404	CL7	C2B-C1B-NB	6.14	114.35	110.23
21	44	406	CL7	C2B-C1B-NB	6.14	114.35	110.23
32	23	421	ZEX	C35-C34-C33	-6.14	118.55	127.31
21	31	409	CL7	C2B-C1B-NB	6.14	114.34	110.23
21	21	418	CL7	C4D-C3D-CAD	-6.13	103.29	107.42
21	4A	403	CL7	C2B-C1B-NB	6.13	114.34	110.23
21	34	414	CL7	C1A-NA-C4A	6.13	110.01	106.30
21	21	404	CL7	C2B-C1B-NB	6.13	114.34	110.23
21	3B	605	CL7	C1A-NA-C4A	6.12	110.01	106.30
21	2C	512	CL7	C2B-C1B-NB	6.12	114.34	110.23
21	34	414	CL7	C2B-C1B-NB	6.12	114.34	110.23
32	43	421	ZEX	C35-C34-C33	-6.12	118.58	127.31
21	33	504	CL7	C2B-C1B-NB	6.12	114.33	110.23
21	41	408	CL7	C2B-C1B-NB	6.12	114.33	110.23
21	21	416	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	3B	612	CL7	C2B-C1B-NB	6.11	114.33	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	504	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	11	420	CL7	C1A-NA-C4A	6.11	110.00	106.30
21	2A	403	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	3A	403	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	44	408	CL7	C2B-C1B-NB	6.11	114.33	110.23
32	33	520	ZEX	C35-C34-C33	-6.11	118.59	127.31
32	42	524	ZEX	C11-C10-C9	-6.11	118.59	127.31
21	42	512	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	44	407	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	42	503	CL7	C2B-C1B-NB	6.11	114.33	110.23
21	32	512	CL7	C2B-C1B-NB	6.10	114.32	110.23
21	42	501	CL7	C4D-C3D-CAD	-6.10	103.31	107.42
21	1B	605	CL7	C1A-NA-C4A	6.10	109.99	106.30
21	12	512	CL7	C2B-C1B-NB	6.10	114.32	110.23
21	33	515	CL7	C2B-C1B-NB	6.10	114.32	110.23
23	4B	619	8CT	C19-C18-C17	-6.10	110.98	123.47
21	32	503	CL7	C2B-C1B-NB	6.10	114.32	110.23
32	13	520	ZEX	C35-C34-C33	-6.10	118.61	127.31
21	43	416	CL7	C2B-C1B-NB	6.10	114.32	110.23
21	31	415	CL7	C1A-NA-C4A	6.10	109.99	106.30
21	11	418	CL7	C4D-C3D-CAD	-6.09	103.32	107.42
21	14	406	CL7	C2B-C1B-NB	6.09	114.32	110.23
32	22	524	ZEX	C11-C10-C9	-6.09	118.62	127.31
32	32	524	ZEX	C11-C10-C9	-6.09	118.62	127.31
22	2D	408	PHO	C4D-CHA-CBD	-6.09	105.76	108.52
21	23	416	CL7	C2B-C1B-NB	6.09	114.31	110.23
21	43	405	CL7	C2B-C1B-NB	6.09	114.31	110.23
21	21	408	CL7	C2B-C1B-NB	6.09	114.31	110.23
21	24	406	CL7	C2B-C1B-NB	6.08	114.31	110.23
21	34	406	CL7	C2B-C1B-NB	6.08	114.31	110.23
21	21	419	CL7	C2B-C1B-NB	6.08	114.31	110.23
32	33	519	ZEX	C11-C10-C9	-6.08	118.64	127.31
21	22	512	CL7	C2B-C1B-NB	6.08	114.31	110.23
21	22	501	CL7	C4D-C3D-CAD	-6.08	103.33	107.42
32	12	524	ZEX	C11-C10-C9	-6.08	118.64	127.31
21	24	407	CL7	C2B-C1B-NB	6.08	114.31	110.23
23	3B	618	8CT	C19-C18-C17	-6.07	111.04	123.47
21	14	408	CL7	C2B-C1B-NB	6.07	114.30	110.23
23	1B	618	8CT	C19-C18-C17	-6.07	111.04	123.47
32	13	519	ZEX	C11-C10-C9	-6.07	118.65	127.31
21	11	416	CL7	C2B-C1B-NB	6.07	114.30	110.23
21	41	416	CL7	C2B-C1B-NB	6.07	114.30	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	613	CL7	C2B-C1B-NB	6.07	114.30	110.23
21	21	411	CL7	C2B-C1B-NB	6.07	114.30	110.23
21	31	411	CL7	C2B-C1B-NB	6.06	114.30	110.23
21	31	403	CL7	C1A-NA-C4A	6.06	109.97	106.30
21	41	415	CL7	C1A-NA-C4A	6.06	109.97	106.30
21	12	501	CL7	C4D-C3D-CAD	-6.06	103.34	107.42
23	2B	619	8CT	C19-C18-C17	-6.06	111.06	123.47
21	1B	612	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	41	403	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	41	411	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	12	509	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	44	414	CL7	C2B-C1B-NB	6.06	114.29	110.23
21	11	402	CL7	C2B-C1B-NB	6.05	114.29	110.23
21	41	402	CL7	C2B-C1B-NB	6.05	114.29	110.23
21	14	415	CL7	C1A-NA-C4A	6.05	109.97	106.30
21	11	403	CL7	C2B-C1B-NB	6.05	114.29	110.23
21	31	402	CL7	C2B-C1B-NB	6.05	114.29	110.23
21	13	515	CL7	C2B-C1B-NB	6.05	114.29	110.23
21	4C	501	CL7	C1A-NA-C4A	6.05	109.96	106.30
21	41	420	CL7	C1A-NA-C4A	6.05	109.96	106.30
21	31	403	CL7	C2B-C1B-NB	6.05	114.29	110.23
32	43	420	ZEX	C11-C10-C9	-6.05	118.68	127.31
21	43	406	CL7	C2B-C1B-NB	6.05	114.28	110.23
21	21	403	CL7	C1A-NA-C4A	6.05	109.96	106.30
32	23	420	ZEX	C11-C10-C9	-6.04	118.68	127.31
21	44	410	CL7	C1A-NA-C4A	6.04	109.96	106.30
21	21	420	CL7	C1A-NA-C4A	6.04	109.96	106.30
21	11	411	CL7	C2B-C1B-NB	6.04	114.28	110.23
21	32	509	CL7	C2B-C1B-NB	6.04	114.28	110.23
21	1C	509	CL7	C2B-C1B-NB	6.04	114.28	110.23
21	11	404	CL7	C2B-C1B-NB	6.04	114.28	110.23
22	4D	408	PHO	C4D-CHA-CBD	-6.03	105.79	108.52
21	32	501	CL7	C4D-C3D-CAD	-6.03	103.36	107.42
21	13	509	CL7	C2B-C1B-NB	6.03	114.28	110.23
21	11	408	CL7	C2B-C1B-NB	6.03	114.27	110.23
21	3C	509	CL7	C2B-C1B-NB	6.03	114.27	110.23
21	2C	511	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	34	410	CL7	C1A-NA-C4A	6.02	109.95	106.30
21	14	410	CL7	C1A-NA-C4A	6.02	109.94	106.30
21	2B	604	CL7	C1A-NA-C4A	6.02	109.94	106.30
21	22	509	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	23	405	CL7	C2B-C1B-NB	6.02	114.27	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	501	CL7	C1A-NA-C4A	6.02	109.94	106.30
21	23	410	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	3C	502	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	3C	511	CL7	C2B-C1B-NB	6.02	114.27	110.23
21	11	403	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	21	415	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	41	403	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	14	407	CL7	C2B-C1B-NB	6.01	114.26	110.23
21	4C	511	CL7	C2B-C1B-NB	6.01	114.26	110.23
21	21	403	CL7	C2B-C1B-NB	6.01	114.26	110.23
21	44	415	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	2C	509	CL7	C2B-C1B-NB	6.00	114.26	110.23
21	24	415	CL7	C1A-NA-C4A	6.00	109.93	106.30
21	34	415	CL7	C1A-NA-C4A	6.00	109.93	106.30
21	11	415	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	4C	509	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	24	410	CL7	C1A-NA-C4A	6.00	109.93	106.30
21	21	402	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	23	406	CL7	C2B-C1B-NB	6.00	114.25	110.23
21	11	415	CL7	C1A-NA-C4A	5.99	109.93	106.30
21	1B	603	CL7	C1A-NA-C4A	5.99	109.93	106.30
21	4D	404	CL7	C1A-NA-C4A	5.98	109.92	106.30
22	3D	408	PHO	C4D-CHA-CBD	-5.98	105.81	108.52
21	31	415	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	34	407	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	11	412	CL7	C1A-NA-C4A	5.98	109.92	106.30
21	34	409	CL7	C1A-NA-C4A	5.98	109.92	106.30
21	43	410	CL7	C2B-C1B-NB	5.98	114.24	110.23
21	42	509	CL7	C2B-C1B-NB	5.97	114.24	110.23
21	14	409	CL7	C1A-NA-C4A	5.97	109.92	106.30
21	2C	502	CL7	C2B-C1B-NB	5.97	114.24	110.23
21	33	509	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	41	415	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	2D	404	CL7	C1A-NA-C4A	5.97	109.92	106.30
21	3D	404	CL7	C1A-NA-C4A	5.97	109.92	106.30
21	4C	502	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	14	405	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	32	514	CL7	C2B-C1B-NB	5.97	114.23	110.23
21	33	504	CL7	C1A-NA-C4A	5.97	109.91	106.30
21	1C	511	CL7	C2B-C1B-NB	5.96	114.23	110.23
21	11	406	CL7	C2B-C1B-NB	5.96	114.23	110.23
21	41	413	CL7	C2B-C1B-NB	5.95	114.22	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2C	501	CL7	C1A-NA-C4A	5.95	109.91	106.30
21	1C	501	CL7	C2B-C1B-NB	5.95	114.22	110.23
22	1D	408	PHO	C4D-CHA-CBD	-5.95	105.82	108.52
21	1C	501	CL7	C1A-NA-C4A	5.95	109.90	106.30
21	1D	404	CL7	C1A-NA-C4A	5.95	109.90	106.30
23	4B	620	8CT	C19-C20-C21	-5.94	118.83	127.31
23	1B	619	8CT	C19-C20-C21	-5.94	118.83	127.31
21	32	501	CL7	C1A-NA-C4A	5.94	109.90	106.30
21	2C	501	CL7	C2B-C1B-NB	5.94	114.22	110.23
21	3C	501	CL7	C2B-C1B-NB	5.94	114.22	110.23
23	2B	620	8CT	C19-C20-C21	-5.94	118.83	127.31
21	21	415	CL7	C2B-C1B-NB	5.94	114.21	110.23
21	4C	501	CL7	C2B-C1B-NB	5.94	114.21	110.23
21	43	415	CL7	C1A-NA-C4A	5.94	109.89	106.30
21	1C	505	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	3B	603	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	1C	502	CL7	C2B-C1B-NB	5.93	114.21	110.23
21	33	505	CL7	C2B-C1B-NB	5.93	114.21	110.23
21	24	409	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	12	514	CL7	C2B-C1B-NB	5.93	114.21	110.23
21	21	406	CL7	C2B-C1B-NB	5.93	114.21	110.23
21	2C	505	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	3C	505	CL7	C2B-C1B-NB	5.93	114.20	110.23
21	24	405	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	44	405	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	23	405	CL7	C1A-NA-C4A	5.92	109.89	106.30
23	3B	619	8CT	C19-C20-C21	-5.92	118.86	127.31
21	41	406	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	21	406	CL7	C1A-NA-C4A	5.92	109.89	106.30
21	13	505	CL7	C2B-C1B-NB	5.92	114.20	110.23
21	31	406	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	11	413	CL7	C2B-C1B-NB	5.91	114.20	110.23
21	22	514	CL7	C2B-C1B-NB	5.91	114.20	110.23
21	4B	604	CL7	C1A-NA-C4A	5.91	109.88	106.30
21	42	514	CL7	C2B-C1B-NB	5.91	114.19	110.23
21	31	413	CL7	C2B-C1B-NB	5.91	114.19	110.23
21	1B	601	CL7	C1A-NA-C4A	5.91	109.88	106.30
21	21	413	CL7	C2B-C1B-NB	5.91	114.19	110.23
21	1D	405	CL7	C1A-NA-C4A	5.91	109.88	106.30
21	4D	405	CL7	C1A-NA-C4A	5.91	109.88	106.30
21	14	406	CL7	C1A-NA-C4A	5.90	109.88	106.30
21	33	514	CL7	C1A-NA-C4A	5.90	109.87	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	501	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	11	406	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	41	406	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	23	404	CL7	C2B-C1B-NB	5.89	114.18	110.23
21	43	404	CL7	C2B-C1B-NB	5.89	114.18	110.23
21	4C	505	CL7	C2B-C1B-NB	5.89	114.18	110.23
21	44	409	CL7	C1A-NA-C4A	5.89	109.86	106.30
21	34	405	CL7	C2B-C1B-NB	5.89	114.18	110.23
21	2C	511	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	3D	405	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	2B	602	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	23	415	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	3B	601	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	21	412	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	44	406	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	24	406	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	34	406	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	13	504	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	43	405	CL7	C1A-NA-C4A	5.88	109.86	106.30
23	1A	404	8CT	C10-C11-C12	-5.87	117.36	126.23
21	4C	505	CL7	C1A-NA-C4A	5.87	109.86	106.30
23	4A	404	8CT	C10-C11-C12	-5.87	117.36	126.23
21	13	514	CL7	C1A-NA-C4A	5.87	109.86	106.30
21	31	406	CL7	C2B-C1B-NB	5.87	114.17	110.23
21	22	501	CL7	C1A-NA-C4A	5.87	109.85	106.30
23	3A	404	8CT	C10-C11-C12	-5.86	117.37	126.23
21	13	516	CL7	C1A-NA-C4A	5.86	109.85	106.30
21	22	501	CL7	C2B-C1B-NB	5.86	114.16	110.23
21	1C	504	CL7	C1A-NA-C4A	5.86	109.85	106.30
21	3C	505	CL7	C1A-NA-C4A	5.85	109.84	106.30
21	4B	602	CL7	C1A-NA-C4A	5.85	109.84	106.30
23	2A	404	8CT	C10-C11-C12	-5.85	117.40	126.23
32	13	522	ZEX	C28-C27-C26	-5.85	117.10	127.09
21	23	411	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	2C	517	CL7	C4D-C3D-CAD	-5.84	103.49	107.42
21	22	513	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	32	513	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	32	501	CL7	C2B-C1B-NB	5.84	114.15	110.23
21	13	510	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	2D	405	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	43	411	CL7	C1A-NA-C4A	5.84	109.84	106.30
32	23	423	ZEX	C28-C27-C26	-5.84	117.12	127.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	501	CL7	C1A-NA-C4A	5.84	109.83	106.30
21	13	514	CL7	C2B-C1B-NB	5.83	114.14	110.23
21	11	418	CL7	C1A-NA-C4A	5.83	109.83	106.30
23	1C	515	8CT	C04-C03-C02	-5.83	114.40	122.61
23	4C	515	8CT	C04-C03-C02	-5.83	114.40	122.61
21	1C	505	CL7	C2B-C1B-NB	5.83	114.14	110.23
21	43	414	CL7	C1A-NA-C4A	5.83	109.83	106.30
21	2C	505	CL7	C2B-C1B-NB	5.82	114.14	110.23
21	42	501	CL7	C2B-C1B-NB	5.82	114.14	110.23
21	4C	511	CL7	C1A-NA-C4A	5.82	109.83	106.30
21	44	410	CL7	C2B-C1B-NB	5.82	114.14	110.23
21	3C	511	CL7	C1A-NA-C4A	5.82	109.82	106.30
21	33	503	CL7	C2B-C1B-NB	5.82	114.13	110.23
21	12	501	CL7	C2B-C1B-NB	5.82	114.13	110.23
21	13	503	CL7	C2B-C1B-NB	5.82	114.13	110.23
21	23	407	CL7	C2B-C1B-NB	5.82	114.13	110.23
21	41	412	CL7	C1A-NA-C4A	5.82	109.82	106.30
21	1C	512	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	12	513	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	31	412	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	43	417	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	1C	511	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	42	513	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	24	410	CL7	C2B-C1B-NB	5.81	114.13	110.23
23	2C	515	8CT	C04-C03-C02	-5.81	114.43	122.61
23	1B	619	8CT	C14-C13-C12	-5.80	119.03	127.31
23	4B	620	8CT	C14-C13-C12	-5.80	119.03	127.31
21	2C	508	CL7	C1A-NA-C4A	5.80	109.81	106.30
32	43	423	ZEX	C28-C27-C26	-5.80	117.18	127.09
21	21	418	CL7	C1A-NA-C4A	5.80	109.81	106.30
21	41	418	CL7	C1A-NA-C4A	5.80	109.81	106.30
32	21	421	ZEX	C28-C27-C26	-5.80	117.19	127.09
32	31	421	ZEX	C28-C27-C26	-5.80	117.19	127.09
32	33	522	ZEX	C28-C27-C26	-5.80	117.19	127.09
21	1C	517	CL7	C4D-C3D-CAD	-5.80	103.52	107.42
21	43	415	CL7	C2B-C1B-NB	5.80	114.12	110.23
21	14	410	CL7	C2B-C1B-NB	5.79	114.11	110.23
21	4C	512	CL7	C1A-NA-C4A	5.79	109.81	106.30
21	33	514	CL7	C2B-C1B-NB	5.79	114.11	110.23
23	3B	619	8CT	C14-C13-C12	-5.79	119.05	127.31
23	3C	515	8CT	C04-C03-C02	-5.79	114.46	122.61
21	4C	517	CL7	C4D-C3D-CAD	-5.79	103.53	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	417	CL7	C1A-NA-C4A	5.79	109.80	106.30
21	33	516	CL7	C1A-NA-C4A	5.79	109.80	106.30
32	41	421	ZEX	C28-C27-C26	-5.79	117.20	127.09
21	33	513	CL7	C1A-NA-C4A	5.78	109.80	106.30
21	13	506	CL7	C2B-C1B-NB	5.78	114.11	110.23
21	3B	614	CL7	C1A-NA-C4A	5.78	109.80	106.30
23	2B	620	8CT	C14-C13-C12	-5.78	119.07	127.31
21	33	510	CL7	C1A-NA-C4A	5.77	109.80	106.30
21	1C	508	CL7	C1A-NA-C4A	5.77	109.80	106.30
21	2B	615	CL7	C1A-NA-C4A	5.77	109.80	106.30
32	11	421	ZEX	C28-C27-C26	-5.77	117.23	127.09
21	32	508	CL7	C1A-NA-C4A	5.77	109.79	106.30
21	12	507	CL7	C2B-C1B-NB	5.76	114.09	110.23
21	34	410	CL7	C2B-C1B-NB	5.76	114.09	110.23
31	3F	101	HEM	CHC-C4B-NB	5.76	130.68	124.42
23	1K	101	8CT	C19-C20-C21	-5.76	119.09	127.31
21	2C	504	CL7	C1A-NA-C4A	5.76	109.79	106.30
23	3K	101	8CT	C19-C20-C21	-5.76	119.09	127.31
21	23	409	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	3C	503	CL7	C1A-NA-C4A	5.75	109.78	106.30
21	4C	502	CL7	C4D-C3D-CAD	-5.75	103.55	107.42
31	4F	101	HEM	CHC-C4B-NB	5.75	130.67	124.42
21	42	515	CL7	C1A-NA-C4A	5.75	109.78	106.30
21	3C	512	CL7	C1A-NA-C4A	5.75	109.78	106.30
21	32	502	CL7	C1A-NA-C4A	5.75	109.78	106.30
21	23	415	CL7	C2B-C1B-NB	5.74	114.08	110.23
21	12	502	CL7	C1A-NA-C4A	5.74	109.78	106.30
21	4C	504	CL7	C1A-NA-C4A	5.74	109.78	106.30
21	4B	612	CL7	C1A-NA-C4A	5.74	109.78	106.30
31	2F	101	HEM	CHC-C4B-NB	5.74	130.65	124.42
21	3C	502	CL7	C4D-C3D-CAD	-5.74	103.56	107.42
21	1B	614	CL7	C1A-NA-C4A	5.74	109.77	106.30
21	43	407	CL7	C2B-C1B-NB	5.73	114.08	110.23
21	1B	608	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	22	516	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	32	516	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	42	502	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	3C	517	CL7	C4D-C3D-CAD	-5.73	103.56	107.42
21	2B	609	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	2B	613	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	2C	502	CL7	C4D-C3D-CAD	-5.73	103.56	107.42
21	3C	504	CL7	C1A-NA-C4A	5.73	109.77	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	34	404	CL7	C1A-NA-C4A	5.72	109.77	106.30
21	42	512	CL7	C1A-NA-C4A	5.72	109.77	106.30
31	1F	101	HEM	CHC-C4B-NB	5.72	130.63	124.42
23	2K	101	8CT	C19-C20-C21	-5.72	119.15	127.31
21	22	502	CL7	C1A-NA-C4A	5.72	109.76	106.30
21	23	414	CL7	C1A-NA-C4A	5.72	109.76	106.30
32	44	403	ZEX	C15-C14-C13	-5.72	119.15	127.31
23	2C	515	8CT	C35-C30-C29	-5.72	105.47	112.70
21	1B	605	CL7	C2B-C1B-NB	5.72	114.06	110.23
21	42	505	CL7	C2B-C1B-NB	5.71	114.06	110.23
21	22	515	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	32	515	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	33	506	CL7	C2B-C1B-NB	5.71	114.06	110.23
23	4K	101	8CT	C19-C20-C21	-5.71	119.16	127.31
21	31	418	CL7	C1A-NA-C4A	5.71	109.76	106.30
23	1C	515	8CT	C35-C30-C29	-5.71	105.48	112.70
32	24	403	ZEX	C15-C14-C13	-5.71	119.16	127.31
32	34	403	ZEX	C15-C14-C13	-5.71	119.16	127.31
21	13	507	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	2B	612	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	21	409	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	12	515	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	13	508	CL7	C1A-NA-C4A	5.71	109.76	106.30
21	12	512	CL7	C1A-NA-C4A	5.71	109.75	106.30
21	13	513	CL7	C1A-NA-C4A	5.71	109.75	106.30
21	14	413	CL7	C1A-NA-C4A	5.71	109.75	106.30
23	3B	618	8CT	C18-C17-C16	-5.70	119.17	127.31
21	4B	609	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	11	409	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	41	409	CL7	C1A-NA-C4A	5.70	109.75	106.30
23	2B	619	8CT	C18-C17-C16	-5.70	119.18	127.31
21	2C	512	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	32	505	CL7	C2B-C1B-NB	5.70	114.05	110.23
23	4B	619	8CT	C18-C17-C16	-5.70	119.18	127.31
23	4C	515	8CT	C35-C30-C29	-5.70	105.50	112.70
21	1C	513	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	4C	513	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	42	516	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	23	408	CL7	C1A-NA-C4A	5.69	109.75	106.30
21	31	407	CL7	C1A-NA-C4A	5.69	109.75	106.30
21	33	508	CL7	C1A-NA-C4A	5.69	109.75	106.30
21	12	505	CL7	C2B-C1B-NB	5.69	114.05	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	615	CL7	C1A-NA-C4A	5.69	109.75	106.30
21	12	505	CL7	C1-C2-C3	5.69	135.88	126.04
21	32	507	CL7	C2B-C1B-NB	5.69	114.04	110.23
21	1C	502	CL7	C4D-C3D-CAD	-5.69	103.59	107.42
21	44	413	CL7	C1A-NA-C4A	5.69	109.74	106.30
21	1C	503	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	31	408	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	41	405	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	22	507	CL7	C2B-C1B-NB	5.68	114.04	110.23
21	3B	605	CL7	C2B-C1B-NB	5.68	114.04	110.23
23	3C	515	8CT	C35-C30-C29	-5.68	105.52	112.70
21	42	514	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	11	404	CL7	C1A-NA-C4A	5.68	109.74	106.30
23	1B	618	8CT	C18-C17-C16	-5.68	119.21	127.31
21	42	505	CL7	C1-C2-C3	5.68	135.86	126.04
21	4B	613	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	42	507	CL7	C2B-C1B-NB	5.67	114.04	110.23
21	3C	508	CL7	C1A-NA-C4A	5.67	109.74	106.30
21	34	408	CL7	C1A-NA-C4A	5.67	109.74	106.30
32	14	403	ZEX	C15-C14-C13	-5.67	119.21	127.31
21	22	508	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	24	408	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	21	404	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	32	510	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	31	404	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	4C	508	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	4B	606	CL7	C2B-C1B-NB	5.67	114.03	110.23
21	24	404	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	42	508	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	11	407	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	24	413	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	4C	503	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	3B	608	CL7	C1A-NA-C4A	5.66	109.73	106.30
21	21	416	CL7	C4D-C3D-CAD	-5.66	103.61	107.42
21	22	505	CL7	C1-C2-C3	5.66	135.83	126.04
21	32	505	CL7	C1-C2-C3	5.66	135.83	126.04
21	22	505	CL7	C2B-C1B-NB	5.66	114.03	110.23
21	2C	513	CL7	C1A-NA-C4A	5.66	109.73	106.30
21	22	512	CL7	C1A-NA-C4A	5.66	109.73	106.30
21	42	507	CL7	C1A-NA-C4A	5.66	109.73	106.30
21	12	508	CL7	C1A-NA-C4A	5.65	109.72	106.30
21	22	514	CL7	C1A-NA-C4A	5.65	109.72	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1B	611	CL7	C1A-NA-C4A	5.65	109.72	106.30
32	22	522	ZEX	C27-C28-C29	-5.65	117.70	126.23
21	12	514	CL7	C1A-NA-C4A	5.65	109.72	106.30
21	44	408	CL7	C1A-NA-C4A	5.65	109.72	106.30
21	21	405	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	33	507	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	1B	612	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	14	408	CL7	C1A-NA-C4A	5.64	109.72	106.30
32	42	522	ZEX	C27-C28-C29	-5.64	117.71	126.23
21	21	407	CL7	C1A-NA-C4A	5.64	109.72	106.30
32	12	522	ZEX	C27-C28-C29	-5.64	117.72	126.23
21	22	504	CL7	C1A-NA-C4A	5.64	109.71	106.30
21	42	506	CL7	C4D-C3D-CAD	-5.64	103.63	107.42
21	44	405	CL7	C4D-C3D-CAD	-5.63	103.63	107.42
21	2B	606	CL7	C2B-C1B-NB	5.63	114.01	110.23
21	12	507	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	11	405	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	44	404	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	32	504	CL7	C1A-NA-C4A	5.62	109.71	106.30
21	43	408	CL7	C1A-NA-C4A	5.62	109.71	106.30
21	32	506	CL7	C4D-C3D-CAD	-5.62	103.64	107.42
21	3B	611	CL7	C1A-NA-C4A	5.62	109.70	106.30
21	3B	612	CL7	C1A-NA-C4A	5.62	109.70	106.30
21	1C	502	CL7	C1A-NA-C4A	5.62	109.70	106.30
21	2C	507	CL7	C1A-NA-C4A	5.62	109.70	106.30
23	2B	618	8CT	C18-C17-C16	-5.62	119.30	127.31
32	32	522	ZEX	C27-C28-C29	-5.61	117.75	126.23
21	12	504	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	2C	503	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	42	504	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	33	507	CL7	C2B-C1B-NB	5.61	113.99	110.23
21	12	516	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	43	409	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	11	416	CL7	C4D-C3D-CAD	-5.61	103.64	107.42
21	33	506	CL7	C4D-C3D-CAD	-5.61	103.64	107.42
21	43	408	CL7	C4D-C3D-CAD	-5.61	103.64	107.42
23	1B	617	8CT	C18-C17-C16	-5.61	119.31	127.31
23	4B	618	8CT	C18-C17-C16	-5.61	119.31	127.31
21	11	408	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	34	413	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	31	409	CL7	C1A-NA-C4A	5.61	109.69	106.30
21	41	407	CL7	C1A-NA-C4A	5.61	109.69	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	506	CL7	C4D-C3D-CAD	-5.60	103.65	107.42
21	32	512	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	43	407	CL7	C4D-C3D-CAD	-5.60	103.65	107.42
23	3B	617	8CT	C18-C17-C16	-5.60	119.32	127.31
21	1C	506	CL7	C2B-C1B-NB	5.60	113.98	110.23
21	21	408	CL7	C1A-NA-C4A	5.59	109.69	106.30
21	3C	513	CL7	C1A-NA-C4A	5.59	109.69	106.30
21	24	405	CL7	C4D-C3D-CAD	-5.59	103.66	107.42
21	2C	506	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	4C	506	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	32	515	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	4C	507	CL7	C1A-NA-C4A	5.59	109.69	106.30
21	13	507	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	43	408	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	24	416	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	34	416	CL7	C2B-C1B-NB	5.59	113.98	110.23
21	41	416	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	4C	502	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	31	416	CL7	C4D-C3D-CAD	-5.58	103.66	107.42
21	14	416	CL7	C2B-C1B-NB	5.58	113.97	110.23
21	41	412	CL7	C2B-C1B-NB	5.58	113.97	110.23
21	44	416	CL7	C2B-C1B-NB	5.58	113.97	110.23
21	3C	507	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	34	405	CL7	C4D-C3D-CAD	-5.58	103.67	107.42
21	22	506	CL7	C4D-C3D-CAD	-5.57	103.67	107.42
21	23	407	CL7	C4D-C3D-CAD	-5.57	103.67	107.42
21	12	510	CL7	C1A-NA-C4A	5.57	109.67	106.30
21	14	404	CL7	C1A-NA-C4A	5.57	109.67	106.30
21	21	412	CL7	C2B-C1B-NB	5.57	113.96	110.23
21	1C	507	CL7	C1A-NA-C4A	5.56	109.67	106.30
21	31	416	CL7	C1A-NA-C4A	5.56	109.67	106.30
23	2C	515	8CT	C24-C25-C26	-5.56	119.38	127.31
23	3C	515	8CT	C24-C25-C26	-5.56	119.38	127.31
21	23	408	CL7	C4D-C3D-CAD	-5.56	103.68	107.42
21	33	509	CL7	C1A-NA-C4A	5.55	109.66	106.30
21	22	515	CL7	C2B-C1B-NB	5.55	113.95	110.23
21	2C	517	CL7	C1A-NA-C4A	5.55	109.66	106.30
21	22	507	CL7	C1A-NA-C4A	5.55	109.66	106.30
21	41	416	CL7	C4D-C3D-CAD	-5.55	103.69	107.42
23	4C	515	8CT	C24-C25-C26	-5.55	119.39	127.31
21	22	510	CL7	C1A-NA-C4A	5.55	109.66	106.30
21	31	412	CL7	C2B-C1B-NB	5.55	113.95	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	506	CL7	C4D-C3D-CAD	-5.55	103.69	107.42
23	1C	515	8CT	C24-C25-C26	-5.54	119.40	127.31
21	2C	502	CL7	C1A-NA-C4A	5.54	109.66	106.30
21	3C	502	CL7	C1A-NA-C4A	5.54	109.66	106.30
21	31	405	CL7	C1A-NA-C4A	5.54	109.65	106.30
21	33	507	CL7	C4D-C3D-CAD	-5.54	103.69	107.42
21	14	405	CL7	C4D-C3D-CAD	-5.53	103.69	107.42
21	32	514	CL7	C1A-NA-C4A	5.53	109.65	106.30
21	34	409	CL7	C2B-C1B-NB	5.53	113.94	110.23
21	3C	506	CL7	C4D-C3D-CAD	-5.53	103.70	107.42
21	1C	506	CL7	C4D-C3D-CAD	-5.52	103.70	107.42
21	31	410	CL7	C1A-NA-C4A	5.52	109.64	106.30
21	42	510	CL7	C1A-NA-C4A	5.52	109.64	106.30
23	24	402	8CT	C19-C20-C21	-5.52	119.43	127.31
21	11	412	CL7	C2B-C1B-NB	5.52	113.93	110.23
23	34	402	8CT	C19-C20-C21	-5.52	119.44	127.31
21	13	507	CL7	C4D-C3D-CAD	-5.52	103.71	107.42
21	41	404	CL7	C1A-NA-C4A	5.52	109.64	106.30
21	43	416	CL7	C1A-NA-C4A	5.51	109.64	106.30
21	32	507	CL7	C1A-NA-C4A	5.51	109.64	106.30
21	41	408	CL7	C1A-NA-C4A	5.51	109.64	106.30
23	14	402	8CT	C19-C20-C21	-5.51	119.45	127.31
21	3C	506	CL7	C2B-C1B-NB	5.51	113.92	110.23
21	12	515	CL7	C2B-C1B-NB	5.50	113.92	110.23
21	42	515	CL7	C2B-C1B-NB	5.50	113.92	110.23
21	23	416	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	24	407	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	41	410	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	34	407	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	1C	517	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	4C	517	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	24	409	CL7	C2B-C1B-NB	5.49	113.91	110.23
21	22	506	CL7	C1A-NA-C4A	5.48	109.62	106.30
21	23	408	CL7	C2B-C1B-NB	5.48	113.91	110.23
21	14	409	CL7	C2B-C1B-NB	5.48	113.91	110.23
21	11	416	CL7	C1A-NA-C4A	5.48	109.62	106.30
23	4C	518	8CT	C19-C20-C21	-5.48	119.49	127.31
23	44	402	8CT	C19-C20-C21	-5.48	119.49	127.31
21	4C	506	CL7	C4D-C3D-CAD	-5.48	103.73	107.42
21	43	410	CL7	C1A-NA-C4A	5.47	109.61	106.30
21	3C	506	CL7	C1A-NA-C4A	5.47	109.61	106.30
21	13	515	CL7	C1A-NA-C4A	5.47	109.61	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	511	CL7	C1A-NA-C4A	5.47	109.61	106.30
21	33	515	CL7	C1A-NA-C4A	5.46	109.61	106.30
23	3K	101	8CT	C07-C02-C03	-5.46	114.80	122.73
21	11	415	CL7	C4D-C3D-CAD	-5.46	103.74	107.42
23	1C	518	8CT	C19-C20-C21	-5.46	119.52	127.31
21	3C	517	CL7	C1A-NA-C4A	5.46	109.60	106.30
21	32	511	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	4B	604	CL7	CMD-C2D-C1D	5.45	133.67	125.37
21	12	506	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	44	409	CL7	C2B-C1B-NB	5.45	113.89	110.23
23	3C	518	8CT	C19-C20-C21	-5.45	119.53	127.31
21	21	416	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	23	410	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	42	508	CL7	C2B-C1B-NB	5.44	113.88	110.23
21	2C	506	CL7	C4D-C3D-CAD	-5.44	103.76	107.42
21	41	415	CL7	C4D-C3D-CAD	-5.44	103.76	107.42
21	32	506	CL7	C1A-NA-C4A	5.44	109.59	106.30
21	4C	504	CL7	C4D-C3D-CAD	-5.44	103.76	107.42
21	21	415	CL7	C4D-C3D-CAD	-5.43	103.76	107.42
23	2C	518	8CT	C19-C20-C21	-5.43	119.56	127.31
21	12	511	CL7	C1A-NA-C4A	5.43	109.59	106.30
21	31	415	CL7	C4D-C3D-CAD	-5.43	103.77	107.42
23	2K	101	8CT	C07-C02-C03	-5.43	114.85	122.73
23	1K	101	8CT	C07-C02-C03	-5.43	114.85	122.73
21	12	508	CL7	C2B-C1B-NB	5.43	113.87	110.23
21	34	416	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	13	509	CL7	C1A-NA-C4A	5.42	109.58	106.30
23	4A	404	8CT	C14-C13-C12	-5.42	119.58	127.31
21	42	511	CL7	C1A-NA-C4A	5.42	109.58	106.30
23	4K	101	8CT	C07-C02-C03	-5.42	114.87	122.73
21	4A	403	CL7	C1A-NA-C4A	5.41	109.58	106.30
21	3B	606	CL7	CMD-C2D-C1D	5.41	133.61	125.37
21	2B	604	CL7	CMD-C2D-C1D	5.41	133.60	125.37
21	3B	603	CL7	CMD-C2D-C1D	5.41	133.60	125.37
21	42	506	CL7	C1A-NA-C4A	5.41	109.58	106.30
21	2B	607	CL7	CMD-C2D-C1D	5.41	133.60	125.37
21	23	418	CL7	C1A-NA-C4A	5.41	109.57	106.30
21	24	416	CL7	C1A-NA-C4A	5.41	109.57	106.30
21	1B	603	CL7	CMD-C2D-C1D	5.41	133.60	125.37
21	4B	607	CL7	CMD-C2D-C1D	5.41	133.60	125.37
21	13	517	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	43	418	CL7	C1A-NA-C4A	5.40	109.57	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	419	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	2C	506	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	32	508	CL7	C2B-C1B-NB	5.40	113.85	110.23
21	1C	506	CL7	C1A-NA-C4A	5.39	109.57	106.30
21	4C	506	CL7	C1A-NA-C4A	5.39	109.57	106.30
21	33	517	CL7	C1A-NA-C4A	5.39	109.56	106.30
23	1A	404	8CT	C14-C13-C12	-5.39	119.62	127.31
23	3A	404	8CT	C14-C13-C12	-5.39	119.62	127.31
21	31	419	CL7	C1A-NA-C4A	5.39	109.56	106.30
21	21	410	CL7	C1A-NA-C4A	5.39	109.56	106.30
21	33	501	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	2C	504	CL7	C4D-C3D-CAD	-5.38	103.80	107.42
21	11	410	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	1B	606	CL7	CMD-C2D-C1D	5.38	133.56	125.37
23	4K	101	8CT	C14-C13-C12	-5.38	119.63	127.31
21	3A	403	CL7	C1A-NA-C4A	5.38	109.56	106.30
23	2K	101	8CT	C14-C13-C12	-5.38	119.64	127.31
21	14	407	CL7	C1A-NA-C4A	5.37	109.55	106.30
32	42	519	ZEX	C35-C34-C33	-5.37	119.65	127.31
23	2A	404	8CT	C14-C13-C12	-5.37	119.65	127.31
21	14	416	CL7	C1A-NA-C4A	5.37	109.55	106.30
21	44	416	CL7	C1A-NA-C4A	5.37	109.55	106.30
21	44	407	CL7	C1A-NA-C4A	5.36	109.55	106.30
21	3B	604	CL7	C2B-C1B-NB	5.36	113.83	110.23
21	43	402	CL7	C1A-NA-C4A	5.36	109.55	106.30
23	3K	101	8CT	C14-C13-C12	-5.35	119.67	127.31
32	22	519	ZEX	C35-C34-C33	-5.35	119.67	127.31
32	32	519	ZEX	C35-C34-C33	-5.35	119.67	127.31
21	2A	403	CL7	C1A-NA-C4A	5.35	109.54	106.30
21	22	508	CL7	C2B-C1B-NB	5.35	113.82	110.23
21	1C	509	CL7	C1A-NA-C4A	5.34	109.54	106.30
21	2B	607	CL7	C1A-NA-C4A	5.34	109.54	106.30
21	4B	607	CL7	C1A-NA-C4A	5.34	109.54	106.30
32	12	519	ZEX	C35-C34-C33	-5.34	119.69	127.31
23	1D	406	8CT	C18-C17-C16	-5.34	119.69	127.31
21	21	419	CL7	C1A-NA-C4A	5.34	109.53	106.30
21	23	402	CL7	C1A-NA-C4A	5.34	109.53	106.30
23	2D	406	8CT	C18-C17-C16	-5.34	119.69	127.31
23	1K	101	8CT	C14-C13-C12	-5.33	119.70	127.31
21	2A	401	CL7	C1A-NA-C4A	5.33	109.53	106.30
21	1A	403	CL7	C1A-NA-C4A	5.33	109.53	106.30
21	4B	603	CL7	C1A-NA-C4A	5.33	109.53	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4D	406	8CT	C18-C17-C16	-5.33	119.71	127.31
21	2C	509	CL7	C1A-NA-C4A	5.32	109.52	106.30
21	43	417	CL7	CMD-C2D-C1D	5.32	133.47	125.37
23	3D	406	8CT	C18-C17-C16	-5.32	119.72	127.31
21	23	417	CL7	CMD-C2D-C1D	5.32	133.47	125.37
21	4B	605	CL7	C2B-C1B-NB	5.32	113.80	110.23
21	4C	509	CL7	C1A-NA-C4A	5.32	109.52	106.30
21	2B	605	CL7	C2B-C1B-NB	5.31	113.79	110.23
21	13	501	CL7	C1A-NA-C4A	5.31	109.52	106.30
23	1D	406	8CT	C01-C02-C03	-5.31	118.57	124.53
21	13	516	CL7	CMD-C2D-C1D	5.31	133.46	125.37
21	3B	606	CL7	C1A-NA-C4A	5.31	109.51	106.30
21	1C	504	CL7	C4D-C3D-CAD	-5.31	103.85	107.42
21	2A	407	CL7	CMD-C2D-C1D	5.30	133.45	125.37
21	4A	407	CL7	CMD-C2D-C1D	5.30	133.44	125.37
21	1A	407	CL7	CMD-C2D-C1D	5.30	133.44	125.37
32	13	525	ZEX	C35-C34-C33	-5.30	119.74	127.31
21	3B	602	CL7	C1A-NA-C4A	5.30	109.51	106.30
21	3C	504	CL7	C4D-C3D-CAD	-5.30	103.85	107.42
21	13	518	CL7	C1A-NA-C4A	5.30	109.51	106.30
21	1B	606	CL7	C1A-NA-C4A	5.30	109.51	106.30
23	3D	406	8CT	C01-C02-C03	-5.30	118.58	124.53
21	12	518	CL7	C1A-NA-C4A	5.29	109.51	106.30
32	33	525	ZEX	C35-C34-C33	-5.29	119.76	127.31
21	2B	617	CL7	C1A-NA-C4A	5.29	109.50	106.30
21	33	516	CL7	CMD-C2D-C1D	5.29	133.43	125.37
21	1B	604	CL7	C2B-C1B-NB	5.29	113.78	110.23
21	3B	609	CL7	C1A-NA-C4A	5.29	109.50	106.30
21	41	419	CL7	C1A-NA-C4A	5.29	109.50	106.30
21	3A	407	CL7	CMD-C2D-C1D	5.29	133.42	125.37
21	22	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	1B	602	CL7	C1A-NA-C4A	5.28	109.50	106.30
23	4B	618	8CT	C30-C31-C32	-5.28	114.97	121.47
21	3C	509	CL7	C1A-NA-C4A	5.28	109.50	106.30
23	4D	406	8CT	C01-C02-C03	-5.27	118.61	124.53
32	12	520	ZEX	C27-C28-C29	-5.27	118.27	126.23
21	33	518	CL7	C1A-NA-C4A	5.27	109.49	106.30
23	2D	406	8CT	C01-C02-C03	-5.27	118.61	124.53
32	23	401	ZEX	C35-C34-C33	-5.27	119.79	127.31
23	2B	618	8CT	C30-C31-C32	-5.27	114.99	121.47
21	32	518	CL7	C1A-NA-C4A	5.26	109.49	106.30
21	23	419	CL7	C1A-NA-C4A	5.26	109.49	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	603	CL7	C1A-NA-C4A	5.26	109.49	106.30
21	3A	401	CL7	C1A-NA-C4A	5.26	109.49	106.30
32	23	423	ZEX	C35-C34-C33	-5.26	119.80	127.31
32	33	522	ZEX	C35-C34-C33	-5.26	119.80	127.31
21	1A	401	CL7	C1A-NA-C4A	5.26	109.48	106.30
21	4A	401	CL7	C1A-NA-C4A	5.26	109.48	106.30
21	2B	610	CL7	C1A-NA-C4A	5.26	109.48	106.30
32	13	522	ZEX	C35-C34-C33	-5.25	119.82	127.31
32	43	401	ZEX	C35-C34-C33	-5.25	119.82	127.31
21	22	509	CL7	C1A-NA-C4A	5.25	109.48	106.30
21	42	518	CL7	C1A-NA-C4A	5.25	109.48	106.30
32	42	519	ZEX	C15-C14-C13	-5.24	119.83	127.31
21	14	412	CL7	C1A-NA-C4A	5.24	109.47	106.30
32	32	520	ZEX	C27-C28-C29	-5.24	118.32	126.23
21	4B	617	CL7	C1A-NA-C4A	5.24	109.47	106.30
32	22	520	ZEX	C27-C28-C29	-5.24	118.32	126.23
23	3B	617	8CT	C30-C31-C32	-5.24	115.02	121.47
21	4B	610	CL7	C1A-NA-C4A	5.24	109.47	106.30
32	43	423	ZEX	C35-C34-C33	-5.23	119.84	127.31
32	13	520	ZEX	C27-C28-C29	-5.23	118.33	126.23
23	1B	617	8CT	C30-C31-C32	-5.23	115.03	121.47
21	4B	606	CL7	CMD-C2D-C1D	5.23	133.33	125.37
21	3B	616	CL7	C1A-NA-C4A	5.23	109.47	106.30
32	42	520	ZEX	C27-C28-C29	-5.23	118.33	126.23
32	33	520	ZEX	C27-C28-C29	-5.23	118.34	126.23
21	41	412	CL7	C4D-C3D-CAD	-5.23	103.90	107.42
32	22	519	ZEX	C15-C14-C13	-5.23	119.85	127.31
21	3C	508	CL7	C2B-C1B-NB	5.22	113.73	110.23
21	24	412	CL7	C1A-NA-C4A	5.22	109.46	106.30
21	43	419	CL7	C1A-NA-C4A	5.22	109.46	106.30
32	32	519	ZEX	C15-C14-C13	-5.22	119.86	127.31
21	42	509	CL7	C1A-NA-C4A	5.22	109.46	106.30
21	44	412	CL7	C1A-NA-C4A	5.22	109.46	106.30
21	1B	605	CL7	CMD-C2D-C1D	5.22	133.31	125.37
21	11	417	CL7	C1A-NA-C4A	5.21	109.46	106.30
21	2B	606	CL7	CMD-C2D-C1D	5.21	133.31	125.37
23	3D	406	8CT	C30-C31-C32	-5.21	115.06	121.47
21	22	517	CL7	C1A-NA-C4A	5.21	109.45	106.30
21	31	412	CL7	C4D-C3D-CAD	-5.21	103.92	107.42
21	21	411	CL7	C1A-NA-C4A	5.20	109.45	106.30
21	4B	612	CL7	C2B-C1B-NB	5.20	113.72	110.23
32	43	421	ZEX	C27-C28-C29	-5.20	118.38	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1B	611	CL7	C2B-C1B-NB	5.20	113.72	110.23
21	32	509	CL7	C1A-NA-C4A	5.20	109.45	106.30
21	42	516	CL7	C4D-C3D-CAD	-5.20	103.92	107.42
21	41	409	CL7	C4D-C3D-CAD	-5.20	103.92	107.42
32	23	421	ZEX	C27-C28-C29	-5.20	118.38	126.23
21	44	412	CL7	C4D-C3D-CAD	-5.19	103.92	107.42
21	1B	609	CL7	C1A-NA-C4A	5.19	109.45	106.30
23	4D	406	8CT	C30-C31-C32	-5.19	115.08	121.47
23	2D	406	8CT	C30-C31-C32	-5.19	115.08	121.47
21	4C	508	CL7	C2B-C1B-NB	5.19	113.71	110.23
21	32	503	CL7	CMD-C2D-C1D	5.19	133.28	125.37
21	24	412	CL7	C4D-C3D-CAD	-5.19	103.93	107.42
21	3B	605	CL7	CMD-C2D-C1D	5.19	133.27	125.37
21	4B	608	CL7	C1A-NA-C4A	5.19	109.44	106.30
21	41	417	CL7	C1A-NA-C4A	5.19	109.44	106.30
21	21	403	CL7	C4D-C3D-CAD	-5.19	103.93	107.42
21	31	409	CL7	C4D-C3D-CAD	-5.19	103.93	107.42
32	12	519	ZEX	C15-C14-C13	-5.19	119.91	127.31
21	12	509	CL7	C1A-NA-C4A	5.19	109.44	106.30
21	11	412	CL7	C4D-C3D-CAD	-5.18	103.93	107.42
21	12	503	CL7	CMD-C2D-C1D	5.18	133.26	125.37
21	42	503	CL7	CMD-C2D-C1D	5.18	133.26	125.37
21	32	517	CL7	C1A-NA-C4A	5.18	109.44	106.30
23	1D	406	8CT	C30-C31-C32	-5.18	115.09	121.47
32	21	422	ZEX	C28-C27-C26	-5.18	118.24	127.09
32	31	422	ZEX	C28-C27-C26	-5.18	118.24	127.09
23	4K	101	8CT	C04-C03-C02	-5.18	115.32	122.61
21	21	417	CL7	C1A-NA-C4A	5.18	109.44	106.30
21	31	417	CL7	C1A-NA-C4A	5.18	109.44	106.30
21	32	516	CL7	C4D-C3D-CAD	-5.18	103.94	107.42
21	24	411	CL7	C1A-NA-C4A	5.17	109.43	106.30
21	22	503	CL7	CMD-C2D-C1D	5.17	133.25	125.37
21	31	403	CL7	C4D-C3D-CAD	-5.17	103.94	107.42
21	1C	508	CL7	C2B-C1B-NB	5.17	113.70	110.23
23	1K	101	8CT	C04-C03-C02	-5.17	115.33	122.61
21	14	412	CL7	C4D-C3D-CAD	-5.17	103.94	107.42
21	2C	508	CL7	C2B-C1B-NB	5.17	113.70	110.23
21	1B	616	CL7	C1A-NA-C4A	5.16	109.43	106.30
21	12	516	CL7	C4D-C3D-CAD	-5.16	103.94	107.42
32	11	422	ZEX	C28-C27-C26	-5.16	118.27	127.09
32	41	422	ZEX	C28-C27-C26	-5.16	118.27	127.09
21	3B	609	CL7	CMD-C2D-C1D	5.16	133.23	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4D	402	CL7	C4D-C3D-CAD	-5.16	103.95	107.42
21	3B	611	CL7	C2B-C1B-NB	5.16	113.69	110.23
32	34	403	ZEX	C35-C34-C33	-5.16	119.95	127.31
21	2B	612	CL7	C2B-C1B-NB	5.16	113.69	110.23
21	3D	402	CL7	C4D-C3D-CAD	-5.16	103.95	107.42
23	1B	617	8CT	C01-C02-C03	-5.15	118.75	124.53
23	1C	515	8CT	C18-C17-C16	-5.15	119.96	127.31
21	34	412	CL7	C1A-NA-C4A	5.15	109.42	106.30
21	14	411	CL7	C1A-NA-C4A	5.14	109.41	106.30
21	44	411	CL7	C1A-NA-C4A	5.14	109.41	106.30
21	3B	607	CL7	C1A-NA-C4A	5.14	109.41	106.30
21	1B	609	CL7	CMD-C2D-C1D	5.14	133.20	125.37
21	42	517	CL7	C1A-NA-C4A	5.14	109.41	106.30
21	34	412	CL7	C4D-C3D-CAD	-5.14	103.96	107.42
23	4B	618	8CT	C01-C02-C03	-5.14	118.76	124.53
32	14	403	ZEX	C35-C34-C33	-5.14	119.98	127.31
21	22	512	CL7	C2D-C1D-ND	5.14	113.67	110.23
21	32	512	CL7	C2D-C1D-ND	5.14	113.67	110.23
21	11	411	CL7	C1A-NA-C4A	5.14	109.41	106.30
21	23	413	CL7	C1A-NA-C4A	5.14	109.41	106.30
21	41	411	CL7	C1A-NA-C4A	5.14	109.41	106.30
32	32	522	ZEX	C15-C14-C13	-5.13	119.98	127.31
21	1B	607	CL7	C1A-NA-C4A	5.13	109.41	106.30
32	23	420	ZEX	C7-C8-C9	-5.13	118.48	126.23
21	43	413	CL7	C1A-NA-C4A	5.13	109.41	106.30
23	3B	617	8CT	C01-C02-C03	-5.13	118.77	124.53
21	3D	404	CL7	CMD-C2D-C1D	5.13	133.18	125.37
23	3K	101	8CT	C04-C03-C02	-5.13	115.39	122.61
21	43	416	CL7	C4D-C3D-CAD	-5.13	103.97	107.42
32	13	519	ZEX	C7-C8-C9	-5.13	118.49	126.23
32	43	420	ZEX	C7-C8-C9	-5.13	118.49	126.23
21	4B	610	CL7	CMD-C2D-C1D	5.13	133.18	125.37
23	2B	618	8CT	C01-C02-C03	-5.12	118.77	124.53
23	4C	515	8CT	C18-C17-C16	-5.12	120.00	127.31
21	12	517	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	12	504	CL7	CMD-C2D-C1D	5.12	133.17	125.37
23	2K	101	8CT	C04-C03-C02	-5.12	115.40	122.61
21	22	516	CL7	C4D-C3D-CAD	-5.12	103.97	107.42
21	3B	613	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	11	403	CL7	C4D-C3D-CAD	-5.12	103.97	107.42
21	41	403	CL7	C4D-C3D-CAD	-5.12	103.97	107.42
23	2C	515	8CT	C18-C17-C16	-5.12	120.00	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	504	CL7	CMD-C2D-C1D	5.12	133.16	125.37
32	12	522	ZEX	C15-C14-C13	-5.12	120.00	127.31
21	21	409	CL7	C4D-C3D-CAD	-5.12	103.98	107.42
21	31	411	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	2D	404	CL7	CMD-C2D-C1D	5.11	133.16	125.37
21	42	504	CL7	CMD-C2D-C1D	5.11	133.16	125.37
21	12	512	CL7	C2D-C1D-ND	5.11	113.66	110.23
21	2B	610	CL7	CMD-C2D-C1D	5.11	133.15	125.37
21	11	409	CL7	C4D-C3D-CAD	-5.11	103.98	107.42
21	21	412	CL7	C4D-C3D-CAD	-5.11	103.98	107.42
23	3C	515	8CT	C18-C17-C16	-5.11	120.02	127.31
21	4D	404	CL7	CMD-C2D-C1D	5.11	133.15	125.37
21	33	515	CL7	C4D-C3D-CAD	-5.11	103.98	107.42
32	33	519	ZEX	C7-C8-C9	-5.11	118.52	126.23
21	1B	613	CL7	C1A-NA-C4A	5.11	109.39	106.30
21	1D	404	CL7	CMD-C2D-C1D	5.10	133.14	125.37
32	22	522	ZEX	C15-C14-C13	-5.10	120.03	127.31
32	44	403	ZEX	C35-C34-C33	-5.10	120.03	127.31
32	42	522	ZEX	C15-C14-C13	-5.10	120.03	127.31
21	34	411	CL7	C1A-NA-C4A	5.10	109.39	106.30
21	41	417	CL7	CMD-C2D-C1D	5.10	133.13	125.37
21	42	512	CL7	C2D-C1D-ND	5.10	113.65	110.23
21	22	504	CL7	CMD-C2D-C1D	5.10	133.13	125.37
32	24	403	ZEX	C35-C34-C33	-5.09	120.04	127.31
21	21	417	CL7	CMD-C2D-C1D	5.09	133.13	125.37
21	1D	402	CL7	C4D-C3D-CAD	-5.09	103.99	107.42
21	32	502	CL7	C2B-C1B-NB	5.08	113.64	110.23
21	31	417	CL7	CMD-C2D-C1D	5.08	133.11	125.37
21	3C	505	CL7	CMD-C2D-C1D	5.08	133.11	125.37
21	33	512	CL7	C1A-NA-C4A	5.08	109.38	106.30
21	2B	608	CL7	C1A-NA-C4A	5.07	109.37	106.30
21	2D	402	CL7	C4D-C3D-CAD	-5.07	104.01	107.42
21	4D	402	CL7	C1A-NA-C4A	5.07	109.37	106.30
23	1K	101	8CT	C01-C02-C03	-5.07	118.84	124.53
21	13	515	CL7	C4D-C3D-CAD	-5.07	104.01	107.42
21	2D	402	CL7	C1A-NA-C4A	5.06	109.37	106.30
21	3D	402	CL7	C1A-NA-C4A	5.06	109.37	106.30
21	41	414	CL7	C1A-NA-C4A	5.06	109.36	106.30
21	11	414	CL7	C1A-NA-C4A	5.06	109.36	106.30
21	21	414	CL7	C1A-NA-C4A	5.06	109.36	106.30
21	23	412	CL7	C4D-C3D-CAD	-5.06	104.02	107.42
21	2C	505	CL7	CMD-C2D-C1D	5.06	133.07	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	416	CL7	C4D-C3D-CAD	-5.05	104.02	107.42
21	4C	505	CL7	CMD-C2D-C1D	5.05	133.06	125.37
21	11	417	CL7	CMD-C2D-C1D	5.05	133.06	125.37
23	4K	101	8CT	C01-C02-C03	-5.05	118.86	124.53
21	13	512	CL7	C1A-NA-C4A	5.04	109.35	106.30
21	13	511	CL7	C4D-C3D-CAD	-5.04	104.03	107.42
21	42	502	CL7	C2B-C1B-NB	5.04	113.61	110.23
21	1C	505	CL7	CMD-C2D-C1D	5.03	133.03	125.37
23	2B	620	8CT	C18-C17-C16	-5.03	120.14	127.31
21	21	410	CL7	CMD-C2D-C1D	5.03	133.02	125.37
21	2B	614	CL7	C1A-NA-C4A	5.03	109.34	106.30
21	4B	614	CL7	C1A-NA-C4A	5.03	109.34	106.30
21	24	416	CL7	C4D-C3D-CAD	-5.03	104.04	107.42
21	31	414	CL7	C1A-NA-C4A	5.02	109.34	106.30
32	24	419	ZEX	C35-C34-C33	-5.02	120.14	127.31
23	3K	101	8CT	C01-C02-C03	-5.02	118.89	124.53
21	31	414	CL7	C4D-C3D-CAD	-5.02	104.04	107.42
32	44	418	ZEX	C27-C28-C29	-5.02	118.65	126.23
21	31	410	CL7	CMD-C2D-C1D	5.02	133.01	125.37
21	33	508	CL7	C2B-C1B-NB	5.01	113.59	110.23
32	44	420	ZEX	C15-C14-C13	-5.01	120.16	127.31
21	44	416	CL7	C4D-C3D-CAD	-5.01	104.05	107.42
21	11	410	CL7	CMD-C2D-C1D	5.01	133.00	125.37
21	1D	402	CL7	C1A-NA-C4A	5.01	109.33	106.30
21	32	514	CL7	CMD-C2D-C1D	5.01	133.00	125.37
21	41	410	CL7	CMD-C2D-C1D	5.01	133.00	125.37
23	2B	618	8CT	C24-C25-C26	-5.01	120.16	127.31
32	24	420	ZEX	C15-C14-C13	-5.01	120.17	127.31
21	12	502	CL7	C2B-C1B-NB	5.01	113.59	110.23
32	14	419	ZEX	C35-C34-C33	-5.00	120.17	127.31
32	44	419	ZEX	C35-C34-C33	-5.00	120.17	127.31
21	43	409	CL7	C2B-C1B-NB	5.00	113.58	110.23
23	1B	618	8CT	C14-C13-C12	-5.00	120.18	127.31
23	4B	619	8CT	C14-C13-C12	-5.00	120.18	127.31
32	34	419	ZEX	C35-C34-C33	-5.00	120.18	127.31
23	1B	619	8CT	C18-C17-C16	-4.99	120.18	127.31
21	14	411	CL7	CMD-C2D-C1D	4.99	132.97	125.37
21	41	414	CL7	C4D-C3D-CAD	-4.99	104.06	107.42
23	2B	619	8CT	C14-C13-C12	-4.99	120.19	127.31
21	33	503	CL7	C4D-C3D-CAD	-4.99	104.06	107.42
21	22	514	CL7	CMD-C2D-C1D	4.99	132.96	125.37
23	1C	515	8CT	C19-C20-C21	-4.98	120.20	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4C	515	8CT	C19-C20-C21	-4.98	120.20	127.31
21	22	502	CL7	C2B-C1B-NB	4.98	113.57	110.23
23	1B	617	8CT	C24-C25-C26	-4.98	120.20	127.31
23	3B	619	8CT	C18-C17-C16	-4.98	120.20	127.31
23	2K	101	8CT	C01-C02-C03	-4.98	118.93	124.53
21	33	511	CL7	C4D-C3D-CAD	-4.98	104.07	107.42
21	12	514	CL7	CMD-C2D-C1D	4.98	132.96	125.37
21	42	514	CL7	CMD-C2D-C1D	4.98	132.96	125.37
23	3K	101	8CT	C10-C11-C12	-4.98	118.71	126.23
23	3B	617	8CT	C24-C25-C26	-4.98	120.21	127.31
23	4B	618	8CT	C24-C25-C26	-4.98	120.21	127.31
32	13	519	ZEX	C28-C27-C26	-4.98	118.59	127.09
21	23	404	CL7	C4D-C3D-CAD	-4.97	104.07	107.42
32	14	420	ZEX	C15-C14-C13	-4.97	120.21	127.31
23	4K	101	8CT	C35-C30-C29	-4.97	106.41	112.70
21	12	511	CL7	CMD-C2D-C1D	4.97	132.94	125.37
21	42	511	CL7	CMD-C2D-C1D	4.97	132.94	125.37
21	44	411	CL7	CMD-C2D-C1D	4.97	132.94	125.37
21	23	409	CL7	C2B-C1B-NB	4.97	113.56	110.23
21	14	416	CL7	C4D-C3D-CAD	-4.97	104.08	107.42
21	23	418	CL7	C4D-C3D-CAD	-4.97	104.08	107.42
23	4B	620	8CT	C18-C17-C16	-4.97	120.22	127.31
23	2K	101	8CT	C35-C30-C29	-4.97	106.42	112.70
21	34	416	CL7	C4D-C3D-CAD	-4.97	104.08	107.42
32	43	420	ZEX	C28-C27-C26	-4.97	118.60	127.09
21	32	511	CL7	CMD-C2D-C1D	4.97	132.93	125.37
21	24	411	CL7	CMD-C2D-C1D	4.97	132.93	125.37
21	34	411	CL7	CMD-C2D-C1D	4.97	132.93	125.37
21	22	511	CL7	CMD-C2D-C1D	4.96	132.93	125.37
32	23	420	ZEX	C28-C27-C26	-4.96	118.61	127.09
23	3K	101	8CT	C35-C30-C29	-4.96	106.43	112.70
21	13	517	CL7	C4D-C3D-CAD	-4.96	104.08	107.42
32	24	418	ZEX	C27-C28-C29	-4.96	118.74	126.23
32	34	418	ZEX	C27-C28-C29	-4.96	118.74	126.23
21	43	404	CL7	C4D-C3D-CAD	-4.96	104.08	107.42
32	34	420	ZEX	C15-C14-C13	-4.96	120.23	127.31
23	2A	404	8CT	C18-C17-C16	-4.96	120.23	127.31
23	2K	101	8CT	C10-C11-C12	-4.96	118.75	126.23
23	3C	515	8CT	C19-C20-C21	-4.96	120.24	127.31
23	1C	518	8CT	C14-C13-C12	-4.95	120.24	127.31
32	14	418	ZEX	C27-C28-C29	-4.95	118.75	126.23
32	33	519	ZEX	C28-C27-C26	-4.95	118.63	127.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1K	101	8CT	C35-C30-C29	-4.95	106.44	112.70
21	33	517	CL7	C4D-C3D-CAD	-4.95	104.09	107.42
23	4K	101	8CT	C10-C11-C12	-4.95	118.76	126.23
21	13	503	CL7	C4D-C3D-CAD	-4.95	104.09	107.42
23	2C	515	8CT	C19-C20-C21	-4.94	120.26	127.31
23	3B	618	8CT	C14-C13-C12	-4.94	120.26	127.31
21	43	412	CL7	C4D-C3D-CAD	-4.94	104.09	107.42
21	13	508	CL7	C2B-C1B-NB	4.94	113.54	110.23
23	1K	101	8CT	C10-C11-C12	-4.93	118.78	126.23
23	4A	404	8CT	C18-C17-C16	-4.92	120.28	127.31
21	21	414	CL7	C4D-C3D-CAD	-4.92	104.11	107.42
21	11	414	CL7	C4D-C3D-CAD	-4.92	104.11	107.42
23	3C	518	8CT	C14-C13-C12	-4.92	120.30	127.31
21	32	510	CL7	C4D-C3D-CAD	-4.91	104.11	107.42
23	2C	518	8CT	C14-C13-C12	-4.91	120.30	127.31
23	1A	404	8CT	C18-C17-C16	-4.91	120.30	127.31
21	43	411	CL7	C4D-C3D-CAD	-4.91	104.12	107.42
21	43	418	CL7	C4D-C3D-CAD	-4.91	104.12	107.42
21	23	411	CL7	C4D-C3D-CAD	-4.90	104.12	107.42
21	33	510	CL7	C4D-C3D-CAD	-4.90	104.12	107.42
21	42	503	CL7	C1D-ND-C4D	-4.90	102.86	106.33
23	3A	404	8CT	C18-C17-C16	-4.90	120.32	127.31
23	4C	518	8CT	C14-C13-C12	-4.89	120.33	127.31
21	31	407	CL7	C4D-C3D-CAD	-4.89	104.13	107.42
23	1B	626	8CT	C19-C18-C17	-4.89	113.46	123.47
21	3C	503	CL7	C1D-ND-C4D	-4.88	102.87	106.33
23	2B	601	8CT	C19-C18-C17	-4.88	113.48	123.47
23	3B	626	8CT	C19-C18-C17	-4.88	113.48	123.47
23	4B	601	8CT	C19-C18-C17	-4.88	113.48	123.47
21	1C	509	CL7	CMD-C2D-C1D	4.88	132.80	125.37
21	4C	509	CL7	CMD-C2D-C1D	4.88	132.80	125.37
21	12	512	CL7	C1D-ND-C4D	-4.88	102.87	106.33
21	2C	509	CL7	CMD-C2D-C1D	4.87	132.79	125.37
21	3C	509	CL7	CMD-C2D-C1D	4.87	132.78	125.37
21	13	510	CL7	C4D-C3D-CAD	-4.87	104.14	107.42
21	2B	623	CL7	C1A-NA-C4A	4.87	109.25	106.30
21	2C	503	CL7	C1D-ND-C4D	-4.86	102.88	106.33
31	2F	101	HEM	CHD-C1D-ND	4.86	129.70	124.42
21	1B	606	CL7	C4D-C3D-CAD	-4.86	104.15	107.42
21	22	503	CL7	C1D-ND-C4D	-4.86	102.88	106.33
31	1F	101	HEM	CHD-C1D-ND	4.86	129.70	124.42
21	22	510	CL7	C4D-C3D-CAD	-4.85	104.15	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	605	CL7	CMD-C2D-C1D	4.85	132.76	125.37
21	21	407	CL7	C4D-C3D-CAD	-4.85	104.16	107.42
21	2B	605	CL7	CMD-C2D-C1D	4.85	132.75	125.37
21	11	407	CL7	C4D-C3D-CAD	-4.85	104.16	107.42
21	41	407	CL7	C4D-C3D-CAD	-4.85	104.16	107.42
31	4F	101	HEM	CHD-C1D-ND	4.84	129.68	124.42
21	3B	604	CL7	CMD-C2D-C1D	4.84	132.75	125.37
23	2B	620	8CT	C30-C31-C32	-4.84	115.51	121.47
21	1B	604	CL7	CMD-C2D-C1D	4.83	132.73	125.37
21	3B	614	CL7	C4D-C3D-CAD	-4.83	104.17	107.42
21	1B	610	CL7	CMD-C2D-C1D	4.83	132.73	125.37
21	4B	611	CL7	CMD-C2D-C1D	4.83	132.73	125.37
21	4B	607	CL7	C4D-C3D-CAD	-4.83	104.17	107.42
21	4B	623	CL7	C1A-NA-C4A	4.83	109.22	106.30
21	12	510	CL7	C4D-C3D-CAD	-4.82	104.17	107.42
21	42	510	CL7	C4D-C3D-CAD	-4.82	104.17	107.42
31	3F	101	HEM	CHD-C1D-ND	4.82	129.66	124.42
21	3B	612	CL7	C4D-C3D-CAD	-4.82	104.18	107.42
21	4B	613	CL7	C4D-C3D-CAD	-4.82	104.18	107.42
21	22	512	CL7	C1D-ND-C4D	-4.81	102.92	106.33
21	32	512	CL7	C1D-ND-C4D	-4.81	102.92	106.33
21	2B	611	CL7	CMD-C2D-C1D	4.81	132.70	125.37
21	42	501	CL7	CMD-C2D-C1D	4.81	132.69	125.37
32	14	418	ZEX	C35-C34-C33	-4.81	120.45	127.31
21	1B	612	CL7	C4D-C3D-CAD	-4.81	104.19	107.42
21	43	409	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
23	3B	619	8CT	C30-C31-C32	-4.80	115.56	121.47
23	2B	620	8CT	C10-C11-C12	-4.80	118.98	126.23
23	1B	619	8CT	C30-C31-C32	-4.80	115.56	121.47
23	4B	620	8CT	C30-C31-C32	-4.80	115.56	121.47
21	13	508	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
32	43	421	ZEX	C15-C14-C13	-4.80	120.46	127.31
21	41	415	CL7	C1D-ND-C4D	-4.80	102.93	106.33
23	3B	619	8CT	C10-C11-C12	-4.80	118.98	126.23
21	33	504	CL7	C4D-C3D-CAD	-4.80	104.19	107.42
21	32	503	CL7	C1D-ND-C4D	-4.80	102.93	106.33
21	1B	616	CL7	CMD-C2D-C1D	4.80	132.67	125.37
21	4B	615	CL7	C4D-C3D-CAD	-4.79	104.19	107.42
21	12	501	CL7	CMD-C2D-C1D	4.79	132.67	125.37
21	3B	610	CL7	CMD-C2D-C1D	4.79	132.67	125.37
32	23	421	ZEX	C15-C14-C13	-4.79	120.47	127.31
21	32	501	CL7	CMD-C2D-C1D	4.79	132.66	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	503	CL7	C1D-ND-C4D	-4.79	102.93	106.33
21	42	512	CL7	C1D-ND-C4D	-4.79	102.93	106.33
21	43	405	CL7	C4D-C3D-CAD	-4.79	104.20	107.42
21	31	411	CL7	CMD-C2D-C1D	4.78	132.66	125.37
21	3B	616	CL7	CMD-C2D-C1D	4.78	132.65	125.37
21	1C	503	CL7	C1D-ND-C4D	-4.78	102.94	106.33
21	31	415	CL7	C1D-ND-C4D	-4.78	102.94	106.33
21	4C	503	CL7	C1D-ND-C4D	-4.78	102.94	106.33
21	23	405	CL7	C4D-C3D-CAD	-4.78	104.20	107.42
21	4B	617	CL7	CMD-C2D-C1D	4.78	132.65	125.37
21	3B	622	CL7	C1A-NA-C4A	4.78	109.19	106.30
23	4B	620	8CT	C10-C11-C12	-4.78	119.01	126.23
21	41	411	CL7	CMD-C2D-C1D	4.78	132.65	125.37
23	1B	619	8CT	C10-C11-C12	-4.78	119.02	126.23
21	22	501	CL7	CMD-C2D-C1D	4.77	132.64	125.37
21	2C	510	CL7	C1A-NA-C4A	4.77	109.19	106.30
21	21	411	CL7	CMD-C2D-C1D	4.77	132.64	125.37
21	33	501	CL7	C4D-C3D-CAD	-4.77	104.21	107.42
32	13	520	ZEX	C15-C14-C13	-4.77	120.50	127.31
21	13	504	CL7	C4D-C3D-CAD	-4.77	104.21	107.42
32	33	520	ZEX	C15-C14-C13	-4.76	120.51	127.31
21	3B	605	CL7	C1D-ND-C4D	-4.76	102.95	106.33
32	32	524	ZEX	C35-C34-C33	-4.76	120.52	127.31
32	24	418	ZEX	C35-C34-C33	-4.76	120.52	127.31
21	1B	614	CL7	C4D-C3D-CAD	-4.76	104.22	107.42
21	2B	615	CL7	C4D-C3D-CAD	-4.76	104.22	107.42
21	11	411	CL7	CMD-C2D-C1D	4.76	132.62	125.37
21	2B	617	CL7	CMD-C2D-C1D	4.76	132.61	125.37
21	2B	611	CL7	C1D-ND-C4D	-4.75	102.96	106.33
21	23	402	CL7	C4D-C3D-CAD	-4.75	104.22	107.42
32	34	418	ZEX	C35-C34-C33	-4.75	120.53	127.31
32	22	524	ZEX	C35-C34-C33	-4.75	120.53	127.31
21	2B	613	CL7	C4D-C3D-CAD	-4.75	104.22	107.42
21	1B	622	CL7	C1A-NA-C4A	4.75	109.17	106.30
21	2B	607	CL7	C4D-C3D-CAD	-4.74	104.23	107.42
21	33	503	CL7	C2D-C1D-ND	4.74	113.41	110.23
21	3C	510	CL7	C1A-NA-C4A	4.74	109.17	106.30
32	12	524	ZEX	C35-C34-C33	-4.74	120.55	127.31
32	21	422	ZEX	C27-C28-C29	-4.73	119.08	126.23
32	31	422	ZEX	C27-C28-C29	-4.73	119.08	126.23
32	42	524	ZEX	C35-C34-C33	-4.73	120.56	127.31
21	3C	501	CL7	C2D-C1D-ND	4.73	113.41	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	402	CL7	C4D-C3D-CAD	-4.73	104.23	107.42
21	43	403	CL7	CMD-C2D-C1D	4.73	132.58	125.37
21	3B	606	CL7	C4D-C3D-CAD	-4.73	104.24	107.42
21	41	411	CL7	C4D-C3D-CAD	-4.73	104.24	107.42
21	21	411	CL7	C4D-C3D-CAD	-4.73	104.24	107.42
21	4B	610	CL7	C4D-C3D-CAD	-4.73	104.24	107.42
32	24	403	ZEX	C11-C10-C9	-4.73	120.56	127.31
21	23	412	CL7	CMD-C2D-C1D	4.72	132.56	125.37
21	11	415	CL7	C1D-ND-C4D	-4.72	102.98	106.33
32	44	418	ZEX	C35-C34-C33	-4.72	120.57	127.31
21	13	511	CL7	CMD-C2D-C1D	4.72	132.56	125.37
21	44	406	CL7	CMD-C2D-C1D	4.72	132.56	125.37
32	41	422	ZEX	C27-C28-C29	-4.72	119.11	126.23
21	2B	606	CL7	C1D-ND-C4D	-4.72	102.98	106.33
21	1C	513	CL7	C1D-ND-C4D	-4.72	102.98	106.33
21	11	404	CL7	C1D-ND-C4D	-4.72	102.98	106.33
21	41	404	CL7	C1D-ND-C4D	-4.72	102.98	106.33
21	1C	501	CL7	C2D-C1D-ND	4.72	113.39	110.23
32	14	403	ZEX	C11-C10-C9	-4.71	120.58	127.31
23	1A	404	8CT	C01-C02-C03	-4.71	119.23	124.53
23	4A	404	8CT	C01-C02-C03	-4.71	119.23	124.53
21	2C	513	CL7	C1D-ND-C4D	-4.71	102.99	106.33
21	13	501	CL7	C4D-C3D-CAD	-4.71	104.25	107.42
21	33	508	CL7	C4D-C3D-CAD	-4.71	104.25	107.42
21	24	415	CL7	CMD-C2D-C1D	4.71	132.54	125.37
32	44	403	ZEX	C11-C10-C9	-4.71	120.59	127.31
21	33	502	CL7	CMD-C2D-C1D	4.71	132.54	125.37
21	21	404	CL7	C1D-ND-C4D	-4.71	102.99	106.33
21	31	404	CL7	C1D-ND-C4D	-4.71	102.99	106.33
21	3C	501	CL7	C1D-ND-C4D	-4.71	102.99	106.33
21	33	511	CL7	CMD-C2D-C1D	4.70	132.53	125.37
21	44	415	CL7	CMD-C2D-C1D	4.70	132.53	125.37
21	13	503	CL7	C2D-C1D-ND	4.70	113.39	110.23
21	24	406	CL7	CMD-C2D-C1D	4.70	132.53	125.37
21	4C	501	CL7	C1D-ND-C4D	-4.70	103.00	106.33
21	34	417	CL7	C2B-C1B-NB	4.70	113.38	110.23
23	3A	404	8CT	C01-C02-C03	-4.70	119.25	124.53
23	2B	618	8CT	C07-C02-C03	-4.70	115.91	122.73
23	2A	404	8CT	C01-C02-C03	-4.70	119.25	124.53
21	1C	510	CL7	C1A-NA-C4A	4.70	109.14	106.30
21	4C	510	CL7	C1A-NA-C4A	4.70	109.14	106.30
21	23	403	CL7	CMD-C2D-C1D	4.70	132.52	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	34	415	CL7	CMD-C2D-C1D	4.69	132.52	125.37
21	4B	606	CL7	C1D-ND-C4D	-4.69	103.00	106.33
21	1C	504	CL7	CMD-C2D-C1D	4.69	132.52	125.37
32	34	403	ZEX	C11-C10-C9	-4.69	120.61	127.31
21	3A	407	CL7	C1D-ND-C4D	-4.69	103.00	106.33
21	13	502	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	21	415	CL7	C1D-ND-C4D	-4.69	103.00	106.33
21	13	510	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	14	415	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	43	411	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	1A	407	CL7	C1D-ND-C4D	-4.69	103.00	106.33
32	11	422	ZEX	C27-C28-C29	-4.69	119.15	126.23
21	43	412	CL7	CMD-C2D-C1D	4.69	132.51	125.37
21	14	406	CL7	CMD-C2D-C1D	4.69	132.50	125.37
21	4C	513	CL7	C1D-ND-C4D	-4.68	103.01	106.33
21	2C	504	CL7	CMD-C2D-C1D	4.68	132.50	125.37
21	3C	504	CL7	CMD-C2D-C1D	4.68	132.50	125.37
23	2C	514	8CT	C01-C02-C03	-4.68	119.27	124.53
21	4C	501	CL7	C2D-C1D-ND	4.68	113.37	110.23
21	33	510	CL7	CMD-C2D-C1D	4.68	132.50	125.37
21	2C	501	CL7	C2D-C1D-ND	4.68	113.37	110.23
21	11	405	CL7	C1D-ND-C4D	-4.68	103.01	106.33
21	14	417	CL7	C2B-C1B-NB	4.68	113.37	110.23
21	13	503	CL7	C1D-ND-C4D	-4.68	103.01	106.33
21	1B	601	CL7	CMD-C2D-C1D	4.68	132.49	125.37
23	4C	514	8CT	C01-C02-C03	-4.68	119.28	124.53
21	43	405	CL7	C1D-ND-C4D	-4.68	103.01	106.33
21	14	404	CL7	CMD-C2D-C1D	4.68	132.49	125.37
21	23	411	CL7	CMD-C2D-C1D	4.68	132.49	125.37
21	24	417	CL7	C2B-C1B-NB	4.67	113.37	110.23
21	43	404	CL7	C2D-C1D-ND	4.67	113.37	110.23
21	34	406	CL7	CMD-C2D-C1D	4.67	132.49	125.37
21	3C	513	CL7	C1D-ND-C4D	-4.67	103.02	106.33
21	2C	501	CL7	C1D-ND-C4D	-4.67	103.02	106.33
21	1C	501	CL7	C1D-ND-C4D	-4.67	103.02	106.33
21	3B	601	CL7	CMD-C2D-C1D	4.67	132.48	125.37
21	21	405	CL7	C1D-ND-C4D	-4.67	103.02	106.33
23	3C	514	8CT	C01-C02-C03	-4.67	119.29	124.53
21	3B	610	CL7	C1D-ND-C4D	-4.67	103.02	106.33
21	33	503	CL7	C1D-ND-C4D	-4.67	103.02	106.33
21	4C	504	CL7	CMD-C2D-C1D	4.66	132.47	125.37
21	34	404	CL7	CMD-C2D-C1D	4.66	132.47	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	411	CL7	C4D-C3D-CAD	-4.66	104.28	107.42
21	24	404	CL7	CMD-C2D-C1D	4.66	132.47	125.37
21	31	413	CL7	CMD-C2D-C1D	4.66	132.47	125.37
21	4B	611	CL7	C1D-ND-C4D	-4.66	103.02	106.33
21	4C	511	CL7	C1D-ND-C4D	-4.66	103.02	106.33
21	2B	610	CL7	C4D-C3D-CAD	-4.66	104.28	107.42
32	34	420	ZEX	C11-C10-C9	-4.66	120.66	127.31
23	3B	617	8CT	C07-C02-C03	-4.66	115.97	122.73
21	11	402	CL7	C4D-C3D-CAD	-4.66	104.28	107.42
21	23	409	CL7	C4D-C3D-CAD	-4.66	104.29	107.42
21	4B	602	CL7	CMD-C2D-C1D	4.66	132.46	125.37
23	1B	617	8CT	C07-C02-C03	-4.66	115.97	122.73
23	4B	618	8CT	C07-C02-C03	-4.66	115.97	122.73
21	1B	609	CL7	C4D-C3D-CAD	-4.66	104.29	107.42
21	21	402	CL7	C4D-C3D-CAD	-4.66	104.29	107.42
21	11	411	CL7	C4D-C3D-CAD	-4.65	104.29	107.42
21	11	413	CL7	CMD-C2D-C1D	4.65	132.46	125.37
21	41	413	CL7	CMD-C2D-C1D	4.65	132.46	125.37
21	23	404	CL7	C1D-ND-C4D	-4.65	103.03	106.33
21	1B	605	CL7	C1D-ND-C4D	-4.65	103.03	106.33
21	21	413	CL7	CMD-C2D-C1D	4.65	132.45	125.37
23	1C	514	8CT	C01-C02-C03	-4.65	119.31	124.53
21	3C	502	CL7	CMD-C2D-C1D	4.65	132.45	125.37
21	21	419	CL7	CMD-C2D-C1D	4.65	132.45	125.37
32	24	420	ZEX	C11-C10-C9	-4.64	120.68	127.31
21	41	419	CL7	CMD-C2D-C1D	4.64	132.44	125.37
32	14	420	ZEX	C11-C10-C9	-4.64	120.68	127.31
32	44	420	ZEX	C11-C10-C9	-4.64	120.68	127.31
21	21	404	CL7	CMD-C2D-C1D	4.64	132.44	125.37
21	44	417	CL7	C2B-C1B-NB	4.64	113.34	110.23
21	1B	616	CL7	C4D-C3D-CAD	-4.64	104.30	107.42
23	1B	626	8CT	C01-C02-C03	-4.64	119.32	124.53
21	43	415	CL7	C4D-C3D-CAD	-4.64	104.30	107.42
21	2B	602	CL7	CMD-C2D-C1D	4.64	132.43	125.37
21	34	412	CL7	CMD-C2D-C1D	4.64	132.43	125.37
21	41	402	CL7	C4D-C3D-CAD	-4.64	104.30	107.42
21	2B	611	CL7	C2D-C1D-ND	4.64	113.34	110.23
21	4B	611	CL7	C2D-C1D-ND	4.63	113.34	110.23
21	44	412	CL7	CMD-C2D-C1D	4.63	132.43	125.37
21	4D	402	CL7	CMD-C2D-C1D	4.63	132.42	125.37
21	13	514	CL7	C4D-C3D-CAD	-4.63	104.31	107.42
21	2C	502	CL7	CMD-C2D-C1D	4.63	132.42	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	403	CL7	C4D-C3D-CAD	-4.63	104.31	107.42
23	3C	514	8CT	C19-C20-C21	-4.63	120.71	127.31
21	22	518	CL7	CMD-C2D-C1D	4.63	132.42	125.37
21	44	404	CL7	CMD-C2D-C1D	4.63	132.41	125.37
21	31	419	CL7	CMD-C2D-C1D	4.63	132.41	125.37
23	2B	601	8CT	C01-C02-C03	-4.62	119.33	124.53
21	2A	407	CL7	C1D-ND-C4D	-4.62	103.05	106.33
21	23	404	CL7	C2D-C1D-ND	4.62	113.33	110.23
21	33	518	CL7	CMD-C2D-C1D	4.62	132.41	125.37
21	3B	609	CL7	C4D-C3D-CAD	-4.62	104.31	107.42
21	24	414	CL7	C1D-ND-C4D	-4.62	103.05	106.33
21	24	410	CL7	CMD-C2D-C1D	4.62	132.41	125.37
21	23	419	CL7	CMD-C2D-C1D	4.62	132.40	125.37
21	11	419	CL7	CMD-C2D-C1D	4.62	132.40	125.37
21	31	405	CL7	C1D-ND-C4D	-4.62	103.06	106.33
23	2C	514	8CT	C19-C20-C21	-4.61	120.72	127.31
21	44	415	CL7	O2D-CGD-CBD	4.61	119.47	111.27
21	42	518	CL7	CMD-C2D-C1D	4.61	132.40	125.37
21	13	504	CL7	C1D-ND-C4D	-4.61	103.06	106.33
21	4C	502	CL7	CMD-C2D-C1D	4.61	132.39	125.37
23	1C	514	8CT	C19-C20-C21	-4.61	120.73	127.31
23	4C	514	8CT	C19-C20-C21	-4.61	120.73	127.31
21	33	514	CL7	C4D-C3D-CAD	-4.61	104.32	107.42
21	41	405	CL7	C1D-ND-C4D	-4.61	103.06	106.33
23	3B	626	8CT	C01-C02-C03	-4.61	119.35	124.53
21	4A	407	CL7	C1D-ND-C4D	-4.61	103.06	106.33
21	34	415	CL7	O2D-CGD-CBD	4.61	119.45	111.27
21	1D	402	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	14	410	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	2D	402	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	24	413	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	44	410	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	3D	404	CL7	C1D-ND-C4D	-4.61	103.06	106.33
21	2B	603	CL7	CMD-C2D-C1D	4.61	132.38	125.37
21	23	415	CL7	C4D-C3D-CAD	-4.61	104.32	107.42
21	14	412	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	32	518	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	14	415	CL7	O2D-CGD-CBD	4.60	119.45	111.27
21	3D	402	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	24	414	CL7	C2D-C1D-ND	4.60	113.32	110.23
21	11	404	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	31	404	CL7	CMD-C2D-C1D	4.60	132.38	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	419	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	24	412	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	1C	502	CL7	CMD-C2D-C1D	4.60	132.38	125.37
21	3B	610	CL7	C2D-C1D-ND	4.60	113.32	110.23
21	23	403	CL7	C4D-C3D-CAD	-4.60	104.33	107.42
21	31	413	CL7	C2D-C1D-ND	4.60	113.31	110.23
21	1D	405	CL7	CMD-C2D-C1D	4.60	132.37	125.37
21	34	408	CL7	CMD-C2D-C1D	4.60	132.37	125.37
21	33	502	CL7	C4D-C3D-CAD	-4.60	104.33	107.42
21	43	404	CL7	C1D-ND-C4D	-4.60	103.07	106.33
21	12	518	CL7	CMD-C2D-C1D	4.60	132.37	125.37
21	24	415	CL7	O2D-CGD-CBD	4.60	119.44	111.27
21	2D	404	CL7	C1D-ND-C4D	-4.60	103.07	106.33
21	1B	610	CL7	C2D-C1D-ND	4.60	113.31	110.23
21	14	413	CL7	CMD-C2D-C1D	4.60	132.37	125.37
21	43	410	CL7	CMD-C2D-C1D	4.60	132.37	125.37
21	44	413	CL7	CMD-C2D-C1D	4.60	132.37	125.37
21	2B	623	CL7	CMD-C2D-C1D	4.59	132.37	125.37
21	13	518	CL7	CMD-C2D-C1D	4.59	132.37	125.37
21	4D	405	CL7	CMD-C2D-C1D	4.59	132.36	125.37
21	2C	511	CL7	C1D-ND-C4D	-4.59	103.07	106.33
21	41	413	CL7	C2D-C1D-ND	4.59	113.31	110.23
23	4B	601	8CT	C01-C02-C03	-4.59	119.37	124.53
21	34	414	CL7	C1D-ND-C4D	-4.59	103.08	106.33
21	1B	602	CL7	CMD-C2D-C1D	4.59	132.35	125.37
21	2C	511	CL7	CMD-C2D-C1D	4.59	132.35	125.37
21	41	408	CL7	CMD-C2D-C1D	4.59	132.35	125.37
21	21	413	CL7	C2D-C1D-ND	4.59	113.31	110.23
21	1D	404	CL7	C1D-ND-C4D	-4.58	103.08	106.33
21	31	402	CL7	C4D-C3D-CAD	-4.58	104.33	107.42
21	34	413	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	44	408	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	1B	610	CL7	C1D-ND-C4D	-4.58	103.08	106.33
21	41	413	CL7	C1D-ND-C4D	-4.58	103.08	106.33
21	41	404	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	1B	622	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	34	410	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	14	408	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	4B	603	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	13	501	CL7	C1D-ND-C4D	-4.58	103.08	106.33
21	21	408	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	3C	511	CL7	CMD-C2D-C1D	4.58	132.34	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	511	CL7	CMD-C2D-C1D	4.58	132.34	125.37
21	4B	623	CL7	CMD-C2D-C1D	4.57	132.34	125.37
21	3C	511	CL7	C1D-ND-C4D	-4.57	103.09	106.33
21	23	410	CL7	CMD-C2D-C1D	4.57	132.33	125.37
21	33	509	CL7	CMD-C2D-C1D	4.57	132.33	125.37
21	1C	511	CL7	C1D-ND-C4D	-4.57	103.09	106.33
21	3B	622	CL7	CMD-C2D-C1D	4.57	132.32	125.37
21	22	517	CL7	C4D-C3D-CAD	-4.57	104.35	107.42
21	2B	617	CL7	C1D-ND-C4D	-4.57	103.09	106.33
21	11	413	CL7	C2D-C1D-ND	4.57	113.29	110.23
21	2B	617	CL7	C4D-C3D-CAD	-4.57	104.35	107.42
21	1C	511	CL7	CMD-C2D-C1D	4.56	132.32	125.37
21	3D	405	CL7	CMD-C2D-C1D	4.56	132.32	125.37
23	4B	601	8CT	C24-C23-C21	-4.56	113.60	126.42
21	4B	616	CL7	CMD-C2D-C1D	4.56	132.32	125.37
23	24	402	8CT	C01-C02-C03	-4.56	119.41	124.53
23	34	402	8CT	C01-C02-C03	-4.56	119.41	124.53
21	21	413	CL7	C1D-ND-C4D	-4.56	103.09	106.33
21	31	413	CL7	C1D-ND-C4D	-4.56	103.09	106.33
21	12	517	CL7	C4D-C3D-CAD	-4.56	104.35	107.42
21	13	509	CL7	C4D-C3D-CAD	-4.56	104.35	107.42
21	24	408	CL7	CMD-C2D-C1D	4.56	132.31	125.37
21	31	408	CL7	CMD-C2D-C1D	4.56	132.31	125.37
21	33	504	CL7	C1D-ND-C4D	-4.56	103.10	106.33
23	2B	601	8CT	C24-C23-C21	-4.56	113.61	126.42
23	3B	626	8CT	C24-C23-C21	-4.56	113.61	126.42
21	11	413	CL7	C1D-ND-C4D	-4.56	103.10	106.33
21	41	414	CL7	CMD-C2D-C1D	4.55	132.30	125.37
23	1B	626	8CT	C24-C23-C21	-4.55	113.63	126.42
21	11	414	CL7	CMD-C2D-C1D	4.55	132.30	125.37
21	23	405	CL7	C1D-ND-C4D	-4.55	103.10	106.33
21	1B	607	CL7	C1D-ND-C4D	-4.55	103.10	106.33
32	24	419	ZEX	C8-C7-C6	-4.55	114.43	127.20
21	21	414	CL7	CMD-C2D-C1D	4.55	132.29	125.37
21	31	414	CL7	CMD-C2D-C1D	4.55	132.29	125.37
21	41	418	CL7	CMD-C2D-C1D	4.55	132.29	125.37
21	31	420	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	2B	616	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	43	402	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	11	408	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	13	512	CL7	CMD-C2D-C1D	4.54	132.29	125.37
21	24	414	CL7	C4D-C3D-CAD	-4.54	104.36	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	44	414	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	21	416	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	4B	617	CL7	C4D-C3D-CAD	-4.54	104.36	107.42
23	1C	518	8CT	C01-C02-C03	-4.54	119.43	124.53
21	13	509	CL7	CMD-C2D-C1D	4.54	132.28	125.37
21	2D	405	CL7	CMD-C2D-C1D	4.54	132.28	125.37
32	34	419	ZEX	C8-C7-C6	-4.54	114.46	127.20
21	23	402	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	33	501	CL7	C1D-ND-C4D	-4.54	103.11	106.33
21	11	405	CL7	CMD-C2D-C1D	4.54	132.28	125.37
23	44	402	8CT	C01-C02-C03	-4.54	119.44	124.53
21	21	418	CL7	CMD-C2D-C1D	4.54	132.28	125.37
21	14	414	CL7	C1D-ND-C4D	-4.53	103.11	106.33
21	11	402	CL7	CMD-C2D-C1D	4.53	132.27	125.37
32	14	419	ZEX	C8-C7-C6	-4.53	114.47	127.20
32	44	419	ZEX	C8-C7-C6	-4.53	114.47	127.20
23	2C	518	8CT	C01-C02-C03	-4.53	119.44	124.53
21	3B	615	CL7	CMD-C2D-C1D	4.53	132.27	125.37
21	41	420	CL7	CMD-C2D-C1D	4.53	132.27	125.37
21	31	413	CL7	C4D-C3D-CAD	-4.53	104.37	107.42
23	14	402	8CT	C01-C02-C03	-4.53	119.44	124.53
21	22	503	CL7	C2D-C1D-ND	4.53	113.27	110.23
21	1B	615	CL7	CMD-C2D-C1D	4.53	132.27	125.37
21	3B	602	CL7	CMD-C2D-C1D	4.53	132.27	125.37
21	42	503	CL7	C2D-C1D-ND	4.53	113.27	110.23
21	41	412	CL7	C1D-ND-C4D	-4.53	103.12	106.33
21	14	414	CL7	C4D-C3D-CAD	-4.53	104.37	107.42
21	32	517	CL7	C4D-C3D-CAD	-4.53	104.37	107.42
21	44	414	CL7	C4D-C3D-CAD	-4.53	104.37	107.42
21	21	405	CL7	CMD-C2D-C1D	4.53	132.26	125.37
21	31	405	CL7	CMD-C2D-C1D	4.53	132.26	125.37
21	3C	510	CL7	CMD-C2D-C1D	4.53	132.26	125.37
21	23	413	CL7	CMD-C2D-C1D	4.53	132.26	125.37
21	11	413	CL7	C4D-C3D-CAD	-4.53	104.38	107.42
21	23	410	CL7	C4D-C3D-CAD	-4.53	104.38	107.42
21	31	404	CL7	C4D-C3D-CAD	-4.53	104.38	107.42
21	22	505	CL7	C1D-ND-C4D	-4.52	103.12	106.33
21	2C	510	CL7	CMD-C2D-C1D	4.52	132.26	125.37
21	21	420	CL7	CMD-C2D-C1D	4.52	132.26	125.37
21	13	502	CL7	C4D-C3D-CAD	-4.52	104.38	107.42
21	31	417	CL7	C4D-C3D-CAD	-4.52	104.38	107.42
21	31	418	CL7	CMD-C2D-C1D	4.52	132.25	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	404	CL7	C4D-C3D-CAD	-4.52	104.38	107.42
21	1C	510	CL7	CMD-C2D-C1D	4.52	132.25	125.37
21	4C	510	CL7	CMD-C2D-C1D	4.52	132.25	125.37
21	11	418	CL7	CMD-C2D-C1D	4.52	132.25	125.37
21	23	416	CL7	CMD-C2D-C1D	4.52	132.25	125.37
21	43	416	CL7	CMD-C2D-C1D	4.51	132.25	125.37
21	4B	617	CL7	C1D-ND-C4D	-4.51	103.13	106.33
21	44	414	CL7	C2D-C1D-ND	4.51	113.26	110.23
21	21	417	CL7	C4D-C3D-CAD	-4.51	104.38	107.42
21	41	405	CL7	CMD-C2D-C1D	4.51	132.24	125.37
21	34	414	CL7	C2D-C1D-ND	4.51	113.26	110.23
21	3B	616	CL7	C4D-C3D-CAD	-4.51	104.39	107.42
21	42	517	CL7	C4D-C3D-CAD	-4.51	104.39	107.42
32	24	420	ZEX	C7-C8-C9	-4.51	119.42	126.23
21	31	402	CL7	CMD-C2D-C1D	4.51	132.24	125.37
21	11	406	CL7	C1D-ND-C4D	-4.51	103.13	106.33
21	41	416	CL7	C1D-ND-C4D	-4.51	103.13	106.33
21	11	420	CL7	CMD-C2D-C1D	4.51	132.23	125.37
21	12	505	CL7	C1D-ND-C4D	-4.51	103.13	106.33
21	42	505	CL7	C1D-ND-C4D	-4.51	103.13	106.33
21	33	512	CL7	CMD-C2D-C1D	4.51	132.23	125.37
32	43	423	ZEX	C15-C14-C13	-4.51	120.88	127.31
21	11	412	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	2B	602	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	21	412	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	4D	404	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	1B	605	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	11	404	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	34	414	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	41	404	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	41	406	CL7	C1D-ND-C4D	-4.50	103.14	106.33
21	1A	403	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	4A	403	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	43	413	CL7	CMD-C2D-C1D	4.50	132.22	125.37
23	3C	518	8CT	C01-C02-C03	-4.50	119.48	124.53
21	43	410	CL7	C4D-C3D-CAD	-4.50	104.39	107.42
21	41	402	CL7	CMD-C2D-C1D	4.50	132.22	125.37
21	43	416	CL7	C2D-C1D-ND	4.49	113.25	110.23
21	33	503	CL7	CMD-C2D-C1D	4.49	132.21	125.37
32	14	420	ZEX	C7-C8-C9	-4.49	119.45	126.23
32	32	519	ZEX	C7-C8-C9	-4.49	119.45	126.23
21	3A	403	CL7	CMD-C2D-C1D	4.49	132.21	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4C	518	8CT	C01-C02-C03	-4.49	119.48	124.53
21	33	506	CL7	CMD-C2D-C1D	4.49	132.21	125.37
21	41	413	CL7	C4D-C3D-CAD	-4.49	104.40	107.42
21	31	406	CL7	C1D-ND-C4D	-4.49	103.14	106.33
21	14	416	CL7	CMD-C2D-C1D	4.49	132.20	125.37
21	21	413	CL7	C4D-C3D-CAD	-4.49	104.40	107.42
21	1B	616	CL7	C1D-ND-C4D	-4.49	103.15	106.33
21	2B	608	CL7	C1D-ND-C4D	-4.49	103.15	106.33
21	44	416	CL7	CMD-C2D-C1D	4.49	132.20	125.37
32	44	420	ZEX	C7-C8-C9	-4.49	119.46	126.23
21	4B	616	CL7	C4D-C3D-CAD	-4.49	104.40	107.42
21	33	515	CL7	CMD-C2D-C1D	4.48	132.20	125.37
21	13	503	CL7	CMD-C2D-C1D	4.48	132.20	125.37
21	23	407	CL7	CMD-C2D-C1D	4.48	132.20	125.37
21	31	415	CL7	C2D-C1D-ND	4.48	113.24	110.23
21	11	419	CL7	C1D-ND-C4D	-4.48	103.15	106.33
21	44	406	CL7	C1D-ND-C4D	-4.48	103.15	106.33
21	12	503	CL7	C2D-C1D-ND	4.48	113.24	110.23
21	21	402	CL7	CMD-C2D-C1D	4.48	132.19	125.37
21	11	417	CL7	C4D-C3D-CAD	-4.48	104.41	107.42
21	13	506	CL7	CMD-C2D-C1D	4.48	132.19	125.37
21	43	404	CL7	CMD-C2D-C1D	4.48	132.19	125.37
21	1C	504	CL7	C1D-ND-C4D	-4.48	103.15	106.33
32	12	519	ZEX	C7-C8-C9	-4.48	119.47	126.23
21	21	406	CL7	C1D-ND-C4D	-4.48	103.16	106.33
21	22	506	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	32	505	CL7	C1D-ND-C4D	-4.47	103.16	106.33
21	12	506	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	2A	403	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	24	405	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	4B	602	CL7	C1D-ND-C4D	-4.47	103.16	106.33
21	4B	608	CL7	C1D-ND-C4D	-4.47	103.16	106.33
32	34	420	ZEX	C7-C8-C9	-4.47	119.48	126.23
21	41	417	CL7	C4D-C3D-CAD	-4.47	104.41	107.42
21	3C	503	CL7	CMD-C2D-C1D	4.47	132.18	125.37
21	3C	504	CL7	C1D-ND-C4D	-4.47	103.16	106.33
21	31	416	CL7	C1D-ND-C4D	-4.47	103.16	106.33
32	23	423	ZEX	C15-C14-C13	-4.47	120.93	127.31
21	22	505	CL7	O2A-C1-C2	-4.47	96.89	108.64
21	32	505	CL7	O2A-C1-C2	-4.47	96.89	108.64
21	34	406	CL7	C1D-ND-C4D	-4.47	103.16	106.33
21	13	515	CL7	CMD-C2D-C1D	4.47	132.17	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	414	CL7	CMD-C2D-C1D	4.47	132.17	125.37
21	21	404	CL7	C4D-C3D-CAD	-4.47	104.42	107.42
21	32	516	CL7	CMD-C2D-C1D	4.47	132.17	125.37
21	42	516	CL7	CMD-C2D-C1D	4.46	132.17	125.37
32	13	522	ZEX	C15-C14-C13	-4.46	120.94	127.31
21	2C	503	CL7	CMD-C2D-C1D	4.46	132.17	125.37
21	23	414	CL7	CMD-C2D-C1D	4.46	132.17	125.37
21	32	506	CL7	CMD-C2D-C1D	4.46	132.17	125.37
21	33	513	CL7	CMD-C2D-C1D	4.46	132.17	125.37
21	34	416	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	12	515	CL7	C4D-C3D-CAD	-4.46	104.42	107.42
21	42	515	CL7	C4D-C3D-CAD	-4.46	104.42	107.42
21	1C	503	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	14	414	CL7	C2D-C1D-ND	4.46	113.22	110.23
21	4C	503	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	43	407	CL7	CMD-C2D-C1D	4.46	132.16	125.37
32	33	522	ZEX	C15-C14-C13	-4.46	120.95	127.31
21	2B	612	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	12	516	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	22	516	CL7	CMD-C2D-C1D	4.46	132.16	125.37
21	42	506	CL7	CMD-C2D-C1D	4.45	132.15	125.37
21	31	412	CL7	C1D-ND-C4D	-4.45	103.17	106.33
21	44	405	CL7	CMD-C2D-C1D	4.45	132.15	125.37
32	44	418	ZEX	C11-C10-C9	-4.45	120.95	127.31
21	42	505	CL7	O2A-C1-C2	-4.45	96.93	108.64
32	42	519	ZEX	C7-C8-C9	-4.45	119.51	126.23
21	24	404	CL7	C4D-C3D-CAD	-4.45	104.42	107.42
21	23	404	CL7	CMD-C2D-C1D	4.45	132.15	125.37
21	24	416	CL7	CMD-C2D-C1D	4.45	132.15	125.37
21	32	503	CL7	C2D-C1D-ND	4.45	113.22	110.23
21	1C	508	CL7	C1D-ND-C4D	-4.45	103.17	106.33
21	33	515	CL7	C1D-ND-C4D	-4.45	103.17	106.33
21	1B	611	CL7	CMD-C2D-C1D	4.45	132.15	125.37
21	13	513	CL7	CMD-C2D-C1D	4.45	132.15	125.37
21	41	415	CL7	C2D-C1D-ND	4.45	113.22	110.23
21	23	416	CL7	C2D-C1D-ND	4.45	113.21	110.23
21	3B	611	CL7	CMD-C2D-C1D	4.44	132.14	125.37
21	12	505	CL7	O2A-C1-C2	-4.44	96.95	108.64
21	3B	601	CL7	C1D-ND-C4D	-4.44	103.18	106.33
21	3B	616	CL7	C1D-ND-C4D	-4.44	103.18	106.33
21	24	410	CL7	C1D-ND-C4D	-4.44	103.18	106.33
21	4C	504	CL7	C1D-ND-C4D	-4.44	103.18	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	515	CL7	C4D-C3D-CAD	-4.44	104.43	107.42
21	14	410	CL7	C1D-ND-C4D	-4.44	103.18	106.33
21	4B	612	CL7	CMD-C2D-C1D	4.44	132.13	125.37
21	2C	506	CL7	CMD-C2D-C1D	4.44	132.13	125.37
21	3C	506	CL7	CMD-C2D-C1D	4.44	132.13	125.37
21	3B	615	CL7	C4D-C3D-CAD	-4.44	104.44	107.42
21	34	405	CL7	CMD-C2D-C1D	4.44	132.12	125.37
21	14	417	CL7	C1D-ND-C4D	-4.44	103.18	106.33
21	14	407	CL7	CMD-C2D-C1D	4.44	132.12	125.37
32	43	401	ZEX	C27-C26-C25	-4.43	115.67	122.84
21	1B	601	CL7	C1D-ND-C4D	-4.43	103.19	106.33
21	3B	607	CL7	C1D-ND-C4D	-4.43	103.19	106.33
21	42	502	CL7	C1D-ND-C4D	-4.43	103.19	106.33
21	1B	615	CL7	C4D-C3D-CAD	-4.43	104.44	107.42
32	22	519	ZEX	C7-C8-C9	-4.43	119.54	126.23
32	34	418	ZEX	C11-C10-C9	-4.43	120.99	127.31
22	4A	402	PHO	C4D-CHA-CBD	-4.43	106.51	108.52
21	11	415	CL7	C2D-C1D-ND	4.43	113.20	110.23
21	11	416	CL7	C1D-ND-C4D	-4.43	103.19	106.33
21	24	407	CL7	CMD-C2D-C1D	4.43	132.11	125.37
21	42	505	CL7	CMD-C2D-C1D	4.43	132.11	125.37
23	3B	618	8CT	C04-C03-C02	-4.43	116.38	122.61
21	34	410	CL7	C1D-ND-C4D	-4.42	103.19	106.33
21	2B	606	CL7	C4D-C3D-CAD	-4.42	104.44	107.42
21	4B	608	CL7	CMD-C2D-C1D	4.42	132.11	125.37
22	2A	402	PHO	C4D-CHA-CBD	-4.42	106.52	108.52
21	14	405	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	44	407	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	1B	614	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	3C	508	CL7	C1D-ND-C4D	-4.42	103.19	106.33
21	4B	606	CL7	C4D-C3D-CAD	-4.42	104.44	107.42
32	23	401	ZEX	C27-C26-C25	-4.42	115.69	122.84
21	1B	607	CL7	CMD-C2D-C1D	4.42	132.10	125.37
21	21	419	CL7	C1D-ND-C4D	-4.42	103.19	106.33
21	31	419	CL7	C1D-ND-C4D	-4.42	103.19	106.33
21	34	417	CL7	C1D-ND-C4D	-4.42	103.19	106.33
21	2B	616	CL7	C4D-C3D-CAD	-4.42	104.45	107.42
21	43	416	CL7	C1D-ND-C4D	-4.42	103.20	106.33
21	14	406	CL7	C1D-ND-C4D	-4.42	103.20	106.33
21	32	505	CL7	CMD-C2D-C1D	4.42	132.09	125.37
21	24	417	CL7	C1D-ND-C4D	-4.42	103.20	106.33
21	3B	605	CL7	C4D-C3D-CAD	-4.42	104.45	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	14	418	ZEX	C11-C10-C9	-4.41	121.01	127.31
21	3B	614	CL7	CMD-C2D-C1D	4.41	132.09	125.37
21	2A	401	CL7	C1-C2-C3	-4.41	118.41	126.04
21	2B	608	CL7	CMD-C2D-C1D	4.41	132.09	125.37
21	3B	607	CL7	CMD-C2D-C1D	4.41	132.09	125.37
21	1C	506	CL7	CMD-C2D-C1D	4.41	132.09	125.37
21	33	515	CL7	C2D-C1D-ND	4.41	113.19	110.23
21	11	409	CL7	CMD-C2D-C1D	4.41	132.08	125.37
21	11	411	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	2B	603	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	41	411	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	41	419	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	12	505	CL7	CMD-C2D-C1D	4.41	132.08	125.37
21	22	502	CL7	C1D-ND-C4D	-4.41	103.20	106.33
21	2B	615	CL7	CMD-C2D-C1D	4.40	132.08	125.37
21	2C	504	CL7	C1D-ND-C4D	-4.40	103.21	106.33
23	1B	618	8CT	C04-C03-C02	-4.40	116.41	122.61
23	4B	619	8CT	C04-C03-C02	-4.40	116.41	122.61
32	24	418	ZEX	C11-C10-C9	-4.40	121.03	127.31
21	4C	506	CL7	CMD-C2D-C1D	4.40	132.07	125.37
21	33	514	CL7	CMD-C2D-C1D	4.40	132.07	125.37
21	4B	615	CL7	CMD-C2D-C1D	4.40	132.07	125.37
21	22	502	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	23	412	CL7	CAA-CBA-CGA	-4.40	100.39	113.25
21	4A	401	CL7	C1-C2-C3	-4.40	118.43	126.04
21	12	502	CL7	C1D-ND-C4D	-4.40	103.21	106.33
21	34	404	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	13	511	CL7	CAA-CBA-CGA	-4.40	100.40	113.25
21	33	511	CL7	CAA-CBA-CGA	-4.40	100.40	113.25
21	44	417	CL7	C1D-ND-C4D	-4.40	103.21	106.33
21	32	515	CL7	C4D-C3D-CAD	-4.40	104.46	107.42
21	31	409	CL7	CMD-C2D-C1D	4.40	132.07	125.37
21	34	407	CL7	CMD-C2D-C1D	4.40	132.07	125.37
21	1C	512	CL7	CMD-C2D-C1D	4.40	132.06	125.37
21	4C	512	CL7	CMD-C2D-C1D	4.40	132.06	125.37
21	3B	608	CL7	C1D-ND-C4D	-4.39	103.21	106.33
32	41	422	ZEX	C11-C10-C9	-4.39	121.04	127.31
21	1C	513	CL7	CMD-C2D-C1D	4.39	132.06	125.37
21	3B	611	CL7	C1D-ND-C4D	-4.39	103.21	106.33
21	43	412	CL7	CAA-CBA-CGA	-4.39	100.42	113.25
21	42	511	CL7	C4D-C3D-CAD	-4.39	104.46	107.42
21	13	514	CL7	CMD-C2D-C1D	4.39	132.06	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	504	CL7	CMD-C2D-C1D	4.39	132.06	125.37
21	22	505	CL7	CMD-C2D-C1D	4.39	132.06	125.37
21	23	416	CL7	C1D-ND-C4D	-4.39	103.22	106.33
21	24	406	CL7	C1D-ND-C4D	-4.39	103.22	106.33
21	31	411	CL7	C1D-ND-C4D	-4.39	103.22	106.33
21	33	509	CL7	C4D-C3D-CAD	-4.39	104.47	107.42
21	44	404	CL7	C4D-C3D-CAD	-4.39	104.47	107.42
21	3C	503	CL7	C2D-C1D-ND	4.39	113.17	110.23
21	1B	602	CL7	C1D-ND-C4D	-4.38	103.22	106.33
21	4B	603	CL7	C1D-ND-C4D	-4.38	103.22	106.33
21	41	409	CL7	CMD-C2D-C1D	4.38	132.05	125.37
32	31	422	ZEX	C11-C10-C9	-4.38	121.05	127.31
21	43	402	CL7	CMD-C2D-C1D	4.38	132.04	125.37
32	13	525	ZEX	C27-C26-C25	-4.38	115.76	122.84
21	2C	517	CL7	CMD-C2D-C1D	4.38	132.04	125.37
22	1A	402	PHO	C4D-CHA-CBD	-4.38	106.53	108.52
21	33	512	CL7	C4D-C3D-CAD	-4.38	104.47	107.42
21	13	515	CL7	C1D-ND-C4D	-4.38	103.22	106.33
21	42	513	CL7	C1D-ND-C4D	-4.38	103.22	106.33
21	2B	614	CL7	C4D-C3D-CAD	-4.38	104.47	107.42
21	22	511	CL7	C4D-C3D-CAD	-4.38	104.47	107.42
21	32	511	CL7	C4D-C3D-CAD	-4.38	104.47	107.42
32	33	525	ZEX	C27-C26-C25	-4.38	115.77	122.84
21	12	511	CL7	C4D-C3D-CAD	-4.38	104.47	107.42
21	13	514	CL7	C1D-ND-C4D	-4.38	103.23	106.33
21	21	411	CL7	C1D-ND-C4D	-4.38	103.23	106.33
32	42	524	ZEX	C15-C14-C13	-4.38	121.06	127.31
21	1A	401	CL7	C1-C2-C3	-4.38	118.48	126.04
21	3A	401	CL7	C1-C2-C3	-4.38	118.48	126.04
21	23	415	CL7	CMD-C2D-C1D	4.37	132.03	125.37
21	2C	503	CL7	C2D-C1D-ND	4.37	113.16	110.23
21	23	402	CL7	CMD-C2D-C1D	4.37	132.03	125.37
21	33	501	CL7	CMD-C2D-C1D	4.37	132.03	125.37
23	2B	619	8CT	C04-C03-C02	-4.37	116.45	122.61
32	22	524	ZEX	C15-C14-C13	-4.37	121.07	127.31
21	12	502	CL7	C4D-C3D-CAD	-4.37	104.48	107.42
21	42	502	CL7	C4D-C3D-CAD	-4.37	104.48	107.42
21	13	504	CL7	CMD-C2D-C1D	4.37	132.02	125.37
21	22	513	CL7	C1D-ND-C4D	-4.37	103.23	106.33
21	32	513	CL7	C1D-ND-C4D	-4.37	103.23	106.33
21	2C	513	CL7	CMD-C2D-C1D	4.37	132.02	125.37
32	21	422	ZEX	C11-C10-C9	-4.37	121.08	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2C	512	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	1C	503	CL7	C2D-C1D-ND	4.36	113.16	110.23
21	4C	503	CL7	C2D-C1D-ND	4.36	113.16	110.23
32	21	421	ZEX	C35-C34-C33	-4.36	121.09	127.31
21	1C	517	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	3C	512	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	4C	517	CL7	CMD-C2D-C1D	4.36	132.01	125.37
21	21	415	CL7	C2D-C1D-ND	4.36	113.15	110.23
21	31	420	CL7	C2D-C1D-ND	4.36	113.15	110.23
21	43	412	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	3B	602	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	33	511	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	4B	612	CL7	C1D-ND-C4D	-4.36	103.24	106.33
21	12	517	CL7	C2D-C1D-ND	4.36	113.15	110.23
32	11	422	ZEX	C11-C10-C9	-4.35	121.10	127.31
21	44	410	CL7	C1D-ND-C4D	-4.35	103.24	106.33
32	41	421	ZEX	C35-C34-C33	-4.35	121.10	127.31
21	23	405	CL7	CMD-C2D-C1D	4.35	132.00	125.37
21	21	420	CL7	C2D-C1D-ND	4.35	113.15	110.23
21	32	515	CL7	CMD-C2D-C1D	4.35	132.00	125.37
32	32	524	ZEX	C15-C14-C13	-4.35	121.10	127.31
21	43	405	CL7	CMD-C2D-C1D	4.35	131.99	125.37
21	31	420	CL7	C1D-ND-C4D	-4.35	103.25	106.33
21	31	407	CL7	CMD-C2D-C1D	4.35	131.99	125.37
21	21	407	CL7	CMD-C2D-C1D	4.35	131.99	125.37
21	43	415	CL7	CMD-C2D-C1D	4.35	131.99	125.37
32	12	524	ZEX	C15-C14-C13	-4.35	121.11	127.31
21	3B	613	CL7	C4D-C3D-CAD	-4.35	104.50	107.42
21	23	415	CL7	C1D-ND-C4D	-4.35	103.25	106.33
32	11	421	ZEX	C35-C34-C33	-4.34	121.11	127.31
21	21	409	CL7	CMD-C2D-C1D	4.34	131.99	125.37
21	1A	401	CL7	C1D-ND-C4D	-4.34	103.25	106.33
21	13	501	CL7	CMD-C2D-C1D	4.34	131.98	125.37
21	4C	513	CL7	CMD-C2D-C1D	4.34	131.98	125.37
21	2C	508	CL7	C1D-ND-C4D	-4.34	103.25	106.33
21	3C	517	CL7	CMD-C2D-C1D	4.34	131.98	125.37
21	4B	609	CL7	C1D-ND-C4D	-4.34	103.25	106.33
21	2B	612	CL7	C1D-ND-C4D	-4.34	103.25	106.33
21	12	515	CL7	CMD-C2D-C1D	4.34	131.97	125.37
21	4A	401	CL7	C2D-C1D-ND	4.34	113.14	110.23
32	31	421	ZEX	C35-C34-C33	-4.33	121.13	127.31
21	33	517	CL7	CMD-C2D-C1D	4.33	131.97	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	515	CL7	C2D-C1D-ND	4.33	113.14	110.23
21	2B	623	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	14	415	CL7	C1D-ND-C4D	-4.33	103.26	106.33
21	13	517	CL7	CMD-C2D-C1D	4.33	131.96	125.37
22	3A	402	PHO	C4D-CHA-CBD	-4.33	106.56	108.52
32	44	418	ZEX	C28-C27-C26	-4.32	119.70	127.09
21	34	409	CL7	O2D-CGD-CBD	4.32	118.95	111.27
21	23	413	CL7	C4D-C3D-CAD	-4.32	104.51	107.42
21	1A	401	CL7	C2D-C1D-ND	4.32	113.13	110.23
21	41	420	CL7	C2D-C1D-ND	4.32	113.13	110.23
21	3C	508	CL7	CMD-C2D-C1D	4.32	131.95	125.37
21	13	512	CL7	C4D-C3D-CAD	-4.32	104.51	107.42
21	42	515	CL7	CMD-C2D-C1D	4.32	131.95	125.37
21	1B	611	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	21	420	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	4C	508	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	11	407	CL7	CMD-C2D-C1D	4.32	131.94	125.37
21	41	407	CL7	CMD-C2D-C1D	4.32	131.94	125.37
21	32	502	CL7	C1D-ND-C4D	-4.32	103.27	106.33
21	12	509	CL7	CMD-C2D-C1D	4.32	131.94	125.37
21	3C	513	CL7	CMD-C2D-C1D	4.32	131.94	125.37
21	22	515	CL7	CMD-C2D-C1D	4.31	131.94	125.37
21	41	420	CL7	C1D-ND-C4D	-4.31	103.27	106.33
21	32	502	CL7	C4D-C3D-CAD	-4.31	104.52	107.42
21	22	509	CL7	CMD-C2D-C1D	4.31	131.94	125.37
21	2A	401	CL7	C1D-ND-C4D	-4.31	103.27	106.33
21	3A	401	CL7	C1D-ND-C4D	-4.31	103.27	106.33
21	11	414	CL7	C1D-ND-C4D	-4.31	103.27	106.33
21	1C	508	CL7	CMD-C2D-C1D	4.31	131.93	125.37
21	12	517	CL7	CMD-C2D-C1D	4.31	131.93	125.37
21	23	412	CL7	C1D-ND-C4D	-4.31	103.28	106.33
21	4C	503	CL7	C4D-C3D-CAD	-4.31	104.52	107.42
21	43	413	CL7	C4D-C3D-CAD	-4.31	104.52	107.42
21	24	411	CL7	C3A-C4A-CHB	-4.31	117.31	123.70
21	3C	512	CL7	C2D-C1D-ND	4.30	113.12	110.23
21	13	511	CL7	C1D-ND-C4D	-4.30	103.28	106.33
21	4B	623	CL7	C1D-ND-C4D	-4.30	103.28	106.33
23	3A	404	8CT	C30-C31-C32	-4.30	116.17	121.47
21	42	509	CL7	CMD-C2D-C1D	4.30	131.92	125.37
32	24	418	ZEX	C28-C27-C26	-4.30	119.74	127.09
21	3B	622	CL7	C1D-ND-C4D	-4.30	103.28	106.33
21	1C	512	CL7	C2D-C1D-ND	4.30	113.11	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	512	CL7	C2D-C1D-ND	4.30	113.11	110.23
21	11	420	CL7	O2D-CGD-CBD	4.30	118.91	111.27
21	41	420	CL7	O2D-CGD-CBD	4.30	118.91	111.27
21	2C	512	CL7	C2D-C1D-ND	4.30	113.11	110.23
21	32	507	CL7	CMD-C2D-C1D	4.30	131.91	125.37
21	11	420	CL7	C1D-ND-C4D	-4.29	103.28	106.33
21	42	507	CL7	CMD-C2D-C1D	4.29	131.91	125.37
32	14	403	ZEX	C27-C28-C29	-4.29	119.75	126.23
21	44	409	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	22	509	CL7	C4D-C3D-CAD	-4.29	104.53	107.42
21	32	509	CL7	C4D-C3D-CAD	-4.29	104.53	107.42
21	4C	508	CL7	CMD-C2D-C1D	4.29	131.91	125.37
21	22	507	CL7	CMD-C2D-C1D	4.29	131.90	125.37
21	2B	609	CL7	C1D-ND-C4D	-4.29	103.29	106.33
21	4B	614	CL7	C4D-C3D-CAD	-4.29	104.53	107.42
32	12	520	ZEX	C35-C34-C33	-4.29	121.19	127.31
21	14	409	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	33	507	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	4A	401	CL7	C1D-ND-C4D	-4.29	103.29	106.33
21	43	415	CL7	C1D-ND-C4D	-4.29	103.29	106.33
23	4A	404	8CT	C30-C31-C32	-4.29	116.19	121.47
21	41	414	CL7	C1D-ND-C4D	-4.28	103.29	106.33
21	32	509	CL7	CMD-C2D-C1D	4.28	131.90	125.37
32	24	403	ZEX	C27-C28-C29	-4.28	119.76	126.23
21	2B	614	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	3B	613	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	11	420	CL7	C2D-C1D-ND	4.28	113.10	110.23
21	1B	608	CL7	C1D-ND-C4D	-4.28	103.29	106.33
21	4A	401	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	43	418	CL7	CMD-C2D-C1D	4.28	131.89	125.37
32	44	403	ZEX	C27-C28-C29	-4.28	119.76	126.23
21	44	411	CL7	C3A-C4A-CHB	-4.28	117.34	123.70
21	2C	508	CL7	CMD-C2D-C1D	4.28	131.89	125.37
21	12	513	CL7	C1D-ND-C4D	-4.28	103.29	106.33
21	2B	604	CL7	C1D-ND-C4D	-4.28	103.29	106.33
21	1B	613	CL7	C4D-C3D-CAD	-4.28	104.54	107.42
21	32	508	CL7	C4D-C3D-CAD	-4.28	104.54	107.42
21	42	508	CL7	C4D-C3D-CAD	-4.28	104.54	107.42
21	12	508	CL7	CMD-C2D-C1D	4.28	131.88	125.37
21	4B	602	CL7	C2D-C1D-ND	4.28	113.10	110.23
21	21	414	CL7	C1D-ND-C4D	-4.28	103.30	106.33
21	1A	403	CL7	C4D-C3D-CAD	-4.28	104.54	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	34	418	ZEX	C28-C27-C26	-4.28	119.78	127.09
21	34	411	CL7	C3A-C4A-CHB	-4.28	117.35	123.70
21	22	508	CL7	C4D-C3D-CAD	-4.27	104.54	107.42
21	3B	604	CL7	C4D-C3D-CAD	-4.27	104.54	107.42
32	43	420	ZEX	C18-C5-C6	-4.27	119.73	124.53
21	13	507	CL7	O2D-CGD-CBD	4.27	118.86	111.27
21	31	420	CL7	O2D-CGD-CBD	4.27	118.86	111.27
21	23	408	CL7	O2D-CGD-CBD	4.27	118.86	111.27
21	4B	614	CL7	CMD-C2D-C1D	4.27	131.88	125.37
23	4C	518	8CT	C18-C17-C16	-4.27	121.21	127.31
21	12	509	CL7	C4D-C3D-CAD	-4.27	104.55	107.42
32	34	403	ZEX	C27-C28-C29	-4.27	119.78	126.23
21	12	507	CL7	CMD-C2D-C1D	4.27	131.87	125.37
21	42	517	CL7	CMD-C2D-C1D	4.27	131.87	125.37
23	44	402	8CT	C11-C10-C03	-4.27	115.21	127.20
23	3C	518	8CT	C18-C17-C16	-4.27	121.22	127.31
21	21	420	CL7	O2D-CGD-CBD	4.27	118.85	111.27
32	14	418	ZEX	C28-C27-C26	-4.27	119.80	127.09
21	33	502	CL7	C1A-NA-C4A	4.27	108.88	106.30
21	43	408	CL7	O2D-CGD-CBD	4.27	118.85	111.27
21	1C	503	CL7	C4D-C3D-CAD	-4.27	104.55	107.42
21	3C	503	CL7	C4D-C3D-CAD	-4.27	104.55	107.42
21	24	409	CL7	O2D-CGD-CBD	4.27	118.85	111.27
21	2A	401	CL7	C2D-C1D-ND	4.26	113.09	110.23
21	22	517	CL7	C2D-C1D-ND	4.26	113.09	110.23
21	3A	401	CL7	C2D-C1D-ND	4.26	113.09	110.23
21	33	514	CL7	C1D-ND-C4D	-4.26	103.31	106.33
32	23	421	ZEX	C18-C5-C6	-4.26	119.74	124.53
32	21	422	ZEX	C35-C34-C33	-4.26	121.22	127.31
21	32	517	CL7	CMD-C2D-C1D	4.26	131.86	125.37
21	1B	613	CL7	CMD-C2D-C1D	4.26	131.86	125.37
32	23	420	ZEX	C18-C5-C6	-4.26	119.74	124.53
32	33	519	ZEX	C18-C5-C6	-4.26	119.74	124.53
21	22	513	CL7	CMD-C2D-C1D	4.26	131.86	125.37
23	1A	404	8CT	C30-C31-C32	-4.26	116.23	121.47
21	23	418	CL7	CMD-C2D-C1D	4.26	131.86	125.37
21	42	508	CL7	CMD-C2D-C1D	4.26	131.86	125.37
23	34	402	8CT	C11-C10-C03	-4.26	115.24	127.20
21	31	415	CL7	CMD-C2D-C1D	4.26	131.85	125.37
21	41	415	CL7	CMD-C2D-C1D	4.26	131.85	125.37
21	41	416	CL7	CMD-C2D-C1D	4.26	131.85	125.37
21	42	507	CL7	O2D-CGD-CBD	4.26	118.83	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	24	402	8CT	C11-C10-C03	-4.26	115.25	127.20
21	2B	615	CL7	C3A-C4A-CHB	-4.25	117.39	123.70
21	42	509	CL7	C4D-C3D-CAD	-4.25	104.56	107.42
23	2A	404	8CT	C30-C31-C32	-4.25	116.23	121.47
21	1B	622	CL7	C1D-ND-C4D	-4.25	103.31	106.33
23	2C	518	8CT	C18-C17-C16	-4.25	121.24	127.31
23	1C	518	8CT	C18-C17-C16	-4.25	121.24	127.31
32	13	519	ZEX	C18-C5-C6	-4.25	119.75	124.53
21	41	417	CL7	C1D-ND-C4D	-4.25	103.32	106.33
21	14	411	CL7	C3A-C4A-CHB	-4.25	117.39	123.70
32	43	421	ZEX	C18-C5-C6	-4.25	119.76	124.53
21	11	416	CL7	CMD-C2D-C1D	4.25	131.84	125.37
21	24	415	CL7	C1D-ND-C4D	-4.25	103.32	106.33
21	34	415	CL7	C1D-ND-C4D	-4.25	103.32	106.33
21	44	415	CL7	C1D-ND-C4D	-4.25	103.32	106.33
21	2C	503	CL7	C4D-C3D-CAD	-4.25	104.56	107.42
21	22	507	CL7	O2D-CGD-CBD	4.24	118.81	111.27
21	32	507	CL7	O2D-CGD-CBD	4.24	118.81	111.27
23	14	402	8CT	C11-C10-C03	-4.24	115.28	127.20
21	22	515	CL7	C1D-ND-C4D	-4.24	103.32	106.33
21	24	416	CL7	C1D-ND-C4D	-4.24	103.32	106.33
23	1B	619	8CT	C35-C30-C29	-4.24	107.34	112.70
21	12	513	CL7	CMD-C2D-C1D	4.24	131.83	125.37
21	42	513	CL7	CMD-C2D-C1D	4.24	131.83	125.37
21	12	512	CL7	C4D-C3D-CAD	-4.24	104.57	107.42
21	22	517	CL7	CMD-C2D-C1D	4.24	131.83	125.37
21	1B	601	CL7	C2D-C1D-ND	4.24	113.07	110.23
21	2B	602	CL7	C2D-C1D-ND	4.24	113.07	110.23
21	22	508	CL7	CMD-C2D-C1D	4.24	131.82	125.37
21	32	508	CL7	CMD-C2D-C1D	4.24	131.82	125.37
21	11	407	CL7	C1D-ND-C4D	-4.24	103.32	106.33
21	21	416	CL7	CMD-C2D-C1D	4.24	131.82	125.37
21	13	502	CL7	C1A-NA-C4A	4.24	108.87	106.30
21	23	406	CL7	C1D-ND-C4D	-4.24	103.33	106.33
21	31	417	CL7	C1D-ND-C4D	-4.24	103.33	106.33
21	1B	604	CL7	C4D-C3D-CAD	-4.24	104.57	107.42
21	3A	403	CL7	C4D-C3D-CAD	-4.24	104.57	107.42
21	4B	605	CL7	C4D-C3D-CAD	-4.24	104.57	107.42
32	41	422	ZEX	C35-C34-C33	-4.23	121.27	127.31
21	22	512	CL7	C4D-C3D-CAD	-4.23	104.57	107.42
21	42	512	CL7	C4D-C3D-CAD	-4.23	104.57	107.42
21	32	513	CL7	CMD-C2D-C1D	4.23	131.82	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	507	CL7	O2D-CGD-CBD	4.23	118.79	111.27
21	3B	601	CL7	C2D-C1D-ND	4.23	113.07	110.23
23	3B	618	8CT	C01-C02-C03	-4.23	119.78	124.53
32	32	520	ZEX	C35-C34-C33	-4.23	121.27	127.31
32	42	520	ZEX	C35-C34-C33	-4.23	121.27	127.31
21	11	415	CL7	CMD-C2D-C1D	4.23	131.81	125.37
21	13	512	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	21	409	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	3D	405	CL7	C4D-C3D-CAD	-4.23	104.57	107.42
21	31	414	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	1B	614	CL7	C3A-C4A-CHB	-4.23	117.42	123.70
21	1B	602	CL7	C4D-C3D-CAD	-4.23	104.57	107.42
23	1B	618	8CT	C01-C02-C03	-4.23	119.78	124.53
21	14	416	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	3B	603	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	1A	401	CL7	CMD-C2D-C1D	4.23	131.81	125.37
21	3C	507	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	44	411	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	31	407	CL7	C1D-ND-C4D	-4.23	103.33	106.33
21	14	411	CL7	C1D-ND-C4D	-4.22	103.33	106.33
21	24	411	CL7	C1D-ND-C4D	-4.22	103.33	106.33
21	23	403	CL7	C1A-NA-C4A	4.22	108.86	106.30
32	31	422	ZEX	C35-C34-C33	-4.22	121.28	127.31
21	2B	605	CL7	C4D-C3D-CAD	-4.22	104.58	107.42
21	21	417	CL7	C1D-ND-C4D	-4.22	103.34	106.33
21	33	512	CL7	C1D-ND-C4D	-4.22	103.34	106.33
21	34	416	CL7	C1D-ND-C4D	-4.22	103.34	106.33
21	34	409	CL7	CMD-C2D-C1D	4.22	131.79	125.37
32	13	520	ZEX	C28-C27-C26	-4.22	119.88	127.09
21	11	409	CL7	C1D-ND-C4D	-4.22	103.34	106.33
21	11	412	CL7	C2D-C1D-ND	4.22	113.06	110.23
32	22	520	ZEX	C35-C34-C33	-4.22	121.29	127.31
21	3B	614	CL7	C3A-C4A-CHB	-4.22	117.44	123.70
21	21	415	CL7	CMD-C2D-C1D	4.22	131.79	125.37
23	4B	620	8CT	C35-C30-C29	-4.22	107.37	112.70
21	14	409	CL7	CMD-C2D-C1D	4.22	131.79	125.37
21	44	409	CL7	CMD-C2D-C1D	4.22	131.79	125.37
21	2A	401	CL7	CMD-C2D-C1D	4.21	131.79	125.37
21	23	413	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	31	409	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	34	411	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	3C	512	CL7	C1D-ND-C4D	-4.21	103.34	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	416	CL7	CMD-C2D-C1D	4.21	131.78	125.37
23	3B	619	8CT	C35-C30-C29	-4.21	107.38	112.70
21	12	508	CL7	C4D-C3D-CAD	-4.21	104.59	107.42
21	3C	505	CL7	C4D-C3D-CAD	-4.21	104.59	107.42
21	43	403	CL7	C1A-NA-C4A	4.21	108.85	106.30
21	21	412	CL7	C2D-C1D-ND	4.21	113.06	110.23
21	32	512	CL7	C4D-C3D-CAD	-4.21	104.59	107.42
32	11	422	ZEX	C35-C34-C33	-4.21	121.30	127.31
21	1C	502	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	21	407	CL7	C1D-ND-C4D	-4.21	103.34	106.33
21	4C	502	CL7	C1D-ND-C4D	-4.21	103.34	106.33
32	34	418	ZEX	C7-C8-C9	-4.21	119.88	126.23
21	41	412	CL7	C2D-C1D-ND	4.21	113.05	110.23
21	2A	403	CL7	C4D-C3D-CAD	-4.21	104.59	107.42
32	33	520	ZEX	C18-C5-C6	-4.21	119.81	124.53
21	4B	615	CL7	C3A-C4A-CHB	-4.20	117.46	123.70
21	4B	604	CL7	C1D-ND-C4D	-4.20	103.35	106.33
21	3A	401	CL7	CMD-C2D-C1D	4.20	131.77	125.37
21	12	515	CL7	C1D-ND-C4D	-4.20	103.35	106.33
21	42	515	CL7	C1D-ND-C4D	-4.20	103.35	106.33
23	2B	619	8CT	C01-C02-C03	-4.20	119.81	124.53
23	4B	619	8CT	C01-C02-C03	-4.20	119.81	124.53
21	24	409	CL7	CMD-C2D-C1D	4.20	131.76	125.37
21	41	409	CL7	C1D-ND-C4D	-4.20	103.35	106.33
21	44	416	CL7	C1D-ND-C4D	-4.20	103.35	106.33
21	42	517	CL7	C2D-C1D-ND	4.20	113.05	110.23
23	2B	620	8CT	C35-C30-C29	-4.19	107.40	112.70
21	11	417	CL7	C1D-ND-C4D	-4.19	103.36	106.33
21	32	501	CL7	C1D-ND-C4D	-4.19	103.36	106.33
21	44	407	CL7	C1D-ND-C4D	-4.19	103.36	106.33
32	13	520	ZEX	C18-C5-C6	-4.19	119.82	124.53
21	22	517	CL7	C1D-ND-C4D	-4.19	103.36	106.33
21	4C	507	CL7	C1D-ND-C4D	-4.19	103.36	106.33
32	43	421	ZEX	C28-C27-C26	-4.19	119.94	127.09
21	13	505	CL7	C1D-ND-C4D	-4.19	103.36	106.33
21	2C	512	CL7	C1D-ND-C4D	-4.18	103.36	106.33
21	33	505	CL7	C1D-ND-C4D	-4.18	103.36	106.33
21	42	501	CL7	C1D-ND-C4D	-4.18	103.36	106.33
21	32	517	CL7	C2D-C1D-ND	4.18	113.04	110.23
21	13	512	CL7	C2D-C1D-ND	4.18	113.03	110.23
21	14	415	CL7	C2D-C1D-ND	4.18	113.03	110.23
21	4B	603	CL7	C4D-C3D-CAD	-4.18	104.61	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	13	522	ZEX	C27-C28-C29	-4.18	119.92	126.23
21	4C	512	CL7	C1D-ND-C4D	-4.18	103.37	106.33
32	33	520	ZEX	C28-C27-C26	-4.18	119.95	127.09
21	4A	403	CL7	C4D-C3D-CAD	-4.17	104.61	107.42
32	23	421	ZEX	C28-C27-C26	-4.17	119.96	127.09
21	21	408	CL7	C1D-ND-C4D	-4.17	103.37	106.33
21	41	407	CL7	C1D-ND-C4D	-4.17	103.37	106.33
21	1C	507	CL7	C1D-ND-C4D	-4.17	103.37	106.33
32	23	423	ZEX	C27-C28-C29	-4.17	119.93	126.23
21	43	406	CL7	C1D-ND-C4D	-4.17	103.37	106.33
21	32	515	CL7	C1D-ND-C4D	-4.17	103.37	106.33
21	12	501	CL7	C1D-ND-C4D	-4.17	103.37	106.33
32	24	418	ZEX	C7-C8-C9	-4.17	119.94	126.23
21	11	405	CL7	C2D-C1D-ND	4.17	113.03	110.23
21	2C	502	CL7	C1D-ND-C4D	-4.17	103.38	106.33
21	33	512	CL7	C2D-C1D-ND	4.16	113.02	110.23
21	1C	505	CL7	C4D-C3D-CAD	-4.16	104.62	107.42
21	4D	405	CL7	C4D-C3D-CAD	-4.16	104.62	107.42
32	44	418	ZEX	C7-C8-C9	-4.16	119.94	126.23
23	14	402	8CT	C13-C14-C15	-4.16	110.23	123.22
21	43	413	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	34	417	CL7	C2D-C1D-ND	4.16	113.02	110.23
21	12	502	CL7	CMD-C2D-C1D	4.16	131.71	125.37
21	34	407	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	2B	613	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	42	502	CL7	CMD-C2D-C1D	4.16	131.70	125.37
21	1D	402	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	2C	507	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	3B	602	CL7	C4D-C3D-CAD	-4.16	104.62	107.42
21	13	518	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	1B	603	CL7	C1D-ND-C4D	-4.16	103.38	106.33
21	1B	616	CL7	C2D-C1D-ND	4.15	113.02	110.23
21	24	415	CL7	C2D-C1D-ND	4.15	113.02	110.23
21	31	412	CL7	C2D-C1D-ND	4.15	113.02	110.23
21	2B	607	CL7	C3A-C4A-CHB	-4.15	117.54	123.70
21	11	408	CL7	C1D-ND-C4D	-4.15	103.39	106.33
21	42	509	CL7	C1D-ND-C4D	-4.15	103.39	106.33
21	32	502	CL7	CMD-C2D-C1D	4.15	131.69	125.37
21	2B	603	CL7	C2D-C1D-ND	4.15	113.01	110.23
21	44	406	CL7	C2D-C1D-ND	4.15	113.01	110.23
23	44	402	8CT	C13-C14-C15	-4.15	110.27	123.22
21	4B	617	CL7	C2D-C1D-ND	4.15	113.01	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	603	CL7	C4D-C3D-CAD	-4.15	104.63	107.42
21	1A	401	CL7	C3A-C4A-CHB	-4.15	117.55	123.70
21	4A	401	CL7	C3A-C4A-CHB	-4.15	117.55	123.70
21	14	411	CL7	C4D-C3D-CAD	-4.15	104.63	107.42
23	24	402	8CT	C13-C14-C15	-4.14	110.28	123.22
23	34	402	8CT	C13-C14-C15	-4.14	110.28	123.22
21	2B	617	CL7	C2D-C1D-ND	4.14	113.01	110.23
21	2A	401	CL7	C3A-C4A-CHB	-4.14	117.55	123.70
21	22	510	CL7	CMD-C2D-C1D	4.14	131.68	125.37
32	14	418	ZEX	C7-C8-C9	-4.14	119.98	126.23
21	12	517	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	3C	502	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	14	405	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	31	402	CL7	C1D-ND-C4D	-4.14	103.39	106.33
21	4C	505	CL7	C4D-C3D-CAD	-4.14	104.64	107.42
21	22	502	CL7	CMD-C2D-C1D	4.14	131.67	125.37
21	12	518	CL7	C1D-ND-C4D	-4.14	103.40	106.33
21	42	518	CL7	C1D-ND-C4D	-4.14	103.40	106.33
21	32	514	CL7	C4D-C3D-CAD	-4.14	104.64	107.42
21	1C	512	CL7	C1D-ND-C4D	-4.14	103.40	106.33
21	11	402	CL7	C1D-ND-C4D	-4.14	103.40	106.33
21	22	518	CL7	C1D-ND-C4D	-4.14	103.40	106.33
21	24	405	CL7	C1D-ND-C4D	-4.14	103.40	106.33
21	43	415	CL7	O2D-CGD-CBD	4.13	118.61	111.27
21	13	513	CL7	C1D-ND-C4D	-4.13	103.40	106.33
21	14	407	CL7	C1D-ND-C4D	-4.13	103.40	106.33
21	2D	402	CL7	C1D-ND-C4D	-4.13	103.40	106.33
21	32	518	CL7	C1D-ND-C4D	-4.13	103.40	106.33
21	21	406	CL7	CMD-C2D-C1D	4.13	131.66	125.37
21	34	417	CL7	CMD-C2D-C1D	4.13	131.66	125.37
21	42	510	CL7	CMD-C2D-C1D	4.13	131.66	125.37
21	41	406	CL7	CMD-C2D-C1D	4.13	131.66	125.37
21	1B	602	CL7	C2D-C1D-ND	4.13	113.00	110.23
21	21	403	CL7	C1D-ND-C4D	-4.13	103.40	106.33
32	33	522	ZEX	C27-C28-C29	-4.13	120.00	126.23
21	1B	606	CL7	C3A-C4A-CHB	-4.13	117.58	123.70
21	23	415	CL7	O2D-CGD-CBD	4.13	118.60	111.27
21	23	413	CL7	C2D-C1D-ND	4.12	113.00	110.23
21	12	510	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	11	406	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	33	514	CL7	O2D-CGD-CBD	4.12	118.59	111.27
21	34	405	CL7	C1D-ND-C4D	-4.12	103.41	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	402	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	2D	405	CL7	C4D-C3D-CAD	-4.12	104.65	107.42
21	31	403	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	34	415	CL7	C2D-C1D-ND	4.12	113.00	110.23
32	43	423	ZEX	C27-C28-C29	-4.12	120.01	126.23
21	14	417	CL7	CMD-C2D-C1D	4.12	131.65	125.37
21	11	403	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	41	403	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	23	419	CL7	C3A-C4A-CHB	-4.12	117.59	123.70
21	33	518	CL7	C3A-C4A-CHB	-4.12	117.59	123.70
21	4D	405	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	43	409	CL7	CMD-C2D-C1D	4.12	131.64	125.37
21	1D	405	CL7	C4D-C3D-CAD	-4.12	104.65	107.42
21	4B	607	CL7	C3A-C4A-CHB	-4.12	117.59	123.70
21	43	413	CL7	C2D-C1D-ND	4.12	112.99	110.23
21	22	501	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	22	509	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	32	509	CL7	C1D-ND-C4D	-4.12	103.41	106.33
21	34	406	CL7	C2D-C1D-ND	4.12	112.99	110.23
21	42	505	CL7	O2D-CGD-CBD	4.12	118.58	111.27
21	1B	612	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	33	518	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	2C	505	CL7	C4D-C3D-CAD	-4.11	104.65	107.42
21	33	508	CL7	CMD-C2D-C1D	4.11	131.63	125.37
21	31	408	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	3B	606	CL7	C3A-C4A-CHB	-4.11	117.60	123.70
21	3D	405	CL7	C3A-C4A-CHB	-4.11	117.60	123.70
21	3C	505	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	42	517	CL7	C1D-ND-C4D	-4.11	103.41	106.33
21	4D	402	CL7	C1D-ND-C4D	-4.11	103.42	106.33
21	32	518	CL7	C4D-C3D-CAD	-4.11	104.66	107.42
21	4B	613	CL7	C1D-ND-C4D	-4.11	103.42	106.33
32	12	520	ZEX	C28-C27-C26	-4.11	120.07	127.09
21	11	412	CL7	CMD-C2D-C1D	4.11	131.62	125.37
21	11	418	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	1D	405	CL7	C3A-C4A-CHB	-4.10	117.61	123.70
21	44	417	CL7	CMD-C2D-C1D	4.10	131.62	125.37
21	32	510	CL7	CMD-C2D-C1D	4.10	131.62	125.37
21	32	517	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	21	412	CL7	CMD-C2D-C1D	4.10	131.62	125.37
21	13	514	CL7	O2D-CGD-CBD	4.10	118.56	111.27
23	1B	617	8CT	C14-C13-C12	-4.10	121.46	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	616	CL7	C2D-C1D-ND	4.10	112.98	110.23
21	12	505	CL7	O2D-CGD-CBD	4.10	118.55	111.27
21	44	405	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	12	516	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	3A	401	CL7	C3A-C4A-CHB	-4.10	117.62	123.70
21	22	505	CL7	O2D-CGD-CBD	4.10	118.55	111.27
21	43	419	CL7	C3A-C4A-CHB	-4.10	117.62	123.70
21	23	419	CL7	C1D-ND-C4D	-4.10	103.42	106.33
21	24	417	CL7	CMD-C2D-C1D	4.10	131.61	125.37
21	2C	510	CL7	C1D-ND-C4D	-4.09	103.43	106.33
21	21	418	CL7	O2D-CGD-CBD	4.09	118.54	111.27
21	2C	501	CL7	CMD-C2D-C1D	4.09	131.60	125.37
21	31	418	CL7	C1D-ND-C4D	-4.09	103.43	106.33
23	3B	617	8CT	C14-C13-C12	-4.09	121.47	127.31
32	32	520	ZEX	C28-C27-C26	-4.09	120.10	127.09
21	4C	501	CL7	CMD-C2D-C1D	4.09	131.60	125.37
21	4C	507	CL7	CMD-C2D-C1D	4.09	131.60	125.37
21	31	406	CL7	CMD-C2D-C1D	4.09	131.59	125.37
21	24	409	CL7	C1D-ND-C4D	-4.09	103.43	106.33
21	13	518	CL7	C3A-C4A-CHB	-4.09	117.63	123.70
21	4D	405	CL7	C3A-C4A-CHB	-4.09	117.63	123.70
21	13	508	CL7	CMD-C2D-C1D	4.09	131.59	125.37
21	1D	405	CL7	C1D-ND-C4D	-4.09	103.43	106.33
32	42	520	ZEX	C28-C27-C26	-4.09	120.11	127.09
21	12	503	CL7	C3A-C4A-CHB	-4.08	117.64	123.70
32	44	420	ZEX	C31-C30-C29	-4.08	121.48	127.31
21	1C	501	CL7	CMD-C2D-C1D	4.08	131.59	125.37
21	3D	402	CL7	C1D-ND-C4D	-4.08	103.43	106.33
21	31	410	CL7	C3A-C4A-CHB	-4.08	117.64	123.70
32	13	522	ZEX	C18-C5-C6	-4.08	119.94	124.53
32	23	423	ZEX	C18-C5-C6	-4.08	119.94	124.53
32	33	522	ZEX	C18-C5-C6	-4.08	119.94	124.53
21	32	505	CL7	O2D-CGD-CBD	4.08	118.52	111.27
21	44	417	CL7	C2D-C1D-ND	4.08	112.97	110.23
23	4B	618	8CT	C14-C13-C12	-4.08	121.49	127.31
21	42	514	CL7	C4D-C3D-CAD	-4.08	104.67	107.42
23	1C	518	8CT	C04-C03-C02	-4.08	116.87	122.61
21	1A	401	CL7	CAA-C2A-C1A	-4.08	98.77	112.19
32	43	423	ZEX	C18-C5-C6	-4.08	119.95	124.53
21	2D	405	CL7	C3A-C4A-CHB	-4.08	117.65	123.70
21	21	405	CL7	C2D-C1D-ND	4.08	112.97	110.23
21	31	405	CL7	C2D-C1D-ND	4.08	112.97	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	404	CL7	O2D-CGD-CBD	4.08	118.51	111.27
21	31	412	CL7	CMD-C2D-C1D	4.08	131.58	125.37
23	2B	619	8CT	C13-C14-C15	-4.08	110.50	123.22
21	4A	401	CL7	CAA-C2A-C1A	-4.08	98.78	112.19
21	11	404	CL7	O2D-CGD-CBD	4.07	118.51	111.27
21	11	418	CL7	O2D-CGD-CBD	4.07	118.51	111.27
23	1B	618	8CT	C13-C14-C15	-4.07	110.50	123.22
23	4B	619	8CT	C13-C14-C15	-4.07	110.50	123.22
21	3A	401	CL7	CAA-C2A-C1A	-4.07	98.79	112.19
21	14	409	CL7	C1D-ND-C4D	-4.07	103.44	106.33
21	3B	612	CL7	C1D-ND-C4D	-4.07	103.44	106.33
21	43	419	CL7	C1D-ND-C4D	-4.07	103.44	106.33
21	44	409	CL7	C1D-ND-C4D	-4.07	103.44	106.33
32	22	520	ZEX	C28-C27-C26	-4.07	120.13	127.09
21	23	409	CL7	CMD-C2D-C1D	4.07	131.57	125.37
21	2C	507	CL7	CMD-C2D-C1D	4.07	131.57	125.37
21	34	409	CL7	C1D-ND-C4D	-4.07	103.44	106.33
21	3C	501	CL7	CMD-C2D-C1D	4.07	131.57	125.37
21	14	417	CL7	C2D-C1D-ND	4.07	112.96	110.23
21	3C	501	CL7	C4D-C3D-CAD	-4.07	104.68	107.42
21	4C	508	CL7	C4D-C3D-CAD	-4.07	104.68	107.42
21	4B	603	CL7	C2D-C1D-ND	4.07	112.96	110.23
21	44	415	CL7	C2D-C1D-ND	4.07	112.96	110.23
21	32	503	CL7	C3A-C4A-CHB	-4.07	117.66	123.70
23	2C	518	8CT	C04-C03-C02	-4.07	116.88	122.61
23	3B	618	8CT	C13-C14-C15	-4.07	110.52	123.22
21	41	412	CL7	CMD-C2D-C1D	4.07	131.56	125.37
23	2B	618	8CT	C14-C13-C12	-4.07	121.50	127.31
21	31	418	CL7	O2D-CGD-CBD	4.07	118.50	111.27
21	41	418	CL7	C1D-ND-C4D	-4.07	103.45	106.33
21	4C	501	CL7	C4D-C3D-CAD	-4.07	104.68	107.42
21	24	414	CL7	CMD-C2D-C1D	4.07	131.56	125.37
21	12	514	CL7	C4D-C3D-CAD	-4.06	104.69	107.42
21	22	514	CL7	C4D-C3D-CAD	-4.06	104.69	107.42
21	24	411	CL7	C4D-C3D-CAD	-4.06	104.69	107.42
21	41	410	CL7	C3A-C4A-CHB	-4.06	117.67	123.70
21	1A	403	CL7	C1D-ND-C4D	-4.06	103.45	106.33
21	24	407	CL7	C1D-ND-C4D	-4.06	103.45	106.33
21	33	513	CL7	C1D-ND-C4D	-4.06	103.45	106.33
21	23	411	CL7	C3A-C4A-CHB	-4.06	117.67	123.70
21	1C	508	CL7	C4D-C3D-CAD	-4.06	104.69	107.42
21	14	406	CL7	C2D-C1D-ND	4.06	112.96	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	24	410	CL7	C2D-C1D-ND	4.06	112.96	110.23
21	2A	401	CL7	CAA-C2A-C1A	-4.06	98.83	112.19
21	1C	507	CL7	CMD-C2D-C1D	4.06	131.55	125.37
21	12	509	CL7	C1D-ND-C4D	-4.06	103.45	106.33
21	43	414	CL7	C1D-ND-C4D	-4.06	103.45	106.33
21	44	414	CL7	CMD-C2D-C1D	4.06	131.55	125.37
32	23	401	ZEX	C8-C7-C6	-4.06	115.80	127.20
21	2C	508	CL7	C4D-C3D-CAD	-4.06	104.69	107.42
21	34	411	CL7	C4D-C3D-CAD	-4.06	104.69	107.42
21	2A	407	CL7	C2D-C1D-ND	4.06	112.95	110.23
32	24	420	ZEX	C31-C30-C29	-4.06	121.52	127.31
32	34	420	ZEX	C31-C30-C29	-4.06	121.52	127.31
23	14	402	8CT	C07-C02-C03	-4.06	116.84	122.73
21	3B	606	CL7	CHD-C1D-ND	-4.05	119.97	124.26
32	14	420	ZEX	C31-C30-C29	-4.05	121.52	127.31
21	22	516	CL7	C1D-ND-C4D	-4.05	103.45	106.33
21	23	409	CL7	C1D-ND-C4D	-4.05	103.45	106.33
21	32	516	CL7	C1D-ND-C4D	-4.05	103.45	106.33
21	33	508	CL7	C1D-ND-C4D	-4.05	103.45	106.33
32	43	401	ZEX	C8-C7-C6	-4.05	115.82	127.20
21	2C	511	CL7	C4D-C3D-CAD	-4.05	104.69	107.42
21	2C	506	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	22	503	CL7	C3A-C4A-CHB	-4.05	117.69	123.70
23	24	402	8CT	C07-C02-C03	-4.05	116.85	122.73
23	34	402	8CT	C07-C02-C03	-4.05	116.85	122.73
21	42	516	CL7	C1D-ND-C4D	-4.05	103.46	106.33
32	33	525	ZEX	C8-C7-C6	-4.05	115.83	127.20
21	2A	403	CL7	C1D-ND-C4D	-4.05	103.46	106.33
23	44	402	8CT	C07-C02-C03	-4.05	116.85	122.73
21	21	404	CL7	O2D-CGD-CBD	4.05	118.46	111.27
21	34	414	CL7	CMD-C2D-C1D	4.05	131.53	125.37
21	24	406	CL7	C2D-C1D-ND	4.05	112.95	110.23
21	1C	506	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	4C	506	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	41	408	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	41	411	CL7	C2D-C1D-ND	4.05	112.94	110.23
21	41	416	CL7	C2D-C1D-ND	4.05	112.94	110.23
21	13	516	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	43	417	CL7	C1D-ND-C4D	-4.05	103.46	106.33
21	3C	508	CL7	C4D-C3D-CAD	-4.05	104.70	107.42
23	4C	518	8CT	C04-C03-C02	-4.04	116.92	122.61
21	33	510	CL7	C3A-C4A-CHB	-4.04	117.70	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4K	101	8CT	C19-C18-C17	-4.04	115.19	123.47
21	41	418	CL7	O2D-CGD-CBD	4.04	118.45	111.27
21	3C	507	CL7	CMD-C2D-C1D	4.04	131.53	125.37
21	11	410	CL7	C3A-C4A-CHB	-4.04	117.70	123.70
21	21	410	CL7	C3A-C4A-CHB	-4.04	117.70	123.70
21	21	402	CL7	C1D-ND-C4D	-4.04	103.46	106.33
21	23	412	CL7	C2D-C1D-ND	4.04	112.94	110.23
21	13	510	CL7	C3A-C4A-CHB	-4.04	117.70	123.70
21	41	404	CL7	O2D-CGD-CBD	4.04	118.45	111.27
21	1A	407	CL7	C2D-C1D-ND	4.04	112.94	110.23
21	4C	509	CL7	C4D-C3D-CAD	-4.04	104.70	107.42
21	44	411	CL7	C4D-C3D-CAD	-4.04	104.70	107.42
23	1K	101	8CT	C19-C18-C17	-4.04	115.20	123.47
21	4A	407	CL7	C2D-C1D-ND	4.04	112.94	110.23
21	41	405	CL7	C2D-C1D-ND	4.04	112.94	110.23
21	2D	405	CL7	C1D-ND-C4D	-4.04	103.47	106.33
21	3A	407	CL7	C2D-C1D-ND	4.03	112.94	110.23
23	3K	101	8CT	C19-C18-C17	-4.03	115.21	123.47
21	42	503	CL7	C3A-C4A-CHB	-4.03	117.71	123.70
21	21	418	CL7	C1D-ND-C4D	-4.03	103.47	106.33
23	3C	518	8CT	C07-C02-C03	-4.03	116.88	122.73
21	22	518	CL7	C4D-C3D-CAD	-4.03	104.71	107.42
21	3B	602	CL7	C2D-C1D-ND	4.03	112.94	110.23
21	42	502	CL7	C2D-C1D-ND	4.03	112.94	110.23
32	13	525	ZEX	C8-C7-C6	-4.03	115.88	127.20
21	1C	505	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	13	508	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	22	514	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	3C	506	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	4C	505	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	1C	501	CL7	C4D-C3D-CAD	-4.03	104.71	107.42
21	4B	607	CL7	CHD-C1D-ND	-4.03	119.99	124.26
21	3C	509	CL7	C4D-C3D-CAD	-4.03	104.71	107.42
21	23	405	CL7	C3A-C4A-CHB	-4.03	117.72	123.70
23	2K	101	8CT	C19-C18-C17	-4.03	115.22	123.47
23	2D	406	8CT	C14-C13-C12	-4.03	121.56	127.31
21	1C	509	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	2C	505	CL7	C1D-ND-C4D	-4.03	103.47	106.33
21	24	417	CL7	C2D-C1D-ND	4.03	112.93	110.23
23	4C	518	8CT	C07-C02-C03	-4.03	116.89	122.73
21	21	405	CL7	C4D-C3D-CAD	-4.02	104.71	107.42
21	24	404	CL7	C1D-ND-C4D	-4.02	103.48	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	514	CL7	C1D-ND-C4D	-4.02	103.48	106.33
21	33	516	CL7	C1D-ND-C4D	-4.02	103.48	106.33
21	11	402	CL7	C2D-C1D-ND	4.02	112.93	110.23
21	13	514	CL7	C2D-C1D-ND	4.02	112.93	110.23
21	13	505	CL7	O2D-CGD-CBD	4.02	118.42	111.27
21	43	409	CL7	C1D-ND-C4D	-4.02	103.48	106.33
21	43	411	CL7	C3A-C4A-CHB	-4.02	117.73	123.70
21	1B	608	CL7	CMD-C2D-C1D	4.02	131.49	125.37
21	3B	608	CL7	CMD-C2D-C1D	4.02	131.49	125.37
21	1C	510	CL7	C1D-ND-C4D	-4.02	103.48	106.33
21	14	414	CL7	CMD-C2D-C1D	4.02	131.49	125.37
21	23	406	CL7	O2D-CGD-CBD	4.02	118.41	111.27
23	1D	406	8CT	C14-C13-C12	-4.02	121.58	127.31
21	13	504	CL7	C3A-C4A-CHB	-4.02	117.74	123.70
21	1C	511	CL7	C4D-C3D-CAD	-4.02	104.72	107.42
23	3D	406	8CT	C14-C13-C12	-4.02	121.58	127.31
21	14	413	CL7	C4D-C3D-CAD	-4.02	104.72	107.42
21	44	413	CL7	C4D-C3D-CAD	-4.02	104.72	107.42
23	3C	518	8CT	C04-C03-C02	-4.02	116.96	122.61
32	12	522	ZEX	C27-C26-C25	-4.02	116.35	122.84
23	2C	518	8CT	C07-C02-C03	-4.01	116.90	122.73
21	21	411	CL7	C2D-C1D-ND	4.01	112.92	110.23
21	31	411	CL7	C2D-C1D-ND	4.01	112.92	110.23
21	12	514	CL7	C1D-ND-C4D	-4.01	103.48	106.33
21	3D	405	CL7	C1D-ND-C4D	-4.01	103.48	106.33
21	42	514	CL7	C1D-ND-C4D	-4.01	103.48	106.33
21	12	518	CL7	C4D-C3D-CAD	-4.01	104.72	107.42
21	4C	511	CL7	C4D-C3D-CAD	-4.01	104.72	107.42
21	42	518	CL7	C4D-C3D-CAD	-4.01	104.72	107.42
21	43	412	CL7	C2D-C1D-ND	4.01	112.92	110.23
21	2B	610	CL7	C1D-ND-C4D	-4.01	103.48	106.33
21	2C	501	CL7	C4D-C3D-CAD	-4.01	104.72	107.42
21	24	413	CL7	C4D-C3D-CAD	-4.01	104.72	107.42
21	3C	510	CL7	C1D-ND-C4D	-4.01	103.49	106.33
21	4B	614	CL7	C1D-ND-C4D	-4.01	103.49	106.33
21	44	404	CL7	C1D-ND-C4D	-4.01	103.49	106.33
32	22	522	ZEX	C27-C26-C25	-4.01	116.37	122.84
21	33	511	CL7	C2D-C1D-ND	4.00	112.92	110.23
32	13	519	ZEX	C35-C34-C33	-4.00	121.60	127.31
21	34	413	CL7	C4D-C3D-CAD	-4.00	104.73	107.42
21	11	411	CL7	C2D-C1D-ND	4.00	112.92	110.23
21	43	405	CL7	C2D-C1D-ND	4.00	112.92	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	509	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	31	410	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	4A	403	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	41	410	CL7	C1D-ND-C4D	-4.00	103.49	106.33
32	32	522	ZEX	C27-C26-C25	-4.00	116.37	122.84
21	43	406	CL7	O2D-CGD-CBD	4.00	118.38	111.27
21	4C	509	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	4C	510	CL7	C1D-ND-C4D	-4.00	103.49	106.33
21	33	504	CL7	C3A-C4A-CHB	-4.00	117.77	123.70
21	13	511	CL7	C2D-C1D-ND	3.99	112.91	110.23
21	43	405	CL7	C3A-C4A-CHB	-3.99	117.77	123.70
21	21	416	CL7	C2D-C1D-ND	3.99	112.91	110.23
23	1C	518	8CT	C07-C02-C03	-3.99	116.94	122.73
21	14	410	CL7	C2D-C1D-ND	3.99	112.91	110.23
21	11	403	CL7	C2D-C1D-ND	3.99	112.91	110.23
21	44	410	CL7	C2D-C1D-ND	3.99	112.91	110.23
21	3C	511	CL7	C4D-C3D-CAD	-3.99	104.74	107.42
21	11	407	CL7	C2D-C1D-ND	3.99	112.90	110.23
32	23	420	ZEX	C35-C34-C33	-3.99	121.62	127.31
21	1B	606	CL7	CHD-C1D-ND	-3.99	120.04	124.26
21	33	505	CL7	O2D-CGD-CBD	3.98	118.35	111.27
21	12	502	CL7	C2D-C1D-ND	3.98	112.90	110.23
21	23	414	CL7	C1D-ND-C4D	-3.98	103.51	106.33
21	42	516	CL7	C2D-C1D-ND	3.98	112.90	110.23
21	2B	604	CL7	C3A-C4A-CHB	-3.98	117.79	123.70
21	4B	609	CL7	CMD-C2D-C1D	3.98	131.43	125.37
21	2B	612	CL7	C4D-C3D-CAD	-3.98	104.74	107.42
21	31	402	CL7	C2D-C1D-ND	3.98	112.90	110.23
21	2B	609	CL7	CMD-C2D-C1D	3.97	131.42	125.37
21	33	504	CL7	C2D-C1D-ND	3.97	112.90	110.23
21	4C	511	CL7	C2D-C1D-ND	3.97	112.90	110.23
21	31	405	CL7	C4D-C3D-CAD	-3.97	104.75	107.42
32	42	522	ZEX	C27-C26-C25	-3.97	116.42	122.84
21	12	516	CL7	C2D-C1D-ND	3.97	112.89	110.23
21	11	416	CL7	C2D-C1D-ND	3.97	112.89	110.23
21	32	511	CL7	C2D-C1D-ND	3.97	112.89	110.23
21	41	408	CL7	O2D-CGD-CBD	3.97	118.32	111.27
32	33	519	ZEX	C35-C34-C33	-3.97	121.65	127.31
21	11	410	CL7	C1D-ND-C4D	-3.97	103.52	106.33
32	24	403	ZEX	C27-C26-C25	-3.97	116.43	122.84
21	11	420	CL7	C4D-C3D-CAD	-3.97	104.75	107.42
21	23	414	CL7	C3A-C4A-CHB	-3.97	117.81	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	407	CL7	C2D-C1D-ND	3.96	112.89	110.23
23	4D	406	8CT	C14-C13-C12	-3.96	121.65	127.31
21	3A	407	CL7	C4D-C3D-CAD	-3.96	104.75	107.42
21	41	420	CL7	C4D-C3D-CAD	-3.96	104.75	107.42
21	31	408	CL7	O2D-CGD-CBD	3.96	118.31	111.27
21	1B	603	CL7	C3A-C4A-CHB	-3.96	117.82	123.70
21	33	513	CL7	C3A-C4A-CHB	-3.96	117.82	123.70
21	21	403	CL7	C2D-C1D-ND	3.96	112.89	110.23
21	3B	609	CL7	C1D-ND-C4D	-3.96	103.52	106.33
21	1B	613	CL7	C1D-ND-C4D	-3.96	103.52	106.33
32	43	420	ZEX	C35-C34-C33	-3.96	121.66	127.31
21	11	408	CL7	O2D-CGD-CBD	3.96	118.30	111.27
21	4B	602	CL7	C4D-C3D-CAD	-3.96	104.76	107.42
23	2A	404	8CT	C35-C30-C29	-3.96	107.70	112.70
21	1C	509	CL7	C4D-C3D-CAD	-3.96	104.76	107.42
21	33	514	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	1B	608	CL7	C4D-C3D-CAD	-3.95	104.76	107.42
21	21	407	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	2C	509	CL7	C1D-ND-C4D	-3.95	103.53	106.33
21	34	410	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	2B	607	CL7	CHD-C1D-ND	-3.95	120.07	124.26
21	21	408	CL7	O2D-CGD-CBD	3.95	118.29	111.27
21	2B	602	CL7	C4D-C3D-CAD	-3.95	104.76	107.42
21	3B	601	CL7	C4D-C3D-CAD	-3.95	104.76	107.42
21	4C	509	CL7	C3A-C4A-CHB	-3.95	117.84	123.70
21	13	504	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	4B	604	CL7	C3A-C4A-CHB	-3.95	117.84	123.70
21	34	404	CL7	C1D-ND-C4D	-3.95	103.53	106.33
21	1C	504	CL7	C3A-C4A-CHB	-3.95	117.84	123.70
21	1C	509	CL7	C3A-C4A-CHB	-3.95	117.84	123.70
32	44	403	ZEX	C27-C26-C25	-3.95	116.46	122.84
23	1A	404	8CT	C35-C30-C29	-3.95	107.71	112.70
21	1C	513	CL7	C2D-C1D-ND	3.95	112.88	110.23
21	2C	502	CL7	C2D-C1D-ND	3.95	112.88	110.23
32	14	403	ZEX	C27-C26-C25	-3.95	116.46	122.84
21	44	408	CL7	C1D-ND-C4D	-3.95	103.53	106.33
21	41	403	CL7	C2D-C1D-ND	3.95	112.88	110.23
32	34	403	ZEX	C27-C26-C25	-3.95	116.46	122.84
21	13	513	CL7	C3A-C4A-CHB	-3.95	117.84	123.70
21	3C	509	CL7	C3A-C4A-CHB	-3.95	117.84	123.70
21	1B	611	CL7	C4D-C3D-CAD	-3.94	104.77	107.42
21	3C	504	CL7	C3A-C4A-CHB	-3.94	117.85	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	43	421	ZEX	C7-C8-C9	-3.94	120.28	126.23
21	23	417	CL7	C1D-ND-C4D	-3.94	103.53	106.33
21	34	413	CL7	C1D-ND-C4D	-3.94	103.53	106.33
21	43	414	CL7	C3A-C4A-CHB	-3.94	117.85	123.70
21	1B	609	CL7	C1D-ND-C4D	-3.94	103.54	106.33
21	3A	403	CL7	C1D-ND-C4D	-3.94	103.54	106.33
21	42	506	CL7	C1D-ND-C4D	-3.94	103.54	106.33
21	4B	612	CL7	C4D-C3D-CAD	-3.94	104.77	107.42
21	1B	607	CL7	C2D-C1D-ND	3.94	112.87	110.23
21	23	415	CL7	C2D-C1D-ND	3.94	112.87	110.23
21	3B	606	CL7	O2D-CGD-CBD	3.94	118.26	111.27
21	32	506	CL7	C1D-ND-C4D	-3.94	103.54	106.33
21	1B	614	CL7	C2D-C1D-ND	3.94	112.87	110.23
21	2B	623	CL7	C2D-C1D-ND	3.94	112.87	110.23
21	41	402	CL7	C2D-C1D-ND	3.94	112.87	110.23
23	3A	404	8CT	C35-C30-C29	-3.93	107.73	112.70
23	3B	617	8CT	C10-C11-C12	-3.93	120.29	126.23
21	1B	610	CL7	CAA-CBA-CGA	-3.93	101.76	113.25
21	4B	611	CL7	CAA-CBA-CGA	-3.93	101.76	113.25
21	3B	603	CL7	C3A-C4A-CHB	-3.93	117.86	123.70
21	12	511	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	12	518	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	42	511	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	43	402	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	34	413	CL7	C2D-C1D-ND	3.93	112.87	110.23
32	42	522	ZEX	C1-C6-C5	-3.93	117.08	122.61
21	3B	610	CL7	CAA-CBA-CGA	-3.93	101.77	113.25
32	33	520	ZEX	C7-C8-C9	-3.93	120.30	126.23
21	14	404	CL7	C1D-ND-C4D	-3.93	103.54	106.33
21	31	420	CL7	C4D-C3D-CAD	-3.93	104.78	107.42
21	1B	606	CL7	O2D-CGD-CBD	3.93	118.25	111.27
21	4B	607	CL7	O2D-CGD-CBD	3.93	118.25	111.27
21	4D	405	CL7	C2D-C1D-ND	3.93	112.87	110.23
21	2B	611	CL7	CAA-CBA-CGA	-3.93	101.77	113.25
21	1B	601	CL7	C4D-C3D-CAD	-3.93	104.78	107.42
21	2C	509	CL7	C4D-C3D-CAD	-3.93	104.78	107.42
21	22	518	CL7	C2D-C1D-ND	3.93	112.86	110.23
21	24	413	CL7	C1D-ND-C4D	-3.93	103.55	106.33
21	33	517	CL7	C1D-ND-C4D	-3.93	103.55	106.33
32	22	522	ZEX	C1-C6-C5	-3.93	117.08	122.61
23	4A	404	8CT	C35-C30-C29	-3.93	107.74	112.70
21	4A	407	CL7	C4D-C3D-CAD	-3.93	104.78	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	504	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	32	516	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	42	518	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	12	504	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	44	405	CL7	CAA-CBA-CGA	-3.92	101.79	113.25
21	32	511	CL7	C1D-ND-C4D	-3.92	103.55	106.33
21	42	501	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	24	405	CL7	CAA-CBA-CGA	-3.92	101.79	113.25
21	2B	614	CL7	C1D-ND-C4D	-3.92	103.55	106.33
21	34	405	CL7	CAA-CBA-CGA	-3.92	101.80	113.25
21	3B	622	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	32	501	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	13	516	CL7	C4D-C3D-CAD	-3.92	104.78	107.42
21	13	511	CL7	O2D-CGD-CBD	3.92	118.23	111.27
21	2B	607	CL7	O2D-CGD-CBD	3.92	118.23	111.27
21	2C	509	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	22	502	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	3B	613	CL7	C1D-ND-C4D	-3.92	103.55	106.33
32	12	522	ZEX	C31-C30-C29	-3.92	121.72	127.31
32	41	421	ZEX	C27-C28-C29	-3.92	120.32	126.23
32	32	522	ZEX	C1-C6-C5	-3.92	117.10	122.61
21	23	412	CL7	O2D-CGD-CBD	3.92	118.23	111.27
21	31	416	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	4C	502	CL7	C2D-C1D-ND	3.92	112.86	110.23
21	11	405	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	41	405	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	13	507	CL7	CMD-C2D-C1D	3.91	131.33	125.37
21	43	408	CL7	CMD-C2D-C1D	3.91	131.33	125.37
21	24	413	CL7	C2D-C1D-ND	3.91	112.86	110.23
21	4B	623	CL7	C2D-C1D-ND	3.91	112.86	110.23
21	33	513	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	2C	510	CL7	CAA-CBA-CGA	-3.91	101.82	113.25
21	3C	510	CL7	CAA-CBA-CGA	-3.91	101.82	113.25
21	32	502	CL7	C2D-C1D-ND	3.91	112.86	110.23
21	44	413	CL7	C2D-C1D-ND	3.91	112.86	110.23
21	2B	609	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	23	408	CL7	CMD-C2D-C1D	3.91	131.33	125.37
21	12	508	CL7	C1D-ND-C4D	-3.91	103.56	106.33
32	13	520	ZEX	C7-C8-C9	-3.91	120.32	126.23
21	14	405	CL7	CAA-CBA-CGA	-3.91	101.82	113.25
21	4C	510	CL7	CAA-CBA-CGA	-3.91	101.82	113.25
21	2C	511	CL7	C2D-C1D-ND	3.91	112.85	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	511	CL7	C2D-C1D-ND	3.91	112.85	110.23
21	4B	608	CL7	C2D-C1D-ND	3.91	112.85	110.23
21	32	504	CL7	C3A-C4A-CHB	-3.91	117.90	123.70
21	1A	407	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	23	414	CL7	C4D-C3D-CAD	-3.91	104.79	107.42
21	3B	611	CL7	C4D-C3D-CAD	-3.90	104.79	107.42
21	43	412	CL7	O2D-CGD-CBD	3.90	118.20	111.27
21	3C	502	CL7	C2D-C1D-ND	3.90	112.85	110.23
21	21	410	CL7	C1D-ND-C4D	-3.90	103.56	106.33
23	2B	618	8CT	C10-C11-C12	-3.90	120.34	126.23
21	22	511	CL7	C2D-C1D-ND	3.90	112.85	110.23
21	33	511	CL7	O2D-CGD-CBD	3.90	118.20	111.27
21	42	504	CL7	C3A-C4A-CHB	-3.90	117.91	123.70
21	2B	615	CL7	C2D-C1D-ND	3.90	112.85	110.23
21	3B	614	CL7	C2D-C1D-ND	3.90	112.85	110.23
21	33	507	CL7	CMD-C2D-C1D	3.90	131.31	125.37
21	21	420	CL7	C4D-C3D-CAD	-3.90	104.80	107.42
32	21	421	ZEX	C27-C28-C29	-3.90	120.34	126.23
32	31	421	ZEX	C27-C28-C29	-3.90	120.34	126.23
21	41	407	CL7	C2D-C1D-ND	3.90	112.84	110.23
21	24	411	CL7	CHD-C1D-ND	-3.90	120.13	124.26
21	44	411	CL7	CHD-C1D-ND	-3.90	120.13	124.26
32	12	522	ZEX	C1-C6-C5	-3.90	117.13	122.61
21	1C	510	CL7	CAA-CBA-CGA	-3.90	101.87	113.25
21	2C	504	CL7	C3A-C4A-CHB	-3.90	117.92	123.70
32	22	522	ZEX	C31-C30-C29	-3.90	121.75	127.31
21	1C	511	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	22	513	CL7	C3A-C4A-CHB	-3.89	117.92	123.70
21	13	513	CL7	C4D-C3D-CAD	-3.89	104.80	107.42
21	24	408	CL7	C4D-C3D-CAD	-3.89	104.80	107.42
21	14	408	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	14	408	CL7	C4D-C3D-CAD	-3.89	104.80	107.42
21	14	413	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	22	516	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	21	402	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	44	415	CL7	C4D-C3D-CAD	-3.89	104.80	107.42
21	12	511	CL7	C1D-ND-C4D	-3.89	103.57	106.33
21	42	511	CL7	C1D-ND-C4D	-3.89	103.57	106.33
23	1B	617	8CT	C10-C11-C12	-3.89	120.36	126.23
21	21	408	CL7	C3A-C4A-CHB	-3.89	117.93	123.70
32	32	522	ZEX	C31-C30-C29	-3.89	121.76	127.31
21	31	403	CL7	C2D-C1D-ND	3.89	112.84	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	417	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	23	405	CL7	C2D-C1D-ND	3.89	112.84	110.23
21	14	411	CL7	CHD-C1D-ND	-3.89	120.14	124.26
21	4B	610	CL7	C1D-ND-C4D	-3.89	103.57	106.33
21	12	506	CL7	C1D-ND-C4D	-3.89	103.58	106.33
21	2C	513	CL7	C2D-C1D-ND	3.88	112.84	110.23
21	14	413	CL7	C1D-ND-C4D	-3.88	103.58	106.33
21	22	504	CL7	C3A-C4A-CHB	-3.88	117.94	123.70
21	1D	405	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	1C	502	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	21	417	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	11	408	CL7	C3A-C4A-CHB	-3.88	117.94	123.70
21	1D	404	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	13	501	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	23	402	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	33	501	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	22	508	CL7	C1D-ND-C4D	-3.88	103.58	106.33
21	32	508	CL7	C1D-ND-C4D	-3.88	103.58	106.33
32	23	421	ZEX	C7-C8-C9	-3.88	120.38	126.23
21	43	415	CL7	C2D-C1D-ND	3.88	112.83	110.23
32	11	421	ZEX	C27-C28-C29	-3.88	120.38	126.23
21	42	508	CL7	C1D-ND-C4D	-3.88	103.58	106.33
21	2A	407	CL7	C4D-C3D-CAD	-3.88	104.81	107.42
21	4C	513	CL7	C2D-C1D-ND	3.88	112.83	110.23
21	34	408	CL7	C4D-C3D-CAD	-3.87	104.81	107.42
23	3D	406	8CT	C25-C24-C23	-3.87	111.13	123.22
21	42	512	CL7	CHD-C4C-C3C	-3.87	118.66	124.94
21	34	411	CL7	CHD-C1D-ND	-3.87	120.16	124.26
21	13	510	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	43	411	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	44	408	CL7	C2D-C1D-ND	3.87	112.83	110.23
23	4D	406	8CT	C25-C24-C23	-3.87	111.14	123.22
21	4B	616	CL7	C1D-ND-C4D	-3.87	103.58	106.33
21	44	413	CL7	C1D-ND-C4D	-3.87	103.58	106.33
21	32	518	CL7	C2D-C1D-ND	3.87	112.83	110.23
21	22	512	CL7	CHD-C4C-C3C	-3.87	118.67	124.94
21	32	512	CL7	CHD-C4C-C3C	-3.87	118.67	124.94
21	43	413	CL7	C3A-C4A-CHB	-3.87	117.96	123.70
21	23	413	CL7	C3A-C4A-CHB	-3.87	117.96	123.70
21	4B	609	CL7	C4D-C3D-CAD	-3.87	104.82	107.42
21	12	510	CL7	C1D-ND-C4D	-3.87	103.59	106.33
21	24	412	CL7	C1D-ND-C4D	-3.87	103.59	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	42	522	ZEX	C31-C30-C29	-3.87	121.79	127.31
21	14	408	CL7	C1D-ND-C4D	-3.87	103.59	106.33
21	14	410	CL7	C4D-C3D-CAD	-3.87	104.82	107.42
21	23	417	CL7	C4D-C3D-CAD	-3.86	104.82	107.42
21	33	516	CL7	C4D-C3D-CAD	-3.86	104.82	107.42
21	1B	622	CL7	C2D-C1D-ND	3.86	112.82	110.23
23	2D	406	8CT	C25-C24-C23	-3.86	111.16	123.22
21	32	503	CL7	CED-O2D-CGD	-3.86	107.20	115.94
21	1C	508	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	2B	608	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	3B	607	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	14	412	CL7	C1D-ND-C4D	-3.86	103.59	106.33
21	22	511	CL7	C1D-ND-C4D	-3.86	103.59	106.33
21	12	512	CL7	CHD-C4C-C3C	-3.86	118.68	124.94
21	1B	611	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	31	409	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	13	506	CL7	C3A-C4A-CHB	-3.86	117.97	123.70
21	22	510	CL7	C1D-ND-C4D	-3.86	103.59	106.33
21	43	417	CL7	C4D-C3D-CAD	-3.86	104.82	107.42
21	43	418	CL7	C1D-ND-C4D	-3.86	103.59	106.33
21	31	408	CL7	C3A-C4A-CHB	-3.86	117.98	123.70
21	42	513	CL7	C3A-C4A-CHB	-3.86	117.98	123.70
21	2D	404	CL7	C2D-C1D-ND	3.86	112.82	110.23
21	12	513	CL7	C3A-C4A-CHB	-3.85	117.98	123.70
21	23	407	CL7	C3A-C4A-CHB	-3.85	117.98	123.70
21	22	501	CL7	C2D-C1D-ND	3.85	112.82	110.23
21	12	503	CL7	CED-O2D-CGD	-3.85	107.22	115.94
21	42	503	CL7	CED-O2D-CGD	-3.85	107.22	115.94
21	32	513	CL7	C3A-C4A-CHB	-3.85	117.98	123.70
21	1B	614	CL7	CAA-C2A-C3A	-3.85	102.23	112.78
21	4B	615	CL7	CAA-C2A-C3A	-3.85	102.23	112.78
23	4B	618	8CT	C10-C11-C12	-3.85	120.41	126.23
23	1D	406	8CT	C25-C24-C23	-3.85	111.19	123.22
21	3D	405	CL7	C2D-C1D-ND	3.85	112.81	110.23
21	22	506	CL7	C1D-ND-C4D	-3.85	103.60	106.33
21	33	512	CL7	C3A-C4A-CHB	-3.85	117.99	123.70
21	43	407	CL7	C3A-C4A-CHB	-3.85	117.99	123.70
21	12	512	CL7	O2D-CGD-CBD	3.85	118.11	111.27
21	2A	403	CL7	CHD-C4C-C3C	-3.85	118.70	124.94
21	3A	403	CL7	CHD-C4C-C3C	-3.85	118.70	124.94
21	13	507	CL7	C1D-ND-C4D	-3.85	103.60	106.33
21	31	417	CL7	C2D-C1D-ND	3.85	112.81	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	614	CL7	CAA-C2A-C3A	-3.85	102.25	112.78
21	32	512	CL7	O2D-CGD-CBD	3.85	118.10	111.27
21	34	408	CL7	C1D-ND-C4D	-3.85	103.60	106.33
21	34	408	CL7	C2D-C1D-ND	3.85	112.81	110.23
21	43	410	CL7	C1D-ND-C4D	-3.84	103.60	106.33
21	3C	513	CL7	C2D-C1D-ND	3.84	112.81	110.23
21	3D	404	CL7	C2D-C1D-ND	3.84	112.81	110.23
21	4B	615	CL7	C2D-C1D-ND	3.84	112.81	110.23
21	43	410	CL7	C2D-C1D-ND	3.84	112.81	110.23
23	4C	515	8CT	C14-C15-C16	-3.84	115.62	126.42
21	11	417	CL7	C2D-C1D-ND	3.84	112.81	110.23
21	3C	508	CL7	C2D-C1D-ND	3.84	112.81	110.23
32	41	421	ZEX	C15-C14-C13	-3.84	121.83	127.31
21	41	408	CL7	C3A-C4A-CHB	-3.84	118.00	123.70
21	3C	507	CL7	C3A-C4A-CHB	-3.84	118.00	123.70
21	1A	403	CL7	CHD-C4C-C3C	-3.84	118.72	124.94
21	22	503	CL7	CED-O2D-CGD	-3.83	107.26	115.94
21	42	512	CL7	O2D-CGD-CBD	3.83	118.08	111.27
23	1C	515	8CT	C14-C15-C16	-3.83	115.64	126.42
21	3B	608	CL7	C4D-C3D-CAD	-3.83	104.84	107.42
21	13	512	CL7	C3A-C4A-CHB	-3.83	118.01	123.70
21	12	501	CL7	C2D-C1D-ND	3.83	112.80	110.23
21	22	512	CL7	O2D-CGD-CBD	3.83	118.08	111.27
21	24	408	CL7	C1D-ND-C4D	-3.83	103.61	106.33
21	3C	507	CL7	O2D-CGD-CBD	3.83	118.08	111.27
21	2C	502	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
21	22	515	CL7	C2D-C1D-ND	3.83	112.80	110.23
21	4C	507	CL7	O2D-CGD-CBD	3.83	118.07	111.27
23	2D	406	8CT	C10-C11-C12	-3.83	120.45	126.23
21	32	515	CL7	C2D-C1D-ND	3.83	112.80	110.23
21	2B	615	CL7	CAA-C2A-C3A	-3.83	102.29	112.78
21	2C	507	CL7	O2D-CGD-CBD	3.83	118.07	111.27
21	2B	612	CL7	C2D-C1D-ND	3.83	112.80	110.23
21	3B	615	CL7	C1D-ND-C4D	-3.83	103.62	106.33
21	34	410	CL7	C4D-C3D-CAD	-3.83	104.84	107.42
21	1C	507	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
21	4C	507	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
21	42	510	CL7	C1D-ND-C4D	-3.82	103.62	106.33
23	2C	515	8CT	C14-C15-C16	-3.82	115.67	126.42
21	4A	403	CL7	CHD-C4C-C3C	-3.82	118.74	124.94
21	43	414	CL7	C4D-C3D-CAD	-3.82	104.85	107.42
32	23	401	ZEX	C15-C14-C13	-3.82	121.86	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	44	418	ZEX	C18-C5-C6	-3.82	120.24	124.53
23	3D	406	8CT	C10-C11-C12	-3.82	120.46	126.23
21	3B	611	CL7	C2D-C1D-ND	3.82	112.79	110.23
21	3C	508	CL7	O2D-CGD-CBD	3.82	118.06	111.27
21	2C	507	CL7	C3A-C4A-CHB	-3.82	118.03	123.70
21	33	510	CL7	C2D-C1D-ND	3.82	112.79	110.23
21	44	408	CL7	C4D-C3D-CAD	-3.82	104.85	107.42
23	1D	406	8CT	C10-C11-C12	-3.82	120.46	126.23
21	22	507	CL7	C3A-C4A-CHB	-3.82	118.03	123.70
21	2C	508	CL7	O2D-CGD-CBD	3.82	118.05	111.27
23	3C	515	8CT	C14-C15-C16	-3.82	115.69	126.42
23	3B	617	8CT	C04-C03-C02	-3.82	117.24	122.61
32	33	525	ZEX	C15-C14-C13	-3.82	121.86	127.31
21	3C	502	CL7	C3A-C4A-CHB	-3.82	118.04	123.70
21	33	517	CL7	C2D-C1D-ND	3.82	112.79	110.23
23	1B	617	8CT	C04-C03-C02	-3.81	117.24	122.61
23	4B	618	8CT	C04-C03-C02	-3.81	117.24	122.61
32	31	422	ZEX	C15-C14-C13	-3.81	121.87	127.31
21	1C	502	CL7	C3A-C4A-CHB	-3.81	118.04	123.70
21	4C	502	CL7	C3A-C4A-CHB	-3.81	118.04	123.70
21	11	409	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	3B	608	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	41	409	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	43	406	CL7	CMD-C2D-C1D	3.81	131.18	125.37
32	13	525	ZEX	C15-C14-C13	-3.81	121.87	127.31
21	3B	606	CL7	C1D-ND-C4D	-3.81	103.63	106.33
21	24	412	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	3B	605	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	3C	504	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	3C	506	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	11	406	CL7	C4D-C3D-CAD	-3.81	104.86	107.42
21	11	414	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	4B	606	CL7	C2D-C1D-ND	3.81	112.79	110.23
21	4C	508	CL7	O2D-CGD-CBD	3.81	118.04	111.27
23	2B	618	8CT	C04-C03-C02	-3.81	117.25	122.61
21	1C	508	CL7	O2D-CGD-CBD	3.81	118.04	111.27
23	4D	406	8CT	C10-C11-C12	-3.81	120.48	126.23
21	33	506	CL7	C3A-C4A-CHB	-3.81	118.05	123.70
21	4C	504	CL7	C2D-C1D-ND	3.81	112.78	110.23
21	31	417	CL7	CHD-C1D-ND	-3.81	120.23	124.26
32	11	421	ZEX	C15-C14-C13	-3.81	121.88	127.31
21	42	507	CL7	C3A-C4A-CHB	-3.81	118.05	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	505	CL7	CMD-C2D-C1D	3.81	131.16	125.37
21	44	410	CL7	C4D-C3D-CAD	-3.81	104.86	107.42
21	13	509	CL7	C1D-ND-C4D	-3.80	103.63	106.33
21	43	408	CL7	C1D-ND-C4D	-3.80	103.63	106.33
21	11	417	CL7	CHD-C1D-ND	-3.80	120.23	124.26
27	1B	624	DGD	O2G-C1B-C2B	3.80	119.70	111.50
21	34	404	CL7	C3A-C4A-CHB	-3.80	118.05	123.70
32	43	401	ZEX	C15-C14-C13	-3.80	121.88	127.31
21	24	408	CL7	C2D-C1D-ND	3.80	112.78	110.23
21	14	415	CL7	C4D-C3D-CAD	-3.80	104.86	107.42
21	41	406	CL7	C4D-C3D-CAD	-3.80	104.86	107.42
27	4B	625	DGD	O2G-C1B-C2B	3.80	119.69	111.50
21	1C	504	CL7	C2D-C1D-ND	3.80	112.78	110.23
21	2C	506	CL7	C2D-C1D-ND	3.80	112.78	110.23
21	3A	407	CL7	CHD-C1D-ND	-3.80	120.23	124.26
27	2B	625	DGD	O2G-C1B-C2B	3.80	119.69	111.50
32	21	421	ZEX	C15-C14-C13	-3.80	121.89	127.31
21	13	505	CL7	CMD-C2D-C1D	3.80	131.15	125.37
21	1C	507	CL7	O2D-CGD-CBD	3.80	118.02	111.27
32	31	421	ZEX	C15-C14-C13	-3.80	121.89	127.31
21	4B	612	CL7	C2D-C1D-ND	3.80	112.78	110.23
21	43	404	CL7	CHD-C4C-C3C	-3.80	118.79	124.94
21	4B	611	CL7	O2D-CGD-CBD	3.80	118.01	111.27
21	23	418	CL7	C1D-ND-C4D	-3.80	103.64	106.33
21	12	507	CL7	C3A-C4A-CHB	-3.79	118.07	123.70
21	13	509	CL7	C2D-C1D-ND	3.79	112.78	110.23
27	3B	624	DGD	O2G-C1B-C2B	3.79	119.68	111.50
21	14	412	CL7	C2D-C1D-ND	3.79	112.78	110.23
21	41	417	CL7	CHD-C1D-ND	-3.79	120.24	124.26
21	23	411	CL7	C2D-C1D-ND	3.79	112.77	110.23
32	34	418	ZEX	C18-C5-C6	-3.79	120.27	124.53
21	44	412	CL7	C2D-C1D-ND	3.79	112.77	110.23
32	24	418	ZEX	C18-C5-C6	-3.79	120.27	124.53
21	11	418	CL7	C2D-C1D-ND	3.79	112.77	110.23
21	1C	510	CL7	CHD-C1D-ND	-3.79	120.25	124.26
32	11	422	ZEX	C15-C14-C13	-3.79	121.91	127.31
32	21	422	ZEX	C15-C14-C13	-3.79	121.91	127.31
21	12	515	CL7	C2D-C1D-ND	3.79	112.77	110.23
21	42	515	CL7	C2D-C1D-ND	3.79	112.77	110.23
21	23	408	CL7	C1D-ND-C4D	-3.79	103.65	106.33
21	33	507	CL7	C1D-ND-C4D	-3.79	103.65	106.33
21	4B	607	CL7	C1D-ND-C4D	-3.79	103.65	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	34	420	ZEX	C35-C34-C33	-3.79	121.91	127.31
31	2F	101	HEM	CHA-C4D-ND	3.78	129.04	124.37
21	2D	405	CL7	C2D-C1D-ND	3.78	112.77	110.23
21	2C	510	CL7	CHD-C1D-ND	-3.78	120.25	124.26
31	1F	101	HEM	CHA-C4D-ND	3.78	129.04	124.37
32	33	519	ZEX	C15-C35-C34	-3.78	115.72	123.47
32	41	422	ZEX	C15-C14-C13	-3.78	121.91	127.31
32	13	519	ZEX	C15-C35-C34	-3.78	115.72	123.47
21	1B	622	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	23	403	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	4B	623	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	13	517	CL7	C1D-ND-C4D	-3.78	103.65	106.33
31	3F	101	HEM	CHA-C4D-ND	3.78	129.04	124.37
21	14	404	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	44	404	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
32	14	418	ZEX	C18-C5-C6	-3.78	120.28	124.53
21	2B	616	CL7	C1D-ND-C4D	-3.78	103.65	106.33
21	34	408	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	44	408	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
21	33	503	CL7	CHD-C4C-C3C	-3.78	118.82	124.94
21	21	409	CL7	C2D-C1D-ND	3.78	112.76	110.23
21	41	418	CL7	C2D-C1D-ND	3.78	112.76	110.23
21	13	503	CL7	CHD-C4C-C3C	-3.78	118.82	124.94
21	13	518	CL7	C2D-C1D-ND	3.78	112.76	110.23
21	42	506	CL7	C2D-C1D-ND	3.78	112.76	110.23
31	2F	101	HEM	C1B-NB-C4B	3.77	108.97	105.07
21	13	502	CL7	C3A-C4A-CHB	-3.77	118.10	123.70
21	21	417	CL7	CHD-C1D-ND	-3.77	120.26	124.26
21	31	407	CL7	C3A-C4A-CHB	-3.77	118.10	123.70
21	1B	608	CL7	C2D-C1D-ND	3.77	112.76	110.23
21	22	518	CL7	C3A-C4A-CHB	-3.77	118.10	123.70
21	23	406	CL7	CMD-C2D-C1D	3.77	131.11	125.37
21	34	413	CL7	C3A-C4A-CHB	-3.77	118.10	123.70
21	21	404	CL7	C1-C2-C3	3.77	132.56	126.04
21	41	414	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	1B	610	CL7	O2D-CGD-CBD	3.77	117.97	111.27
21	33	509	CL7	C1D-ND-C4D	-3.77	103.66	106.33
32	43	420	ZEX	C15-C35-C34	-3.77	115.75	123.47
21	23	419	CL7	C2D-C1D-ND	3.77	112.76	110.23
21	33	518	CL7	C2D-C1D-ND	3.77	112.76	110.23
21	2B	623	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	3B	622	CL7	C3A-C4A-CHB	-3.77	118.11	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1B	607	CL7	CHD-C1D-ND	-3.77	120.27	124.26
21	4C	510	CL7	CHD-C1D-ND	-3.77	120.27	124.26
21	4A	407	CL7	CHD-C1D-ND	-3.77	120.27	124.26
21	24	404	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	24	413	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	31	402	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	4B	605	CL7	C1D-ND-C4D	-3.77	103.66	106.33
32	44	420	ZEX	C35-C34-C33	-3.77	121.94	127.31
21	2B	606	CL7	C2D-C1D-ND	3.76	112.76	110.23
21	23	410	CL7	C2D-C1D-ND	3.76	112.76	110.23
21	24	405	CL7	C2D-C1D-ND	3.76	112.76	110.23
23	4B	601	8CT	C39-C16-C17	-3.76	117.65	122.92
21	23	410	CL7	C1D-ND-C4D	-3.76	103.66	106.33
21	32	510	CL7	C1D-ND-C4D	-3.76	103.66	106.33
21	32	507	CL7	C3A-C4A-CHB	-3.76	118.11	123.70
31	4F	101	HEM	CHA-C4D-ND	3.76	129.01	124.37
21	2B	611	CL7	O2D-CGD-CBD	3.76	117.95	111.27
21	3B	610	CL7	O2D-CGD-CBD	3.76	117.95	111.27
21	14	413	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	32	518	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	41	419	CL7	C2D-C1D-ND	3.76	112.75	110.23
32	14	420	ZEX	C35-C34-C33	-3.76	121.94	127.31
21	3B	604	CL7	O2D-CGD-CBD	3.76	117.95	111.27
21	12	518	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	1B	615	CL7	C1D-ND-C4D	-3.76	103.66	106.33
21	2B	605	CL7	C1D-ND-C4D	-3.76	103.66	106.33
21	4D	404	CL7	C2D-C1D-ND	3.76	112.75	110.23
23	1B	626	8CT	C39-C16-C17	-3.76	117.66	122.92
21	11	407	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	41	407	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	13	510	CL7	C1D-ND-C4D	-3.76	103.67	106.33
21	31	404	CL7	C1-C2-C3	3.76	132.54	126.04
21	13	518	CL7	C4D-C3D-CAD	-3.76	104.89	107.42
21	32	506	CL7	C2D-C1D-ND	3.76	112.75	110.23
21	14	408	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	3C	503	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
32	23	420	ZEX	C15-C35-C34	-3.76	115.78	123.47
21	23	404	CL7	CHD-C4C-C3C	-3.76	118.85	124.94
21	24	415	CL7	C4D-C3D-CAD	-3.76	104.89	107.42
21	34	415	CL7	C4D-C3D-CAD	-3.76	104.89	107.42
23	2B	601	8CT	C39-C16-C17	-3.75	117.66	122.92
23	3B	626	8CT	C39-C16-C17	-3.75	117.66	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	405	CL7	C1-C2-C3	3.75	132.54	126.04
21	2A	407	CL7	CHD-C1D-ND	-3.75	120.28	124.26
21	12	506	CL7	C2D-C1D-ND	3.75	112.75	110.23
21	2C	504	CL7	C2D-C1D-ND	3.75	112.75	110.23
31	4F	101	HEM	C1B-NB-C4B	3.75	108.95	105.07
23	1B	619	8CT	C01-C02-C03	-3.75	120.31	124.53
23	4B	620	8CT	C01-C02-C03	-3.75	120.31	124.53
21	34	412	CL7	C1D-ND-C4D	-3.75	103.67	106.33
21	2C	503	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
31	1F	101	HEM	C1B-NB-C4B	3.75	108.95	105.07
21	43	418	CL7	C2D-C1D-ND	3.75	112.75	110.23
32	24	420	ZEX	C35-C34-C33	-3.75	121.95	127.31
32	44	419	ZEX	C31-C30-C29	-3.75	121.95	127.31
21	24	408	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	41	414	CL7	C2D-C1D-ND	3.75	112.75	110.23
21	3B	609	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	33	502	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	34	405	CL7	C1-C2-C3	3.75	132.53	126.04
21	33	518	CL7	C4D-C3D-CAD	-3.75	104.90	107.42
21	11	404	CL7	C1-C2-C3	3.75	132.53	126.04
31	3F	101	HEM	C1B-NB-C4B	3.75	108.94	105.07
21	1A	407	CL7	CHD-C1D-ND	-3.75	120.29	124.26
21	21	414	CL7	C3A-C4A-CHB	-3.75	118.14	123.70
21	42	518	CL7	C3A-C4A-CHB	-3.75	118.14	123.70
21	44	412	CL7	C1D-ND-C4D	-3.74	103.67	106.33
21	21	419	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	31	418	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	31	419	CL7	C2D-C1D-ND	3.74	112.74	110.23
32	14	419	ZEX	C31-C30-C29	-3.74	121.97	127.31
21	3C	506	CL7	C3A-C4A-CHB	-3.74	118.14	123.70
21	43	403	CL7	C3A-C4A-CHB	-3.74	118.14	123.70
21	2B	605	CL7	O2D-CGD-CBD	3.74	117.92	111.27
21	4B	605	CL7	O2D-CGD-CBD	3.74	117.92	111.27
32	34	419	ZEX	C31-C30-C29	-3.74	121.97	127.31
21	11	419	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	31	414	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	1B	604	CL7	O2D-CGD-CBD	3.74	117.92	111.27
21	1B	606	CL7	C1D-ND-C4D	-3.74	103.68	106.33
21	2B	607	CL7	C1D-ND-C4D	-3.74	103.68	106.33
21	12	510	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	22	506	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	4C	508	CL7	C2D-C1D-ND	3.74	112.74	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	407	CL7	C3A-C4A-CHB	-3.74	118.15	123.70
21	31	406	CL7	C4D-C3D-CAD	-3.74	104.90	107.42
21	44	413	CL7	C3A-C4A-CHB	-3.74	118.15	123.70
21	22	503	CL7	CAA-CBA-CGA	-3.74	102.33	113.25
21	41	402	CL7	C3A-C4A-CHB	-3.74	118.15	123.70
21	32	503	CL7	CAA-CBA-CGA	-3.74	102.33	113.25
21	21	414	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	41	404	CL7	C1-C2-C3	3.74	132.51	126.04
21	32	503	CL7	CHD-C4C-C3C	-3.74	118.88	124.94
23	1B	619	8CT	C24-C23-C21	-3.74	115.92	126.42
21	22	517	CL7	C3A-C4A-CHB	-3.74	118.15	123.70
23	1K	101	8CT	C24-C25-C26	-3.74	121.98	127.31
21	1B	605	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	22	510	CL7	C2D-C1D-ND	3.74	112.74	110.23
21	1B	604	CL7	C1D-ND-C4D	-3.74	103.68	106.33
21	43	411	CL7	C1D-ND-C4D	-3.73	103.68	106.33
21	33	509	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	4B	609	CL7	C2D-C1D-ND	3.73	112.73	110.23
23	4K	101	8CT	C24-C25-C26	-3.73	121.98	127.31
21	21	406	CL7	C4D-C3D-CAD	-3.73	104.91	107.42
21	23	419	CL7	C4D-C3D-CAD	-3.73	104.91	107.42
21	1C	506	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	2B	613	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	4C	506	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	42	503	CL7	CAA-CBA-CGA	-3.73	102.35	113.25
21	1C	503	CL7	C3A-C4A-CHB	-3.73	118.17	123.70
23	3B	617	8CT	C19-C20-C21	-3.73	121.99	127.31
21	43	419	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	3C	510	CL7	CHD-C1D-ND	-3.73	120.31	124.26
32	12	522	ZEX	C31-C32-C33	-3.73	115.94	126.42
32	42	522	ZEX	C31-C32-C33	-3.73	115.94	126.42
21	11	414	CL7	C3A-C4A-CHB	-3.73	118.17	123.70
21	21	418	CL7	C2D-C1D-ND	3.73	112.73	110.23
21	12	503	CL7	CAA-CBA-CGA	-3.73	102.36	113.25
23	4B	620	8CT	C24-C23-C21	-3.73	115.95	126.42
21	34	412	CL7	C2D-C1D-ND	3.72	112.73	110.23
21	24	412	CL7	CHD-C1D-ND	-3.72	120.31	124.26
21	43	417	CL7	CHD-C1D-ND	-3.72	120.31	124.26
21	24	405	CL7	C1-C2-C3	3.72	132.48	126.04
21	44	405	CL7	C1-C2-C3	3.72	132.48	126.04
23	2B	620	8CT	C24-C23-C21	-3.72	115.95	126.42
21	2C	508	CL7	C2D-C1D-ND	3.72	112.73	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	402	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
21	21	402	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
21	14	412	CL7	CHD-C1D-ND	-3.72	120.32	124.26
23	3C	514	8CT	C10-C11-C12	-3.72	120.61	126.23
21	42	503	CL7	CHD-C4C-C3C	-3.72	118.91	124.94
23	2B	620	8CT	C01-C02-C03	-3.72	120.35	124.53
23	4C	514	8CT	C10-C11-C12	-3.72	120.62	126.23
21	4B	608	CL7	CHD-C1D-ND	-3.72	120.32	124.26
21	3B	604	CL7	C1D-ND-C4D	-3.72	103.69	106.33
21	4B	610	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
21	12	503	CL7	CHD-C4C-C3C	-3.72	118.92	124.94
23	3B	619	8CT	C24-C23-C21	-3.72	115.98	126.42
21	4B	613	CL7	C2D-C1D-ND	3.72	112.72	110.23
21	1B	614	CL7	C1D-ND-C4D	-3.71	103.70	106.33
21	13	517	CL7	C2D-C1D-ND	3.71	112.72	110.23
32	32	522	ZEX	C31-C32-C33	-3.71	115.98	126.42
21	2B	609	CL7	C2D-C1D-ND	3.71	112.72	110.23
21	3B	612	CL7	C2D-C1D-ND	3.71	112.72	110.23
21	43	419	CL7	C4D-C3D-CAD	-3.71	104.92	107.42
21	44	411	CL7	C2D-C1D-ND	3.71	112.72	110.23
21	3B	622	CL7	O2D-CGD-CBD	3.71	117.86	111.27
23	4B	618	8CT	C19-C20-C21	-3.71	122.02	127.31
21	2C	506	CL7	C3A-C4A-CHB	-3.71	118.19	123.70
21	1B	622	CL7	O2D-CGD-CBD	3.71	117.86	111.27
21	4C	503	CL7	C3A-C4A-CHB	-3.71	118.20	123.70
23	2K	101	8CT	C24-C25-C26	-3.71	122.02	127.31
23	3K	101	8CT	C24-C25-C26	-3.71	122.02	127.31
21	2B	608	CL7	CHD-C1D-ND	-3.71	120.33	124.26
21	3B	607	CL7	CHD-C1D-ND	-3.71	120.33	124.26
21	3C	513	CL7	C3A-C4A-CHB	-3.71	118.20	123.70
21	31	414	CL7	C3A-C4A-CHB	-3.71	118.20	123.70
21	42	510	CL7	C2D-C1D-ND	3.71	112.72	110.23
21	32	517	CL7	C3A-C4A-CHB	-3.70	118.20	123.70
21	34	411	CL7	O2A-C1-C2	-3.70	98.90	108.64
32	12	520	ZEX	C15-C14-C13	-3.70	122.03	127.31
23	2C	514	8CT	C10-C11-C12	-3.70	120.64	126.23
23	2B	620	8CT	C11-C10-C03	-3.70	116.80	127.20
21	44	411	CL7	O2A-C1-C2	-3.70	98.90	108.64
21	13	507	CL7	C2D-C1D-ND	3.70	112.71	110.23
21	43	408	CL7	C2D-C1D-ND	3.70	112.71	110.23
21	22	503	CL7	CHD-C4C-C3C	-3.70	118.94	124.94
23	1C	514	8CT	C10-C11-C12	-3.70	120.64	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	613	CL7	O2D-CGD-CBD	3.70	117.84	111.27
21	3B	612	CL7	O2D-CGD-CBD	3.70	117.84	111.27
21	14	411	CL7	O2A-C1-C2	-3.70	98.92	108.64
21	33	516	CL7	CHD-C1D-ND	-3.70	120.34	124.26
21	2B	623	CL7	O2D-CGD-CBD	3.70	117.84	111.27
21	44	412	CL7	CHD-C1D-ND	-3.70	120.34	124.26
21	24	410	CL7	C4D-C3D-CAD	-3.70	104.93	107.42
32	22	522	ZEX	C31-C32-C33	-3.70	116.03	126.42
23	3B	619	8CT	C01-C02-C03	-3.70	120.38	124.53
23	2K	101	8CT	C18-C17-C16	-3.70	122.03	127.31
23	3K	101	8CT	C18-C17-C16	-3.70	122.03	127.31
23	4B	620	8CT	C11-C10-C03	-3.70	116.82	127.20
21	4B	623	CL7	O2D-CGD-CBD	3.70	117.83	111.27
23	4K	101	8CT	C18-C17-C16	-3.69	122.04	127.31
32	42	520	ZEX	C15-C14-C13	-3.69	122.04	127.31
23	1B	617	8CT	C19-C20-C21	-3.69	122.04	127.31
32	24	419	ZEX	C31-C30-C29	-3.69	122.04	127.31
23	1B	619	8CT	C11-C10-C03	-3.69	116.83	127.20
21	42	508	CL7	C2D-C1D-ND	3.69	112.71	110.23
21	1C	506	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
21	4C	506	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
21	42	517	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
21	4B	613	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	1C	513	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
21	4C	513	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
21	33	511	CL7	CHD-C4C-C3C	-3.69	118.96	124.94
21	13	516	CL7	CHD-C1D-ND	-3.69	120.35	124.26
23	3B	619	8CT	C11-C10-C03	-3.69	116.84	127.20
21	4C	501	CL7	CHD-C4C-C3C	-3.69	118.96	124.94
21	21	411	CL7	C3A-C4A-CHB	-3.69	118.23	123.70
21	12	506	CL7	C3A-C4A-CHB	-3.69	118.23	123.70
21	24	411	CL7	O2A-C1-C2	-3.69	98.95	108.64
23	2B	618	8CT	C19-C20-C21	-3.69	122.05	127.31
21	32	510	CL7	C2D-C1D-ND	3.68	112.70	110.23
21	43	417	CL7	C7-C6-C5	-3.68	103.35	113.36
21	23	411	CL7	C1D-ND-C4D	-3.68	103.72	106.33
21	33	510	CL7	C1D-ND-C4D	-3.68	103.72	106.33
32	22	520	ZEX	C15-C14-C13	-3.68	122.05	127.31
32	32	520	ZEX	C15-C14-C13	-3.68	122.05	127.31
21	1B	612	CL7	O2D-CGD-CBD	3.68	117.81	111.27
21	11	420	CL7	C3A-C4A-CHB	-3.68	118.23	123.70
21	23	417	CL7	C7-C6-C5	-3.68	103.36	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1K	101	8CT	C18-C17-C16	-3.68	122.06	127.31
21	43	407	CL7	C1D-ND-C4D	-3.68	103.72	106.33
21	2B	610	CL7	C3A-C4A-CHB	-3.68	118.24	123.70
21	4D	404	CL7	O2D-CGD-CBD	3.68	117.81	111.27
21	23	417	CL7	CHD-C1D-ND	-3.68	120.36	124.26
21	14	411	CL7	C2D-C1D-ND	3.68	112.70	110.23
21	44	405	CL7	C2D-C1D-ND	3.68	112.70	110.23
21	11	411	CL7	C3A-C4A-CHB	-3.68	118.24	123.70
21	43	412	CL7	CHD-C4C-C3C	-3.68	118.98	124.94
21	1B	612	CL7	C2D-C1D-ND	3.68	112.70	110.23
21	14	409	CL7	C3A-C4A-CHB	-3.68	118.25	123.70
21	11	403	CL7	CMD-C2D-C1D	3.67	130.97	125.37
21	22	512	CL7	CMD-C2D-C1D	3.67	130.97	125.37
21	32	512	CL7	CMD-C2D-C1D	3.67	130.97	125.37
21	22	504	CL7	C1D-ND-C4D	-3.67	103.72	106.33
21	43	414	CL7	C2D-C1D-ND	3.67	112.69	110.23
21	1B	609	CL7	C3A-C4A-CHB	-3.67	118.25	123.70
32	42	520	ZEX	C11-C10-C9	-3.67	122.07	127.31
21	44	412	CL7	O2D-CGD-CBD	3.67	117.79	111.27
21	34	412	CL7	CHD-C1D-ND	-3.67	120.37	124.26
21	33	516	CL7	C7-C6-C5	-3.67	103.39	113.36
21	13	517	CL7	C3A-C4A-CHB	-3.67	118.25	123.70
21	2C	501	CL7	CHD-C4C-C3C	-3.67	118.99	124.94
21	13	516	CL7	C7-C6-C5	-3.67	103.40	113.36
21	32	506	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	31	420	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	31	411	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	1A	403	CL7	C2D-C1D-ND	3.67	112.69	110.23
21	23	408	CL7	C2D-C1D-ND	3.67	112.69	110.23
21	33	507	CL7	C2D-C1D-ND	3.67	112.69	110.23
21	13	506	CL7	C1D-ND-C4D	-3.67	103.73	106.33
21	1C	501	CL7	CHD-C4C-C3C	-3.66	119.00	124.94
21	21	403	CL7	CMD-C2D-C1D	3.66	130.95	125.37
21	31	403	CL7	CMD-C2D-C1D	3.66	130.95	125.37
21	2C	513	CL7	C3A-C4A-CHB	-3.66	118.26	123.70
23	1C	518	8CT	C10-C11-C12	-3.66	120.70	126.23
21	14	412	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	12	517	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	24	409	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	34	409	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	31	406	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	2D	404	CL7	O2D-CGD-CBD	3.66	117.77	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3D	404	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	23	412	CL7	CHD-C4C-C3C	-3.66	119.01	124.94
21	11	406	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	32	511	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	13	513	CL7	C2D-C1D-ND	3.66	112.68	110.23
21	14	405	CL7	C2D-C1D-ND	3.66	112.68	110.23
21	23	418	CL7	C2D-C1D-ND	3.66	112.68	110.23
21	41	411	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	3C	501	CL7	CHD-C4C-C3C	-3.66	119.01	124.94
21	12	504	CL7	C1D-ND-C4D	-3.66	103.74	106.33
21	4A	407	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	41	420	CL7	C3A-C4A-CHB	-3.66	118.27	123.70
21	22	506	CL7	C3A-C4A-CHB	-3.66	118.28	123.70
27	3C	516	DGD	O2G-C1B-C2B	3.65	119.38	111.50
21	13	508	CL7	C1-C2-C3	3.65	132.36	126.04
21	12	508	CL7	C2D-C1D-ND	3.65	112.68	110.23
21	13	511	CL7	CHD-C4C-C3C	-3.65	119.02	124.94
21	3B	602	CL7	O2D-CGD-CBD	3.65	117.76	111.27
21	41	403	CL7	CMD-C2D-C1D	3.65	130.93	125.37
21	12	512	CL7	CMD-C2D-C1D	3.65	130.93	125.37
21	24	412	CL7	O2D-CGD-CBD	3.65	117.76	111.27
21	34	412	CL7	O2D-CGD-CBD	3.65	117.76	111.27
21	3B	610	CL7	C4D-C3D-CAD	-3.65	104.96	107.42
21	24	411	CL7	C2D-C1D-ND	3.65	112.68	110.23
21	3B	613	CL7	C2D-C1D-ND	3.65	112.68	110.23
21	12	511	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
21	1B	613	CL7	C2D-C1D-ND	3.65	112.68	110.23
21	4B	614	CL7	C2D-C1D-ND	3.65	112.68	110.23
32	12	520	ZEX	C11-C10-C9	-3.65	122.10	127.31
21	43	409	CL7	C1-C2-C3	3.65	132.35	126.04
21	14	415	CL7	C3A-C4A-CHB	-3.65	118.29	123.70
21	3D	404	CL7	C4D-C3D-CAD	-3.65	104.97	107.42
21	22	508	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	32	508	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	1D	404	CL7	O2D-CGD-CBD	3.64	117.74	111.27
21	34	405	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	34	411	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	32	504	CL7	C1D-ND-C4D	-3.64	103.75	106.33
27	4C	516	DGD	O2G-C1B-C2B	3.64	119.35	111.50
21	42	512	CL7	CMD-C2D-C1D	3.64	130.91	125.37
21	41	406	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	2B	615	CL7	C1D-ND-C4D	-3.64	103.75	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	420	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	44	409	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	2A	407	CL7	O2D-CGD-CBD	3.64	117.73	111.27
21	33	508	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	2B	603	CL7	O2D-CGD-CBD	3.64	117.73	111.27
21	23	418	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	2B	614	CL7	C2D-C1D-ND	3.64	112.67	110.23
21	3B	614	CL7	C1D-ND-C4D	-3.63	103.75	106.33
21	42	506	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	42	511	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	23	409	CL7	C1-C2-C3	3.63	132.33	126.04
21	33	508	CL7	C1-C2-C3	3.63	132.33	126.04
21	22	511	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
32	32	520	ZEX	C11-C10-C9	-3.63	122.12	127.31
21	2B	603	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	3B	602	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	4B	603	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	42	504	CL7	C1D-ND-C4D	-3.63	103.75	106.33
23	1B	626	8CT	C30-C31-C32	-3.63	117.00	121.47
32	44	419	ZEX	C27-C28-C29	-3.63	120.75	126.23
32	14	419	ZEX	C27-C28-C29	-3.63	120.75	126.23
21	43	404	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	14	406	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	3D	402	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	33	506	CL7	C1D-ND-C4D	-3.63	103.76	106.33
23	34	402	8CT	C24-C25-C26	-3.63	122.13	127.31
32	24	419	ZEX	C27-C28-C29	-3.63	120.75	126.23
21	43	418	CL7	C3A-C4A-CHB	-3.63	118.32	123.70
21	4B	603	CL7	O2D-CGD-CBD	3.63	117.71	111.27
21	4B	615	CL7	C1D-ND-C4D	-3.63	103.76	106.33
27	2C	516	DGD	O2G-C1B-C2B	3.63	119.31	111.50
21	11	411	CL7	CHD-C1D-ND	-3.63	120.42	124.26
21	41	411	CL7	CHD-C1D-ND	-3.63	120.42	124.26
21	1B	602	CL7	C3A-C4A-CHB	-3.62	118.32	123.70
21	33	517	CL7	C3A-C4A-CHB	-3.62	118.32	123.70
23	3B	626	8CT	C30-C31-C32	-3.62	117.01	121.47
21	3A	407	CL7	O2D-CGD-CBD	3.62	117.70	111.27
21	11	414	CL7	CAC-C3C-C4C	-3.62	118.98	124.68
21	23	416	CL7	O2D-CGD-CBD	3.62	117.70	111.27
21	13	503	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
21	41	418	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
21	21	411	CL7	CHD-C1D-ND	-3.62	120.43	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4C	518	8CT	C10-C11-C12	-3.62	120.77	126.23
21	1C	517	CL7	O2D-CGD-CBD	3.62	117.69	111.27
21	4C	517	CL7	O2D-CGD-CBD	3.62	117.69	111.27
21	23	407	CL7	C1D-ND-C4D	-3.61	103.77	106.33
21	41	417	CL7	CHD-C4C-C3C	-3.61	119.08	124.94
21	32	501	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	33	503	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	33	513	CL7	C2D-C1D-ND	3.61	112.65	110.23
21	11	417	CL7	CHD-C4C-C3C	-3.61	119.08	124.94
21	21	406	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	2A	407	CL7	O2A-C1-C2	-3.61	99.14	108.64
27	1C	516	DGD	O2G-C1B-C2B	3.61	119.28	111.50
21	21	417	CL7	CHD-C4C-C3C	-3.61	119.08	124.94
21	1B	602	CL7	O2D-CGD-CBD	3.61	117.69	111.27
21	2D	402	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	3A	407	CL7	O2A-C1-C2	-3.61	99.14	108.64
32	34	419	ZEX	C27-C28-C29	-3.61	120.78	126.23
21	2A	403	CL7	C2D-C1D-ND	3.61	112.65	110.23
21	23	414	CL7	C2D-C1D-ND	3.61	112.65	110.23
21	3D	404	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	1A	407	CL7	O2A-C1-C2	-3.61	99.15	108.64
32	22	520	ZEX	C11-C10-C9	-3.61	122.16	127.31
21	3C	517	CL7	O2D-CGD-CBD	3.61	117.68	111.27
21	33	505	CL7	C7-C6-C5	-3.61	103.56	113.36
21	1A	407	CL7	O2D-CGD-CBD	3.61	117.68	111.27
21	31	411	CL7	CHD-C1D-ND	-3.61	120.44	124.26
23	3C	518	8CT	C10-C11-C12	-3.61	120.78	126.23
21	43	409	CL7	C2D-C1D-ND	3.61	112.65	110.23
21	4A	407	CL7	O2A-C1-C2	-3.61	99.16	108.64
21	3C	517	CL7	C1D-ND-C4D	-3.61	103.77	106.33
21	41	414	CL7	CAC-C3C-C4C	-3.61	119.00	124.68
21	21	404	CL7	C2D-C1D-ND	3.61	112.65	110.23
21	23	404	CL7	C3A-C4A-CHB	-3.60	118.35	123.70
21	31	414	CL7	CAC-C3C-C4C	-3.60	119.01	124.68
23	14	402	8CT	C24-C25-C26	-3.60	122.17	127.31
23	44	402	8CT	C24-C25-C26	-3.60	122.17	127.31
23	2C	518	8CT	C10-C11-C12	-3.60	120.79	126.23
21	21	414	CL7	CAC-C3C-C4C	-3.60	119.01	124.68
21	24	406	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	4D	404	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	4A	403	CL7	C4C-C3C-C2C	-3.60	102.44	107.13
21	24	407	CL7	C3A-C4A-CHB	-3.60	118.36	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	34	407	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	13	515	CL7	O2D-CGD-CBD	3.60	117.66	111.27
21	14	407	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	44	407	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	41	414	CL7	CHD-C1D-ND	-3.60	120.45	124.26
21	4B	611	CL7	C4D-C3D-CAD	-3.60	105.00	107.42
21	1D	404	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	2C	517	CL7	O2D-CGD-CBD	3.60	117.66	111.27
23	2B	601	8CT	C30-C31-C32	-3.60	117.04	121.47
21	24	415	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	23	406	CL7	C7-C6-C5	-3.60	103.59	113.36
21	34	415	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
23	4B	619	8CT	C07-C02-C03	-3.60	117.51	122.73
21	21	414	CL7	CHD-C1D-ND	-3.60	120.45	124.26
21	23	409	CL7	C2D-C1D-ND	3.59	112.64	110.23
21	4C	512	CL7	C3A-C4A-CHB	-3.59	118.36	123.70
21	42	501	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
23	4B	601	8CT	C30-C31-C32	-3.59	117.05	121.47
21	2A	403	CL7	C4C-C3C-C2C	-3.59	102.44	107.13
21	13	505	CL7	C7-C6-C5	-3.59	103.60	113.36
21	43	406	CL7	C7-C6-C5	-3.59	103.60	113.36
21	43	416	CL7	O2D-CGD-CBD	3.59	117.65	111.27
21	11	415	CL7	CHD-C4C-C3C	-3.59	119.12	124.94
21	2B	614	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	3B	613	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	4B	611	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
23	1C	515	8CT	C01-C02-C07	3.59	120.51	113.62
23	4C	515	8CT	C01-C02-C07	3.59	120.51	113.62
21	31	417	CL7	CHD-C4C-C3C	-3.59	119.12	124.94
21	11	417	CL7	C3A-C4A-CHB	-3.59	118.38	123.70
21	41	420	CL7	CHD-C4C-C3C	-3.59	119.13	124.94
21	1D	402	CL7	CHD-C1D-ND	-3.59	120.46	124.26
21	4D	402	CL7	CHD-C1D-ND	-3.59	120.46	124.26
21	24	412	CL7	C3A-C4A-CHB	-3.59	118.38	123.70
21	2D	404	CL7	C3A-C4A-CHB	-3.58	118.38	123.70
21	42	510	CL7	C3A-C4A-CHB	-3.58	118.38	123.70
21	33	515	CL7	O2D-CGD-CBD	3.58	117.64	111.27
21	11	414	CL7	CHD-C1D-ND	-3.58	120.46	124.26
21	2D	402	CL7	CHD-C1D-ND	-3.58	120.47	124.26
21	24	416	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	21	418	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	44	415	CL7	C3A-C4A-CHB	-3.58	118.39	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	24	402	8CT	C24-C25-C26	-3.58	122.20	127.31
21	22	501	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	34	406	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	12	501	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	44	406	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	2C	510	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	1A	403	CL7	C4C-C3C-C2C	-3.58	102.46	107.13
23	3C	515	8CT	C07-C02-C03	-3.58	117.54	122.73
21	13	507	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	43	408	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	13	501	CL7	CHD-C1D-ND	-3.58	120.47	124.26
32	23	401	ZEX	C10-C11-C12	-3.58	112.06	123.22
32	33	525	ZEX	C10-C11-C12	-3.58	112.06	123.22
21	14	416	CL7	C2D-C1D-ND	3.58	112.63	110.23
21	1C	517	CL7	C1D-ND-C4D	-3.58	103.80	106.33
21	2C	517	CL7	C1D-ND-C4D	-3.58	103.80	106.33
21	1B	610	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
23	1C	515	8CT	C07-C02-C03	-3.57	117.54	122.73
23	4C	515	8CT	C07-C02-C03	-3.57	117.54	122.73
21	14	412	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
21	31	417	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
21	3A	403	CL7	C4C-C3C-C2C	-3.57	102.47	107.13
21	13	512	CL7	O2D-CGD-CBD	3.57	117.62	111.27
32	12	520	ZEX	C35-C15-C14	-3.57	116.15	123.47
21	2B	611	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
21	4C	517	CL7	C1D-ND-C4D	-3.57	103.80	106.33
21	31	418	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
21	23	402	CL7	CHD-C1D-ND	-3.57	120.47	124.26
21	43	402	CL7	CHD-C1D-ND	-3.57	120.48	124.26
21	33	512	CL7	O2D-CGD-CBD	3.57	117.61	111.27
21	31	420	CL7	CHD-C4C-C3C	-3.57	119.15	124.94
21	34	416	CL7	C2D-C1D-ND	3.57	112.62	110.23
21	4B	616	CL7	C2D-C1D-ND	3.57	112.62	110.23
21	11	418	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
21	23	410	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
23	2B	619	8CT	C07-C02-C03	-3.57	117.55	122.73
21	1D	404	CL7	C4D-C3D-CAD	-3.57	105.02	107.42
21	4D	404	CL7	C4D-C3D-CAD	-3.57	105.02	107.42
21	43	413	CL7	O2D-CGD-CBD	3.57	117.61	111.27
21	11	409	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	21	416	CL7	O2D-CGD-CBD	3.57	117.61	111.27
21	31	416	CL7	C3A-C4A-CHB	-3.57	118.41	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	13	525	ZEX	C10-C11-C12	-3.57	112.09	123.22
21	1B	610	CL7	C4D-C3D-CAD	-3.57	105.02	107.42
21	31	415	CL7	CHD-C4C-C3C	-3.56	119.16	124.94
32	32	520	ZEX	C35-C15-C14	-3.56	116.17	123.47
21	3C	512	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	3B	616	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	3A	403	CL7	C2D-C1D-ND	3.56	112.62	110.23
21	2B	617	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	4B	614	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	31	410	CL7	C4D-C3D-CAD	-3.56	105.02	107.42
21	31	414	CL7	CHD-C1D-ND	-3.56	120.48	124.26
23	2C	515	8CT	C01-C02-C07	3.56	120.46	113.62
23	2C	515	8CT	C07-C02-C03	-3.56	117.56	122.73
32	43	401	ZEX	C10-C11-C12	-3.56	112.10	123.22
21	2C	512	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	11	410	CL7	C4D-C3D-CAD	-3.56	105.03	107.42
21	21	415	CL7	CHD-C4C-C3C	-3.56	119.17	124.94
21	1C	512	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	32	510	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	3D	402	CL7	CHD-C1D-ND	-3.56	120.49	124.26
21	1D	402	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	11	403	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	34	410	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	41	403	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	44	416	CL7	C2D-C1D-ND	3.56	112.62	110.23
23	1B	618	8CT	C07-C02-C03	-3.56	117.56	122.73
21	1B	613	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	21	403	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	21	409	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	4D	402	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	13	508	CL7	C2D-C1D-ND	3.56	112.62	110.23
21	43	403	CL7	C1D-ND-C4D	-3.56	103.81	106.33
21	44	412	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	22	510	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	24	410	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	3C	501	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
23	3C	515	8CT	C01-C02-C07	3.56	120.45	113.62
21	44	410	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	31	416	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	33	507	CL7	C3A-C4A-CHB	-3.55	118.42	123.70
21	22	507	CL7	C1D-ND-C4D	-3.55	103.81	106.33
21	32	507	CL7	C1D-ND-C4D	-3.55	103.81	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	416	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	1B	616	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
21	31	404	CL7	C2D-C1D-ND	3.55	112.61	110.23
21	21	420	CL7	CHD-C4C-C3C	-3.55	119.18	124.94
21	41	409	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
32	42	520	ZEX	C35-C15-C14	-3.55	116.20	123.47
21	41	415	CL7	CHD-C4C-C3C	-3.55	119.18	124.94
21	4A	403	CL7	C2D-C1D-ND	3.55	112.61	110.23
21	23	413	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	41	417	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
21	33	505	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	4B	612	CL7	CHD-C1D-ND	-3.55	120.50	124.26
21	2D	404	CL7	C4D-C3D-CAD	-3.55	105.03	107.42
32	22	520	ZEX	C35-C15-C14	-3.55	116.20	123.47
21	21	418	CL7	CHD-C4C-C3C	-3.55	119.19	124.94
21	1C	510	CL7	C2D-C1D-ND	3.55	112.61	110.23
21	3B	615	CL7	C2D-C1D-ND	3.55	112.61	110.23
21	3C	510	CL7	C2D-C1D-ND	3.55	112.61	110.23
21	33	501	CL7	CHD-C1D-ND	-3.55	120.50	124.26
21	21	417	CL7	C3A-C4A-CHB	-3.55	118.44	123.70
21	11	416	CL7	O2D-CGD-CBD	3.55	117.57	111.27
21	14	407	CL7	C2D-C1D-ND	3.55	112.61	110.23
21	3B	610	CL7	C3A-C4A-CHB	-3.55	118.44	123.70
21	43	410	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	11	418	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	11	420	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	3D	404	CL7	CHD-C1D-ND	-3.54	120.51	124.26
21	21	416	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	3C	517	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
23	3B	618	8CT	C07-C02-C03	-3.54	117.59	122.73
21	44	407	CL7	C2D-C1D-ND	3.54	112.61	110.23
21	11	416	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	13	505	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	43	406	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	11	404	CL7	CHD-C1D-ND	-3.54	120.51	124.26
21	41	404	CL7	CHD-C1D-ND	-3.54	120.51	124.26
21	41	418	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	2C	501	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	31	403	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	31	418	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	2B	612	CL7	CHD-C1D-ND	-3.54	120.51	124.26
21	1C	501	CL7	C3A-C4A-CHB	-3.54	118.45	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	617	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	23	406	CL7	CHD-C4C-C3C	-3.54	119.20	124.94
21	14	410	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	34	415	CL7	CHD-C4C-C3C	-3.54	119.21	124.94
21	41	410	CL7	C2D-C1D-ND	3.54	112.60	110.23
21	2D	404	CL7	CHD-C1D-ND	-3.54	120.51	124.26
21	3B	611	CL7	CHD-C1D-ND	-3.53	120.52	124.26
21	4A	403	CL7	CAC-C3C-C4C	-3.53	119.11	124.68
21	34	412	CL7	C3A-C4A-CHB	-3.53	118.45	123.70
22	2A	402	PHO	C2B-C1B-NB	-3.53	107.09	109.53
21	34	409	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	1D	404	CL7	CHD-C1D-ND	-3.53	120.52	124.26
21	13	509	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	23	408	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	31	409	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	11	404	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	22	509	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	32	509	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	41	404	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	1B	611	CL7	CHD-C1D-ND	-3.53	120.52	124.26
21	12	510	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	2B	611	CL7	C4D-C3D-CAD	-3.53	105.05	107.42
21	4B	608	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	2B	610	CL7	CHD-C1D-ND	-3.53	120.52	124.26
21	31	419	CL7	CHD-C1D-ND	-3.53	120.52	124.26
22	3A	402	PHO	C2B-C1B-NB	-3.53	107.09	109.53
21	14	415	CL7	CHD-C4C-C3C	-3.53	119.22	124.94
21	44	415	CL7	CHD-C4C-C3C	-3.53	119.22	124.94
21	21	410	CL7	C2D-C1D-ND	3.53	112.60	110.23
21	12	507	CL7	C1D-ND-C4D	-3.53	103.83	106.33
21	2A	403	CL7	CAC-C3C-C4C	-3.53	119.13	124.68
21	11	410	CL7	C2D-C1D-ND	3.52	112.59	110.23
21	2C	517	CL7	C2D-C1D-ND	3.52	112.59	110.23
21	4C	501	CL7	C3A-C4A-CHB	-3.52	118.47	123.70
21	41	416	CL7	C3A-C4A-CHB	-3.52	118.47	123.70
21	34	416	CL7	CHD-C4C-C3C	-3.52	119.23	124.94
21	4C	517	CL7	CMA-C3A-C2A	-3.52	107.87	116.10
21	12	513	CL7	O2D-CGD-CBD	3.52	117.53	111.27
21	1A	403	CL7	CAC-C3C-C4C	-3.52	119.13	124.68
21	43	415	CL7	CHD-C4C-C3C	-3.52	119.23	124.94
21	4D	404	CL7	CHD-C1D-ND	-3.52	120.53	124.26
32	43	421	ZEX	C31-C32-C33	-3.52	116.52	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	24	414	CL7	CHD-C4C-C3C	-3.52	119.23	124.94
21	43	416	CL7	C3A-C4A-CHB	-3.52	118.47	123.70
21	4C	510	CL7	C2D-C1D-ND	3.52	112.59	110.23
32	23	421	ZEX	C31-C32-C33	-3.52	116.53	126.42
21	24	415	CL7	CHD-C4C-C3C	-3.52	119.23	124.94
32	13	520	ZEX	C31-C32-C33	-3.52	116.53	126.42
32	33	520	ZEX	C31-C32-C33	-3.52	116.53	126.42
21	13	505	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
21	4C	517	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
21	43	406	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
21	13	515	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
21	2B	616	CL7	C2D-C1D-ND	3.51	112.59	110.23
21	23	412	CL7	C3A-C4A-CHB	-3.51	118.48	123.70
21	33	511	CL7	C3A-C4A-CHB	-3.51	118.48	123.70
21	13	502	CL7	C1D-ND-C4D	-3.51	103.84	106.33
21	43	412	CL7	C3A-C4A-CHB	-3.51	118.49	123.70
21	11	419	CL7	CHD-C1D-ND	-3.51	120.54	124.26
21	33	509	CL7	C3A-C4A-CHB	-3.51	118.49	123.70
21	41	410	CL7	C4D-C3D-CAD	-3.51	105.06	107.42
21	33	514	CL7	CHD-C4C-C3C	-3.51	119.25	124.94
21	22	513	CL7	O2D-CGD-CBD	3.51	117.51	111.27
21	32	513	CL7	O2D-CGD-CBD	3.51	117.51	111.27
21	3C	517	CL7	CMA-C3A-C2A	-3.51	107.91	116.10
21	13	501	CL7	C3A-C4A-CHB	-3.51	118.49	123.70
21	23	402	CL7	C3A-C4A-CHB	-3.51	118.49	123.70
21	14	416	CL7	CHD-C4C-C3C	-3.51	119.25	124.94
21	1C	517	CL7	CMA-C3A-C2A	-3.51	107.91	116.10
21	23	415	CL7	CHD-C4C-C3C	-3.51	119.25	124.94
32	32	524	ZEX	C27-C28-C29	-3.51	120.94	126.23
32	22	524	ZEX	C27-C28-C29	-3.51	120.94	126.23
21	3C	517	CL7	C2D-C1D-ND	3.51	112.58	110.23
32	14	420	ZEX	C27-C28-C29	-3.50	120.94	126.23
21	24	416	CL7	CHD-C4C-C3C	-3.50	119.26	124.94
22	1A	402	PHO	C2B-C1B-NB	-3.50	107.11	109.53
22	4A	402	PHO	C2B-C1B-NB	-3.50	107.11	109.53
21	2C	517	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
21	34	407	CL7	CMA-C3A-C2A	-3.50	107.92	116.10
21	43	402	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
21	31	404	CL7	CHD-C1D-ND	-3.50	120.55	124.26
21	42	507	CL7	C1D-ND-C4D	-3.50	103.85	106.33
21	21	419	CL7	CHD-C1D-ND	-3.50	120.55	124.26
21	33	501	CL7	C3A-C4A-CHB	-3.50	118.50	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1B	601	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
21	13	511	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
21	1C	517	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
32	12	524	ZEX	C27-C28-C29	-3.50	120.95	126.23
32	42	524	ZEX	C27-C28-C29	-3.50	120.95	126.23
21	44	414	CL7	CHD-C4C-C3C	-3.50	119.27	124.94
21	42	513	CL7	O2D-CGD-CBD	3.50	117.48	111.27
21	1B	607	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
32	12	519	ZEX	C18-C5-C6	-3.50	120.60	124.53
21	2C	517	CL7	CMA-C3A-C2A	-3.50	107.94	116.10
21	21	404	CL7	CHD-C1D-ND	-3.50	120.56	124.26
21	23	403	CL7	C1D-ND-C4D	-3.50	103.85	106.33
21	34	407	CL7	C2D-C1D-ND	3.49	112.58	110.23
21	14	414	CL7	CHD-C4C-C3C	-3.49	119.28	124.94
21	3A	403	CL7	CAC-C3C-C4C	-3.49	119.18	124.68
21	33	505	CL7	C3A-C4A-CHB	-3.49	118.52	123.70
21	24	407	CL7	CMA-C3A-C2A	-3.49	107.95	116.10
32	22	519	ZEX	C18-C5-C6	-3.49	120.61	124.53
21	14	407	CL7	CMA-C3A-C2A	-3.49	107.95	116.10
21	41	419	CL7	CHD-C1D-ND	-3.49	120.56	124.26
21	44	407	CL7	CMA-C3A-C2A	-3.49	107.96	116.10
21	42	509	CL7	C2D-C1D-ND	3.49	112.57	110.23
21	44	416	CL7	CHD-C4C-C3C	-3.49	119.28	124.94
21	3B	609	CL7	CHD-C1D-ND	-3.49	120.56	124.26
21	21	410	CL7	C4D-C3D-CAD	-3.49	105.07	107.42
21	31	414	CL7	CHD-C4C-C3C	-3.49	119.29	124.94
21	2B	608	CL7	C3A-C4A-CHB	-3.49	118.53	123.70
21	33	515	CL7	C3A-C4A-CHB	-3.49	118.53	123.70
21	23	416	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	4A	403	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	32	505	CL7	CHD-C4C-C3C	-3.48	119.29	124.94
21	1B	615	CL7	C2D-C1D-ND	3.48	112.57	110.23
21	12	505	CL7	CHD-C4C-C3C	-3.48	119.29	124.94
21	3B	601	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	33	502	CL7	C1D-ND-C4D	-3.48	103.86	106.33
21	13	514	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	3B	607	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
23	1C	515	8CT	C01-C02-C03	-3.48	120.62	124.53
23	4C	515	8CT	C01-C02-C03	-3.48	120.62	124.53
21	14	409	CL7	C2D-C1D-ND	3.48	112.56	110.23
21	44	409	CL7	C2D-C1D-ND	3.48	112.56	110.23
21	34	414	CL7	CHD-C4C-C3C	-3.48	119.30	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	42	519	ZEX	C18-C5-C6	-3.48	120.62	124.53
21	13	514	CL7	CHD-C4C-C3C	-3.48	119.30	124.94
21	4B	610	CL7	CHD-C1D-ND	-3.48	120.57	124.26
21	3C	510	CL7	CHC-C1C-NC	-3.48	121.26	124.45
21	1C	517	CL7	C2D-C1D-ND	3.48	112.56	110.23
21	4C	517	CL7	C2D-C1D-ND	3.48	112.56	110.23
32	34	420	ZEX	C27-C28-C29	-3.48	120.98	126.23
21	44	414	CL7	CHC-C1C-NC	-3.48	121.26	124.45
21	33	514	CL7	C3A-C4A-CHB	-3.48	118.54	123.70
21	44	407	CL7	CHD-C4C-C3C	-3.48	119.31	124.94
21	23	415	CL7	C3A-C4A-CHB	-3.48	118.54	123.70
21	4B	602	CL7	C3A-C4A-CHB	-3.47	118.54	123.70
21	31	410	CL7	C2D-C1D-ND	3.47	112.56	110.23
21	1B	608	CL7	O2D-CGD-CBD	3.47	117.44	111.27
21	3B	605	CL7	CHD-C1D-ND	-3.47	120.58	124.26
32	32	519	ZEX	C18-C5-C6	-3.47	120.63	124.53
21	4B	617	CL7	CHD-C1D-ND	-3.47	120.58	124.26
21	41	414	CL7	CHD-C4C-C3C	-3.47	119.31	124.94
21	42	505	CL7	CHD-C4C-C3C	-3.47	119.31	124.94
32	12	519	ZEX	C2-C3-C4	3.47	115.05	110.30
21	3B	608	CL7	O2D-CGD-CBD	3.47	117.43	111.27
21	22	505	CL7	CHD-C4C-C3C	-3.47	119.32	124.94
21	21	414	CL7	CHD-C4C-C3C	-3.47	119.32	124.94
21	2B	602	CL7	C3A-C4A-CHB	-3.47	118.56	123.70
21	11	414	CL7	CHD-C4C-C3C	-3.47	119.32	124.94
32	44	420	ZEX	C27-C28-C29	-3.47	121.00	126.23
21	31	413	CL7	CHD-C4C-C3C	-3.47	119.32	124.94
21	11	406	CL7	C2D-C1D-ND	3.47	112.56	110.23
23	2C	515	8CT	C01-C02-C03	-3.46	120.64	124.53
21	2A	403	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
21	23	406	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
21	2B	609	CL7	O2D-CGD-CBD	3.46	117.42	111.27
21	4B	604	CL7	CHD-C1D-ND	-3.46	120.60	124.26
21	24	409	CL7	C2D-C1D-ND	3.46	112.55	110.23
21	43	415	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
21	43	413	CL7	CHD-C4C-C3C	-3.46	119.34	124.94
21	2B	604	CL7	CHD-C1D-ND	-3.46	120.60	124.26
21	12	509	CL7	C2D-C1D-ND	3.46	112.55	110.23
21	12	516	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
21	24	407	CL7	CHD-C4C-C3C	-3.45	119.34	124.94
21	4B	623	CL7	CHD-C1D-ND	-3.45	120.60	124.26
21	41	413	CL7	CHB-C1B-NB	-3.45	120.60	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	44	403	ZEX	C18-C5-C6	-3.45	120.65	124.53
21	13	516	CL7	C2D-C1D-ND	3.45	112.55	110.23
21	43	417	CL7	C2D-C1D-ND	3.45	112.55	110.23
32	34	419	ZEX	C18-C5-C4	3.45	120.75	114.36
32	24	420	ZEX	C27-C28-C29	-3.45	121.02	126.23
21	4B	609	CL7	O2D-CGD-CBD	3.45	117.40	111.27
21	32	511	CL7	CHD-C4C-C3C	-3.45	119.34	124.94
21	41	406	CL7	C2D-C1D-ND	3.45	112.55	110.23
21	14	407	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	34	417	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	1B	609	CL7	CHD-C1D-ND	-3.45	120.61	124.26
21	11	403	CL7	O2D-CGD-CBD	3.45	117.40	111.27
21	44	417	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	1A	403	CL7	C3A-C4A-CHB	-3.45	118.58	123.70
21	41	413	CL7	CHD-C4C-C3C	-3.45	119.35	124.94
21	2C	511	CL7	O2D-CGD-CBD	3.45	117.39	111.27
21	4B	616	CL7	O2D-CGD-CBD	3.45	117.39	111.27
21	4A	401	CL7	C4-C3-C5	3.45	121.07	115.27
21	2B	606	CL7	CHD-C1D-ND	-3.45	120.61	124.26
21	34	409	CL7	CHB-C1B-NB	-3.45	120.61	124.26
21	41	403	CL7	O2D-CGD-CBD	3.45	117.39	111.27
21	21	406	CL7	C2D-C1D-ND	3.45	112.54	110.23
32	44	419	ZEX	C18-C5-C4	3.45	120.74	114.36
32	34	403	ZEX	C18-C5-C6	-3.45	120.66	124.53
21	31	414	CL7	O2D-CGD-CBD	3.45	117.39	111.27
21	11	405	CL7	CHD-C1D-ND	-3.44	120.61	124.26
21	2B	623	CL7	CHD-C1D-ND	-3.44	120.61	124.26
21	3C	511	CL7	O2D-CGD-CBD	3.44	117.39	111.27
21	24	417	CL7	CHD-C4C-C3C	-3.44	119.36	124.94
32	32	519	ZEX	C2-C3-C4	3.44	115.02	110.30
23	3A	404	8CT	C04-C03-C02	-3.44	117.76	122.61
21	1C	509	CL7	C2D-C1D-ND	3.44	112.54	110.23
21	4C	509	CL7	C2D-C1D-ND	3.44	112.54	110.23
21	31	405	CL7	CHD-C1D-ND	-3.44	120.61	124.26
23	3C	515	8CT	C01-C02-C03	-3.44	120.66	124.53
21	3C	506	CL7	CHD-C4C-C3C	-3.44	119.36	124.94
21	1C	510	CL7	CHC-C1C-NC	-3.44	121.29	124.45
21	4C	510	CL7	CHC-C1C-NC	-3.44	121.29	124.45
21	2B	617	CL7	CHD-C1D-ND	-3.44	120.61	124.26
21	11	413	CL7	CHD-C4C-C3C	-3.44	119.36	124.94
21	34	414	CL7	CHC-C1C-NC	-3.44	121.29	124.45
21	43	406	CL7	C2D-C1D-ND	3.44	112.54	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	414	CL7	O2D-CGD-CBD	3.44	117.38	111.27
21	13	512	CL7	CHD-C4C-C3C	-3.44	119.36	124.94
21	14	412	CL7	CHD-C4C-C3C	-3.44	119.36	124.94
21	4B	606	CL7	CHD-C1D-ND	-3.44	120.62	124.26
21	34	412	CL7	CHD-C4C-C3C	-3.44	119.36	124.94
21	24	407	CL7	C2D-C1D-ND	3.44	112.54	110.23
21	3C	507	CL7	C2D-C1D-ND	3.44	112.54	110.23
21	3A	403	CL7	C3A-C4A-CHB	-3.44	118.60	123.70
21	11	413	CL7	CHB-C1B-NB	-3.44	120.62	124.26
21	14	414	CL7	CHC-C1C-NC	-3.44	121.30	124.45
21	24	412	CL7	CHD-C4C-C3C	-3.44	119.37	124.94
23	4A	404	8CT	C04-C03-C02	-3.43	117.78	122.61
23	4B	620	8CT	C01-C02-C07	3.43	120.21	113.62
21	21	413	CL7	CHD-C4C-C3C	-3.43	119.37	124.94
21	3C	509	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	22	516	CL7	C3A-C4A-CHB	-3.43	118.61	123.70
21	2B	616	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	2B	616	CL7	C3A-C4A-CHB	-3.43	118.61	123.70
21	4B	616	CL7	C3A-C4A-CHB	-3.43	118.61	123.70
21	2B	604	CL7	C2D-C1D-ND	3.43	112.53	110.23
21	34	407	CL7	CHD-C4C-C3C	-3.43	119.38	124.94
21	42	511	CL7	CHD-C4C-C3C	-3.43	119.38	124.94
21	1A	401	CL7	C4-C3-C5	3.43	121.04	115.27
21	21	403	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	22	513	CL7	C2D-C1D-ND	3.43	112.53	110.23
23	1A	404	8CT	C04-C03-C02	-3.43	117.78	122.61
21	11	414	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	41	414	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	3B	611	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	44	406	CL7	C4D-C3D-CAD	-3.43	105.11	107.42
21	31	403	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	23	406	CL7	C2D-C1D-ND	3.43	112.53	110.23
32	22	519	ZEX	C2-C3-C4	3.43	114.99	110.30
21	33	512	CL7	CHD-C4C-C3C	-3.43	119.39	124.94
21	1C	511	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	4C	511	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	41	405	CL7	CHD-C1D-ND	-3.43	120.63	124.26
23	34	402	8CT	C18-C17-C16	-3.42	122.42	127.31
21	2C	510	CL7	CHC-C1C-NC	-3.42	121.31	124.45
21	34	405	CL7	CHD-C1D-ND	-3.42	120.63	124.26
21	4C	507	CL7	C2D-C1D-ND	3.42	112.53	110.23
21	42	516	CL7	C3A-C4A-CHB	-3.42	118.62	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	413	CL7	CHD-C4C-C3C	-3.42	119.39	124.94
21	1B	622	CL7	CHD-C1D-ND	-3.42	120.64	124.26
21	1B	615	CL7	O2D-CGD-CBD	3.42	117.35	111.27
21	2C	506	CL7	CHD-C4C-C3C	-3.42	119.39	124.94
23	2A	404	8CT	C04-C03-C02	-3.42	117.80	122.61
23	1B	626	8CT	C15-C16-C17	3.42	124.19	118.94
21	3B	615	CL7	O2D-CGD-CBD	3.42	117.34	111.27
21	12	511	CL7	CHD-C4C-C3C	-3.42	119.40	124.94
21	44	412	CL7	CHD-C4C-C3C	-3.42	119.40	124.94
21	31	415	CL7	C3A-C4A-CHB	-3.42	118.62	123.70
21	2A	401	CL7	C4-C3-C5	3.42	121.02	115.27
21	1C	506	CL7	CHD-C4C-C3C	-3.42	119.40	124.94
21	4C	506	CL7	CHD-C4C-C3C	-3.42	119.40	124.94
21	4B	604	CL7	C2D-C1D-ND	3.42	112.52	110.23
32	14	419	ZEX	C18-C5-C4	3.42	120.69	114.36
32	24	419	ZEX	C18-C5-C4	3.42	120.69	114.36
32	33	520	ZEX	C11-C12-C13	-3.42	116.82	126.42
21	1B	616	CL7	CHD-C1D-ND	-3.42	120.64	124.26
23	3B	619	8CT	C01-C02-C07	3.42	120.18	113.62
21	24	414	CL7	CHC-C1C-NC	-3.42	121.31	124.45
21	22	511	CL7	CHD-C4C-C3C	-3.42	119.40	124.94
23	1B	619	8CT	C01-C02-C07	3.42	120.18	113.62
21	14	417	CL7	CHD-C4C-C3C	-3.41	119.41	124.94
21	4B	604	CL7	C4D-C3D-CAD	-3.41	105.12	107.42
32	42	519	ZEX	C2-C3-C4	3.41	114.98	110.30
21	13	505	CL7	C2D-C1D-ND	3.41	112.52	110.23
21	4B	605	CL7	C2D-C1D-ND	3.41	112.52	110.23
21	1B	611	CL7	O2D-CGD-CBD	3.41	117.33	111.27
21	3A	401	CL7	C4-C3-C5	3.41	121.01	115.27
21	11	415	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
21	21	417	CL7	O2D-CGD-CBD	3.41	117.33	111.27
21	24	405	CL7	CHD-C1D-ND	-3.41	120.65	124.26
21	1C	511	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
23	24	402	8CT	C18-C17-C16	-3.41	122.44	127.31
21	1B	605	CL7	CHD-C1D-ND	-3.41	120.65	124.26
21	21	405	CL7	CHD-C1D-ND	-3.41	120.65	124.26
21	23	403	CL7	CHD-C1D-ND	-3.41	120.65	124.26
32	23	421	ZEX	C11-C12-C13	-3.41	116.84	126.42
21	1A	407	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
21	3B	615	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
23	3B	619	8CT	C07-C02-C03	-3.41	117.78	122.73
21	32	516	CL7	C3A-C4A-CHB	-3.41	118.65	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	415	CL7	C3A-C4A-CHB	-3.40	118.65	123.70
21	1B	603	CL7	CHD-C1D-ND	-3.40	120.65	124.26
32	13	520	ZEX	C11-C12-C13	-3.40	116.85	126.42
21	4B	612	CL7	O2D-CGD-CBD	3.40	117.32	111.27
21	43	415	CL7	C4C-C3C-C2C	-3.40	102.69	107.13
21	33	505	CL7	C2D-C1D-ND	3.40	112.51	110.23
23	14	402	8CT	C18-C17-C16	-3.40	122.45	127.31
23	44	402	8CT	C18-C17-C16	-3.40	122.45	127.31
21	41	402	CL7	CHD-C4C-C3C	-3.40	119.42	124.94
21	43	403	CL7	CHD-C1D-ND	-3.40	120.66	124.26
32	14	403	ZEX	C18-C5-C6	-3.40	120.71	124.53
21	3B	622	CL7	CHD-C1D-ND	-3.40	120.66	124.26
21	31	402	CL7	CHD-C4C-C3C	-3.40	119.43	124.94
21	3B	612	CL7	CHC-C1C-NC	-3.40	121.33	124.45
21	2C	507	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	14	409	CL7	CHB-C1B-NB	-3.40	120.66	124.26
21	44	405	CL7	CHD-C1D-ND	-3.40	120.66	124.26
21	4C	511	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	44	409	CL7	CHB-C1B-NB	-3.40	120.66	124.26
32	43	421	ZEX	C11-C12-C13	-3.40	116.87	126.42
21	3C	511	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	1B	615	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	2A	407	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
23	2B	601	8CT	C15-C16-C17	3.40	124.15	118.94
23	3B	626	8CT	C15-C16-C17	3.40	124.15	118.94
21	32	513	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	42	505	CL7	C2D-C1D-ND	3.40	112.51	110.23
21	41	417	CL7	O2D-CGD-CBD	3.39	117.30	111.27
21	21	413	CL7	CHB-C1B-NB	-3.39	120.66	124.26
32	24	403	ZEX	C18-C5-C6	-3.39	120.72	124.53
21	2B	613	CL7	C3A-C4A-CHB	-3.39	118.67	123.70
23	4B	620	8CT	C07-C02-C03	-3.39	117.81	122.73
21	2D	405	CL7	O2D-CGD-CBD	3.39	117.29	111.27
21	3D	405	CL7	O2D-CGD-CBD	3.39	117.29	111.27
23	2B	618	8CT	C11-C10-C03	-3.39	117.68	127.20
21	11	402	CL7	CHD-C4C-C3C	-3.39	119.44	124.94
21	11	417	CL7	O2D-CGD-CBD	3.39	117.29	111.27
23	2B	620	8CT	C01-C02-C07	3.39	120.13	113.62
21	2B	612	CL7	O2D-CGD-CBD	3.39	117.29	111.27
21	4A	407	CL7	C3A-C4A-CHB	-3.39	118.67	123.70
23	3B	617	8CT	C11-C10-C03	-3.39	117.69	127.20
21	3B	616	CL7	CHD-C1D-ND	-3.39	120.67	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	415	CL7	C3A-C4A-CHB	-3.39	118.67	123.70
21	4B	613	CL7	CHC-C1C-NC	-3.39	121.34	124.45
21	1D	405	CL7	O2D-CGD-CBD	3.39	117.29	111.27
21	2C	511	CL7	C3A-C4A-CHB	-3.39	118.67	123.70
21	44	414	CL7	O2D-CGD-CBD	3.39	117.29	111.27
21	14	405	CL7	CHD-C1D-ND	-3.39	120.67	124.26
23	4B	601	8CT	C15-C16-C17	3.39	124.14	118.94
21	13	502	CL7	CHD-C1D-ND	-3.39	120.67	124.26
21	42	513	CL7	C2D-C1D-ND	3.38	112.50	110.23
21	33	502	CL7	CHD-C1D-ND	-3.38	120.67	124.26
21	3B	603	CL7	CHD-C1D-ND	-3.38	120.67	124.26
21	2B	605	CL7	C2D-C1D-ND	3.38	112.50	110.23
23	1B	617	8CT	C11-C10-C03	-3.38	117.70	127.20
21	23	417	CL7	C2D-C1D-ND	3.38	112.50	110.23
21	21	402	CL7	CHD-C4C-C3C	-3.38	119.46	124.94
21	22	515	CL7	C3A-C4A-CHB	-3.38	118.68	123.70
23	2B	601	8CT	C14-C15-C16	-3.38	116.92	126.42
23	3B	626	8CT	C14-C15-C16	-3.38	116.92	126.42
23	4B	601	8CT	C14-C15-C16	-3.38	116.92	126.42
21	23	415	CL7	C4C-C3C-C2C	-3.38	102.72	107.13
21	1B	603	CL7	C4D-C3D-CAD	-3.38	105.15	107.42
21	33	516	CL7	C2D-C1D-ND	3.38	112.50	110.23
21	14	414	CL7	O2D-CGD-CBD	3.38	117.27	111.27
21	1B	612	CL7	C3A-C4A-CHB	-3.38	118.69	123.70
21	4B	613	CL7	C3A-C4A-CHB	-3.38	118.69	123.70
21	4D	405	CL7	O2D-CGD-CBD	3.37	117.27	111.27
21	3A	407	CL7	C3A-C4A-CHB	-3.37	118.69	123.70
21	31	406	CL7	C2D-C1D-ND	3.37	112.49	110.23
21	44	406	CL7	CHD-C1D-ND	-3.37	120.69	124.26
21	1C	503	CL7	CHD-C4C-C3C	-3.37	119.48	124.94
21	1C	507	CL7	C2D-C1D-ND	3.37	112.49	110.23
21	24	413	CL7	CHD-C4C-C3C	-3.37	119.48	124.94
21	33	503	CL7	C7-C6-C5	-3.37	104.21	113.36
32	41	422	ZEX	C18-C5-C4	3.37	120.59	114.36
21	24	409	CL7	CHB-C1B-NB	-3.37	120.69	124.26
21	1D	404	CL7	CAA-CBA-CGA	-3.37	103.41	113.25
21	14	413	CL7	CHD-C4C-C3C	-3.37	119.48	124.94
21	34	413	CL7	CHD-C4C-C3C	-3.37	119.48	124.94
21	44	413	CL7	CHD-C4C-C3C	-3.37	119.48	124.94
21	32	515	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
21	31	417	CL7	O2D-CGD-CBD	3.37	117.25	111.27
21	2B	614	CL7	CHD-C4C-C3C	-3.37	119.48	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	612	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
23	1B	626	8CT	C14-C15-C16	-3.37	116.96	126.42
21	13	517	CL7	O2D-CGD-CBD	3.37	117.25	111.27
21	33	514	CL7	C4C-C3C-C2C	-3.37	102.74	107.13
21	3D	404	CL7	CAA-CBA-CGA	-3.37	103.42	113.25
21	24	404	CL7	C2D-C1D-ND	3.37	112.49	110.23
21	2D	404	CL7	CAA-CBA-CGA	-3.36	103.42	113.25
23	1B	619	8CT	C07-C02-C03	-3.36	117.85	122.73
21	1C	508	CL7	CHD-C1D-ND	-3.36	120.70	124.26
21	22	505	CL7	C2D-C1D-ND	3.36	112.49	110.23
21	13	503	CL7	C7-C6-C5	-3.36	104.23	113.36
21	4D	404	CL7	CAA-CBA-CGA	-3.36	103.43	113.25
21	42	515	CL7	C3A-C4A-CHB	-3.36	118.71	123.70
32	23	423	ZEX	C19-C9-C10	-3.36	118.21	122.92
32	33	522	ZEX	C19-C9-C10	-3.36	118.21	122.92
21	3B	612	CL7	CHD-C4C-C3C	-3.36	119.49	124.94
23	4B	618	8CT	C11-C10-C03	-3.36	117.76	127.20
21	34	406	CL7	C4D-C3D-CAD	-3.36	105.16	107.42
21	12	515	CL7	C3A-C4A-CHB	-3.36	118.71	123.70
21	2C	503	CL7	CHD-C4C-C3C	-3.36	119.49	124.94
21	23	404	CL7	C7-C6-C5	-3.36	104.23	113.36
32	13	522	ZEX	C19-C9-C10	-3.36	118.22	122.92
21	11	406	CL7	C7-C6-C5	-3.36	104.24	113.36
21	23	417	CL7	C3A-C4A-CHB	-3.36	118.72	123.70
23	2B	620	8CT	C07-C02-C03	-3.36	117.85	122.73
21	2C	512	CL7	CHC-C1C-NC	-3.36	121.37	124.45
21	13	518	CL7	CHD-C1D-ND	-3.36	120.70	124.26
21	3B	613	CL7	CHD-C4C-C3C	-3.36	119.50	124.94
21	33	517	CL7	O2D-CGD-CBD	3.36	117.23	111.27
21	1C	512	CL7	CHC-C1C-NC	-3.35	121.37	124.45
21	2C	509	CL7	C2D-C1D-ND	3.35	112.48	110.23
21	31	406	CL7	C7-C6-C5	-3.35	104.25	113.36
21	24	414	CL7	O2D-CGD-CBD	3.35	117.23	111.27
21	3C	502	CL7	CHD-C4C-C3C	-3.35	119.50	124.94
21	33	516	CL7	C3A-C4A-CHB	-3.35	118.72	123.70
21	34	406	CL7	CHD-C1D-ND	-3.35	120.71	124.26
21	43	404	CL7	C7-C6-C5	-3.35	104.26	113.36
21	3C	503	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
21	23	418	CL7	O2D-CGD-CBD	3.35	117.22	111.27
21	34	414	CL7	O2D-CGD-CBD	3.35	117.22	111.27
21	1A	407	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
21	43	418	CL7	O2D-CGD-CBD	3.35	117.22	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	508	CL7	CHD-C1D-ND	-3.35	120.71	124.26
21	43	417	CL7	C3A-C4A-CHB	-3.35	118.73	123.70
32	43	423	ZEX	C19-C9-C10	-3.35	118.23	122.92
32	42	520	ZEX	C18-C5-C6	-3.35	120.77	124.53
21	31	413	CL7	CHB-C1B-NB	-3.35	120.71	124.26
21	4B	613	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
32	21	422	ZEX	C18-C5-C4	3.35	120.56	114.36
21	12	505	CL7	C2D-C1D-ND	3.35	112.48	110.23
21	34	404	CL7	C2D-C1D-ND	3.35	112.48	110.23
21	1B	612	CL7	CHC-C1C-NC	-3.35	121.38	124.45
21	4C	512	CL7	CHC-C1C-NC	-3.35	121.38	124.45
21	43	408	CL7	CHC-C1C-NC	-3.35	121.38	124.45
23	2C	514	8CT	C35-C30-C29	-3.35	108.47	112.70
21	1C	502	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
21	3B	610	CL7	CHD-C4C-C3C	-3.35	119.51	124.94
32	31	422	ZEX	C18-C5-C4	3.35	120.56	114.36
21	4B	612	CL7	C3A-C4A-CHB	-3.35	118.73	123.70
21	1B	613	CL7	CHD-C4C-C3C	-3.34	119.52	124.94
21	22	501	CL7	CHC-C1C-NC	-3.34	121.38	124.45
21	21	407	CL7	CHD-C1D-ND	-3.34	120.72	124.26
21	31	407	CL7	CHD-C1D-ND	-3.34	120.72	124.26
21	3B	603	CL7	C2D-C1D-ND	3.34	112.47	110.23
21	11	407	CL7	CHD-C1D-ND	-3.34	120.72	124.26
21	2B	604	CL7	C4D-C3D-CAD	-3.34	105.17	107.42
21	3B	603	CL7	C4D-C3D-CAD	-3.34	105.17	107.42
21	33	507	CL7	CHC-C1C-NC	-3.34	121.38	124.45
21	2B	613	CL7	CHD-C4C-C3C	-3.34	119.52	124.94
21	21	406	CL7	C7-C6-C5	-3.34	104.29	113.36
21	41	406	CL7	C7-C6-C5	-3.34	104.29	113.36
21	3B	604	CL7	C2D-C1D-ND	3.34	112.47	110.23
23	1C	514	8CT	C35-C30-C29	-3.34	108.48	112.70
21	1B	610	CL7	CHD-C4C-C3C	-3.34	119.53	124.94
21	2A	407	CL7	CHD-C4C-C3C	-3.34	119.53	124.94
23	2D	406	8CT	C01-C02-C07	3.34	120.03	113.62
21	1B	604	CL7	C2D-C1D-ND	3.34	112.47	110.23
32	11	422	ZEX	C18-C5-C4	3.34	120.54	114.36
21	4C	503	CL7	CHD-C4C-C3C	-3.34	119.53	124.94
21	2B	613	CL7	CHC-C1C-NC	-3.34	121.39	124.45
21	1B	612	CL7	CHD-C4C-C3C	-3.34	119.53	124.94
21	2C	507	CL7	C7-C6-C5	-3.34	104.30	113.36
21	12	504	CL7	O2D-CGD-CBD	3.34	117.19	111.27
21	1B	603	CL7	C2D-C1D-ND	3.34	112.47	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	513	CL7	C2D-C1D-ND	3.34	112.47	110.23
23	4C	514	8CT	C01-C02-C07	3.34	120.02	113.62
32	23	421	ZEX	C18-C5-C4	3.34	120.53	114.36
21	13	514	CL7	C4C-C3C-C2C	-3.33	102.78	107.13
21	42	509	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	3A	407	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
23	2C	514	8CT	C01-C02-C07	3.33	120.02	113.62
21	12	509	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	24	407	CL7	C4D-C3D-CAD	-3.33	105.18	107.42
21	11	419	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	13	516	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	21	406	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
32	32	520	ZEX	C18-C5-C6	-3.33	120.79	124.53
21	1C	507	CL7	C7-C6-C5	-3.33	104.31	113.36
21	14	405	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
31	2F	101	HEM	CHB-C1B-NB	3.33	128.48	124.37
21	22	509	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	32	509	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	14	406	CL7	C4D-C3D-CAD	-3.33	105.18	107.42
23	3C	514	8CT	C01-C02-C07	3.33	120.01	113.62
21	11	406	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
21	31	406	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
21	4A	407	CL7	CHD-C4C-C3C	-3.33	119.54	124.94
21	43	418	CL7	CHD-C1D-ND	-3.33	120.73	124.26
21	24	405	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
23	4C	514	8CT	C35-C30-C29	-3.33	108.49	112.70
21	43	405	CL7	CHD-C1D-ND	-3.33	120.73	124.26
21	41	406	CL7	CHD-C4C-C3C	-3.33	119.55	124.94
21	43	402	CL7	CHD-C4C-C3C	-3.33	119.55	124.94
21	11	413	CL7	CMA-C3A-C2A	-3.33	108.33	116.10
21	41	413	CL7	CMA-C3A-C2A	-3.33	108.33	116.10
21	2C	508	CL7	CHD-C1D-ND	-3.33	120.73	124.26
21	1B	611	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	21	413	CL7	CMA-C3A-C2A	-3.33	108.34	116.10
21	24	406	CL7	C4D-C3D-CAD	-3.33	105.18	107.42
21	14	408	CL7	CHD-C4C-C3C	-3.33	119.55	124.94
21	24	408	CL7	CHD-C4C-C3C	-3.33	119.55	124.94
23	1D	406	8CT	C01-C02-C07	3.32	120.00	113.62
21	4B	609	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
21	41	416	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	4B	611	CL7	C7-C6-C5	-3.32	104.33	113.36
21	14	404	CL7	C2D-C1D-ND	3.32	112.46	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	611	CL7	C7-C6-C5	-3.32	104.33	113.36
21	3B	610	CL7	C7-C6-C5	-3.32	104.33	113.36
21	42	505	CL7	CHB-C1B-NB	-3.32	120.74	124.26
21	23	402	CL7	CHD-C4C-C3C	-3.32	119.55	124.94
21	2B	612	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
21	3B	611	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
21	12	504	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	31	413	CL7	CMA-C3A-C2A	-3.32	108.35	116.10
23	4D	406	8CT	C01-C02-C07	3.32	120.00	113.62
21	23	414	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
21	4C	502	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
21	4B	603	CL7	CHD-C1D-ND	-3.32	120.74	124.26
21	11	403	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
21	43	414	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
23	3D	406	8CT	C01-C02-C07	3.32	120.00	113.62
32	43	421	ZEX	C18-C5-C4	3.32	120.51	114.36
21	3C	507	CL7	C7-C6-C5	-3.32	104.34	113.36
21	2B	606	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
32	12	520	ZEX	C18-C5-C6	-3.32	120.80	124.53
32	33	520	ZEX	C18-C5-C4	3.32	120.50	114.36
21	4B	614	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
21	23	408	CL7	CHC-C1C-NC	-3.32	121.40	124.45
21	11	405	CL7	C3A-C4A-CHB	-3.32	118.78	123.70
21	32	505	CL7	CHB-C1B-NB	-3.32	120.74	124.26
21	12	514	CL7	O2D-CGD-CBD	3.32	117.16	111.27
21	34	417	CL7	CMB-C2B-C1B	3.32	130.42	125.37
21	44	406	CL7	CHD-C4C-C3C	-3.32	119.56	124.94
21	21	416	CL7	CHD-C1D-ND	-3.32	120.75	124.26
31	1F	101	HEM	CHB-C1B-NB	3.32	128.46	124.37
23	1A	404	8CT	C07-C02-C03	-3.32	117.92	122.73
21	23	419	CL7	CHD-C1D-ND	-3.32	120.75	124.26
21	4C	507	CL7	C7-C6-C5	-3.32	104.36	113.36
21	4B	613	CL7	CMD-C2D-C1D	3.32	130.42	125.37
21	4B	611	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
21	31	415	CL7	O2D-CGD-CBD	3.31	117.16	111.27
21	21	415	CL7	O2D-CGD-CBD	3.31	117.16	111.27
21	1C	506	CL7	CHD-C1D-ND	-3.31	120.75	124.26
21	4C	506	CL7	CHD-C1D-ND	-3.31	120.75	124.26
21	31	403	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
23	3C	514	8CT	C35-C30-C29	-3.31	108.51	112.70
21	2B	603	CL7	CHD-C1D-ND	-3.31	120.75	124.26
21	11	415	CL7	O2D-CGD-CBD	3.31	117.15	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	514	CL7	O2D-CGD-CBD	3.31	117.15	111.27
21	41	415	CL7	O2D-CGD-CBD	3.31	117.15	111.27
21	2C	502	CL7	CHD-C4C-C3C	-3.31	119.57	124.94
32	41	422	ZEX	C31-C30-C29	-3.31	122.58	127.31
21	24	406	CL7	CHD-C1D-ND	-3.31	120.75	124.26
32	22	520	ZEX	C18-C5-C6	-3.31	120.81	124.53
21	22	505	CL7	CHB-C1B-NB	-3.31	120.75	124.26
21	4C	508	CL7	CHD-C1D-ND	-3.31	120.75	124.26
21	41	404	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	14	417	CL7	CMB-C2B-C1B	3.31	130.41	125.37
21	32	504	CL7	O2D-CGD-CBD	3.31	117.15	111.27
21	1B	610	CL7	C7-C6-C5	-3.31	104.37	113.36
21	34	408	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
23	1C	514	8CT	C01-C02-C07	3.31	119.97	113.62
21	1B	608	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	44	405	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	33	515	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	1C	512	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	13	501	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	3C	506	CL7	CHD-C1D-ND	-3.31	120.76	124.26
23	2D	406	8CT	C11-C10-C03	-3.31	117.92	127.20
21	21	404	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	33	501	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
32	13	520	ZEX	C18-C5-C4	3.31	120.48	114.36
21	11	404	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	33	513	CL7	CHD-C4C-C3C	-3.31	119.58	124.94
21	33	517	CL7	CHD-C1D-ND	-3.31	120.76	124.26
21	32	516	CL7	C7-C6-C5	-3.30	104.38	113.36
21	22	504	CL7	O2D-CGD-CBD	3.30	117.14	111.27
21	24	406	CL7	CHD-C4C-C3C	-3.30	119.58	124.94
21	34	406	CL7	CHD-C4C-C3C	-3.30	119.58	124.94
21	3C	513	CL7	CHD-C1D-ND	-3.30	120.76	124.26
21	32	505	CL7	C2D-C1D-ND	3.30	112.45	110.23
21	12	516	CL7	C7-C6-C5	-3.30	104.39	113.36
32	21	422	ZEX	C31-C30-C29	-3.30	122.59	127.31
31	4F	101	HEM	CHB-C1B-NB	3.30	128.45	124.37
21	4D	402	CL7	O2D-CGD-CBD	3.30	117.14	111.27
21	44	408	CL7	CHD-C4C-C3C	-3.30	119.58	124.94
21	41	419	CL7	C3A-C4A-CHB	-3.30	118.80	123.70
21	41	403	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
23	4D	406	8CT	C11-C10-C03	-3.30	117.93	127.20
31	3F	101	HEM	CHB-C1B-NB	3.30	128.45	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	404	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
21	12	501	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	42	501	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	24	414	CL7	CHD-C1D-ND	-3.30	120.76	124.26
21	44	404	CL7	C2D-C1D-ND	3.30	112.44	110.23
21	44	416	CL7	C3A-C4A-CHB	-3.30	118.80	123.70
21	3C	512	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	2B	611	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
21	2A	407	CL7	C7-C6-C5	-3.30	104.40	113.36
23	3D	406	8CT	C11-C10-C03	-3.30	117.94	127.20
21	14	406	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
21	4C	511	CL7	CHD-C4C-C3C	-3.30	119.59	124.94
21	33	504	CL7	CHD-C1D-ND	-3.30	120.77	124.26
21	1B	605	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
21	14	416	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
21	12	508	CL7	O2D-CGD-CBD	3.30	117.13	111.27
21	42	508	CL7	O2D-CGD-CBD	3.30	117.13	111.27
21	14	411	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	42	504	CL7	CHD-C1D-ND	-3.30	120.77	124.26
21	3B	605	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
23	3A	404	8CT	C07-C02-C03	-3.30	117.94	122.73
21	2B	613	CL7	CMD-C2D-C1D	3.30	130.39	125.37
21	13	504	CL7	CHD-C1D-ND	-3.30	120.77	124.26
21	4C	511	CL7	CHD-C1D-ND	-3.30	120.77	124.26
23	1D	406	8CT	C11-C10-C03	-3.30	117.94	127.20
21	34	405	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
21	21	403	CL7	CHD-C4C-C3C	-3.30	119.60	124.94
21	44	417	CL7	CMB-C2B-C1B	3.30	130.39	125.37
21	1B	602	CL7	CHD-C1D-ND	-3.29	120.77	124.26
21	21	419	CL7	C3A-C4A-CHB	-3.29	118.81	123.70
21	31	419	CL7	C3A-C4A-CHB	-3.29	118.81	123.70
21	33	505	CL7	C4C-C3C-C2C	-3.29	102.83	107.13
21	3B	612	CL7	CMD-C2D-C1D	3.29	130.39	125.37
21	22	513	CL7	CHD-C1D-ND	-3.29	120.77	124.26
21	32	513	CL7	CHD-C1D-ND	-3.29	120.77	124.26
21	43	419	CL7	CHD-C1D-ND	-3.29	120.77	124.26
21	22	508	CL7	C3A-C4A-CHB	-3.29	118.81	123.70
21	22	514	CL7	O2D-CGD-CBD	3.29	117.12	111.27
21	3B	605	CL7	CMB-C2B-C1B	3.29	130.38	125.37
32	13	525	ZEX	C27-C28-C29	-3.29	121.26	126.23
21	4D	405	CL7	CHD-C4C-C3C	-3.29	119.61	124.94
21	3B	601	CL7	O2D-CGD-CBD	3.29	117.11	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	504	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	24	416	CL7	C3A-C4A-CHB	-3.29	118.82	123.70
21	2B	602	CL7	O2D-CGD-CBD	3.29	117.11	111.27
21	4B	602	CL7	O2D-CGD-CBD	3.29	117.11	111.27
21	41	407	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	3B	608	CL7	C3A-C4A-CHB	-3.29	118.82	123.70
21	42	504	CL7	O2D-CGD-CBD	3.29	117.11	111.27
32	44	418	ZEX	C39-C29-C30	-3.29	118.32	122.92
21	4C	509	CL7	CHC-C1C-NC	-3.29	121.43	124.45
21	1C	513	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	2B	602	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	22	516	CL7	C7-C6-C5	-3.29	104.43	113.36
21	22	503	CL7	C4D-C3D-CAD	-3.29	105.21	107.42
21	33	518	CL7	CHD-C1D-ND	-3.29	120.78	124.26
32	31	422	ZEX	C31-C30-C29	-3.29	122.62	127.31
32	23	401	ZEX	C27-C28-C29	-3.29	121.27	126.23
23	2A	404	8CT	C07-C02-C03	-3.29	117.96	122.73
21	3B	602	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	44	414	CL7	CHD-C1D-ND	-3.29	120.78	124.26
21	42	516	CL7	C7-C6-C5	-3.29	104.44	113.36
21	13	515	CL7	CHD-C4C-C3C	-3.29	119.61	124.94
21	3A	407	CL7	C7-C6-C5	-3.28	104.44	113.36
21	1A	407	CL7	C7-C6-C5	-3.28	104.44	113.36
21	3C	509	CL7	C7-C6-C5	-3.28	104.44	113.36
21	21	405	CL7	C3A-C4A-CHB	-3.28	118.83	123.70
30	2D	407	PL9	C7-C3-C4	3.28	119.55	116.88
21	13	507	CL7	CHC-C1C-NC	-3.28	121.44	124.45
32	13	522	ZEX	C35-C15-C14	-3.28	116.75	123.47
21	14	406	CL7	CHD-C1D-ND	-3.28	120.78	124.26
21	33	506	CL7	C2D-C1D-ND	3.28	112.43	110.23
32	22	520	ZEX	C31-C30-C29	-3.28	122.62	127.31
21	4B	606	CL7	CMB-C2B-C1B	3.28	130.37	125.37
21	2C	506	CL7	CHD-C1D-ND	-3.28	120.78	124.26
21	32	514	CL7	CHD-C1D-ND	-3.28	120.78	124.26
21	34	414	CL7	CHD-C1D-ND	-3.28	120.78	124.26
21	3C	511	CL7	CHD-C4C-C3C	-3.28	119.62	124.94
21	32	508	CL7	C3A-C4A-CHB	-3.28	118.83	123.70
21	32	501	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	2B	609	CL7	C3A-C4A-CHB	-3.28	118.83	123.70
21	32	514	CL7	O2D-CGD-CBD	3.28	117.10	111.27
21	13	513	CL7	CHD-C4C-C3C	-3.28	119.62	124.94
21	1C	509	CL7	C7-C6-C5	-3.28	104.45	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	509	CL7	C7-C6-C5	-3.28	104.45	113.36
21	1D	402	CL7	O2D-CGD-CBD	3.28	117.09	111.27
21	34	407	CL7	C4D-C3D-CAD	-3.28	105.22	107.42
21	4A	407	CL7	C7-C6-C5	-3.28	104.46	113.36
21	4C	512	CL7	CHD-C4C-C3C	-3.28	119.63	124.94
21	14	414	CL7	CHD-C1D-ND	-3.28	120.79	124.26
32	34	418	ZEX	C39-C29-C30	-3.28	118.33	122.92
21	11	416	CL7	CHD-C1D-ND	-3.28	120.79	124.26
21	32	518	CL7	CHD-C1D-ND	-3.28	120.79	124.26
21	1D	405	CL7	CHD-C4C-C3C	-3.28	119.63	124.94
23	4A	404	8CT	C07-C02-C03	-3.28	117.98	122.73
21	2C	505	CL7	C3A-C4A-CHB	-3.27	118.84	123.70
21	34	416	CL7	C3A-C4A-CHB	-3.27	118.84	123.70
21	2C	509	CL7	CHD-C4C-C3C	-3.27	119.63	124.94
30	3D	407	PL9	C7-C3-C4	3.27	119.54	116.88
21	4B	606	CL7	C3A-C4A-CHB	-3.27	118.84	123.70
21	1B	612	CL7	CMD-C2D-C1D	3.27	130.35	125.37
21	41	418	CL7	CHC-C1C-NC	-3.27	121.45	124.45
21	33	502	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	1C	509	CL7	CHD-C4C-C3C	-3.27	119.63	124.94
21	43	407	CL7	C2D-C1D-ND	3.27	112.43	110.23
32	24	418	ZEX	C39-C29-C30	-3.27	118.34	122.92
21	13	502	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	43	403	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	41	405	CL7	C3A-C4A-CHB	-3.27	118.84	123.70
21	23	416	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
21	4C	509	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
21	2C	509	CL7	CHC-C1C-NC	-3.27	121.45	124.45
21	1B	601	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	13	506	CL7	C2D-C1D-ND	3.27	112.42	110.23
21	12	508	CL7	C3A-C4A-CHB	-3.27	118.85	123.70
21	42	508	CL7	C3A-C4A-CHB	-3.27	118.85	123.70
21	4B	623	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
32	43	423	ZEX	C35-C15-C14	-3.27	116.78	123.47
23	1B	626	8CT	C35-C30-C29	3.27	116.83	112.70
21	2C	509	CL7	C7-C6-C5	-3.27	104.48	113.36
21	3D	402	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	43	416	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
21	12	505	CL7	CHB-C1B-NB	-3.27	120.80	124.26
32	23	423	ZEX	C35-C15-C14	-3.27	116.78	123.47
21	21	418	CL7	CHC-C1C-NC	-3.27	121.45	124.45
21	44	407	CL7	C4D-C3D-CAD	-3.27	105.22	107.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	416	CL7	CHD-C1D-ND	-3.27	120.80	124.26
21	2C	512	CL7	CHD-C4C-C3C	-3.27	119.64	124.94
21	23	403	CL7	O2D-CGD-CBD	3.27	117.07	111.27
21	41	410	CL7	CHD-C1D-ND	-3.27	120.80	124.26
32	11	422	ZEX	C31-C30-C29	-3.27	122.65	127.31
21	22	508	CL7	O2D-CGD-CBD	3.27	117.07	111.27
21	32	508	CL7	O2D-CGD-CBD	3.27	117.07	111.27
21	23	407	CL7	C2D-C1D-ND	3.27	112.42	110.23
21	1C	505	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	24	417	CL7	CMB-C2B-C1B	3.26	130.34	125.37
21	2C	503	CL7	CHD-C1D-ND	-3.26	120.80	124.26
21	2C	505	CL7	O2D-CGD-CBD	3.26	117.07	111.27
21	3C	505	CL7	O2D-CGD-CBD	3.26	117.07	111.27
21	2C	511	CL7	CHD-C4C-C3C	-3.26	119.65	124.94
21	2B	606	CL7	CMB-C2B-C1B	3.26	130.34	125.37
23	2B	601	8CT	C35-C30-C29	3.26	116.83	112.70
23	3B	626	8CT	C35-C30-C29	3.26	116.83	112.70
21	1C	504	CL7	CHD-C4C-C3C	-3.26	119.65	124.94
23	4B	601	8CT	C35-C30-C29	3.26	116.83	112.70
21	24	407	CL7	CHC-C1C-NC	-3.26	121.46	124.45
21	42	503	CL7	C4D-C3D-CAD	-3.26	105.23	107.42
21	3C	513	CL7	O2D-CGD-CBD	3.26	117.06	111.27
21	42	513	CL7	CHD-C1D-ND	-3.26	120.80	124.26
21	22	511	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	1B	605	CL7	CMB-C2B-C1B	3.26	130.34	125.37
21	31	405	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	4C	505	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	12	513	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	23	418	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	41	404	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	23	406	CL7	C4C-C3C-C2C	-3.26	102.88	107.13
21	11	404	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
23	2C	514	8CT	C11-C10-C03	-3.26	118.05	127.20
23	3C	514	8CT	C11-C10-C03	-3.26	118.05	127.20
21	3C	512	CL7	CHD-C4C-C3C	-3.26	119.66	124.94
21	12	514	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	1B	605	CL7	CHD-C4C-C3C	-3.26	119.66	124.94
21	1C	510	CL7	C3A-C4A-CHB	-3.26	118.87	123.70
21	2C	513	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	33	518	CL7	CHD-C4C-C3C	-3.26	119.66	124.94
21	2B	611	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	2C	511	CL7	CHD-C1D-ND	-3.26	120.81	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	511	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	32	506	CL7	CHD-C1D-ND	-3.26	120.81	124.26
21	3C	509	CL7	CHD-C4C-C3C	-3.25	119.66	124.94
32	32	520	ZEX	C31-C30-C29	-3.25	122.67	127.31
32	33	522	ZEX	C35-C15-C14	-3.25	116.81	123.47
21	2B	623	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	1C	509	CL7	CHC-C1C-NC	-3.25	121.46	124.45
21	11	418	CL7	CHC-C1C-NC	-3.25	121.46	124.45
21	21	410	CL7	CHD-C1D-ND	-3.25	120.81	124.26
21	1B	607	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	13	505	CL7	C4C-C3C-C2C	-3.25	102.89	107.13
21	43	406	CL7	C4C-C3C-C2C	-3.25	102.89	107.13
21	1C	511	CL7	CHD-C1D-ND	-3.25	120.81	124.26
21	3C	503	CL7	CHD-C1D-ND	-3.25	120.81	124.26
21	2C	513	CL7	O2D-CGD-CBD	3.25	117.05	111.27
21	2C	510	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	4C	513	CL7	CHD-C1D-ND	-3.25	120.81	124.26
21	4C	505	CL7	O2D-CGD-CBD	3.25	117.05	111.27
21	33	504	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	4C	503	CL7	CHD-C1D-ND	-3.25	120.82	124.26
21	3C	509	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	12	514	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	2D	402	CL7	O2D-CGD-CBD	3.25	117.04	111.27
32	12	520	ZEX	C31-C30-C29	-3.25	122.67	127.31
23	1C	514	8CT	C11-C10-C03	-3.25	118.08	127.20
21	2B	608	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	3B	607	CL7	CHD-C4C-C3C	-3.25	119.67	124.94
21	3B	609	CL7	C2D-C1D-ND	3.25	112.41	110.23
21	22	514	CL7	CHD-C1D-ND	-3.25	120.82	124.26
21	42	518	CL7	CHD-C1D-ND	-3.25	120.82	124.26
21	3C	505	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	24	412	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	2D	405	CL7	CHD-C4C-C3C	-3.25	119.68	124.94
21	43	405	CL7	CHD-C4C-C3C	-3.25	119.68	124.94
32	14	418	ZEX	C39-C29-C30	-3.25	118.38	122.92
21	31	413	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	43	409	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
32	13	522	ZEX	C1-C2-C3	-3.25	106.31	113.64
32	42	520	ZEX	C31-C30-C29	-3.25	122.68	127.31
32	33	525	ZEX	C27-C28-C29	-3.25	121.33	126.23
21	34	407	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	34	414	CL7	C3A-C4A-CHB	-3.25	118.88	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	602	CL7	CHD-C1D-ND	-3.25	120.82	124.26
21	32	503	CL7	C4D-C3D-CAD	-3.25	105.24	107.42
21	4B	608	CL7	CHD-C4C-C3C	-3.24	119.68	124.94
21	23	405	CL7	CHD-C1D-ND	-3.24	120.82	124.26
21	23	409	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	33	508	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	42	514	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	3B	622	CL7	CHD-C4C-C3C	-3.24	119.68	124.94
21	42	506	CL7	CHD-C1D-ND	-3.24	120.82	124.26
22	2D	408	PHO	C2B-C1B-NB	-3.24	107.29	109.53
32	43	401	ZEX	C27-C28-C29	-3.24	121.33	126.23
21	32	514	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	13	518	CL7	CHD-C4C-C3C	-3.24	119.68	124.94
21	14	414	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	4C	510	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	11	411	CL7	O2D-CGD-CBD	3.24	117.03	111.27
30	1D	407	PL9	C7-C3-C4	3.24	119.51	116.88
30	4D	407	PL9	C7-C3-C4	3.24	119.51	116.88
23	4C	514	8CT	C11-C10-C03	-3.24	118.10	127.20
21	32	511	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	31	404	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	21	404	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	3B	601	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	1C	503	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	22	514	CL7	C3A-C4A-CHB	-3.24	118.89	123.70
21	2C	504	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	23	405	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	3C	504	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	1C	506	CL7	CHC-C1C-NC	-3.24	121.48	124.45
21	22	518	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	31	410	CL7	CHD-C1D-ND	-3.24	120.83	124.26
21	1C	511	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	4C	513	CL7	O2D-CGD-CBD	3.24	117.02	111.27
21	34	404	CL7	O2D-CGD-CBD	3.24	117.02	111.27
21	14	407	CL7	CHC-C1C-NC	-3.24	121.48	124.45
21	44	407	CL7	CHC-C1C-NC	-3.24	121.48	124.45
21	4C	504	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	43	419	CL7	CHD-C4C-C3C	-3.24	119.69	124.94
21	31	418	CL7	CHC-C1C-NC	-3.24	121.48	124.45
21	3D	405	CL7	CHD-C4C-C3C	-3.23	119.70	124.94
21	41	411	CL7	O2D-CGD-CBD	3.23	117.02	111.27
21	1C	513	CL7	O2D-CGD-CBD	3.23	117.01	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1A	401	CL7	CAA-CBA-CGA	-3.23	103.80	113.25
21	13	517	CL7	CHD-C1D-ND	-3.23	120.83	124.26
21	4B	606	CL7	CHD-C4C-C3C	-3.23	119.70	124.94
21	1B	601	CL7	CHD-C1D-ND	-3.23	120.83	124.26
21	11	410	CL7	CHD-C1D-ND	-3.23	120.83	124.26
21	12	518	CL7	CHD-C4C-C3C	-3.23	119.70	124.94
21	11	411	CL7	CHD-C4C-C3C	-3.23	119.70	124.94
21	44	404	CL7	O2D-CGD-CBD	3.23	117.01	111.27
21	44	414	CL7	C3A-C4A-CHB	-3.23	118.91	123.70
21	31	411	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	14	409	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	2C	508	CL7	CHD-C4C-C3C	-3.23	119.71	124.94
21	42	501	CL7	CHD-C1D-ND	-3.23	120.84	124.26
21	13	504	CL7	CHD-C4C-C3C	-3.23	119.71	124.94
21	12	515	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	1B	622	CL7	CHD-C4C-C3C	-3.23	119.71	124.94
21	12	518	CL7	CHD-C1D-ND	-3.23	120.84	124.26
21	32	501	CL7	CHD-C1D-ND	-3.23	120.84	124.26
21	32	504	CL7	CHD-C1D-ND	-3.23	120.84	124.26
21	2A	407	CL7	CAA-CBA-CGA	-3.23	103.83	113.25
21	2B	606	CL7	CHD-C4C-C3C	-3.22	119.71	124.94
32	23	423	ZEX	C1-C2-C3	-3.22	106.36	113.64
21	24	404	CL7	O2D-CGD-CBD	3.22	117.00	111.27
21	24	414	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
23	2B	618	8CT	C14-C15-C16	-3.22	117.36	126.42
21	31	414	CL7	C4C-C3C-C2C	-3.22	102.93	107.13
21	22	515	CL7	O2D-CGD-CBD	3.22	117.00	111.27
21	3B	605	CL7	CHD-C4C-C3C	-3.22	119.72	124.94
21	2A	401	CL7	CAA-CBA-CGA	-3.22	103.84	113.25
21	3A	401	CL7	CAA-CBA-CGA	-3.22	103.84	113.25
21	32	510	CL7	CHD-C4C-C3C	-3.22	119.72	124.94
21	31	402	CL7	CHC-C1C-NC	-3.22	121.49	124.45
21	42	511	CL7	CHD-C1D-ND	-3.22	120.85	124.26
21	13	508	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
23	4B	618	8CT	C14-C15-C16	-3.22	117.37	126.42
21	24	409	CL7	CMB-C2B-C1B	3.22	130.28	125.37
21	44	409	CL7	CHC-C1C-NC	-3.22	121.49	124.45
21	42	518	CL7	O2D-CGD-CBD	3.22	116.99	111.27
21	31	402	CL7	CHD-C1D-ND	-3.22	120.85	124.26
21	44	406	CL7	O2D-CGD-CBD	3.22	116.99	111.27
21	21	413	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
21	1B	613	CL7	CHD-C1D-ND	-3.22	120.85	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	514	CL7	CHD-C1D-ND	-3.22	120.85	124.26
32	33	522	ZEX	C1-C2-C3	-3.22	106.38	113.64
21	34	406	CL7	O2D-CGD-CBD	3.22	116.99	111.27
21	4A	401	CL7	CAA-CBA-CGA	-3.22	103.85	113.25
21	41	412	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
21	1A	407	CL7	CAA-CBA-CGA	-3.22	103.85	113.25
21	4A	407	CL7	CAA-CBA-CGA	-3.22	103.85	113.25
21	42	512	CL7	C3A-C4A-CHB	-3.22	118.93	123.70
32	43	423	ZEX	C1-C2-C3	-3.22	106.38	113.64
21	21	411	CL7	O2D-CGD-CBD	3.22	116.98	111.27
21	3B	606	CL7	C2D-C1D-ND	3.22	112.39	110.23
21	23	411	CL7	CHD-C4C-C3C	-3.22	119.73	124.94
21	3A	401	CL7	CHD-C4C-C3C	-3.22	119.73	124.94
21	33	517	CL7	CHD-C4C-C3C	-3.22	119.73	124.94
21	12	506	CL7	CHD-C1D-ND	-3.22	120.85	124.26
21	34	409	CL7	CMB-C2B-C1B	3.22	130.27	125.37
21	34	411	CL7	CHC-C1C-NC	-3.21	121.50	124.45
21	34	412	CL7	CHC-C1C-NC	-3.21	121.50	124.45
21	1B	615	CL7	CHB-C1B-NB	-3.21	120.86	124.26
21	14	412	CL7	CHC-C1C-NC	-3.21	121.50	124.45
21	32	518	CL7	O2D-CGD-CBD	3.21	116.98	111.27
21	22	518	CL7	CHD-C4C-C3C	-3.21	119.73	124.94
21	21	411	CL7	CHD-C4C-C3C	-3.21	119.73	124.94
21	32	518	CL7	CHD-C4C-C3C	-3.21	119.73	124.94
21	22	518	CL7	C7-C6-C5	-3.21	104.64	113.36
21	12	511	CL7	CHD-C1D-ND	-3.21	120.86	124.26
21	3B	613	CL7	CHD-C1D-ND	-3.21	120.86	124.26
21	1C	505	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	14	404	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	33	510	CL7	CHD-C4C-C3C	-3.21	119.74	124.94
21	2C	508	CL7	C3A-C4A-CHB	-3.21	118.94	123.70
21	44	409	CL7	CMB-C2B-C1B	3.21	130.25	125.37
21	3C	510	CL7	C3A-C4A-CHB	-3.21	118.94	123.70
21	21	408	CL7	C7-C6-C5	-3.21	104.65	113.36
21	42	518	CL7	CHD-C4C-C3C	-3.21	119.74	124.94
21	12	518	CL7	C7-C6-C5	-3.21	104.65	113.36
21	4B	616	CL7	CHB-C1B-NB	-3.21	120.86	124.26
21	44	411	CL7	CHC-C1C-NC	-3.21	121.51	124.45
21	42	515	CL7	O2D-CGD-CBD	3.20	116.96	111.27
21	24	406	CL7	O2D-CGD-CBD	3.20	116.96	111.27
21	31	411	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	22	501	CL7	CHD-C1D-ND	-3.20	120.86	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	510	CL7	C7-C6-C5	-3.20	104.66	113.36
21	42	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	13	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
22	4D	408	PHO	C2B-C1B-NB	-3.20	107.31	109.53
21	21	414	CL7	C4C-C3C-C2C	-3.20	102.95	107.13
21	12	510	CL7	C7-C6-C5	-3.20	104.66	113.36
21	44	412	CL7	CHC-C1C-NC	-3.20	121.51	124.45
21	3B	610	CL7	CHD-C1D-ND	-3.20	120.87	124.26
21	11	412	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	41	414	CL7	C4C-C3C-C2C	-3.20	102.95	107.13
21	23	419	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	32	518	CL7	C7-C6-C5	-3.20	104.67	113.36
21	34	409	CL7	CHC-C1C-NC	-3.20	121.51	124.45
21	32	512	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	32	502	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	4A	401	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	34	412	CL7	CAA-CBA-CGA	-3.20	103.90	113.25
21	4B	607	CL7	C2D-C1D-ND	3.20	112.38	110.23
21	4B	610	CL7	C2D-C1D-ND	3.20	112.38	110.23
21	31	412	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
23	3B	617	8CT	C14-C15-C16	-3.20	117.43	126.42
21	3A	407	CL7	CAA-CBA-CGA	-3.20	103.90	113.25
21	31	408	CL7	C7-C6-C5	-3.20	104.67	113.36
21	44	412	CL7	CAA-CBA-CGA	-3.20	103.91	113.25
23	1B	617	8CT	C14-C15-C16	-3.20	117.43	126.42
21	2B	617	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	23	418	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
21	3C	510	CL7	CHD-C4C-C3C	-3.20	119.75	124.94
23	1B	626	8CT	C01-C02-C07	3.20	119.76	113.62
23	3B	626	8CT	C01-C02-C07	3.20	119.76	113.62
21	2C	506	CL7	CHC-C1C-NC	-3.20	121.52	124.45
21	3C	506	CL7	CHC-C1C-NC	-3.20	121.52	124.45
21	42	517	CL7	CHD-C4C-C3C	-3.20	119.76	124.94
21	22	506	CL7	CHD-C1D-ND	-3.20	120.87	124.26
21	22	509	CL7	CHD-C1D-ND	-3.20	120.87	124.26
21	32	509	CL7	CHD-C1D-ND	-3.20	120.87	124.26
21	12	503	CL7	C4D-C3D-CAD	-3.20	105.27	107.42
21	1C	510	CL7	CHD-C4C-C3C	-3.20	119.76	124.94
21	13	517	CL7	CHD-C4C-C3C	-3.20	119.76	124.94
21	11	413	CL7	C3A-C4A-CHB	-3.20	118.96	123.70
21	14	412	CL7	CAA-CBA-CGA	-3.20	103.92	113.25
21	32	510	CL7	C7-C6-C5	-3.19	104.69	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	414	CL7	C4C-C3C-C2C	-3.19	102.96	107.13
21	2B	616	CL7	CHB-C1B-NB	-3.19	120.88	124.26
21	2B	610	CL7	C2D-C1D-ND	3.19	112.37	110.23
21	32	515	CL7	O2D-CGD-CBD	3.19	116.94	111.27
21	14	406	CL7	O2D-CGD-CBD	3.19	116.94	111.27
21	4C	508	CL7	C3A-C4A-CHB	-3.19	118.96	123.70
21	22	510	CL7	C7-C6-C5	-3.19	104.69	113.36
21	42	518	CL7	C7-C6-C5	-3.19	104.69	113.36
21	11	402	CL7	CHD-C1D-ND	-3.19	120.88	124.26
21	41	411	CL7	CHD-C4C-C3C	-3.19	119.77	124.94
21	11	408	CL7	C7-C6-C5	-3.19	104.70	113.36
21	11	408	CL7	CAA-CBA-CGA	-3.19	103.93	113.25
21	1C	508	CL7	C3A-C4A-CHB	-3.19	118.97	123.70
21	3C	508	CL7	C3A-C4A-CHB	-3.19	118.97	123.70
21	41	413	CL7	C3A-C4A-CHB	-3.19	118.97	123.70
21	21	408	CL7	CAA-CBA-CGA	-3.19	103.94	113.25
21	41	403	CL7	CHB-C1B-NB	-3.19	120.88	124.26
21	24	412	CL7	CAA-CBA-CGA	-3.19	103.94	113.25
21	22	517	CL7	CHD-C1D-ND	-3.19	120.88	124.26
21	1B	607	CL7	C7-C6-C5	-3.19	104.70	113.36
21	1C	508	CL7	CHD-C4C-C3C	-3.19	119.77	124.94
21	3C	508	CL7	CHD-C4C-C3C	-3.19	119.77	124.94
21	41	408	CL7	C7-C6-C5	-3.19	104.71	113.36
21	12	517	CL7	CHD-C1D-ND	-3.19	120.88	124.26
21	21	412	CL7	C3A-C4A-CHB	-3.19	118.97	123.70
21	3B	611	CL7	C7-C6-C5	-3.19	104.71	113.36
21	13	507	CL7	CHD-C4C-C3C	-3.19	119.78	124.94
21	22	502	CL7	CHD-C4C-C3C	-3.19	119.78	124.94
21	3B	616	CL7	CHD-C4C-C3C	-3.19	119.78	124.94
21	14	407	CL7	C4D-C3D-CAD	-3.18	105.28	107.42
21	31	408	CL7	CAA-CBA-CGA	-3.18	103.95	113.25
21	2C	510	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	4B	608	CL7	C7-C6-C5	-3.18	104.71	113.36
21	1B	611	CL7	C7-C6-C5	-3.18	104.72	113.36
23	2B	601	8CT	C01-C02-C07	3.18	119.73	113.62
21	12	501	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	12	517	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	4B	614	CL7	CHD-C1D-ND	-3.18	120.89	124.26
21	2B	612	CL7	C7-C6-C5	-3.18	104.72	113.36
21	22	501	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	12	518	CL7	O2D-CGD-CBD	3.18	116.92	111.27
21	23	414	CL7	O2D-CGD-CBD	3.18	116.92	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	414	CL7	O2D-CGD-CBD	3.18	116.92	111.27
21	14	409	CL7	CMB-C2B-C1B	3.18	130.21	125.37
21	22	503	CL7	CHD-C1D-ND	-3.18	120.89	124.26
21	1B	609	CL7	C2D-C1D-ND	3.18	112.36	110.23
21	43	418	CL7	CHD-C4C-C3C	-3.18	119.78	124.94
21	1A	401	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	22	510	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	4B	617	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	22	518	CL7	O2D-CGD-CBD	3.18	116.92	111.27
21	2B	607	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	32	517	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	43	411	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
32	13	522	ZEX	C8-C7-C6	-3.18	118.28	127.20
21	24	411	CL7	CHC-C1C-NC	-3.18	121.53	124.45
21	2B	608	CL7	C7-C6-C5	-3.18	104.73	113.36
21	4B	611	CL7	CHD-C1D-ND	-3.18	120.89	124.26
23	3B	617	8CT	C18-C19-C20	-3.18	116.97	123.47
21	2A	401	CL7	CHD-C4C-C3C	-3.18	119.79	124.94
21	22	512	CL7	C3A-C4A-CHB	-3.18	118.99	123.70
21	21	403	CL7	CHB-C1B-NB	-3.17	120.90	124.26
21	31	403	CL7	CHB-C1B-NB	-3.17	120.90	124.26
21	42	503	CL7	CHD-C1D-ND	-3.17	120.90	124.26
21	12	510	CL7	CHD-C4C-C3C	-3.17	119.79	124.94
21	41	408	CL7	CAA-CBA-CGA	-3.17	103.98	113.25
21	24	409	CL7	CHC-C1C-NC	-3.17	121.54	124.45
21	1B	616	CL7	CHD-C4C-C3C	-3.17	119.79	124.94
21	12	502	CL7	CHD-C4C-C3C	-3.17	119.80	124.94
21	12	501	CL7	CHD-C1D-ND	-3.17	120.90	124.26
21	32	515	CL7	CMB-C2B-C1B	3.17	130.20	125.37
21	12	512	CL7	C3A-C4A-CHB	-3.17	118.99	123.70
21	4C	508	CL7	CHD-C4C-C3C	-3.17	119.80	124.94
21	22	517	CL7	CHD-C4C-C3C	-3.17	119.80	124.94
21	3B	615	CL7	CHB-C1B-NB	-3.17	120.90	124.26
21	43	404	CL7	CMB-C2B-C1B	3.17	130.20	125.37
23	2C	518	8CT	C24-C23-C21	-3.17	117.51	126.42
21	32	503	CL7	CHD-C1D-ND	-3.17	120.90	124.26
21	22	509	CL7	CHC-C1C-NC	-3.17	121.54	124.45
21	12	515	CL7	CHD-C4C-C3C	-3.17	119.80	124.94
21	23	417	CL7	O2D-CGD-CBD	3.17	116.90	111.27
21	42	509	CL7	CHD-C1D-ND	-3.17	120.90	124.26
23	2B	618	8CT	C18-C19-C20	-3.17	116.99	123.47
21	33	507	CL7	CHD-C4C-C3C	-3.17	119.81	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	607	CL7	C7-C6-C5	-3.17	104.76	113.36
32	43	423	ZEX	C8-C7-C6	-3.17	118.31	127.20
22	3D	408	PHO	C2B-C1B-NB	-3.17	107.34	109.53
21	13	513	CL7	O2D-CGD-CBD	3.17	116.89	111.27
32	33	522	ZEX	C8-C7-C6	-3.17	118.31	127.20
21	4B	612	CL7	C7-C6-C5	-3.16	104.76	113.36
21	11	402	CL7	CHC-C1C-NC	-3.16	121.55	124.45
21	41	402	CL7	CHC-C1C-NC	-3.16	121.55	124.45
21	4C	506	CL7	CHC-C1C-NC	-3.16	121.55	124.45
21	13	508	CL7	C7-C6-C5	-3.16	104.77	113.36
21	1B	606	CL7	CHD-C4C-C3C	-3.16	119.81	124.94
21	2B	614	CL7	CHD-C1D-ND	-3.16	120.91	124.26
23	4B	618	8CT	C18-C19-C20	-3.16	117.00	123.47
21	3B	606	CL7	CHD-C4C-C3C	-3.16	119.81	124.94
32	14	419	ZEX	C3-C4-C5	-3.16	105.56	111.85
21	23	409	CL7	C7-C6-C5	-3.16	104.77	113.36
21	12	515	CL7	CMB-C2B-C1B	3.16	130.18	125.37
32	24	419	ZEX	C3-C4-C5	-3.16	105.56	111.85
21	43	409	CL7	C7-C6-C5	-3.16	104.78	113.36
21	4B	607	CL7	CHD-C4C-C3C	-3.16	119.82	124.94
21	33	503	CL7	CMB-C2B-C1B	3.16	130.18	125.37
21	42	502	CL7	CHD-C1D-ND	-3.16	120.91	124.26
21	32	506	CL7	C7-C6-C5	-3.16	104.78	113.36
23	4B	601	8CT	C01-C02-C07	3.16	119.68	113.62
21	2B	614	CL7	CHC-C1C-NC	-3.16	121.55	124.45
21	11	403	CL7	CHB-C1B-NB	-3.16	120.91	124.26
21	22	515	CL7	CMB-C2B-C1B	3.16	130.18	125.37
21	42	506	CL7	C7-C6-C5	-3.16	104.78	113.36
21	41	415	CL7	CHD-C1D-ND	-3.16	120.92	124.26
21	43	408	CL7	CHD-C4C-C3C	-3.16	119.82	124.94
21	44	410	CL7	CHD-C4C-C3C	-3.16	119.82	124.94
21	32	517	CL7	CHD-C1D-ND	-3.16	120.92	124.26
32	23	423	ZEX	C8-C7-C6	-3.16	118.34	127.20
21	33	508	CL7	C7-C6-C5	-3.15	104.79	113.36
21	23	408	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
21	1B	610	CL7	CHD-C1D-ND	-3.15	120.92	124.26
21	22	506	CL7	C7-C6-C5	-3.15	104.79	113.36
21	32	515	CL7	CHD-C4C-C3C	-3.15	119.83	124.94
21	31	415	CL7	CHD-C1D-ND	-3.15	120.92	124.26
21	32	514	CL7	C2D-C1D-ND	3.15	112.34	110.23
21	33	513	CL7	O2D-CGD-CBD	3.15	116.87	111.27
23	4C	518	8CT	C24-C23-C21	-3.15	117.56	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1B	618	8CT	C27-C26-C28	3.15	123.04	118.08
23	1C	518	8CT	C24-C23-C21	-3.15	117.56	126.42
22	1D	408	PHO	C2B-C1B-NB	-3.15	107.35	109.53
32	13	525	ZEX	C35-C15-C14	-3.15	117.02	123.47
21	12	506	CL7	C7-C6-C5	-3.15	104.81	113.36
21	24	410	CL7	O2D-CGD-CBD	3.15	116.86	111.27
21	33	516	CL7	O2D-CGD-CBD	3.15	116.86	111.27
21	4C	510	CL7	CHD-C4C-C3C	-3.15	119.84	124.94
21	1C	502	CL7	CHD-C1D-ND	-3.15	120.93	124.26
23	1B	617	8CT	C18-C19-C20	-3.15	117.03	123.47
32	34	419	ZEX	C3-C4-C5	-3.15	105.59	111.85
21	42	502	CL7	CHD-C4C-C3C	-3.15	119.84	124.94
21	12	503	CL7	CHD-C1D-ND	-3.14	120.93	124.26
21	21	408	CL7	C2D-C1D-ND	3.14	112.34	110.23
23	3C	518	8CT	C24-C23-C21	-3.14	117.58	126.42
21	1B	602	CL7	CHD-C4C-C3C	-3.14	119.84	124.94
21	42	515	CL7	CMB-C2B-C1B	3.14	130.16	125.37
21	43	402	CL7	O2D-CGD-CBD	3.14	116.85	111.27
21	12	509	CL7	CHD-C4C-C3C	-3.14	119.84	124.94
21	42	509	CL7	CHD-C4C-C3C	-3.14	119.84	124.94
21	23	402	CL7	O2D-CGD-CBD	3.14	116.85	111.27
23	2B	619	8CT	C27-C26-C28	3.14	123.03	118.08
21	23	404	CL7	CMB-C2B-C1B	3.14	130.15	125.37
21	41	402	CL7	CHD-C1D-ND	-3.14	120.93	124.26
21	13	503	CL7	CMB-C2B-C1B	3.14	130.15	125.37
21	42	501	CL7	CHD-C4C-C3C	-3.14	119.85	124.94
21	21	402	CL7	CHC-C1C-NC	-3.14	121.57	124.45
21	43	409	CL7	CHD-C1D-ND	-3.14	120.93	124.26
21	1B	606	CL7	C2D-C1D-ND	3.14	112.34	110.23
21	13	518	CL7	O2D-CGD-CBD	3.14	116.84	111.27
21	4B	614	CL7	CHC-C1C-NC	-3.14	121.57	124.45
21	14	410	CL7	CHD-C4C-C3C	-3.14	119.85	124.94
21	12	509	CL7	CHD-C1D-ND	-3.14	120.94	124.26
32	44	419	ZEX	C3-C4-C5	-3.14	105.61	111.85
32	33	525	ZEX	C35-C15-C14	-3.14	117.05	123.47
21	2B	603	CL7	CHD-C4C-C3C	-3.14	119.86	124.94
21	13	516	CL7	O2D-CGD-CBD	3.14	116.84	111.27
21	23	419	CL7	O2D-CGD-CBD	3.14	116.84	111.27
21	21	403	CL7	CHC-C1C-NC	-3.14	121.57	124.45
21	32	503	CL7	CHC-C1C-NC	-3.14	121.57	124.45
21	3C	504	CL7	CHD-C1D-ND	-3.14	120.94	124.26
21	42	505	CL7	C3A-C4A-CHB	-3.13	119.05	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1C	517	CL7	CHD-C1D-ND	-3.13	120.94	124.26
21	4C	517	CL7	CHD-C1D-ND	-3.13	120.94	124.26
32	43	401	ZEX	C35-C15-C14	-3.13	117.06	123.47
21	44	406	CL7	C7-C6-C5	-3.13	104.85	113.36
21	33	501	CL7	O2D-CGD-CBD	3.13	116.84	111.27
21	24	410	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	34	410	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	42	515	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	43	419	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	32	509	CL7	CHC-C1C-NC	-3.13	121.58	124.45
21	4C	504	CL7	CHD-C1D-ND	-3.13	120.94	124.26
23	3B	618	8CT	C27-C26-C28	3.13	123.01	118.08
21	3B	602	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	32	501	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	13	509	CL7	CHD-C4C-C3C	-3.13	119.86	124.94
21	12	502	CL7	CHD-C1D-ND	-3.13	120.94	124.26
21	43	417	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	3B	604	CL7	C3A-C4A-CHB	-3.13	119.06	123.70
21	42	517	CL7	CHD-C1D-ND	-3.13	120.94	124.26
32	12	519	ZEX	C11-C10-C9	-3.13	122.84	127.31
21	22	502	CL7	CHD-C1D-ND	-3.13	120.94	124.26
21	23	410	CL7	CHD-C4C-C3C	-3.13	119.87	124.94
21	1B	613	CL7	CHC-C1C-NC	-3.13	121.58	124.45
21	12	516	CL7	CHD-C1D-ND	-3.13	120.95	124.26
21	2C	517	CL7	CHC-C1C-NC	-3.13	121.58	124.45
21	3C	517	CL7	CHD-C1D-ND	-3.13	120.95	124.26
21	2B	605	CL7	C3A-C4A-CHB	-3.13	119.06	123.70
21	13	501	CL7	O2D-CGD-CBD	3.12	116.82	111.27
21	21	402	CL7	CHD-C1D-ND	-3.12	120.95	124.26
21	22	509	CL7	CHD-C4C-C3C	-3.12	119.88	124.94
21	24	406	CL7	C7-C6-C5	-3.12	104.88	113.36
23	4B	619	8CT	C27-C26-C28	3.12	122.99	118.08
21	34	406	CL7	C7-C6-C5	-3.12	104.88	113.36
21	14	406	CL7	C7-C6-C5	-3.12	104.89	113.36
21	22	515	CL7	CHD-C4C-C3C	-3.12	119.88	124.94
21	2B	607	CL7	C2D-C1D-ND	3.12	112.32	110.23
21	2C	502	CL7	CHD-C1D-ND	-3.12	120.95	124.26
21	4B	604	CL7	C7-C6-C5	-3.12	104.89	113.36
21	11	405	CL7	CHD-C4C-C3C	-3.12	119.89	124.94
21	1C	507	CL7	C3B-C2B-C1B	-3.12	103.40	107.16
21	12	503	CL7	CHC-C1C-NC	-3.12	121.59	124.45
21	43	416	CL7	CHC-C1C-NC	-3.12	121.59	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	24	404	CL7	CHD-C1D-ND	-3.12	120.96	124.26
32	23	401	ZEX	C35-C15-C14	-3.12	117.09	123.47
21	1C	507	CL7	CHD-C4C-C3C	-3.12	119.89	124.94
21	1B	605	CL7	CHB-C1B-NB	-3.12	120.96	124.26
21	24	416	CL7	CHD-C1D-ND	-3.11	120.96	124.26
21	33	518	CL7	O2D-CGD-CBD	3.11	116.80	111.27
21	4B	603	CL7	CHD-C4C-C3C	-3.11	119.89	124.94
21	34	410	CL7	O2D-CGD-CBD	3.11	116.80	111.27
21	3B	603	CL7	C7-C6-C5	-3.11	104.91	113.36
21	33	508	CL7	CHD-C1D-ND	-3.11	120.96	124.26
21	34	411	CL7	CHD-C4C-C3C	-3.11	119.89	124.94
21	2C	517	CL7	CHD-C1D-ND	-3.11	120.96	124.26
21	23	412	CL7	O2A-C1-C2	-3.11	100.46	108.64
21	33	511	CL7	O2A-C1-C2	-3.11	100.46	108.64
21	23	409	CL7	CHD-C1D-ND	-3.11	120.96	124.26
21	44	408	CL7	CHD-C1D-ND	-3.11	120.96	124.26
21	1B	604	CL7	C3A-C4A-CHB	-3.11	119.08	123.70
21	4B	605	CL7	C3A-C4A-CHB	-3.11	119.08	123.70
21	11	415	CL7	CHD-C1D-ND	-3.11	120.97	124.26
21	4C	502	CL7	CHD-C1D-ND	-3.11	120.97	124.26
21	42	516	CL7	CHD-C1D-ND	-3.11	120.97	124.26
21	2B	604	CL7	C7-C6-C5	-3.11	104.92	113.36
32	33	519	ZEX	C27-C26-C25	-3.11	117.82	122.84
32	22	519	ZEX	C11-C10-C9	-3.11	122.88	127.31
32	14	418	ZEX	C15-C35-C34	-3.11	117.11	123.47
21	41	405	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
21	32	505	CL7	C3A-C4A-CHB	-3.11	119.09	123.70
21	14	410	CL7	O2D-CGD-CBD	3.11	116.79	111.27
21	4B	606	CL7	O2D-CGD-CBD	3.11	116.79	111.27
32	24	419	ZEX	C11-C10-C9	-3.11	122.88	127.31
32	34	419	ZEX	C11-C10-C9	-3.11	122.88	127.31
21	32	509	CL7	CHD-C4C-C3C	-3.11	119.90	124.94
21	1B	603	CL7	C7-C6-C5	-3.11	104.92	113.36
32	34	418	ZEX	C15-C35-C34	-3.11	117.11	123.47
21	11	415	CL7	CHC-C1C-NC	-3.11	121.60	124.45
21	3B	613	CL7	CHC-C1C-NC	-3.11	121.60	124.45
21	41	415	CL7	CHC-C1C-NC	-3.11	121.60	124.45
21	21	415	CL7	CHD-C1D-ND	-3.10	120.97	124.26
32	23	420	ZEX	C27-C26-C25	-3.10	117.82	122.84
21	44	415	CL7	C4C-C3C-C2C	-3.10	103.08	107.13
21	21	412	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
21	11	403	CL7	CHC-C1C-NC	-3.10	121.60	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	511	CL7	O2A-C1-C2	-3.10	100.48	108.64
21	2B	602	CL7	CHB-C1B-NB	-3.10	120.97	124.26
21	32	509	CL7	C7-C6-C5	-3.10	104.94	113.36
21	43	403	CL7	C2D-C1D-ND	3.10	112.31	110.23
21	32	502	CL7	CHD-C1D-ND	-3.10	120.97	124.26
21	34	404	CL7	CHD-C1D-ND	-3.10	120.97	124.26
21	44	404	CL7	CHD-C1D-ND	-3.10	120.97	124.26
21	4C	507	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
21	44	411	CL7	CHD-C4C-C3C	-3.10	119.91	124.94
32	23	421	ZEX	C1-C2-C3	-3.10	106.64	113.64
21	12	507	CL7	C3B-C2B-C1B	-3.10	103.42	107.16
21	14	405	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	21	403	CL7	CHD-C1D-ND	-3.10	120.98	124.26
21	22	505	CL7	C3A-C4A-CHB	-3.10	119.10	123.70
21	44	405	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	2B	606	CL7	O2D-CGD-CBD	3.10	116.77	111.27
21	3B	605	CL7	O2D-CGD-CBD	3.10	116.77	111.27
32	42	519	ZEX	C11-C10-C9	-3.10	122.89	127.31
21	3C	509	CL7	CHD-C1D-ND	-3.10	120.98	124.26
21	33	509	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	34	405	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	43	412	CL7	O2A-C1-C2	-3.10	100.50	108.64
21	33	515	CL7	CHC-C1C-NC	-3.10	121.61	124.45
21	3C	507	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	34	415	CL7	C4C-C3C-C2C	-3.10	103.09	107.13
21	14	415	CL7	CHD-C1D-ND	-3.10	120.98	124.26
21	2C	507	CL7	C3B-C2B-C1B	-3.10	103.42	107.16
21	21	419	CL7	CHD-C4C-C3C	-3.10	119.92	124.94
21	12	509	CL7	CHC-C1C-NC	-3.09	121.61	124.45
21	42	509	CL7	CHC-C1C-NC	-3.09	121.61	124.45
21	43	410	CL7	CHD-C4C-C3C	-3.09	119.92	124.94
21	3C	506	CL7	O2A-CGA-O1A	-3.09	115.79	123.59
32	32	519	ZEX	C11-C10-C9	-3.09	122.90	127.31
21	11	403	CL7	CHD-C1D-ND	-3.09	120.98	124.26
21	34	410	CL7	CHD-C1D-ND	-3.09	120.98	124.26
21	22	503	CL7	CHC-C1C-NC	-3.09	121.61	124.45
32	33	520	ZEX	C1-C2-C3	-3.09	106.66	113.64
21	34	416	CL7	CHD-C1D-ND	-3.09	120.98	124.26
21	34	413	CL7	O2D-CGD-CBD	3.09	116.76	111.27
21	3C	502	CL7	CHD-C1D-ND	-3.09	120.98	124.26
21	4B	606	CL7	CHB-C1B-NB	-3.09	120.98	124.26
21	1C	506	CL7	O2A-CGA-O1A	-3.09	115.79	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	506	CL7	O2A-CGA-O1A	-3.09	115.79	123.59
21	32	502	CL7	C3A-C4A-CHB	-3.09	119.11	123.70
32	24	418	ZEX	C15-C35-C34	-3.09	117.14	123.47
21	2C	507	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	21	405	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	24	405	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
32	44	419	ZEX	C11-C10-C9	-3.09	122.90	127.31
21	1B	610	CL7	CHC-C1C-NC	-3.09	121.61	124.45
21	13	514	CL7	CHD-C1D-ND	-3.09	120.99	124.26
32	13	519	ZEX	C27-C26-C25	-3.09	117.85	122.84
21	32	516	CL7	CHD-C4C-C3C	-3.09	119.93	124.94
21	21	415	CL7	CHC-C1C-NC	-3.09	121.62	124.45
21	43	416	CL7	CHD-C1D-ND	-3.09	120.99	124.26
21	44	410	CL7	O2D-CGD-CBD	3.09	116.75	111.27
21	24	415	CL7	C4C-C3C-C2C	-3.09	103.10	107.13
21	12	513	CL7	CMB-C2B-C1B	3.09	130.07	125.37
32	13	522	ZEX	C30-C31-C32	-3.09	113.58	123.22
21	1B	605	CL7	O2D-CGD-CBD	3.09	116.75	111.27
21	24	417	CL7	CHC-C1C-NC	-3.09	121.62	124.45
21	22	513	CL7	CHB-C1B-NB	-3.09	120.99	124.26
21	22	516	CL7	CHD-C1D-ND	-3.09	120.99	124.26
32	33	522	ZEX	C30-C31-C32	-3.09	113.59	123.22
21	11	412	CL7	CHD-C4C-C3C	-3.09	119.94	124.94
21	41	412	CL7	CHD-C4C-C3C	-3.09	119.94	124.94
21	22	509	CL7	C7-C6-C5	-3.09	104.98	113.36
21	42	509	CL7	C7-C6-C5	-3.09	104.98	113.36
32	13	520	ZEX	C1-C2-C3	-3.09	106.67	113.64
32	43	421	ZEX	C1-C2-C3	-3.09	106.67	113.64
21	31	415	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	12	509	CL7	C7-C6-C5	-3.08	104.98	113.36
21	4B	602	CL7	CHB-C1B-NB	-3.08	120.99	124.26
21	3C	517	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	1C	517	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	21	419	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	4C	517	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	43	411	CL7	CHD-C1D-ND	-3.08	120.99	124.26
21	31	412	CL7	CHD-C4C-C3C	-3.08	119.94	124.94
21	3C	507	CL7	CAA-CBA-CGA	-3.08	104.25	113.25
21	23	416	CL7	CHC-C1C-NC	-3.08	121.62	124.45
32	34	403	ZEX	C31-C32-C33	-3.08	117.76	126.42
21	14	417	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	3B	613	CL7	O2D-CGD-CBD	3.08	116.74	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2D	406	8CT	C07-C02-C03	-3.08	118.26	122.73
32	23	423	ZEX	C30-C31-C32	-3.08	113.61	123.22
21	1D	402	CL7	C2D-C1D-ND	3.08	112.30	110.23
21	4D	402	CL7	C2D-C1D-ND	3.08	112.30	110.23
21	12	516	CL7	CHD-C4C-C3C	-3.08	119.95	124.94
21	14	411	CL7	CHD-C4C-C3C	-3.08	119.95	124.94
21	31	405	CL7	CHD-C4C-C3C	-3.08	119.95	124.94
21	34	417	CL7	CHC-C1C-NC	-3.08	121.63	124.45
21	24	411	CL7	CHD-C4C-C3C	-3.08	119.95	124.94
21	14	416	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	23	416	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	33	515	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	44	416	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	43	411	CL7	C7-C6-C5	-3.08	105.00	113.36
21	3C	507	CL7	CHD-C1D-ND	-3.08	121.00	124.26
21	14	415	CL7	C4C-C3C-C2C	-3.08	103.12	107.13
21	24	413	CL7	O2D-CGD-CBD	3.07	116.73	111.27
21	1C	507	CL7	CAA-CBA-CGA	-3.07	104.27	113.25
21	4C	507	CL7	CAA-CBA-CGA	-3.07	104.27	113.25
21	43	407	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	12	514	CL7	C2D-C1D-ND	3.07	112.29	110.23
21	42	514	CL7	C2D-C1D-ND	3.07	112.29	110.23
21	13	503	CL7	CHC-C1C-NC	-3.07	121.63	124.45
21	42	513	CL7	CHB-C1B-NB	-3.07	121.00	124.26
21	4B	609	CL7	CHD-C4C-C3C	-3.07	119.96	124.94
21	1B	613	CL7	O2D-CGD-CBD	3.07	116.73	111.27
23	1C	518	8CT	C11-C10-C03	-3.07	118.57	127.20
21	13	510	CL7	C7-C6-C5	-3.07	105.01	113.36
21	42	503	CL7	CHC-C1C-NC	-3.07	121.63	124.45
21	22	501	CL7	CMB-C2B-C1B	3.07	130.05	125.37
21	1C	509	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	13	508	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	2C	504	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	4B	605	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	4C	509	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	42	508	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	12	505	CL7	C3A-C4A-CHB	-3.07	119.14	123.70
21	13	506	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	13	510	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	14	408	CL7	CHD-C1D-ND	-3.07	121.00	124.26
21	23	411	CL7	C7-C6-C5	-3.07	105.02	113.36
21	4C	507	CL7	C3B-C2B-C1B	-3.07	103.45	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	507	CL7	C3B-C2B-C1B	-3.07	103.45	107.16
32	43	420	ZEX	C27-C26-C25	-3.07	117.88	122.84
32	14	403	ZEX	C31-C32-C33	-3.07	117.79	126.42
32	44	403	ZEX	C31-C32-C33	-3.07	117.79	126.42
21	14	410	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	3C	512	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	4B	611	CL7	CHC-C1C-NC	-3.07	121.63	124.45
21	2C	507	CL7	CAA-CBA-CGA	-3.07	104.28	113.25
21	1C	512	CL7	O2D-CGD-CBD	3.07	116.72	111.27
21	1C	504	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	34	408	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	44	410	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	31	419	CL7	CHD-C4C-C3C	-3.07	119.97	124.94
21	33	506	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	3C	507	CL7	C3B-C2B-C1B	-3.07	103.46	107.16
21	11	419	CL7	CHD-C4C-C3C	-3.07	119.97	124.94
21	41	419	CL7	CHD-C4C-C3C	-3.07	119.97	124.94
32	43	423	ZEX	C30-C31-C32	-3.07	113.64	123.22
21	33	510	CL7	C7-C6-C5	-3.07	105.03	113.36
21	14	404	CL7	CHD-C1D-ND	-3.07	121.01	124.26
21	3B	605	CL7	CHB-C1B-NB	-3.07	121.01	124.26
21	2C	513	CL7	CHD-C4C-C3C	-3.07	119.97	124.94
21	2B	614	CL7	O2D-CGD-CBD	3.07	116.72	111.27
21	2C	512	CL7	O2D-CGD-CBD	3.07	116.72	111.27
21	2B	606	CL7	CHB-C1B-NB	-3.07	121.01	124.26
21	21	406	CL7	CHB-C1B-NB	-3.07	121.01	124.26
21	21	407	CL7	CHD-C4C-C3C	-3.06	119.97	124.94
21	42	516	CL7	CHD-C4C-C3C	-3.06	119.97	124.94
21	3B	610	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	41	403	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	12	502	CL7	C3A-C4A-CHB	-3.06	119.15	123.70
21	22	502	CL7	C3A-C4A-CHB	-3.06	119.15	123.70
21	2C	506	CL7	O2A-CGA-O1A	-3.06	115.86	123.59
23	34	402	8CT	C05-C04-C03	3.06	115.20	110.48
32	13	522	ZEX	C11-C12-C13	-3.06	117.81	126.42
21	22	513	CL7	CMB-C2B-C1B	3.06	130.03	125.37
21	32	513	CL7	CMB-C2B-C1B	3.06	130.03	125.37
32	24	403	ZEX	C31-C32-C33	-3.06	117.81	126.42
32	44	418	ZEX	C15-C35-C34	-3.06	117.20	123.47
21	1B	604	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	32	501	CL7	CMB-C2B-C1B	3.06	130.03	125.37
21	41	408	CL7	C2D-C1D-ND	3.06	112.28	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	403	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	34	411	CL7	C3B-C2B-C1B	-3.06	103.47	107.16
21	1B	601	CL7	CHB-C1B-NB	-3.06	121.02	124.26
21	1B	614	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
21	31	407	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
21	22	516	CL7	O2D-CGD-CBD	3.06	116.70	111.27
21	23	407	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	33	509	CL7	C7-C6-C5	-3.06	105.06	113.36
21	2C	508	CL7	CAA-CBA-CGA	-3.06	104.32	113.25
21	24	411	CL7	C3B-C2B-C1B	-3.06	103.47	107.16
32	24	420	ZEX	C30-C31-C32	-3.06	113.68	123.22
21	4B	614	CL7	O2D-CGD-CBD	3.06	116.70	111.27
23	4D	406	8CT	C07-C02-C03	-3.06	118.29	122.73
21	24	410	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	34	415	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	41	406	CL7	CHB-C1B-NB	-3.06	121.02	124.26
21	4C	513	CL7	CHD-C4C-C3C	-3.06	119.98	124.94
31	1F	101	HEM	CBA-CAA-C2A	-3.06	104.14	112.63
21	33	512	CL7	CHD-C1D-ND	-3.06	121.02	124.26
21	32	507	CL7	C3B-C2B-C1B	-3.06	103.47	107.16
21	31	403	CL7	CHC-C1C-NC	-3.06	121.65	124.45
21	1B	602	CL7	O2A-CGA-CBA	3.05	121.49	111.91
21	42	502	CL7	C3A-C4A-CHB	-3.05	119.17	123.70
21	1C	501	CL7	O2D-CGD-CBD	3.05	116.69	111.27
21	12	513	CL7	CHB-C1B-NB	-3.05	121.02	124.26
21	3B	601	CL7	CHB-C1B-NB	-3.05	121.02	124.26
32	43	423	ZEX	C11-C12-C13	-3.05	117.84	126.42
21	2B	605	CL7	CHD-C4C-C3C	-3.05	119.99	124.94
21	13	502	CL7	C2D-C1D-ND	3.05	112.28	110.23
21	41	414	CL7	CHC-C1C-NC	-3.05	121.65	124.45
21	11	407	CL7	CHD-C4C-C3C	-3.05	119.99	124.94
21	2B	615	CL7	CHD-C4C-C3C	-3.05	119.99	124.94
21	24	408	CL7	CHD-C1D-ND	-3.05	121.03	124.26
21	32	513	CL7	CHB-C1B-NB	-3.05	121.03	124.26
21	14	413	CL7	O2D-CGD-CBD	3.05	116.69	111.27
21	4C	512	CL7	O2D-CGD-CBD	3.05	116.69	111.27
21	44	413	CL7	O2D-CGD-CBD	3.05	116.69	111.27
32	34	420	ZEX	C30-C31-C32	-3.05	113.69	123.22
21	23	404	CL7	CHC-C1C-NC	-3.05	121.65	124.45
21	33	503	CL7	CHC-C1C-NC	-3.05	121.65	124.45
21	2C	507	CL7	CHD-C1D-ND	-3.05	121.03	124.26
21	24	415	CL7	CHD-C1D-ND	-3.05	121.03	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	615	CL7	CHD-C1D-ND	-3.05	121.03	124.26
21	12	516	CL7	O2D-CGD-CBD	3.05	116.69	111.27
21	41	407	CL7	CHD-C4C-C3C	-3.05	119.99	124.94
21	41	419	CL7	CHC-C1C-NC	-3.05	121.65	124.45
21	13	505	CL7	C4D-C3D-CAD	-3.05	105.37	107.42
21	43	406	CL7	C4D-C3D-CAD	-3.05	105.37	107.42
21	2C	501	CL7	O2D-CGD-CBD	3.05	116.69	111.27
21	3C	501	CL7	O2D-CGD-CBD	3.05	116.69	111.27
21	22	514	CL7	C2D-C1D-ND	3.05	112.28	110.23
23	2C	514	8CT	C25-C24-C23	-3.05	113.70	123.22
32	44	420	ZEX	C30-C31-C32	-3.05	113.70	123.22
21	32	516	CL7	CHD-C1D-ND	-3.05	121.03	124.26
23	44	402	8CT	C05-C04-C03	3.05	115.17	110.48
21	4D	402	CL7	CHC-C1C-NC	-3.05	121.65	124.45
21	11	412	CL7	O2D-CGD-CBD	3.05	116.68	111.27
21	23	403	CL7	C2D-C1D-ND	3.05	112.28	110.23
21	4B	603	CL7	O2A-CGA-CBA	3.05	121.47	111.91
23	24	402	8CT	C05-C04-C03	3.05	115.17	110.48
21	31	403	CL7	CHD-C1D-ND	-3.05	121.03	124.26
21	4B	605	CL7	CHD-C4C-C3C	-3.05	120.00	124.94
21	43	410	CL7	C7-C6-C5	-3.05	105.09	113.36
32	14	419	ZEX	C11-C10-C9	-3.05	122.96	127.31
23	3D	406	8CT	C07-C02-C03	-3.05	118.31	122.73
21	44	411	CL7	C3B-C2B-C1B	-3.05	103.48	107.16
21	2B	603	CL7	O2A-CGA-CBA	3.04	121.46	111.91
21	21	414	CL7	CHC-C1C-NC	-3.04	121.66	124.45
23	3C	514	8CT	C25-C24-C23	-3.04	113.72	123.22
21	2B	605	CL7	CHD-C1D-ND	-3.04	121.03	124.26
21	23	415	CL7	CHD-C1D-ND	-3.04	121.03	124.26
21	22	516	CL7	CHD-C4C-C3C	-3.04	120.00	124.94
21	21	412	CL7	O2D-CGD-CBD	3.04	116.68	111.27
21	3B	602	CL7	O2A-CGA-CBA	3.04	121.46	111.91
21	12	504	CL7	CAA-CBA-CGA	-3.04	104.43	112.51
21	31	418	CL7	C7-C6-C5	-3.04	105.09	113.36
21	4B	615	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	31	412	CL7	O2D-CGD-CBD	3.04	116.67	111.27
32	33	522	ZEX	C11-C12-C13	-3.04	117.87	126.42
31	4F	101	HEM	CBA-CAA-C2A	-3.04	104.17	112.63
21	2C	508	CL7	CMB-C2B-C1B	3.04	130.00	125.37
21	32	504	CL7	CAA-CBA-CGA	-3.04	104.43	112.51
31	2F	101	HEM	CBA-CAA-C2A	-3.04	104.18	112.63
23	4C	514	8CT	C25-C24-C23	-3.04	113.72	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	502	CL7	C2D-C1D-ND	3.04	112.27	110.23
32	41	421	ZEX	C11-C10-C9	-3.04	122.97	127.31
21	42	516	CL7	O2D-CGD-CBD	3.04	116.67	111.27
32	11	422	ZEX	C21-C22-C23	-3.04	107.11	113.69
32	23	423	ZEX	C11-C12-C13	-3.04	117.88	126.42
21	13	509	CL7	C7-C6-C5	-3.04	105.10	113.36
31	3F	101	HEM	CBA-CAA-C2A	-3.04	104.18	112.63
21	22	509	CL7	CAA-CBA-CGA	-3.04	104.37	113.25
23	14	402	8CT	C05-C04-C03	3.04	115.16	110.48
23	4C	518	8CT	C11-C10-C03	-3.04	118.67	127.20
21	13	515	CL7	CHC-C1C-NC	-3.04	121.66	124.45
32	14	420	ZEX	C30-C31-C32	-3.04	113.73	123.22
21	12	506	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	2B	604	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	3B	604	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	42	501	CL7	CMB-C2B-C1B	3.04	130.00	125.37
23	3C	518	8CT	C11-C10-C03	-3.04	118.67	127.20
21	11	408	CL7	C2D-C1D-ND	3.04	112.27	110.23
21	3B	608	CL7	CHD-C4C-C3C	-3.04	120.01	124.94
21	1C	508	CL7	CMB-C2B-C1B	3.04	130.00	125.37
31	1F	101	HEM	C4C-NC-C1C	3.04	108.32	105.35
32	41	422	ZEX	C21-C22-C23	-3.04	107.11	113.69
21	2D	402	CL7	C2D-C1D-ND	3.04	112.27	110.23
21	23	411	CL7	CHD-C1D-ND	-3.04	121.04	124.26
21	3D	405	CL7	CHD-C1D-ND	-3.04	121.04	124.26
21	33	510	CL7	CHD-C1D-ND	-3.04	121.04	124.26
21	14	411	CL7	C3B-C2B-C1B	-3.04	103.50	107.16
21	3B	614	CL7	CHD-C4C-C3C	-3.04	120.02	124.94
23	1D	406	8CT	C07-C02-C03	-3.04	118.32	122.73
21	23	410	CL7	C7-C6-C5	-3.04	105.11	113.36
32	21	422	ZEX	C21-C22-C23	-3.04	107.11	113.69
21	41	418	CL7	C7-C6-C5	-3.04	105.11	113.36
21	4C	501	CL7	O2D-CGD-CBD	3.04	116.66	111.27
21	32	509	CL7	CAA-CBA-CGA	-3.04	104.38	113.25
21	42	513	CL7	CMB-C2B-C1B	3.03	129.99	125.37
21	1C	508	CL7	CAA-CBA-CGA	-3.03	104.39	113.25
21	4C	508	CL7	CAA-CBA-CGA	-3.03	104.39	113.25
21	11	412	CL7	CHD-C1D-ND	-3.03	121.05	124.26
21	13	515	CL7	CHD-C1D-ND	-3.03	121.05	124.26
21	41	412	CL7	CHD-C1D-ND	-3.03	121.05	124.26
23	1C	514	8CT	C25-C24-C23	-3.03	113.75	123.22
21	2B	611	CL7	CHC-C1C-NC	-3.03	121.67	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2C	518	8CT	C11-C10-C03	-3.03	118.68	127.20
21	3C	512	CL7	O2D-CGD-CBD	3.03	116.66	111.27
21	11	406	CL7	CHB-C1B-NB	-3.03	121.05	124.26
21	13	501	CL7	CHC-C1C-NC	-3.03	121.67	124.45
21	12	509	CL7	CAA-CBA-CGA	-3.03	104.39	113.25
21	12	501	CL7	CMB-C2B-C1B	3.03	129.99	125.37
32	22	520	ZEX	C30-C31-C32	-3.03	113.75	123.22
22	1D	408	PHO	CMA-C3A-C4A	-3.03	107.74	114.38
21	3D	402	CL7	C2D-C1D-ND	3.03	112.26	110.23
21	22	504	CL7	CAA-CBA-CGA	-3.03	104.46	112.51
21	4C	508	CL7	CMB-C2B-C1B	3.03	129.99	125.37
21	42	504	CL7	CAA-CBA-CGA	-3.03	104.46	112.51
21	3C	508	CL7	CAA-CBA-CGA	-3.03	104.40	113.25
21	2B	616	CL7	CHD-C1D-ND	-3.03	121.05	124.26
21	22	515	CL7	CHD-C1D-ND	-3.03	121.05	124.26
32	42	520	ZEX	C30-C31-C32	-3.03	113.76	123.22
32	22	520	ZEX	C1-C2-C3	-3.03	106.80	113.64
32	32	520	ZEX	C30-C31-C32	-3.03	113.76	123.22
32	31	422	ZEX	C21-C22-C23	-3.03	107.13	113.69
21	13	512	CL7	CHD-C1D-ND	-3.03	121.05	124.26
21	1B	604	CL7	CHD-C4C-C3C	-3.03	120.03	124.94
21	2B	605	CL7	C4-C3-C5	3.03	120.36	115.27
21	13	503	CL7	CHD-C1D-ND	-3.03	121.05	124.26
21	31	402	CL7	CHB-C1B-NB	-3.03	121.05	124.26
21	11	402	CL7	CHB-C1B-NB	-3.03	121.05	124.26
21	21	418	CL7	C7-C6-C5	-3.03	105.14	113.36
22	3D	408	PHO	CMA-C3A-C4A	-3.03	107.75	114.38
21	4B	616	CL7	CHD-C1D-ND	-3.02	121.06	124.26
21	42	515	CL7	CHD-C1D-ND	-3.02	121.06	124.26
21	33	501	CL7	CHC-C1C-NC	-3.02	121.67	124.45
21	1C	507	CL7	CHD-C1D-ND	-3.02	121.06	124.26
21	22	508	CL7	CHD-C4C-C3C	-3.02	120.04	124.94
21	42	509	CL7	CAA-CBA-CGA	-3.02	104.42	113.25
21	23	407	CL7	CHB-C1B-NB	-3.02	121.06	124.26
21	1C	517	CL7	CHD-C4C-C3C	-3.02	120.04	124.94
21	31	406	CL7	CHB-C1B-NB	-3.02	121.06	124.26
32	44	420	ZEX	C10-C11-C12	-3.02	113.79	123.22
21	11	409	CL7	O2D-CGD-CBD	3.02	116.64	111.27
21	33	503	CL7	CHD-C1D-ND	-3.02	121.06	124.26
21	23	402	CL7	CHC-C1C-NC	-3.02	121.68	124.45
21	3B	613	CL7	CAA-CBA-CGA	-3.02	104.43	113.25
32	24	420	ZEX	C10-C11-C12	-3.02	113.79	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	502	CL7	CHB-C1B-NB	-3.02	121.06	124.26
21	44	415	CL7	CHD-C1D-ND	-3.02	121.06	124.26
21	11	418	CL7	C7-C6-C5	-3.02	105.16	113.36
22	2D	408	PHO	CMA-C3A-C4A	-3.02	107.76	114.38
21	3B	603	CL7	CHD-C4C-C3C	-3.02	120.05	124.94
21	3C	508	CL7	CMB-C2B-C1B	3.02	129.97	125.37
21	2D	402	CL7	CHC-C1C-NC	-3.02	121.68	124.45
21	1C	513	CL7	CHD-C4C-C3C	-3.02	120.05	124.94
21	32	505	CL7	C4D-C3D-CAD	-3.02	105.39	107.42
21	3B	604	CL7	C4-C3-C5	3.02	120.35	115.27
21	31	409	CL7	O2D-CGD-CBD	3.02	116.63	111.27
21	12	508	CL7	CHD-C1D-ND	-3.02	121.06	124.26
21	2B	609	CL7	CHD-C4C-C3C	-3.02	120.05	124.94
21	4C	517	CL7	CHD-C4C-C3C	-3.02	120.05	124.94
32	12	520	ZEX	C30-C31-C32	-3.02	113.80	123.22
21	14	408	CL7	CHC-C1C-NC	-3.02	121.68	124.45
21	3B	604	CL7	CHD-C1D-ND	-3.02	121.06	124.26
32	12	520	ZEX	C3-C4-C5	-3.02	105.84	111.85
23	34	402	8CT	C19-C18-C17	-3.02	117.29	123.47
21	22	505	CL7	C4D-C3D-CAD	-3.02	105.39	107.42
21	22	507	CL7	C3B-C2B-C1B	-3.02	103.52	107.16
21	41	412	CL7	O2D-CGD-CBD	3.02	116.63	111.27
21	1B	613	CL7	CAA-CBA-CGA	-3.02	104.44	113.25
21	11	412	CL7	CHC-C1C-NC	-3.02	121.68	124.45
21	41	409	CL7	O2D-CGD-CBD	3.01	116.62	111.27
21	1D	405	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	43	415	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	33	510	CL7	CHC-C1C-NC	-3.01	121.68	124.45
21	44	417	CL7	CHC-C1C-NC	-3.01	121.68	124.45
21	2B	610	CL7	CHD-C4C-C3C	-3.01	120.05	124.94
21	1B	604	CL7	C4-C3-C5	3.01	120.34	115.27
21	1B	601	CL7	CHD-C4C-C3C	-3.01	120.05	124.94
21	42	506	CL7	CHD-C4C-C3C	-3.01	120.05	124.94
21	21	417	CL7	C4C-C3C-C2C	-3.01	103.20	107.13
21	13	514	CL7	CHC-C1C-NC	-3.01	121.69	124.45
21	41	412	CL7	CHC-C1C-NC	-3.01	121.69	124.45
21	43	415	CL7	CHC-C1C-NC	-3.01	121.69	124.45
32	21	422	ZEX	C3-C4-C5	-3.01	105.85	111.85
21	21	409	CL7	O2D-CGD-CBD	3.01	116.62	111.27
21	32	516	CL7	O2D-CGD-CBD	3.01	116.62	111.27
21	3B	609	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
22	4D	408	PHO	CMA-C3A-C4A	-3.01	107.78	114.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	14	420	ZEX	C10-C11-C12	-3.01	113.82	123.22
21	12	517	CL7	O2D-CGD-CBD	3.01	116.62	111.27
21	33	514	CL7	CHC-C1C-NC	-3.01	121.69	124.45
21	24	417	CL7	O2D-CGD-CBD	3.01	116.62	111.27
21	11	414	CL7	CHC-C1C-NC	-3.01	121.69	124.45
21	3D	402	CL7	CHC-C1C-NC	-3.01	121.69	124.45
32	34	420	ZEX	C10-C11-C12	-3.01	113.82	123.22
21	22	508	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	32	508	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	2B	602	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	4B	605	CL7	C4-C3-C5	3.01	120.33	115.27
21	22	506	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	3C	513	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	2C	512	CL7	CHD-C1D-ND	-3.01	121.07	124.26
32	11	422	ZEX	C3-C4-C5	-3.01	105.86	111.85
32	41	422	ZEX	C3-C4-C5	-3.01	105.86	111.85
31	3F	101	HEM	C4C-NC-C1C	3.01	108.30	105.35
21	1B	608	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	2C	509	CL7	CHD-C1D-ND	-3.01	121.07	124.26
21	1B	609	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	32	506	CL7	CHD-C4C-C3C	-3.01	120.06	124.94
21	33	511	CL7	C4C-C3C-C2C	-3.01	103.21	107.13
21	31	408	CL7	C2D-C1D-ND	3.01	112.25	110.23
32	31	421	ZEX	C11-C10-C9	-3.01	123.02	127.31
21	24	408	CL7	CHC-C1C-NC	-3.01	121.69	124.45
21	1C	502	CL7	C4C-C3C-C2C	-3.01	103.21	107.13
21	11	417	CL7	C4C-C3C-C2C	-3.01	103.21	107.13
21	41	417	CL7	C4C-C3C-C2C	-3.01	103.21	107.13
21	42	508	CL7	CHD-C4C-C3C	-3.01	120.07	124.94
21	2D	405	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	23	413	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	31	412	CL7	CHD-C1D-ND	-3.00	121.08	124.26
21	34	408	CL7	CHC-C1C-NC	-3.00	121.69	124.45
21	4D	405	CL7	CHD-C1D-ND	-3.00	121.08	124.26
32	12	520	ZEX	C1-C2-C3	-3.00	106.86	113.64
21	4B	614	CL7	CAA-CBA-CGA	-3.00	104.48	113.25
21	23	412	CL7	C7-C6-C5	-3.00	105.20	113.36
21	42	512	CL7	CHC-C1C-NC	-3.00	121.69	124.45
21	4B	610	CL7	CHD-C4C-C3C	-3.00	120.07	124.94
21	3C	505	CL7	CHB-C1B-NB	-3.00	121.08	124.26
21	22	517	CL7	O2D-CGD-CBD	3.00	116.60	111.27
21	2B	614	CL7	CAA-CBA-CGA	-3.00	104.48	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	42	520	ZEX	C3-C4-C5	-3.00	105.87	111.85
21	31	417	CL7	C4C-C3C-C2C	-3.00	103.21	107.13
21	4B	603	CL7	CAA-C2A-C1A	-3.00	102.31	112.19
32	32	520	ZEX	C1-C2-C3	-3.00	106.86	113.64
21	43	412	CL7	C7-C6-C5	-3.00	105.21	113.36
32	31	422	ZEX	C3-C4-C5	-3.00	105.88	111.85
21	42	505	CL7	C4D-C3D-CAD	-3.00	105.40	107.42
21	31	412	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	43	402	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	32	502	CL7	C7-C6-C5	-3.00	105.21	113.36
23	2B	618	8CT	C01-C02-C07	3.00	119.38	113.62
21	31	415	CL7	CHB-C1B-NB	-3.00	121.08	124.26
21	43	404	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	12	508	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
23	44	402	8CT	C19-C18-C17	-3.00	117.33	123.47
32	21	421	ZEX	C11-C10-C9	-3.00	123.03	127.31
21	21	415	CL7	CHB-C1B-NB	-3.00	121.08	124.26
21	12	514	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
21	32	508	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
21	32	514	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
32	32	520	ZEX	C3-C4-C5	-3.00	105.88	111.85
23	24	402	8CT	C19-C18-C17	-3.00	117.33	123.47
21	13	511	CL7	C7-C6-C5	-3.00	105.22	113.36
21	33	511	CL7	C7-C6-C5	-3.00	105.22	113.36
21	22	514	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
32	11	421	ZEX	C11-C10-C9	-3.00	123.03	127.31
21	42	514	CL7	CHD-C4C-C3C	-3.00	120.08	124.94
21	12	512	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	22	512	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	23	404	CL7	CHB-C1B-NB	-3.00	121.09	124.26
21	4C	507	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	41	413	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	3C	502	CL7	C4C-C3C-C2C	-2.99	103.22	107.13
21	2C	503	CL7	CHC-C1C-NC	-2.99	121.70	124.45
21	44	408	CL7	CHC-C1C-NC	-2.99	121.70	124.45
21	23	404	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	41	415	CL7	CHB-C1B-NB	-2.99	121.09	124.26
23	3B	617	8CT	C01-C02-C07	2.99	119.37	113.62
21	2C	517	CL7	CHD-C4C-C3C	-2.99	120.09	124.94
21	3C	517	CL7	CHD-C4C-C3C	-2.99	120.09	124.94
21	44	417	CL7	O2D-CGD-CBD	2.99	116.58	111.27
21	23	412	CL7	C4C-C3C-C2C	-2.99	103.23	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	413	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	13	518	CL7	CHC-C1C-NC	-2.99	121.70	124.45
23	3B	626	8CT	C07-C02-C03	-2.99	118.39	122.73
21	31	408	CL7	C3B-C2B-C1B	-2.99	103.55	107.16
32	22	520	ZEX	C3-C4-C5	-2.99	105.90	111.85
32	42	520	ZEX	C1-C2-C3	-2.99	106.89	113.64
21	3B	602	CL7	CAA-C2A-C1A	-2.99	102.35	112.19
21	13	506	CL7	CHB-C1B-NB	-2.99	121.09	124.26
23	14	402	8CT	C19-C18-C17	-2.99	117.35	123.47
21	1B	602	CL7	CAA-C2A-C1A	-2.99	102.35	112.19
21	31	419	CL7	CHC-C1C-NC	-2.99	121.71	124.45
21	3B	601	CL7	CHD-C4C-C3C	-2.99	120.09	124.94
23	1B	626	8CT	C07-C02-C03	-2.99	118.39	122.73
21	33	514	CL7	CHD-C1D-ND	-2.99	121.09	124.26
32	33	522	ZEX	C7-C8-C9	-2.99	121.72	126.23
21	1B	615	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	43	404	CL7	CHD-C1D-ND	-2.99	121.09	124.26
21	11	419	CL7	CHC-C1C-NC	-2.99	121.71	124.45
21	33	512	CL7	CHC-C1C-NC	-2.99	121.71	124.45
32	13	522	ZEX	C7-C8-C9	-2.99	121.72	126.23
21	3B	603	CL7	CHC-C1C-NC	-2.99	121.71	124.45
21	43	407	CL7	CHB-C1B-NB	-2.99	121.09	124.26
21	32	517	CL7	O2D-CGD-CBD	2.99	116.58	111.27
21	4B	602	CL7	CHD-C4C-C3C	-2.99	120.10	124.94
21	14	417	CL7	O2D-CGD-CBD	2.99	116.57	111.27
21	43	413	CL7	CHD-C1D-ND	-2.99	121.10	124.26
32	43	423	ZEX	C7-C8-C9	-2.99	121.72	126.23
21	2B	603	CL7	CAA-C2A-C1A	-2.99	102.37	112.19
21	34	414	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	22	502	CL7	C7-C6-C5	-2.98	105.25	113.36
21	23	406	CL7	C4D-C3D-CAD	-2.98	105.41	107.42
21	1B	603	CL7	CHD-C4C-C3C	-2.98	120.11	124.94
21	21	409	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	3A	401	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	41	408	CL7	C3B-C2B-C1B	-2.98	103.56	107.16
32	41	421	ZEX	C27-C26-C25	-2.98	118.02	122.84
21	11	415	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	13	513	CL7	CHD-C1D-ND	-2.98	121.10	124.26
21	4C	505	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	42	502	CL7	C7-C6-C5	-2.98	105.27	113.36
21	13	512	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	21	402	CL7	CHB-C1B-NB	-2.98	121.10	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	24	414	CL7	CHB-C1B-NB	-2.98	121.10	124.26
21	21	412	CL7	CHD-C1D-ND	-2.98	121.11	124.26
21	12	502	CL7	C7-C6-C5	-2.98	105.27	113.36
21	21	416	CL7	CHD-C4C-C3C	-2.98	120.11	124.94
21	13	511	CL7	C4C-C3C-C2C	-2.98	103.25	107.13
21	43	412	CL7	C4C-C3C-C2C	-2.98	103.25	107.13
21	1C	512	CL7	CHD-C1D-ND	-2.98	121.11	124.26
21	31	409	CL7	CHD-C1D-ND	-2.98	121.11	124.26
21	4C	512	CL7	CHD-C1D-ND	-2.98	121.11	124.26
21	21	410	CL7	CHD-C4C-C3C	-2.98	120.12	124.94
21	4B	604	CL7	CHD-C4C-C3C	-2.98	120.12	124.94
21	12	505	CL7	C4D-C3D-CAD	-2.98	105.42	107.42
21	42	502	CL7	O2D-CGD-CBD	2.97	116.55	111.27
21	12	502	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	11	413	CL7	CHD-C1D-ND	-2.97	121.11	124.26
21	42	502	CL7	CHB-C1B-NB	-2.97	121.11	124.26
21	41	410	CL7	CHD-C4C-C3C	-2.97	120.12	124.94
21	41	409	CL7	CHD-C1D-ND	-2.97	121.11	124.26
32	11	421	ZEX	C27-C26-C25	-2.97	118.03	122.84
21	32	507	CL7	C2D-C1D-ND	2.97	112.22	110.23
23	4B	618	8CT	C01-C02-C07	2.97	119.33	113.62
32	21	421	ZEX	C27-C26-C25	-2.97	118.04	122.84
32	31	421	ZEX	C27-C26-C25	-2.97	118.04	122.84
21	34	417	CL7	O2D-CGD-CBD	2.97	116.55	111.27
21	43	413	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	43	418	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	12	515	CL7	CHD-C1D-ND	-2.97	121.11	124.26
21	41	402	CL7	CHB-C1B-NB	-2.97	121.11	124.26
32	31	421	ZEX	C39-C29-C30	-2.97	118.76	122.92
23	1B	617	8CT	C01-C02-C07	2.97	119.32	113.62
21	1C	503	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	21	412	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	31	414	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	1A	401	CL7	CHD-C1D-ND	-2.97	121.11	124.26
21	32	515	CL7	CHD-C1D-ND	-2.97	121.11	124.26
21	3B	604	CL7	CMB-C2B-C1B	2.97	129.89	125.37
21	43	417	CL7	CHD-C4C-C3C	-2.97	120.12	124.94
21	3A	401	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	22	502	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	1D	402	CL7	CHC-C1C-NC	-2.97	121.73	124.45
23	1C	515	8CT	C40-C12-C13	-2.97	118.77	122.92
21	2C	505	CL7	CHB-C1B-NB	-2.97	121.12	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	502	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	34	404	CL7	CHD-C4C-C3C	-2.97	120.13	124.94
21	11	410	CL7	C7-C6-C5	-2.97	105.30	113.36
21	33	505	CL7	C4D-C3D-CAD	-2.97	105.42	107.42
21	1A	401	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	42	517	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	11	410	CL7	CHD-C4C-C3C	-2.97	120.13	124.94
21	4B	616	CL7	CHD-C4C-C3C	-2.97	120.13	124.94
21	23	405	CL7	O2D-CGD-CBD	2.97	116.54	111.27
21	1C	508	CL7	O2A-CGA-CBA	2.96	121.21	111.91
21	4C	502	CL7	C4C-C3C-C2C	-2.96	103.26	107.13
21	22	507	CL7	C2D-C1D-ND	2.96	112.22	110.23
32	23	423	ZEX	C7-C8-C9	-2.96	121.76	126.23
21	31	410	CL7	C7-C6-C5	-2.96	105.31	113.36
21	11	409	CL7	CHD-C1D-ND	-2.96	121.12	124.26
21	2A	401	CL7	CHD-C1D-ND	-2.96	121.12	124.26
21	24	406	CL7	CAA-CBA-CGA	-2.96	104.59	113.25
21	32	512	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	13	517	CL7	C3B-C2B-C1B	-2.96	103.59	107.16
21	3C	508	CL7	O2A-CGA-CBA	2.96	121.20	111.91
21	4B	612	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	22	505	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	32	510	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	24	404	CL7	CHD-C4C-C3C	-2.96	120.14	124.94
21	33	516	CL7	CHD-C4C-C3C	-2.96	120.14	124.94
21	43	411	CL7	CHC-C1C-NC	-2.96	121.73	124.45
23	2C	515	8CT	C40-C12-C13	-2.96	118.78	122.92
21	14	411	CL7	O2D-CGD-CBD	2.96	116.53	111.27
21	22	501	CL7	O2D-CGD-CBD	2.96	116.53	111.27
23	2B	601	8CT	C07-C02-C03	-2.96	118.44	122.73
21	12	510	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	21	417	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	4B	604	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	42	510	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	14	414	CL7	CHB-C1B-NB	-2.96	121.13	124.26
21	4C	508	CL7	O2A-CGA-CBA	2.96	121.19	111.91
21	12	502	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	3A	403	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	42	501	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	31	413	CL7	CHD-C1D-ND	-2.96	121.13	124.26
21	22	511	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	3B	611	CL7	CHC-C1C-NC	-2.96	121.74	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	419	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	33	517	CL7	C3B-C2B-C1B	-2.96	103.59	107.16
23	4B	601	8CT	C07-C02-C03	-2.96	118.44	122.73
21	31	410	CL7	CHD-C4C-C3C	-2.96	120.15	124.94
21	2C	502	CL7	C4C-C3C-C2C	-2.96	103.27	107.13
21	41	410	CL7	C7-C6-C5	-2.95	105.33	113.36
21	34	406	CL7	CAA-CBA-CGA	-2.95	104.62	113.25
21	21	410	CL7	C7-C6-C5	-2.95	105.34	113.36
21	1B	615	CL7	CHD-C4C-C3C	-2.95	120.15	124.94
21	12	505	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	4C	503	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	4B	610	CL7	O2D-CGD-CBD	2.95	116.51	111.27
21	34	406	CL7	CHC-C1C-NC	-2.95	121.74	124.45
32	11	421	ZEX	C18-C5-C6	-2.95	121.22	124.53
23	3C	515	8CT	C40-C12-C13	-2.95	118.79	122.92
21	44	411	CL7	O2D-CGD-CBD	2.95	116.51	111.27
21	14	404	CL7	CHD-C4C-C3C	-2.95	120.16	124.94
21	43	404	CL7	CHB-C1B-NB	-2.95	121.14	124.26
21	3C	503	CL7	CHC-C1C-NC	-2.95	121.75	124.45
31	2F	101	HEM	C4C-NC-C1C	2.95	108.23	105.35
21	23	411	CL7	CHC-C1C-NC	-2.95	121.75	124.45
21	3B	622	CL7	CHC-C1C-NC	-2.95	121.75	124.45
21	32	505	CL7	CHC-C1C-NC	-2.95	121.75	124.45
21	2A	401	CL7	O2D-CGD-CBD	2.95	116.50	111.27
31	4F	101	HEM	C4C-NC-C1C	2.95	108.23	105.35
21	41	416	CL7	CHD-C4C-C3C	-2.95	120.16	124.94
21	44	406	CL7	CAA-CBA-CGA	-2.94	104.65	113.25
21	23	415	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	14	406	CL7	CAA-CBA-CGA	-2.94	104.65	113.25
21	4A	401	CL7	CHD-C1D-ND	-2.94	121.14	124.26
21	2B	610	CL7	O2D-CGD-CBD	2.94	116.50	111.27
21	33	507	CL7	C7-C6-C5	-2.94	105.37	113.36
21	14	405	CL7	O2D-CGD-CBD	2.94	116.50	111.27
21	23	418	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	23	419	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	33	518	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	44	406	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	1B	607	CL7	O2D-CGD-CBD	2.94	116.50	111.27
21	24	411	CL7	O2D-CGD-CBD	2.94	116.50	111.27
21	1C	505	CL7	CHB-C1B-NB	-2.94	121.14	124.26
21	33	513	CL7	CHD-C1D-ND	-2.94	121.14	124.26
21	2B	604	CL7	CHC-C1C-NC	-2.94	121.75	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	417	CL7	CHD-C4C-C3C	-2.94	120.17	124.94
21	22	501	CL7	CHB-C1B-NB	-2.94	121.14	124.26
21	23	414	CL7	CHD-C1D-ND	-2.94	121.14	124.26
21	32	501	CL7	CHB-C1B-NB	-2.94	121.14	124.26
21	44	414	CL7	CHB-C1B-NB	-2.94	121.14	124.26
21	41	407	CL7	O2D-CGD-CBD	2.94	116.49	111.27
21	22	510	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	4B	608	CL7	CHC-C1C-NC	-2.94	121.75	124.45
32	32	524	ZEX	C1-C6-C5	-2.94	118.47	122.61
21	43	408	CL7	C7-C6-C5	-2.94	105.38	113.36
21	22	502	CL7	CHB-C1B-NB	-2.94	121.15	124.26
21	2C	508	CL7	O2A-CGA-CBA	2.94	121.13	111.91
21	11	416	CL7	CHD-C4C-C3C	-2.94	120.18	124.94
21	31	419	CL7	CHB-C1B-NB	-2.94	121.15	124.26
21	24	405	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	31	417	CL7	CHC-C1C-NC	-2.94	121.75	124.45
23	4C	515	8CT	C40-C12-C13	-2.94	118.81	122.92
21	1B	604	CL7	CMB-C2B-C1B	2.94	129.84	125.37
21	2B	612	CL7	CHC-C1C-NC	-2.94	121.76	124.45
21	13	507	CL7	C7-C6-C5	-2.94	105.39	113.36
21	34	411	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	32	501	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	23	405	CL7	C7-C6-C5	-2.93	105.39	113.36
21	44	405	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	12	501	CL7	CHB-C1B-NB	-2.93	121.15	124.26
21	33	506	CL7	CHB-C1B-NB	-2.93	121.15	124.26
21	42	501	CL7	CHB-C1B-NB	-2.93	121.15	124.26
21	23	408	CL7	C7-C6-C5	-2.93	105.39	113.36
21	1C	508	CL7	C1-C2-C3	2.93	131.12	126.04
21	23	418	CL7	C3B-C2B-C1B	-2.93	103.62	107.16
21	42	507	CL7	C2D-C1D-ND	2.93	112.20	110.23
21	2B	623	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	23	413	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	1B	609	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	3B	609	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	2B	605	CL7	CMB-C2B-C1B	2.93	129.84	125.37
21	42	512	CL7	CHD-C1D-ND	-2.93	121.15	124.26
21	2B	616	CL7	CHD-C4C-C3C	-2.93	120.19	124.94
32	12	520	ZEX	C2-C3-C4	-2.93	106.29	110.30
32	42	520	ZEX	C2-C3-C4	-2.93	106.29	110.30
21	1B	603	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	14	412	CL7	C7-C6-C5	-2.93	105.40	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4A	401	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	31	416	CL7	CHD-C4C-C3C	-2.93	120.19	124.94
21	11	408	CL7	C3B-C2B-C1B	-2.93	103.62	107.16
21	44	404	CL7	CHD-C4C-C3C	-2.93	120.19	124.94
21	13	504	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	43	405	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	4B	623	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	13	503	CL7	CHB-C1B-NB	-2.93	121.16	124.26
21	3C	503	CL7	CHB-C1B-NB	-2.93	121.16	124.26
21	32	504	CL7	CMB-C2B-C1B	2.93	129.83	125.37
21	3B	615	CL7	CHD-C4C-C3C	-2.93	120.19	124.94
21	2C	505	CL7	CHD-C4C-C3C	-2.93	120.19	124.94
21	34	417	CL7	CHD-C1D-ND	-2.93	121.16	124.26
21	43	414	CL7	CHD-C1D-ND	-2.93	121.16	124.26
21	33	504	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	32	512	CL7	CHD-C1D-ND	-2.93	121.16	124.26
21	44	417	CL7	CHD-C1D-ND	-2.93	121.16	124.26
21	1A	403	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	2A	403	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	4A	403	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	44	412	CL7	C7-C6-C5	-2.93	105.42	113.36
21	13	513	CL7	CHC-C1C-NC	-2.92	121.77	124.45
32	22	522	ZEX	C18-C5-C4	2.92	119.77	114.36
21	4C	506	CL7	CMB-C2B-C1B	2.92	129.82	125.37
32	22	520	ZEX	C2-C3-C4	-2.92	106.30	110.30
21	1B	614	CL7	C3B-C2B-C1B	-2.92	103.63	107.16
21	4B	615	CL7	C3B-C2B-C1B	-2.92	103.63	107.16
21	31	407	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	13	516	CL7	CHD-C4C-C3C	-2.92	120.20	124.94
21	21	419	CL7	CHB-C1B-NB	-2.92	121.16	124.26
32	42	522	ZEX	C18-C5-C4	2.92	119.77	114.36
21	12	501	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	21	410	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	4B	605	CL7	CMB-C2B-C1B	2.92	129.82	125.37
32	21	421	ZEX	C18-C5-C6	-2.92	121.25	124.53
32	31	421	ZEX	C18-C5-C6	-2.92	121.25	124.53
21	43	405	CL7	C7-C6-C5	-2.92	105.43	113.36
21	1B	607	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	33	517	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	13	504	CL7	C7-C6-C5	-2.92	105.43	113.36
32	21	421	ZEX	C39-C29-C30	-2.92	118.83	122.92
21	1B	611	CL7	CHC-C1C-NC	-2.92	121.77	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	517	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	41	417	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	14	417	CL7	CHD-C1D-ND	-2.92	121.17	124.26
21	4C	513	CL7	CHB-C1B-NB	-2.92	121.17	124.26
21	24	406	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	24	412	CL7	C7-C6-C5	-2.92	105.43	113.36
21	11	407	CL7	O2D-CGD-CBD	2.92	116.45	111.27
21	34	405	CL7	O2D-CGD-CBD	2.92	116.45	111.27
21	24	405	CL7	O2D-CGD-CBD	2.92	116.45	111.27
21	22	504	CL7	CMB-C2B-C1B	2.92	129.81	125.37
23	1B	618	8CT	C25-C24-C23	-2.92	114.12	123.22
21	3B	616	CL7	O2D-CGD-CBD	2.92	116.45	111.27
32	22	524	ZEX	C1-C6-C5	-2.92	118.51	122.61
21	41	420	CL7	CHD-C1D-ND	-2.92	121.17	124.26
21	42	504	CL7	CMB-C2B-C1B	2.92	129.81	125.37
21	21	408	CL7	C3B-C2B-C1B	-2.91	103.64	107.16
21	43	418	CL7	C3B-C2B-C1B	-2.91	103.64	107.16
21	33	504	CL7	C7-C6-C5	-2.91	105.44	113.36
21	24	409	CL7	CHD-C1D-ND	-2.91	121.17	124.26
21	41	419	CL7	CHB-C1B-NB	-2.91	121.17	124.26
21	2B	608	CL7	O2D-CGD-CBD	2.91	116.44	111.27
21	2C	510	CL7	C7-C6-C5	-2.91	105.45	113.36
21	1B	614	CL7	CHD-C1D-ND	-2.91	121.17	124.26
21	22	505	CL7	CHD-C1D-ND	-2.91	121.17	124.26
21	34	409	CL7	CHD-C1D-ND	-2.91	121.17	124.26
21	12	511	CL7	CHC-C1C-NC	-2.91	121.78	124.45
23	2B	620	8CT	C19-C18-C17	-2.91	117.51	123.47
21	31	420	CL7	CHD-C1D-ND	-2.91	121.17	124.26
21	14	405	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	23	410	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	44	405	CL7	CHC-C1C-NC	-2.91	121.78	124.45
32	42	524	ZEX	C1-C6-C5	-2.91	118.51	122.61
21	34	412	CL7	C7-C6-C5	-2.91	105.45	113.36
21	12	505	CL7	CHD-C1D-ND	-2.91	121.17	124.26
32	32	520	ZEX	C2-C3-C4	-2.91	106.32	110.30
23	4B	620	8CT	C19-C18-C17	-2.91	117.51	123.47
31	4F	101	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
21	1B	616	CL7	O2D-CGD-CBD	2.91	116.44	111.27
21	4B	617	CL7	O2D-CGD-CBD	2.91	116.44	111.27
23	3B	618	8CT	C25-C24-C23	-2.91	114.13	123.22
21	13	510	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	2B	608	CL7	CHC-C1C-NC	-2.91	121.78	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	607	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	22	512	CL7	CHD-C1D-ND	-2.91	121.18	124.26
21	41	410	CL7	O2D-CGD-CBD	2.91	116.44	111.27
21	14	406	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	44	413	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	3C	505	CL7	CHD-C4C-C3C	-2.91	120.22	124.94
21	4C	503	CL7	CHB-C1B-NB	-2.91	121.18	124.26
21	21	407	CL7	O2D-CGD-CBD	2.91	116.44	111.27
32	12	522	ZEX	C18-C5-C4	2.91	119.74	114.36
21	32	517	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	21	420	CL7	CHD-C1D-ND	-2.91	121.18	124.26
31	2F	101	HEM	CHD-C1D-C2D	-2.91	120.44	124.98
23	4B	619	8CT	C25-C24-C23	-2.91	114.15	123.22
27	2B	625	DGD	O1G-C1A-C2A	2.91	121.03	111.91
32	41	421	ZEX	C39-C29-C30	-2.91	118.85	122.92
21	21	419	CL7	O2D-CGD-CBD	2.90	116.43	111.27
21	1B	622	CL7	CHC-C1C-NC	-2.90	121.78	124.45
21	3B	607	CL7	O2D-CGD-CBD	2.90	116.43	111.27
21	4B	608	CL7	O2D-CGD-CBD	2.90	116.43	111.27
21	2B	612	CL7	CHD-C4C-C3C	-2.90	120.23	124.94
31	1F	101	HEM	CHD-C1D-C2D	-2.90	120.44	124.98
21	23	414	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	33	513	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	2C	508	CL7	C1-C2-C3	2.90	131.06	126.04
21	3C	508	CL7	C1-C2-C3	2.90	131.06	126.04
21	1C	503	CL7	CHB-C1B-NB	-2.90	121.18	124.26
21	2C	513	CL7	CHB-C1B-NB	-2.90	121.19	124.26
21	41	418	CL7	CHD-C1D-ND	-2.90	121.19	124.26
21	2C	506	CL7	CMB-C2B-C1B	2.90	129.79	125.37
21	14	416	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	34	405	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	14	409	CL7	CHD-C1D-ND	-2.90	121.19	124.26
21	44	409	CL7	CHD-C1D-ND	-2.90	121.19	124.26
21	2B	616	CL7	CAA-CBA-CGA	-2.90	104.78	113.25
23	2B	619	8CT	C25-C24-C23	-2.90	114.17	123.22
21	11	419	CL7	O2D-CGD-CBD	2.90	116.42	111.27
21	41	419	CL7	O2D-CGD-CBD	2.90	116.42	111.27
21	12	504	CL7	CMB-C2B-C1B	2.90	129.78	125.37
21	3C	510	CL7	C7-C6-C5	-2.90	105.49	113.36
23	1B	619	8CT	C19-C18-C17	-2.90	117.54	123.47
21	11	410	CL7	O2D-CGD-CBD	2.90	116.42	111.27
21	3B	615	CL7	CAA-CBA-CGA	-2.90	104.78	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	515	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	1B	606	CL7	C3B-C2B-C1B	-2.90	103.66	107.16
21	4B	607	CL7	C3B-C2B-C1B	-2.90	103.66	107.16
21	1B	615	CL7	CAA-CBA-CGA	-2.90	104.79	113.25
21	3B	608	CL7	C3B-C2B-C1B	-2.90	103.67	107.16
21	43	408	CL7	CMB-C2B-C1B	2.90	129.78	125.37
32	32	522	ZEX	C18-C5-C4	2.90	119.72	114.36
21	4B	616	CL7	CAA-CBA-CGA	-2.90	104.79	113.25
27	1B	624	DGD	O1G-C1A-C2A	2.90	121.00	111.91
21	31	418	CL7	CHD-C1D-ND	-2.90	121.19	124.26
21	2B	617	CL7	O2D-CGD-CBD	2.89	116.41	111.27
21	1C	510	CL7	C7-C6-C5	-2.89	105.50	113.36
21	4C	510	CL7	C7-C6-C5	-2.89	105.50	113.36
21	42	505	CL7	CHC-C1C-NC	-2.89	121.79	124.45
21	21	406	CL7	O2D-CGD-CBD	2.89	116.41	111.27
21	11	417	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	12	512	CL7	CHD-C1D-ND	-2.89	121.19	124.26
21	13	508	CL7	CHD-C4C-C3C	-2.89	120.25	124.94
21	2B	615	CL7	C3B-C2B-C1B	-2.89	103.67	107.16
21	3B	614	CL7	C3B-C2B-C1B	-2.89	103.67	107.16
21	33	503	CL7	CHB-C1B-NB	-2.89	121.19	124.26
21	23	406	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	22	517	CL7	CMB-C2B-C1B	2.89	129.77	125.37
21	3C	513	CL7	CHB-C1B-NB	-2.89	121.20	124.26
21	41	407	CL7	CHC-C1C-NC	-2.89	121.80	124.45
27	4B	625	DGD	O1G-C1A-C2A	2.89	120.98	111.91
21	2C	503	CL7	CHB-C1B-NB	-2.89	121.20	124.26
21	22	510	CL7	O2D-CGD-CBD	2.89	116.40	111.27
21	34	413	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	2B	609	CL7	C3B-C2B-C1B	-2.89	103.67	107.16
21	1C	513	CL7	CMB-C2B-C1B	2.89	129.77	125.37
27	3B	624	DGD	O1G-C1A-C2A	2.89	120.97	111.91
21	24	409	CL7	CHD-C4C-C3C	-2.89	120.26	124.94
21	11	419	CL7	CHB-C1B-NB	-2.89	121.20	124.26
21	14	415	CL7	CHB-C1B-NB	-2.89	121.20	124.26
21	12	513	CL7	C3B-C2B-C1B	-2.89	103.67	107.16
21	14	413	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	42	512	CL7	CHB-C1B-NB	-2.89	121.20	124.26
21	4B	609	CL7	C3B-C2B-C1B	-2.89	103.68	107.16
32	41	421	ZEX	C18-C5-C6	-2.89	121.29	124.53
21	13	509	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	32	511	CL7	CHC-C1C-NC	-2.89	121.80	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	410	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	24	417	CL7	CHD-C1D-ND	-2.89	121.20	124.26
21	32	517	CL7	CMB-C2B-C1B	2.89	129.76	125.37
31	3F	101	HEM	CHD-C1D-C2D	-2.88	120.47	124.98
21	23	412	CL7	O2A-CGA-O1A	-2.88	116.31	123.59
21	1C	513	CL7	CHB-C1B-NB	-2.88	121.20	124.26
23	3B	619	8CT	C19-C18-C17	-2.88	117.56	123.47
32	14	403	ZEX	C15-C35-C34	-2.88	117.56	123.47
21	1C	506	CL7	CMB-C2B-C1B	2.88	129.76	125.37
21	12	507	CL7	C2D-C1D-ND	2.88	112.17	110.23
21	13	507	CL7	CMB-C2B-C1B	2.88	129.76	125.37
21	12	515	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	12	517	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	13	505	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	43	406	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	1B	608	CL7	C3B-C2B-C1B	-2.88	103.68	107.16
21	2B	607	CL7	C3B-C2B-C1B	-2.88	103.68	107.16
21	3B	614	CL7	CHD-C1D-ND	-2.88	121.21	124.26
32	11	421	ZEX	C39-C29-C30	-2.88	118.89	122.92
21	12	510	CL7	O2D-CGD-CBD	2.88	116.39	111.27
21	23	409	CL7	O2D-CGD-CBD	2.88	116.39	111.27
21	33	507	CL7	CMB-C2B-C1B	2.88	129.76	125.37
21	24	414	CL7	CMB-C2B-C1B	2.88	129.76	125.37
21	1C	505	CL7	CHD-C4C-C3C	-2.88	120.27	124.94
21	31	410	CL7	O2D-CGD-CBD	2.88	116.39	111.27
23	2D	406	8CT	C22-C21-C20	-2.88	118.89	122.92
21	12	504	CL7	C2D-C1D-ND	2.88	112.16	110.23
21	1A	403	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	42	511	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	44	408	CL7	CAA-CBA-CGA	-2.88	104.86	112.51
32	12	524	ZEX	C1-C6-C5	-2.88	118.56	122.61
21	43	414	CL7	CHC-C1C-NC	-2.88	121.81	124.45
32	13	520	ZEX	C19-C9-C10	-2.88	118.89	122.92
21	23	409	CL7	CHD-C4C-C3C	-2.88	120.27	124.94
21	22	517	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	12	517	CL7	CMB-C2B-C1B	2.88	129.75	125.37
21	14	416	CL7	CMA-C3A-C2A	-2.88	109.38	116.10
21	3C	506	CL7	CMB-C2B-C1B	2.88	129.75	125.37
21	14	409	CL7	CHD-C4C-C3C	-2.88	120.28	124.94
21	44	409	CL7	CHD-C4C-C3C	-2.88	120.28	124.94
21	11	409	CL7	CHD-C4C-C3C	-2.88	120.28	124.94
21	32	505	CL7	CHD-C1D-ND	-2.88	121.21	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	419	CL7	O2D-CGD-CBD	2.88	116.38	111.27
21	33	512	CL7	C7-C6-C5	-2.88	105.55	113.36
21	11	407	CL7	CHC-C1C-NC	-2.88	121.81	124.45
32	33	520	ZEX	C19-C9-C10	-2.88	118.89	122.92
21	12	507	CL7	CHC-C1C-NC	-2.87	121.81	124.45
21	4C	508	CL7	C1-C2-C3	2.87	131.01	126.04
21	3B	611	CL7	CHD-C4C-C3C	-2.87	120.28	124.94
32	24	419	ZEX	C27-C26-C25	-2.87	118.19	122.84
21	42	505	CL7	CHD-C1D-ND	-2.87	121.21	124.26
23	2B	618	8CT	C35-C30-C29	-2.87	109.07	112.70
21	32	516	CL7	CHC-C1C-NC	-2.87	121.81	124.45
21	3B	606	CL7	C3B-C2B-C1B	-2.87	103.69	107.16
21	2C	513	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	3C	513	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	11	420	CL7	CHD-C1D-ND	-2.87	121.22	124.26
21	21	409	CL7	CHD-C4C-C3C	-2.87	120.28	124.94
21	31	409	CL7	CHD-C4C-C3C	-2.87	120.28	124.94
21	2C	511	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	3C	511	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	4B	604	CL7	CHB-C1B-NB	-2.87	121.22	124.26
21	13	511	CL7	O2A-CGA-O1A	-2.87	116.34	123.59
32	34	403	ZEX	C15-C35-C34	-2.87	117.59	123.47
21	4C	505	CL7	CHD-C4C-C3C	-2.87	120.28	124.94
23	1B	617	8CT	C35-C30-C29	-2.87	109.07	112.70
23	4B	618	8CT	C35-C30-C29	-2.87	109.07	112.70
21	23	413	CL7	C7-C6-C5	-2.87	105.56	113.36
21	22	512	CL7	CHB-C1B-NB	-2.87	121.22	124.26
21	33	508	CL7	CHD-C4C-C3C	-2.87	120.29	124.94
21	4B	612	CL7	CHD-C4C-C3C	-2.87	120.29	124.94
21	23	408	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	11	418	CL7	CHD-C1D-ND	-2.87	121.22	124.26
21	4B	615	CL7	CHD-C1D-ND	-2.87	121.22	124.26
21	14	414	CL7	CMB-C2B-C1B	2.87	129.74	125.37
21	3A	403	CL7	CHC-C1C-NC	-2.87	121.82	124.45
21	34	409	CL7	CHD-C4C-C3C	-2.87	120.29	124.94
32	44	403	ZEX	C15-C35-C34	-2.87	117.60	123.47
23	3D	406	8CT	C22-C21-C20	-2.87	118.91	122.92
21	2B	615	CL7	CHD-C1D-ND	-2.87	121.22	124.26
21	14	408	CL7	CAA-CBA-CGA	-2.87	104.90	112.51
32	44	419	ZEX	C27-C26-C25	-2.87	118.21	122.84
21	44	417	CL7	CHB-C1B-NB	-2.87	121.22	124.26
21	31	406	CL7	O2D-CGD-CBD	2.87	116.36	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	510	CL7	O2D-CGD-CBD	2.87	116.36	111.27
21	42	517	CL7	CHC-C1C-NC	-2.87	121.82	124.45
21	1B	614	CL7	O2D-CGD-CBD	2.86	116.36	111.27
21	13	516	CL7	C3B-C2B-C1B	-2.86	103.70	107.16
21	3C	501	CL7	CHD-C1D-ND	-2.86	121.22	124.26
21	12	503	CL7	C7-C6-C5	-2.86	105.58	113.36
21	1B	611	CL7	CHD-C4C-C3C	-2.86	120.30	124.94
21	43	412	CL7	O2A-CGA-O1A	-2.86	116.37	123.59
21	21	407	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	4A	403	CL7	CHC-C1C-NC	-2.86	121.82	124.45
32	14	420	ZEX	C1-C6-C5	-2.86	118.58	122.61
21	34	408	CL7	CAA-CBA-CGA	-2.86	104.91	112.51
21	24	416	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	34	416	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	42	510	CL7	CHD-C1D-ND	-2.86	121.23	124.26
21	24	408	CL7	CAA-CBA-CGA	-2.86	104.92	112.51
21	13	508	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	33	511	CL7	O2A-CGA-O1A	-2.86	116.37	123.59
21	22	503	CL7	C7-C6-C5	-2.86	105.59	113.36
21	12	509	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	24	416	CL7	CMA-C3A-C2A	-2.86	109.43	116.10
21	34	416	CL7	CMA-C3A-C2A	-2.86	109.43	116.10
21	4C	511	CL7	CMB-C2B-C1B	2.86	129.72	125.37
21	24	417	CL7	CHB-C1B-NB	-2.86	121.23	124.26
21	4C	513	CL7	CMB-C2B-C1B	2.86	129.72	125.37
21	3C	505	CL7	C2D-C1D-ND	2.86	112.15	110.23
21	2A	403	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	22	507	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	32	507	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	32	515	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	44	416	CL7	CMA-C3A-C2A	-2.86	109.43	116.10
21	32	503	CL7	C7-C6-C5	-2.86	105.60	113.36
21	33	507	CL7	C3B-C2B-C1B	-2.86	103.71	107.16
21	11	406	CL7	O2D-CGD-CBD	2.86	116.34	111.27
21	41	406	CL7	O2D-CGD-CBD	2.86	116.34	111.27
21	41	420	CL7	CHB-C1B-NB	-2.86	121.23	124.26
21	44	417	CL7	C4C-C3C-C2C	-2.86	103.41	107.13
21	32	502	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	43	417	CL7	C3B-C2B-C1B	-2.86	103.72	107.16
23	4C	515	8CT	C30-C31-C32	-2.85	117.95	121.47
27	1B	624	DGD	C2G-O2G-C1B	-2.85	110.76	117.79
27	3B	624	DGD	C2G-O2G-C1B	-2.85	110.76	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	406	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
32	14	419	ZEX	C27-C26-C25	-2.85	118.23	122.84
21	3B	614	CL7	O2D-CGD-CBD	2.85	116.34	111.27
21	12	512	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	13	512	CL7	C7-C6-C5	-2.85	105.61	113.36
21	43	413	CL7	C7-C6-C5	-2.85	105.61	113.36
21	4B	602	CL7	CHC-C1C-NC	-2.85	121.83	124.45
21	32	509	CL7	O2D-CGD-CBD	2.85	116.34	111.27
21	43	409	CL7	CHD-C4C-C3C	-2.85	120.32	124.94
21	3B	603	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	13	507	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
21	43	408	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
21	42	507	CL7	CHC-C1C-NC	-2.85	121.83	124.45
21	42	517	CL7	CMB-C2B-C1B	2.85	129.71	125.37
21	1B	603	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	33	511	CL7	CHD-C1D-ND	-2.85	121.24	124.26
21	44	415	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	1C	511	CL7	CMB-C2B-C1B	2.85	129.71	125.37
23	1D	406	8CT	C22-C21-C20	-2.85	118.93	122.92
23	4D	406	8CT	C22-C21-C20	-2.85	118.93	122.92
21	42	503	CL7	C7-C6-C5	-2.85	105.62	113.36
32	24	403	ZEX	C15-C35-C34	-2.85	117.64	123.47
32	44	420	ZEX	C1-C6-C5	-2.85	118.60	122.61
21	33	508	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	32	504	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	11	404	CL7	C7-C6-C5	-2.85	105.62	113.36
21	41	404	CL7	C7-C6-C5	-2.85	105.62	113.36
21	4B	603	CL7	CHC-C1C-NC	-2.85	121.84	124.45
21	41	409	CL7	CHD-C4C-C3C	-2.85	120.32	124.94
21	23	417	CL7	C3B-C2B-C1B	-2.85	103.72	107.16
21	24	417	CL7	C4C-C3C-C2C	-2.85	103.41	107.13
21	32	510	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	34	405	CL7	CHB-C1B-NB	-2.85	121.24	124.26
32	14	420	ZEX	C35-C15-C14	-2.85	117.64	123.47
21	41	405	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	31	404	CL7	C7-C6-C5	-2.85	105.63	113.36
21	21	405	CL7	O2D-CGD-CBD	2.85	116.33	111.27
27	4B	625	DGD	C2G-O2G-C1B	-2.85	110.78	117.79
21	1C	504	CL7	CHB-C1B-NB	-2.85	121.24	124.26
21	23	412	CL7	CHD-C1D-ND	-2.85	121.24	124.26
21	12	502	CL7	CHC-C1C-NC	-2.85	121.84	124.45
21	2B	603	CL7	CHC-C1C-NC	-2.85	121.84	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	602	CL7	CHC-C1C-NC	-2.85	121.84	124.45
21	42	502	CL7	CHC-C1C-NC	-2.85	121.84	124.45
21	42	515	CL7	CHC-C1C-NC	-2.85	121.84	124.45
21	4B	615	CL7	O2D-CGD-CBD	2.85	116.32	111.27
21	22	507	CL7	CHB-C1B-NB	-2.85	121.25	124.26
23	1C	515	8CT	C30-C31-C32	-2.84	117.97	121.47
32	41	422	ZEX	C30-C31-C32	-2.84	114.34	123.22
27	2B	625	DGD	C2G-O2G-C1B	-2.84	110.79	117.79
32	44	419	ZEX	C18-C5-C6	-2.84	121.33	124.53
21	21	404	CL7	C7-C6-C5	-2.84	105.64	113.36
21	22	510	CL7	CHD-C1D-ND	-2.84	121.25	124.26
21	21	420	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	42	509	CL7	O2D-CGD-CBD	2.84	116.32	111.27
21	43	409	CL7	O2D-CGD-CBD	2.84	116.32	111.27
21	32	513	CL7	C3B-C2B-C1B	-2.84	103.73	107.16
21	33	506	CL7	C3B-C4B-NB	2.84	113.15	110.52
21	44	414	CL7	CMB-C2B-C1B	2.84	129.70	125.37
21	12	507	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	42	515	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	41	411	CL7	CHC-C1C-NC	-2.84	121.84	124.45
21	1D	402	CL7	CHD-C4C-C3C	-2.84	120.33	124.94
21	1C	511	CL7	CHC-C1C-NC	-2.84	121.84	124.45
32	24	419	ZEX	C18-C5-C6	-2.84	121.34	124.53
32	34	419	ZEX	C18-C5-C6	-2.84	121.34	124.53
21	14	417	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	22	515	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	24	415	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	32	512	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	32	515	CL7	CHB-C1B-NB	-2.84	121.25	124.26
32	24	420	ZEX	C35-C15-C14	-2.84	117.66	123.47
21	1B	602	CL7	CHC-C1C-NC	-2.84	121.84	124.45
21	21	411	CL7	CHC-C1C-NC	-2.84	121.84	124.45
21	24	413	CL7	CHC-C1C-NC	-2.84	121.84	124.45
21	34	417	CL7	CHB-C1B-NB	-2.84	121.25	124.26
32	21	422	ZEX	C30-C31-C32	-2.84	114.36	123.22
21	22	509	CL7	O2D-CGD-CBD	2.84	116.31	111.27
21	22	517	CL7	C3B-C2B-C1B	-2.84	103.74	107.16
21	33	516	CL7	C3B-C2B-C1B	-2.84	103.74	107.16
32	43	421	ZEX	C19-C9-C10	-2.84	118.95	122.92
21	34	415	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	41	409	CL7	CHB-C1B-NB	-2.84	121.25	124.26
21	43	414	CL7	CHB-C1B-NB	-2.84	121.25	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	510	CL7	CHD-C1D-ND	-2.84	121.25	124.26
23	3C	514	8CT	C19-C18-C17	-2.84	117.67	123.47
21	31	407	CL7	CHC-C1C-NC	-2.84	121.85	124.45
21	41	404	CL7	CHC-C1C-NC	-2.84	121.85	124.45
21	3D	402	CL7	CHD-C4C-C3C	-2.84	120.34	124.94
21	21	418	CL7	CHD-C1D-ND	-2.84	121.25	124.26
32	24	420	ZEX	C1-C6-C5	-2.84	118.62	122.61
21	31	420	CL7	CHB-C1B-NB	-2.83	121.26	124.26
32	43	421	ZEX	C8-C7-C6	-2.83	119.24	127.20
23	3B	617	8CT	C35-C30-C29	-2.83	109.12	112.70
21	43	410	CL7	O2D-CGD-CBD	2.83	116.30	111.27
21	11	405	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	2B	615	CL7	O2D-CGD-CBD	2.83	116.30	111.27
21	34	417	CL7	C4C-C3C-C2C	-2.83	103.43	107.13
21	22	516	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	33	505	CL7	CHC-C1C-NC	-2.83	121.85	124.45
23	1D	406	8CT	C04-C03-C02	-2.83	118.62	122.61
21	43	403	CL7	CHD-C4C-C3C	-2.83	120.35	124.94
32	23	421	ZEX	C19-C9-C10	-2.83	118.96	122.92
32	44	420	ZEX	C35-C15-C14	-2.83	117.67	123.47
21	1C	508	CL7	O2A-CGA-O1A	-2.83	116.44	123.59
32	11	422	ZEX	C30-C31-C32	-2.83	114.38	123.22
21	44	416	CL7	CHC-C1C-NC	-2.83	121.85	124.45
21	33	509	CL7	O2D-CGD-CBD	2.83	116.30	111.27
21	4C	509	CL7	O2D-CGD-CBD	2.83	116.30	111.27
21	12	517	CL7	C3B-C2B-C1B	-2.83	103.74	107.16
21	22	513	CL7	C3B-C2B-C1B	-2.83	103.74	107.16
21	22	504	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	32	516	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	13	509	CL7	O2D-CGD-CBD	2.83	116.30	111.27
21	32	517	CL7	C3B-C2B-C1B	-2.83	103.75	107.16
21	12	504	CL7	CHB-C1B-NB	-2.83	121.26	124.26
21	11	405	CL7	O2D-CGD-CBD	2.83	116.30	111.27
21	21	406	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	31	405	CL7	O2D-CGD-CBD	2.83	116.29	111.27
21	21	416	CL7	CMB-C2B-C1B	2.83	129.68	125.37
21	34	414	CL7	CMB-C2B-C1B	2.83	129.68	125.37
21	12	516	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	4C	503	CL7	O2D-CGD-CBD	2.83	116.29	111.27
21	3C	508	CL7	O2A-CGA-O1A	-2.83	116.46	123.59
21	12	510	CL7	CHD-C1D-ND	-2.83	121.27	124.26
21	13	511	CL7	CHD-C1D-ND	-2.83	121.27	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	517	CL7	C3B-C2B-C1B	-2.83	103.75	107.16
32	34	420	ZEX	C35-C15-C14	-2.83	117.69	123.47
21	23	406	CL7	C3B-C2B-C1B	-2.83	103.75	107.16
32	33	520	ZEX	C8-C7-C6	-2.83	119.27	127.20
21	1C	505	CL7	CHD-C1D-ND	-2.83	121.27	124.26
21	12	516	CL7	CHB-C1B-NB	-2.83	121.27	124.26
21	3B	612	CL7	CAA-CBA-CGA	-2.82	105.00	113.25
21	1C	509	CL7	O2D-CGD-CBD	2.82	116.29	111.27
21	2D	402	CL7	CHD-C4C-C3C	-2.82	120.36	124.94
21	1B	603	CL7	C3B-C2B-C1B	-2.82	103.75	107.16
21	1C	517	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	4D	405	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	12	515	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	2B	605	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	3B	604	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	33	516	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	24	416	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	33	502	CL7	CHD-C4C-C3C	-2.82	120.36	124.94
21	11	406	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	2D	405	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	24	405	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	3D	405	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	31	406	CL7	C4-C3-C5	2.82	120.02	115.27
21	4D	402	CL7	CHD-C4C-C3C	-2.82	120.37	124.94
23	4C	514	8CT	C19-C18-C17	-2.82	117.70	123.47
21	42	506	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	3C	509	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	3B	608	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	3C	511	CL7	CHC-C1C-NC	-2.82	121.86	124.45
23	2D	406	8CT	C04-C03-C02	-2.82	118.64	122.61
21	43	407	CL7	CHD-C4C-C3C	-2.82	120.37	124.94
21	42	504	CL7	CHB-C1B-NB	-2.82	121.27	124.26
32	34	419	ZEX	C27-C26-C25	-2.82	118.28	122.84
21	11	420	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	2C	513	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	22	502	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	31	404	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	2C	509	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	2B	604	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	21	409	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	44	405	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	3D	404	CL7	CHD-C4C-C3C	-2.82	120.37	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	610	CL7	C7-C6-C5	-2.82	105.70	113.36
32	13	520	ZEX	C8-C7-C6	-2.82	119.29	127.20
21	11	418	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	2B	613	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	31	405	CL7	CHB-C1B-NB	-2.82	121.27	124.26
21	14	405	CL7	CHB-C1B-NB	-2.82	121.28	124.26
21	4C	501	CL7	CHD-C1D-ND	-2.82	121.28	124.26
21	4C	504	CL7	CHB-C1B-NB	-2.82	121.28	124.26
21	2C	503	CL7	C7-C6-C5	-2.82	105.71	113.36
21	3C	513	CL7	CHC-C1C-NC	-2.82	121.87	124.45
21	31	411	CL7	CHC-C1C-NC	-2.82	121.87	124.45
21	4C	511	CL7	CHC-C1C-NC	-2.82	121.87	124.45
21	33	506	CL7	CHD-C4C-C3C	-2.82	120.37	124.94
32	31	422	ZEX	C30-C31-C32	-2.82	114.43	123.22
32	23	420	ZEX	C19-C9-C10	-2.82	118.98	122.92
21	4D	402	CL7	C3B-C2B-C1B	-2.82	103.76	107.16
21	42	513	CL7	C3B-C2B-C1B	-2.82	103.76	107.16
21	21	404	CL7	CHC-C1C-NC	-2.82	121.87	124.45
21	33	509	CL7	CHC-C1C-NC	-2.82	121.87	124.45
21	4B	605	CL7	CHC-C1C-NC	-2.82	121.87	124.45
21	4B	613	CL7	CAA-CBA-CGA	-2.81	105.03	113.25
21	2C	505	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	32	514	CL7	C4C-C3C-C2C	-2.81	103.46	107.13
23	14	402	8CT	C14-C13-C12	-2.81	123.29	127.31
21	2B	613	CL7	CAA-CBA-CGA	-2.81	105.03	113.25
21	3B	612	CL7	C3B-C2B-C1B	-2.81	103.76	107.16
21	43	412	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	33	505	CL7	C3B-C2B-C1B	-2.81	103.77	107.16
21	2C	508	CL7	O2A-CGA-O1A	-2.81	116.49	123.59
21	21	408	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	3C	504	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	32	507	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	43	417	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	2B	604	CL7	C3B-C2B-C1B	-2.81	103.77	107.16
21	1C	513	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	2C	511	CL7	CHC-C1C-NC	-2.81	121.87	124.45
23	1C	514	8CT	C19-C18-C17	-2.81	117.71	123.47
21	3B	612	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	4C	505	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	2B	613	CL7	C3B-C2B-C1B	-2.81	103.77	107.16
21	11	408	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	42	504	CL7	C2D-C1D-ND	2.81	112.12	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	405	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	31	408	CL7	CHD-C1D-ND	-2.81	121.28	124.26
21	12	514	CL7	C4C-C3C-C2C	-2.81	103.46	107.13
21	42	502	CL7	CAA-CBA-CGA	-2.81	105.04	113.25
32	34	420	ZEX	C1-C6-C5	-2.81	118.66	122.61
21	21	420	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	11	414	CL7	C3B-C2B-C1B	-2.81	103.77	107.16
21	4C	503	CL7	C7-C6-C5	-2.81	105.73	113.36
21	41	406	CL7	C4-C3-C5	2.81	120.00	115.27
21	2C	503	CL7	O2D-CGD-CBD	2.81	116.26	111.27
21	3C	503	CL7	O2D-CGD-CBD	2.81	116.26	111.27
21	1B	609	CL7	C7-C6-C5	-2.81	105.73	113.36
23	2C	515	8CT	C30-C31-C32	-2.81	118.01	121.47
21	42	516	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	11	416	CL7	CMB-C2B-C1B	2.81	129.65	125.37
23	4D	406	8CT	C04-C03-C02	-2.81	118.66	122.61
23	3C	515	8CT	C30-C31-C32	-2.81	118.01	121.47
21	32	506	CL7	CHB-C1B-NB	-2.81	121.28	124.26
21	3C	503	CL7	C7-C6-C5	-2.81	105.73	113.36
21	2C	504	CL7	CHB-C1B-NB	-2.81	121.29	124.26
32	14	419	ZEX	C18-C5-C6	-2.81	121.38	124.53
21	23	410	CL7	O2D-CGD-CBD	2.81	116.25	111.27
21	31	416	CL7	CMB-C2B-C1B	2.81	129.64	125.37
21	1D	405	CL7	CHB-C1B-NB	-2.81	121.29	124.26
21	42	507	CL7	CHB-C1B-NB	-2.81	121.29	124.26
21	13	502	CL7	CHD-C4C-C3C	-2.81	120.39	124.94
21	1B	612	CL7	CAA-CBA-CGA	-2.81	105.06	113.25
32	23	421	ZEX	C8-C7-C6	-2.81	119.32	127.20
21	34	416	CL7	O2D-CGD-CBD	2.80	116.25	111.27
21	22	514	CL7	C4C-C3C-C2C	-2.80	103.47	107.13
21	12	510	CL7	CMB-C2B-C1B	2.80	129.64	125.37
21	13	506	CL7	CHD-C4C-C3C	-2.80	120.39	124.94
21	3A	407	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	4C	508	CL7	O2A-CGA-O1A	-2.80	116.52	123.59
21	23	408	CL7	C3B-C2B-C1B	-2.80	103.78	107.16
21	2C	501	CL7	CHD-C1D-ND	-2.80	121.29	124.26
21	32	502	CL7	CAA-CBA-CGA	-2.80	105.06	113.25
21	22	504	CL7	C2D-C1D-ND	2.80	112.11	110.23
21	11	409	CL7	CHB-C1B-NB	-2.80	121.29	124.26
21	44	416	CL7	O2D-CGD-CBD	2.80	116.25	111.27
21	4B	605	CL7	CHB-C1B-NB	-2.80	121.29	124.26
23	2C	514	8CT	C19-C18-C17	-2.80	117.73	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1C	503	CL7	C7-C6-C5	-2.80	105.75	113.36
21	24	409	CL7	C4C-C3C-C2C	-2.80	103.48	107.13
21	14	416	CL7	O2D-CGD-CBD	2.80	116.24	111.27
21	22	516	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	33	503	CL7	CAA-CBA-CGA	-2.80	105.07	113.25
21	21	406	CL7	C4-C3-C5	2.80	119.98	115.27
21	3B	609	CL7	C7-C6-C5	-2.80	105.76	113.36
21	11	406	CL7	C4-C3-C5	2.80	119.98	115.27
21	23	403	CL7	CHD-C4C-C3C	-2.80	120.40	124.94
23	1B	626	8CT	C23-C21-C20	2.80	123.23	118.94
21	1B	612	CL7	CHB-C1B-NB	-2.80	121.30	124.26
21	12	502	CL7	CAA-CBA-CGA	-2.80	105.08	113.25
21	41	416	CL7	CMB-C2B-C1B	2.80	129.63	125.37
21	43	407	CL7	C3B-C4B-NB	2.80	113.11	110.52
21	21	418	CL7	CHB-C1B-NB	-2.80	121.30	124.26
21	23	412	CL7	O2A-CGA-CBA	2.80	120.69	111.91
21	31	420	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	43	412	CL7	O2A-CGA-CBA	2.80	120.68	111.91
32	31	422	ZEX	C35-C15-C14	-2.80	117.75	123.47
21	1B	604	CL7	CHB-C1B-NB	-2.80	121.30	124.26
21	13	505	CL7	C3B-C2B-C1B	-2.79	103.79	107.16
21	3B	616	CL7	C3B-C2B-C1B	-2.79	103.79	107.16
21	2B	609	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	2D	404	CL7	CHD-C4C-C3C	-2.79	120.41	124.94
21	4B	610	CL7	C7-C6-C5	-2.79	105.77	113.36
21	12	506	CL7	CHB-C1B-NB	-2.79	121.30	124.26
21	33	512	CL7	CHB-C1B-NB	-2.79	121.30	124.26
21	1D	404	CL7	CHD-C4C-C3C	-2.79	120.41	124.94
21	4D	404	CL7	CHD-C4C-C3C	-2.79	120.41	124.94
21	11	415	CL7	C4C-C3C-C2C	-2.79	103.49	107.13
23	44	402	8CT	C14-C13-C12	-2.79	123.33	127.31
21	2B	605	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	42	516	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	41	420	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	33	511	CL7	O2A-CGA-CBA	2.79	120.67	111.91
21	14	408	CL7	O2D-CGD-CBD	2.79	116.23	111.27
21	13	503	CL7	CAA-CBA-CGA	-2.79	105.09	113.25
21	11	406	CL7	CHD-C1D-ND	-2.79	121.30	124.26
23	1B	626	8CT	C27-C26-C25	-2.79	119.01	122.92
23	3D	406	8CT	C04-C03-C02	-2.79	118.68	122.61
21	11	411	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	33	504	CL7	CMB-C2B-C1B	2.79	129.62	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	406	CL7	CHD-C1D-ND	-2.79	121.30	124.26
21	1B	608	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	4B	609	CL7	CHC-C1C-NC	-2.79	121.89	124.45
23	2B	601	8CT	C27-C26-C25	-2.79	119.02	122.92
21	2C	505	CL7	C2D-C1D-ND	2.79	112.10	110.23
21	23	407	CL7	CHD-C4C-C3C	-2.79	120.42	124.94
21	13	512	CL7	CHB-C1B-NB	-2.79	121.30	124.26
21	3C	505	CL7	CHD-C1D-ND	-2.79	121.30	124.26
21	34	409	CL7	C4C-C3C-C2C	-2.79	103.49	107.13
21	42	512	CL7	CAC-C3C-C2C	2.79	132.30	127.53
21	42	510	CL7	CMB-C2B-C1B	2.79	129.62	125.37
21	1C	503	CL7	O2D-CGD-CBD	2.79	116.22	111.27
21	11	416	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	23	407	CL7	C3B-C4B-NB	2.79	113.10	110.52
21	1C	501	CL7	CHD-C1D-ND	-2.79	121.31	124.26
21	23	417	CL7	CHB-C1B-NB	-2.79	121.31	124.26
21	3B	615	CL7	C3B-C2B-C1B	-2.79	103.80	107.16
21	1C	505	CL7	C2D-C1D-ND	2.79	112.10	110.23
21	4C	505	CL7	C2D-C1D-ND	2.79	112.10	110.23
21	23	402	CL7	CHB-C1B-NB	-2.79	121.31	124.26
21	33	501	CL7	CHB-C1B-NB	-2.79	121.31	124.26
21	41	408	CL7	CHD-C1D-ND	-2.79	121.31	124.26
21	14	409	CL7	C4C-C3C-C2C	-2.79	103.49	107.13
21	44	409	CL7	C4C-C3C-C2C	-2.79	103.49	107.13
21	22	502	CL7	CAA-CBA-CGA	-2.79	105.11	113.25
21	13	511	CL7	O2A-CGA-CBA	2.79	120.65	111.91
21	43	404	CL7	CAA-CBA-CGA	-2.79	105.11	113.25
21	22	512	CL7	CAC-C3C-C2C	2.79	132.29	127.53
21	34	408	CL7	O2D-CGD-CBD	2.79	116.22	111.27
21	14	417	CL7	C4C-C3C-C2C	-2.79	103.50	107.13
21	32	504	CL7	C2D-C1D-ND	2.78	112.10	110.23
21	3A	407	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
32	13	519	ZEX	C19-C9-C10	-2.78	119.02	122.92
32	43	420	ZEX	C19-C9-C10	-2.78	119.02	122.92
21	3B	606	CL7	CAA-C2A-C3A	-2.78	105.15	112.78
23	3B	626	8CT	C23-C21-C20	2.78	123.21	118.94
21	3B	603	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	2C	504	CL7	O2D-CGD-CBD	2.78	116.22	111.27
21	31	416	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	41	405	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	1B	604	CL7	CHC-C1C-NC	-2.78	121.90	124.45
32	33	519	ZEX	C19-C9-C10	-2.78	119.02	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	510	CL7	O2D-CGD-CBD	2.78	116.21	111.27
21	4B	613	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	33	503	CL7	O2D-CGD-CBD	2.78	116.21	111.27
21	4C	517	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	33	510	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	4B	616	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	31	418	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	4B	613	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	21	414	CL7	C3B-C2B-C1B	-2.78	103.80	107.16
21	31	406	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	31	409	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	32	507	CL7	CAA-CBA-CGA	-2.78	105.13	113.25
21	12	512	CL7	CAC-C3C-C2C	2.78	132.28	127.53
21	22	518	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	41	406	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	13	510	CL7	O2D-CGD-CBD	2.78	116.21	111.27
21	43	411	CL7	O2D-CGD-CBD	2.78	116.21	111.27
21	13	513	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	31	414	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
21	11	420	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	23	414	CL7	CHB-C1B-NB	-2.78	121.31	124.26
21	4B	604	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
21	1B	606	CL7	CAA-C2A-C3A	-2.78	105.17	112.78
21	4B	607	CL7	CAA-C2A-C3A	-2.78	105.17	112.78
21	41	403	CL7	C7-C6-C5	-2.78	105.81	113.36
21	22	507	CL7	CAA-CBA-CGA	-2.78	105.14	113.25
21	31	403	CL7	C7-C6-C5	-2.78	105.82	113.36
21	42	504	CL7	C3B-C2B-C1B	-2.78	103.81	107.16
21	13	501	CL7	CHB-C1B-NB	-2.78	121.32	124.26
21	12	507	CL7	CAA-CBA-CGA	-2.78	105.14	113.25
32	21	422	ZEX	C35-C15-C14	-2.78	117.79	123.47
21	22	506	CL7	CHB-C1B-NB	-2.78	121.32	124.26
21	23	404	CL7	CAA-CBA-CGA	-2.78	105.14	113.25
21	1C	504	CL7	O2D-CGD-CBD	2.78	116.20	111.27
21	4C	504	CL7	O2D-CGD-CBD	2.78	116.20	111.27
21	1B	612	CL7	C3B-C2B-C1B	-2.77	103.81	107.16
21	1B	615	CL7	C3B-C2B-C1B	-2.77	103.81	107.16
21	32	514	CL7	C3B-C2B-C1B	-2.77	103.81	107.16
21	2B	607	CL7	CAA-C2A-C3A	-2.77	105.18	112.78
21	22	510	CL7	CMB-C2B-C1B	2.77	129.59	125.37
21	32	510	CL7	CMB-C2B-C1B	2.77	129.59	125.37
21	42	502	CL7	CMB-C2B-C1B	2.77	129.59	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	504	CL7	O2D-CGD-CBD	2.77	116.20	111.27
21	3B	601	CL7	CHC-C1C-NC	-2.77	121.91	124.45
23	4B	601	8CT	C27-C26-C25	-2.77	119.04	122.92
21	42	514	CL7	C4C-C3C-C2C	-2.77	103.51	107.13
21	1D	402	CL7	C3B-C2B-C1B	-2.77	103.81	107.16
21	1B	601	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	2B	616	CL7	C3B-C2B-C1B	-2.77	103.81	107.16
21	2D	404	CL7	CHB-C1B-NB	-2.77	121.32	124.26
21	3C	517	CL7	CHB-C1B-NB	-2.77	121.32	124.26
21	3D	404	CL7	CHB-C1B-NB	-2.77	121.32	124.26
21	14	417	CL7	C3A-C4A-CHB	-2.77	119.59	123.70
21	21	403	CL7	C7-C6-C5	-2.77	105.83	113.36
21	42	507	CL7	CAA-CBA-CGA	-2.77	105.16	113.25
23	4A	404	8CT	C24-C23-C21	-2.77	118.63	126.42
21	31	415	CL7	C4C-C3C-C2C	-2.77	103.52	107.13
21	41	404	CL7	C4C-C3C-C2C	-2.77	103.52	107.13
21	41	418	CL7	CHB-C1B-NB	-2.77	121.33	124.26
23	3A	404	8CT	C24-C23-C21	-2.77	118.64	126.42
21	1D	405	CL7	C3B-C2B-C1B	-2.77	103.82	107.16
21	42	509	CL7	CMB-C2B-C1B	2.77	129.59	125.37
21	44	408	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	43	413	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	1B	614	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	4A	407	CL7	C3B-C2B-C1B	-2.77	103.82	107.16
21	11	403	CL7	C7-C6-C5	-2.77	105.85	113.36
21	41	416	CL7	CHC-C1C-NC	-2.77	121.91	124.45
32	11	422	ZEX	C35-C15-C14	-2.77	117.81	123.47
21	12	518	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	13	504	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	3B	602	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	42	518	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	43	405	CL7	CHB-C1B-NB	-2.77	121.33	124.26
21	34	416	CL7	C4C-C3C-C2C	-2.77	103.52	107.13
21	11	402	CL7	CMB-C2B-C1B	2.77	129.58	125.37
21	1A	407	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	2A	407	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	24	415	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	11	404	CL7	CHC-C1C-NC	-2.76	121.91	124.45
21	23	403	CL7	CHC-C1C-NC	-2.76	121.91	124.45
21	2D	402	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	23	411	CL7	O2D-CGD-CBD	2.76	116.18	111.27
21	22	509	CL7	CMB-C2B-C1B	2.76	129.58	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	509	CL7	CMB-C2B-C1B	2.76	129.58	125.37
21	2B	602	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	44	415	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	11	404	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	1B	616	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	11	406	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	23	411	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	3D	402	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	4B	617	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	31	402	CL7	CMB-C2B-C1B	2.76	129.58	125.37
23	2B	601	8CT	C05-C04-C03	2.76	114.73	110.48
21	22	518	CL7	CHB-C1B-NB	-2.76	121.33	124.26
21	44	413	CL7	CHB-C1B-NB	-2.76	121.33	124.26
23	2B	601	8CT	C23-C21-C20	2.76	123.18	118.94
21	31	416	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	43	411	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	11	416	CL7	CHB-C1B-NB	-2.76	121.33	124.26
21	41	416	CL7	CHB-C1B-NB	-2.76	121.33	124.26
23	1B	626	8CT	C05-C04-C03	2.76	114.73	110.48
21	3B	604	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	4C	513	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	24	416	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	32	512	CL7	CAC-C3C-C2C	2.76	132.25	127.53
21	34	417	CL7	C3A-C4A-CHB	-2.76	119.61	123.70
21	43	403	CL7	CHC-C1C-NC	-2.76	121.92	124.45
23	1A	404	8CT	C24-C23-C21	-2.76	118.66	126.42
23	2C	514	8CT	C07-C02-C03	-2.76	118.72	122.73
21	13	510	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	21	402	CL7	CMB-C2B-C1B	2.76	129.57	125.37
21	3D	405	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	21	404	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	2C	517	CL7	CMB-C2B-C1B	2.76	129.57	125.37
21	41	402	CL7	CMB-C2B-C1B	2.76	129.57	125.37
21	3C	505	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	24	404	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	13	516	CL7	CHB-C1B-NB	-2.76	121.34	124.26
23	3B	626	8CT	C27-C26-C25	-2.76	119.06	122.92
21	41	410	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
21	41	414	CL7	C3B-C2B-C1B	-2.76	103.83	107.16
23	4B	601	8CT	C23-C21-C20	2.76	123.17	118.94
21	1C	517	CL7	CMB-C2B-C1B	2.76	129.57	125.37
21	13	514	CL7	CMB-C2B-C1B	2.76	129.57	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	517	CL7	CMB-C2B-C1B	2.76	129.57	125.37
21	21	415	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	23	413	CL7	CHB-C1B-NB	-2.76	121.34	124.26
21	31	406	CL7	CHD-C1D-ND	-2.76	121.34	124.26
21	24	417	CL7	C3A-C4A-CHB	-2.76	119.61	123.70
21	32	506	CL7	O2D-CGD-CBD	2.76	116.16	111.27
21	13	506	CL7	C3B-C4B-NB	2.76	113.07	110.52
21	33	514	CL7	CMB-C2B-C1B	2.76	129.56	125.37
23	3C	514	8CT	C07-C02-C03	-2.76	118.73	122.73
23	4C	514	8CT	C07-C02-C03	-2.75	118.73	122.73
21	31	402	CL7	O2D-CGD-CBD	2.75	116.16	111.27
21	32	502	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	41	402	CL7	O2D-CGD-CBD	2.75	116.16	111.27
21	4B	603	CL7	CHB-C1B-NB	-2.75	121.34	124.26
21	31	404	CL7	C4C-C3C-C2C	-2.75	103.54	107.13
21	12	509	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	41	417	CL7	C7-C6-C5	-2.75	105.88	113.36
21	21	416	CL7	CHB-C1B-NB	-2.75	121.34	124.26
21	12	512	CL7	C7-C6-C5	-2.75	105.88	113.36
21	22	506	CL7	C4-C3-C5	2.75	119.90	115.27
23	4C	514	8CT	C18-C17-C16	-2.75	123.38	127.31
21	24	408	CL7	O2D-CGD-CBD	2.75	116.16	111.27
32	41	422	ZEX	C35-C15-C14	-2.75	117.84	123.47
21	42	506	CL7	C4-C3-C5	2.75	119.90	115.27
21	31	410	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
21	33	503	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
21	22	507	CL7	CHD-C4C-C3C	-2.75	120.48	124.94
21	32	507	CL7	CHD-C4C-C3C	-2.75	120.48	124.94
23	3C	514	8CT	C18-C17-C16	-2.75	123.38	127.31
21	2B	616	CL7	C3B-C4B-NB	2.75	113.07	110.52
21	2A	407	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
21	32	504	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
21	43	415	CL7	CMB-C2B-C1B	2.75	129.56	125.37
21	21	402	CL7	O2D-CGD-CBD	2.75	116.16	111.27
21	12	507	CL7	CHD-C4C-C3C	-2.75	120.48	124.94
21	14	413	CL7	CHB-C1B-NB	-2.75	121.35	124.26
23	2A	404	8CT	C24-C23-C21	-2.75	118.69	126.42
21	41	415	CL7	C4C-C3C-C2C	-2.75	103.54	107.13
21	23	404	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
21	42	506	CL7	O2D-CGD-CBD	2.75	116.15	111.27
21	13	503	CL7	C3B-C2B-C1B	-2.75	103.84	107.16
23	24	402	8CT	C14-C13-C12	-2.75	123.39	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	34	402	8CT	C14-C13-C12	-2.75	123.39	127.31
21	32	518	CL7	CHC-C1C-NC	-2.75	121.93	124.45
32	24	419	ZEX	C15-C35-C34	-2.75	117.85	123.47
21	43	402	CL7	CHB-C1B-NB	-2.75	121.35	124.26
21	22	506	CL7	O2D-CGD-CBD	2.75	116.15	111.27
32	44	419	ZEX	C15-C35-C34	-2.75	117.85	123.47
21	14	416	CL7	C4C-C3C-C2C	-2.75	103.55	107.13
21	31	417	CL7	C7-C6-C5	-2.75	105.90	113.36
23	4B	601	8CT	C05-C04-C03	2.75	114.71	110.48
21	22	512	CL7	C7-C6-C5	-2.75	105.90	113.36
23	1C	514	8CT	C07-C02-C03	-2.75	118.75	122.73
21	12	502	CL7	CMB-C2B-C1B	2.75	129.55	125.37
21	23	404	CL7	O2D-CGD-CBD	2.75	116.15	111.27
21	43	404	CL7	O2D-CGD-CBD	2.75	116.15	111.27
21	2B	615	CL7	CHB-C1B-NB	-2.75	121.35	124.26
21	3B	614	CL7	CHB-C1B-NB	-2.75	121.35	124.26
21	23	405	CL7	CMB-C2B-C1B	2.74	129.55	125.37
21	24	413	CL7	CHB-C1B-NB	-2.74	121.35	124.26
21	33	504	CL7	CHB-C1B-NB	-2.74	121.35	124.26
21	4B	615	CL7	CHB-C1B-NB	-2.74	121.35	124.26
23	1B	617	8CT	C25-C24-C23	-2.74	114.66	123.22
21	34	413	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	43	404	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
21	13	504	CL7	CMB-C2B-C1B	2.74	129.55	125.37
21	4B	617	CL7	CAA-CBA-CGA	-2.74	105.23	112.51
21	11	417	CL7	C7-C6-C5	-2.74	105.91	113.36
21	21	406	CL7	CHD-C1D-ND	-2.74	121.35	124.26
23	4B	618	8CT	C25-C24-C23	-2.74	114.66	123.22
23	4C	518	8CT	C19-C18-C17	-2.74	117.86	123.47
21	12	514	CL7	C3B-C2B-C1B	-2.74	103.85	107.16
23	1C	514	8CT	C18-C17-C16	-2.74	123.40	127.31
21	21	417	CL7	C7-C6-C5	-2.74	105.91	113.36
21	12	506	CL7	O2D-CGD-CBD	2.74	116.14	111.27
21	33	513	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	13	503	CL7	O2D-CGD-CBD	2.74	116.14	111.27
21	4B	616	CL7	C3B-C4B-NB	2.74	113.06	110.52
23	2C	514	8CT	C18-C17-C16	-2.74	123.40	127.31
21	13	502	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	43	405	CL7	CMB-C2B-C1B	2.74	129.54	125.37
32	22	524	ZEX	C18-C5-C4	2.74	119.43	114.36
21	2B	613	CL7	CHD-C1D-ND	-2.74	121.36	124.26
21	44	417	CL7	C3A-C4A-CHB	-2.74	119.63	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	502	CL7	CMB-C2B-C1B	2.74	129.54	125.37
21	2B	617	CL7	CAA-CBA-CGA	-2.74	105.24	112.51
21	3B	616	CL7	CAA-CBA-CGA	-2.74	105.24	112.51
23	3B	617	8CT	C25-C24-C23	-2.74	114.67	123.22
21	12	513	CL7	CHD-C4C-C3C	-2.74	120.50	124.94
21	3C	504	CL7	C7-C6-C5	-2.74	105.92	113.36
21	12	506	CL7	C4-C3-C5	2.74	119.88	115.27
21	1D	402	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	22	514	CL7	C3B-C2B-C1B	-2.74	103.86	107.16
21	42	512	CL7	C7-C6-C5	-2.74	105.92	113.36
23	2B	618	8CT	C25-C24-C23	-2.74	114.68	123.22
21	2D	405	CL7	C3B-C2B-C1B	-2.74	103.86	107.16
23	2C	518	8CT	C19-C18-C17	-2.74	117.87	123.47
21	22	513	CL7	CHD-C4C-C3C	-2.74	120.50	124.94
21	4A	401	CL7	CAA-C2A-C3A	-2.74	105.28	112.78
21	4C	517	CL7	CMB-C2B-C1B	2.74	129.54	125.37
21	1A	401	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	2C	517	CL7	CHB-C1B-NB	-2.74	121.36	124.26
21	31	406	CL7	C3B-C2B-C1B	-2.74	103.86	107.16
21	41	406	CL7	C3B-C2B-C1B	-2.74	103.86	107.16
21	4B	615	CL7	CHC-C1C-NC	-2.73	121.94	124.45
32	14	419	ZEX	C15-C35-C34	-2.73	117.87	123.47
21	32	506	CL7	C4-C3-C5	2.73	119.87	115.27
21	4A	401	CL7	CHB-C1B-NB	-2.73	121.36	124.26
32	13	522	ZEX	C27-C26-C25	-2.73	118.42	122.84
21	2B	617	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
21	3A	401	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
21	43	409	CL7	CMB-C2B-C1B	2.73	129.53	125.37
21	2B	615	CL7	C7-C6-C5	-2.73	105.94	113.36
21	34	413	CL7	CHB-C1B-NB	-2.73	121.36	124.26
21	4A	401	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
21	4A	407	CL7	CHC-C1C-NC	-2.73	121.94	124.45
21	1B	616	CL7	CAA-CBA-CGA	-2.73	105.26	112.51
21	22	507	CL7	CHD-C1D-ND	-2.73	121.36	124.26
21	32	507	CL7	CHD-C1D-ND	-2.73	121.36	124.26
21	24	409	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
21	42	514	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
32	31	421	ZEX	C18-C5-C4	2.73	119.42	114.36
21	42	507	CL7	CHD-C4C-C3C	-2.73	120.51	124.94
21	4D	405	CL7	C3B-C2B-C1B	-2.73	103.86	107.16
21	13	501	CL7	C7-C6-C5	-2.73	105.94	113.36
21	32	512	CL7	C7-C6-C5	-2.73	105.94	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	610	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
23	2C	514	8CT	C39-C16-C15	2.73	122.38	118.08
21	2A	401	CL7	CAA-C2A-C3A	-2.73	105.30	112.78
21	3C	517	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	2A	403	CL7	CHD-C1D-ND	-2.73	121.37	124.26
21	4D	404	CL7	CHB-C1B-NB	-2.73	121.37	124.26
21	1C	517	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	31	418	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	44	413	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	43	402	CL7	C7-C6-C5	-2.73	105.95	113.36
21	11	410	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
32	11	421	ZEX	C18-C5-C4	2.73	119.41	114.36
23	1C	514	8CT	C39-C16-C15	2.73	122.37	118.08
21	23	405	CL7	CHB-C1B-NB	-2.73	121.37	124.26
21	2C	509	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	33	512	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	23	402	CL7	C7-C6-C5	-2.73	105.96	113.36
21	23	409	CL7	CMB-C2B-C1B	2.73	129.52	125.37
21	42	513	CL7	CHD-C4C-C3C	-2.73	120.52	124.94
21	2A	401	CL7	CHB-C1B-NB	-2.73	121.37	124.26
21	22	504	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
21	34	409	CL7	C3B-C2B-C1B	-2.73	103.87	107.16
32	34	419	ZEX	C15-C35-C34	-2.72	117.89	123.47
21	13	515	CL7	CMB-C2B-C1B	2.72	129.52	125.37
21	1B	614	CL7	C7-C6-C5	-2.72	105.96	113.36
21	1A	401	CL7	CAA-C2A-C3A	-2.72	105.32	112.78
21	23	415	CL7	CMB-C2B-C1B	2.72	129.52	125.37
21	44	416	CL7	C4C-C3C-C2C	-2.72	103.58	107.13
21	3C	508	CL7	C7-C6-C5	-2.72	105.96	113.36
21	44	407	CL7	C3B-C2B-C1B	-2.72	103.87	107.16
21	4C	508	CL7	C7-C6-C5	-2.72	105.96	113.36
23	3C	518	8CT	C19-C18-C17	-2.72	117.90	123.47
21	23	414	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	3C	509	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	43	414	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	23	417	CL7	CHC-C1C-NC	-2.72	121.95	124.45
23	3B	626	8CT	C05-C04-C03	2.72	114.67	110.48
21	11	402	CL7	O2D-CGD-CBD	2.72	116.11	111.27
21	3A	401	CL7	CAA-C2A-C3A	-2.72	105.33	112.78
21	14	415	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	2C	501	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	13	507	CL7	CHB-C1B-NB	-2.72	121.38	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	414	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	1C	505	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	24	407	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	4C	505	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	41	418	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
32	12	524	ZEX	C18-C5-C4	2.72	119.40	114.36
32	33	522	ZEX	C27-C26-C25	-2.72	118.44	122.84
21	24	415	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	31	413	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	34	415	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	3C	506	CL7	O2D-CGD-CBD	2.72	116.10	111.27
21	31	408	CL7	CHD-C4C-C3C	-2.72	120.53	124.94
21	2B	603	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	11	418	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	44	415	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	43	416	CL7	CMB-C2B-C1B	2.72	129.51	125.37
21	14	407	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	21	416	CL7	CHC-C1C-NC	-2.72	121.96	124.45
21	4C	509	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	1A	403	CL7	CHD-C1D-ND	-2.72	121.38	124.26
21	1D	404	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	33	501	CL7	C7-C6-C5	-2.72	105.98	113.36
21	4B	615	CL7	C7-C6-C5	-2.72	105.98	113.36
21	2B	611	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	12	518	CL7	CHC-C1C-NC	-2.72	121.96	124.45
21	21	410	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
21	32	513	CL7	CHD-C4C-C3C	-2.72	120.54	124.94
21	3D	402	CL7	CHB-C1B-NB	-2.72	121.38	124.26
21	3B	614	CL7	C7-C6-C5	-2.72	105.98	113.36
21	22	503	CL7	C3B-C2B-C1B	-2.72	103.88	107.16
32	32	524	ZEX	C18-C5-C4	2.71	119.39	114.36
21	1C	508	CL7	C7-C6-C5	-2.71	105.99	113.36
32	41	421	ZEX	C18-C5-C4	2.71	119.38	114.36
21	1C	504	CL7	C7-C6-C5	-2.71	105.99	113.36
21	4C	504	CL7	C7-C6-C5	-2.71	105.99	113.36
25	13	523	SQD	O8-S-C6	-2.71	101.42	105.74
21	3A	401	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	1A	407	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	1B	614	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	42	518	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	13	509	CL7	CHD-C1D-ND	-2.71	121.39	124.26
21	3B	608	CL7	CHD-C1D-ND	-2.71	121.39	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	410	CL7	CHD-C1D-ND	-2.71	121.39	124.26
21	14	415	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	44	409	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
23	1C	518	8CT	C19-C18-C17	-2.71	117.92	123.47
32	42	524	ZEX	C18-C5-C4	2.71	119.38	114.36
21	3B	614	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	4D	402	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	1C	505	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	4C	505	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	2C	504	CL7	C7-C6-C5	-2.71	106.00	113.36
23	3C	514	8CT	C39-C16-C15	2.71	122.35	118.08
21	1C	501	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	4C	501	CL7	CHC-C1C-NC	-2.71	121.96	124.45
32	23	423	ZEX	C27-C26-C25	-2.71	118.46	122.84
21	13	518	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	22	514	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	43	413	CL7	C4C-C3C-C2C	-2.71	103.60	107.13
21	1C	509	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	21	408	CL7	CHD-C4C-C3C	-2.71	120.55	124.94
21	1A	401	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	33	507	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	13	516	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	2A	401	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	2C	505	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	11	414	CL7	CHB-C1B-NB	-2.71	121.39	124.26
21	14	409	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	21	406	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
21	23	419	CL7	C3B-C2B-C1B	-2.71	103.89	107.16
25	23	424	SQD	O8-S-C6	-2.71	101.43	105.74
21	11	413	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	4A	401	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	24	413	CL7	C3B-C2B-C1B	-2.71	103.90	107.16
32	21	421	ZEX	C18-C5-C4	2.70	119.37	114.36
25	43	424	SQD	O8-S-C6	-2.70	101.43	105.74
32	43	423	ZEX	C27-C26-C25	-2.70	118.47	122.84
21	3C	510	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	1B	602	CL7	CHB-C1B-NB	-2.70	121.39	124.26
21	23	416	CL7	CMB-C2B-C1B	2.70	129.49	125.37
21	33	515	CL7	CMB-C2B-C1B	2.70	129.49	125.37
21	11	405	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	41	405	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	4C	517	CL7	C3B-C2B-C1B	-2.70	103.90	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2C	508	CL7	C7-C6-C5	-2.70	106.02	113.36
21	12	504	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	14	413	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	4C	503	CL7	CMB-C2B-C1B	2.70	129.48	125.37
21	13	518	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	12	507	CL7	CHD-C1D-ND	-2.70	121.40	124.26
21	32	512	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	42	514	CL7	CHB-C1B-NB	-2.70	121.40	124.26
21	12	510	CL7	O2A-C1-C2	-2.70	101.54	108.64
21	3C	507	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	2C	517	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	21	418	CL7	C3B-C2B-C1B	-2.70	103.90	107.16
21	1C	503	CL7	CMB-C2B-C1B	2.70	129.48	125.37
21	21	408	CL7	CHB-C1B-NB	-2.70	121.40	124.26
21	21	412	CL7	CHB-C1B-NB	-2.70	121.40	124.26
21	11	408	CL7	CHD-C4C-C3C	-2.70	120.57	124.94
21	41	408	CL7	CHD-C4C-C3C	-2.70	120.57	124.94
25	33	523	SQD	O8-S-C6	-2.70	101.44	105.74
21	34	407	CL7	C3B-C2B-C1B	-2.70	103.91	107.16
21	12	503	CL7	CHB-C1B-NB	-2.70	121.40	124.26
21	2C	503	CL7	CMB-C2B-C1B	2.70	129.47	125.37
21	3C	503	CL7	CMB-C2B-C1B	2.70	129.47	125.37
21	3B	615	CL7	C3B-C4B-NB	2.70	113.02	110.52
21	2C	510	CL7	C3B-C2B-C1B	-2.70	103.91	107.16
21	1B	612	CL7	CHD-C1D-ND	-2.69	121.40	124.26
21	42	510	CL7	O2A-C1-C2	-2.69	101.55	108.64
21	1B	605	CL7	CHC-C1C-NC	-2.69	121.98	124.45
21	1C	507	CL7	CHC-C1C-NC	-2.69	121.98	124.45
23	4C	514	8CT	C39-C16-C15	2.69	122.32	118.08
21	1C	510	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	3B	613	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	33	509	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	4B	610	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	4C	510	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	14	404	CL7	CHC-C1C-NC	-2.69	121.98	124.45
21	34	415	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	4B	611	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	2C	506	CL7	O2D-CGD-CBD	2.69	116.05	111.27
21	24	415	CL7	CAC-C3C-C4C	-2.69	120.44	124.68
21	34	413	CL7	CHD-C1D-ND	-2.69	121.41	124.26
21	43	408	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	43	402	CL7	C3B-C2B-C1B	-2.69	103.91	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1A	401	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	31	408	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	2B	602	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	3B	601	CL7	C3B-C2B-C1B	-2.69	103.91	107.16
21	1C	501	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	41	414	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	43	416	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	21	405	CL7	CHC-C1C-NC	-2.69	121.98	124.45
21	22	510	CL7	O2A-C1-C2	-2.69	101.57	108.64
21	32	510	CL7	O2A-C1-C2	-2.69	101.57	108.64
21	34	415	CL7	CAC-C3C-C4C	-2.69	120.44	124.68
21	13	509	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
21	21	413	CL7	CHC-C1C-NC	-2.69	121.98	124.45
21	42	512	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
21	23	406	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	23	419	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	33	518	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	4A	403	CL7	CHD-C1D-ND	-2.69	121.41	124.26
21	33	508	CL7	CMB-C2B-C1B	2.69	129.46	125.37
21	13	508	CL7	CMB-C2B-C1B	2.69	129.46	125.37
21	22	503	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	32	514	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	33	515	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	2B	615	CL7	CHC-C1C-NC	-2.69	121.98	124.45
21	4C	501	CL7	CHB-C1B-NB	-2.69	121.41	124.26
21	43	410	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
21	24	405	CL7	CMB-C2B-C1B	2.69	129.46	125.37
21	12	512	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
21	2A	401	CL7	C3B-C2B-C1B	-2.69	103.92	107.16
21	4C	506	CL7	O2D-CGD-CBD	2.68	116.04	111.27
21	12	514	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	32	503	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	1B	613	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	44	404	CL7	CHC-C1C-NC	-2.68	121.99	124.45
21	31	412	CL7	C1C-C2C-C3C	-2.68	103.02	106.94
21	11	414	CL7	CMB-C2B-C1B	2.68	129.46	125.37
21	23	408	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	42	507	CL7	CHD-C1D-ND	-2.68	121.42	124.26
21	2B	606	CL7	CHC-C1C-NC	-2.68	121.99	124.45
32	14	418	ZEX	C27-C26-C25	-2.68	118.51	122.84
21	1B	603	CL7	O2D-CGD-CBD	2.68	116.03	111.27
21	4B	604	CL7	O2D-CGD-CBD	2.68	116.03	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1B	615	CL7	C3B-C4B-NB	2.68	113.00	110.52
21	31	412	CL7	CHB-C1B-NB	-2.68	121.42	124.26
23	3B	618	8CT	C40-C12-C13	-2.68	119.17	122.92
21	2C	505	CL7	C3B-C2B-C1B	-2.68	103.92	107.16
21	33	502	CL7	CHC-C1C-NC	-2.68	121.99	124.45
32	34	419	ZEX	C7-C8-C9	-2.68	122.18	126.23
21	3A	401	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	3B	609	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	33	513	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	2C	501	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	3C	501	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	1C	506	CL7	O2D-CGD-CBD	2.68	116.03	111.27
21	3C	502	CL7	O2D-CGD-CBD	2.68	116.03	111.27
21	13	512	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	44	405	CL7	CMB-C2B-C1B	2.68	129.45	125.37
21	2B	604	CL7	O2D-CGD-CBD	2.68	116.03	111.27
21	2B	609	CL7	CHD-C1D-ND	-2.68	121.42	124.26
21	2D	402	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	43	419	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	13	513	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	4B	614	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	23	402	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	41	417	CL7	C3B-C2B-C1B	-2.68	103.93	107.16
21	32	510	CL7	CHB-C1B-NB	-2.68	121.42	124.26
21	3C	501	CL7	CHC-C1C-NC	-2.68	121.99	124.45
21	41	412	CL7	C1C-C2C-C3C	-2.68	103.03	106.94
21	1B	608	CL7	CHD-C1D-ND	-2.68	121.42	124.26
21	33	512	CL7	C4C-C3C-C2C	-2.68	103.64	107.13
21	23	410	CL7	CHD-C1D-ND	-2.68	121.42	124.26
23	1C	515	8CT	C19-C18-C17	-2.67	118.00	123.47
21	1C	502	CL7	O2D-CGD-CBD	2.67	116.02	111.27
21	4C	502	CL7	O2D-CGD-CBD	2.67	116.02	111.27
21	41	414	CL7	CMB-C2B-C1B	2.67	129.44	125.37
21	2C	507	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	41	413	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	3B	612	CL7	CHD-C1D-ND	-2.67	121.43	124.26
21	41	412	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	43	417	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	32	518	CL7	CHB-C1B-NB	-2.67	121.43	124.26
32	14	419	ZEX	C7-C8-C9	-2.67	122.20	126.23
32	44	419	ZEX	C7-C8-C9	-2.67	122.20	126.23
21	3A	403	CL7	CHD-C1D-ND	-2.67	121.43	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	503	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	42	503	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	43	419	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	11	412	CL7	C1C-C2C-C3C	-2.67	103.04	106.94
21	14	415	CL7	CAC-C3C-C4C	-2.67	120.47	124.68
21	22	512	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	23	413	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	11	417	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	44	407	CL7	CHB-C1B-NB	-2.67	121.43	124.26
21	34	404	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	21	412	CL7	C1C-C2C-C3C	-2.67	103.04	106.94
21	23	413	CL7	C4C-C3C-C2C	-2.67	103.65	107.13
21	1B	609	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
21	2B	610	CL7	C3B-C2B-C1B	-2.67	103.94	107.16
32	32	524	ZEX	C11-C12-C13	-2.67	118.92	126.42
21	3B	603	CL7	O2D-CGD-CBD	2.67	116.01	111.27
21	4B	613	CL7	CHD-C1D-ND	-2.67	121.43	124.26
21	41	408	CL7	CHB-C1B-NB	-2.67	121.43	124.26
32	42	522	ZEX	C7-C6-C5	2.67	127.93	121.46
21	3B	602	CL7	C7-C6-C5	-2.67	106.11	113.36
21	33	509	CL7	CHD-C1D-ND	-2.67	121.43	124.26
21	43	406	CL7	CAA-CBA-CGA	-2.67	105.46	113.25
23	2C	515	8CT	C19-C18-C17	-2.67	118.01	123.47
32	22	519	ZEX	C28-C29-C30	2.67	123.03	118.94
32	32	519	ZEX	C28-C29-C30	2.67	123.03	118.94
32	22	522	ZEX	C7-C6-C5	2.67	127.92	121.46
32	24	419	ZEX	C7-C8-C9	-2.67	122.21	126.23
21	23	406	CL7	CAA-CBA-CGA	-2.67	105.47	113.25
21	33	505	CL7	CAA-CBA-CGA	-2.67	105.47	113.25
21	1B	612	CL7	C7-C6-C5	-2.67	106.12	113.36
32	34	418	ZEX	C27-C26-C25	-2.66	118.53	122.84
21	2C	511	CL7	CHB-C1B-NB	-2.66	121.44	124.26
21	32	504	CL7	CHD-C4C-C3C	-2.66	120.62	124.94
21	2B	614	CL7	C3B-C2B-C1B	-2.66	103.94	107.16
21	44	415	CL7	CAC-C3C-C4C	-2.66	120.48	124.68
21	31	417	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
21	22	516	CL7	CMB-C2B-C1B	2.66	129.43	125.37
21	4A	401	CL7	CMB-C2B-C1B	2.66	129.43	125.37
21	43	419	CL7	CAA-CBA-CGA	-2.66	105.44	112.51
21	12	510	CL7	CHB-C1B-NB	-2.66	121.44	124.26
21	3B	605	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	33	511	CL7	CHC-C1C-NC	-2.66	122.01	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1B	602	CL7	C7-C6-C5	-2.66	106.13	113.36
21	3C	505	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	42	504	CL7	CHD-C4C-C3C	-2.66	120.62	124.94
21	1B	607	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
21	33	518	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
23	2B	619	8CT	C40-C12-C13	-2.66	119.19	122.92
21	14	405	CL7	CMB-C2B-C1B	2.66	129.42	125.37
21	2C	502	CL7	O2D-CGD-CBD	2.66	116.00	111.27
21	4B	603	CL7	C7-C6-C5	-2.66	106.13	113.36
21	23	416	CL7	CHB-C1B-NB	-2.66	121.44	124.26
23	3C	515	8CT	C19-C18-C17	-2.66	118.03	123.47
21	3C	511	CL7	CHB-C1B-NB	-2.66	121.44	124.26
23	3B	626	8CT	C28-C26-C25	2.66	123.02	118.94
21	3A	403	CL7	C7-C6-C5	-2.66	106.14	113.36
21	23	419	CL7	CAA-CBA-CGA	-2.66	105.45	112.51
21	11	408	CL7	CHB-C1B-NB	-2.66	121.44	124.26
21	1A	403	CL7	C7-C6-C5	-2.66	106.14	113.36
21	21	420	CL7	C4C-C3C-C2C	-2.66	103.66	107.13
21	31	420	CL7	C4C-C3C-C2C	-2.66	103.66	107.13
21	4B	613	CL7	C7-C6-C5	-2.66	106.14	113.36
21	1B	601	CL7	C3B-C2B-C1B	-2.66	103.95	107.16
23	4C	515	8CT	C19-C18-C17	-2.66	118.03	123.47
21	4D	405	CL7	O2D-CGD-O1D	-2.66	118.64	123.84
21	2A	403	CL7	C7-C6-C5	-2.66	106.14	113.36
21	33	504	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	4C	507	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	32	507	CL7	CMB-C2B-C1B	2.66	129.41	125.37
23	3C	518	8CT	C01-C02-C07	2.66	118.72	113.62
21	13	518	CL7	CAA-CBA-CGA	-2.66	105.46	112.51
21	33	518	CL7	CAA-CBA-CGA	-2.66	105.46	112.51
23	1B	618	8CT	C40-C12-C13	-2.66	119.20	122.92
23	4B	619	8CT	C40-C12-C13	-2.66	119.20	122.92
21	33	501	CL7	C3B-C2B-C1B	-2.66	103.96	107.16
23	1A	404	8CT	C13-C14-C15	-2.66	114.93	123.22
21	24	413	CL7	CHD-C1D-ND	-2.66	121.45	124.26
21	31	405	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	3D	405	CL7	O2D-CGD-O1D	-2.66	118.65	123.84
21	23	410	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	3B	607	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	44	413	CL7	CHD-C1D-ND	-2.65	121.45	124.26
23	3A	404	8CT	C13-C14-C15	-2.65	114.93	123.22
21	34	411	CL7	CAA-C2A-C3A	-2.65	105.51	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	613	CL7	C7-C6-C5	-2.65	106.15	113.36
32	12	519	ZEX	C28-C29-C30	2.65	123.01	118.94
32	42	519	ZEX	C28-C29-C30	2.65	123.01	118.94
32	32	522	ZEX	C7-C6-C5	2.65	127.89	121.46
21	2B	608	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	31	405	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
23	1B	626	8CT	C28-C26-C25	2.65	123.01	118.94
21	3B	612	CL7	C7-C6-C5	-2.65	106.15	113.36
21	41	420	CL7	C4C-C3C-C2C	-2.65	103.67	107.13
21	14	411	CL7	CAA-C2A-C3A	-2.65	105.51	112.78
21	44	411	CL7	CAA-C2A-C3A	-2.65	105.51	112.78
23	2A	404	8CT	C13-C14-C15	-2.65	114.94	123.22
23	4A	404	8CT	C13-C14-C15	-2.65	114.94	123.22
21	32	503	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	43	413	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	2B	603	CL7	C7-C6-C5	-2.65	106.16	113.36
21	24	412	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	1B	610	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	4B	602	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	34	414	CL7	CAC-C3C-C2C	2.65	132.06	127.53
21	4B	612	CL7	C1C-C2C-C3C	-2.65	103.07	106.94
21	31	414	CL7	CMB-C2B-C1B	2.65	129.40	125.37
21	24	414	CL7	CAC-C3C-C2C	2.65	132.06	127.53
21	14	412	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	21	417	CL7	C3B-C2B-C1B	-2.65	103.96	107.16
21	11	406	CL7	CMB-C2B-C1B	2.65	129.40	125.37
21	42	510	CL7	CHB-C1B-NB	-2.65	121.45	124.26
21	23	414	CL7	C4C-C3C-C2C	-2.65	103.68	107.13
21	4B	608	CL7	C3B-C2B-C1B	-2.65	103.97	107.16
21	13	505	CL7	CAA-CBA-CGA	-2.65	105.52	113.25
21	2D	405	CL7	O2D-CGD-O1D	-2.65	118.66	123.84
23	4C	518	8CT	C01-C02-C07	2.65	118.70	113.62
21	31	414	CL7	CHB-C1B-NB	-2.65	121.46	124.26
23	4B	601	8CT	C28-C26-C25	2.65	123.00	118.94
21	22	509	CL7	C3B-C2B-C1B	-2.65	103.97	107.16
21	32	509	CL7	C3B-C2B-C1B	-2.65	103.97	107.16
32	44	418	ZEX	C27-C26-C25	-2.65	118.57	122.84
21	24	411	CL7	CAA-C2A-C3A	-2.64	105.53	112.78
21	13	505	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	42	503	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	4A	403	CL7	C7-C6-C5	-2.64	106.18	113.36
21	31	416	CL7	C3B-C2B-C1B	-2.64	103.97	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3A	401	CL7	CMB-C2B-C1B	2.64	129.40	125.37
21	34	405	CL7	CMB-C2B-C1B	2.64	129.40	125.37
21	1B	611	CL7	C1C-C2C-C3C	-2.64	103.08	106.94
32	22	524	ZEX	C11-C12-C13	-2.64	118.99	126.42
21	43	414	CL7	C4C-C3C-C2C	-2.64	103.68	107.13
21	1B	622	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	12	510	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	4B	623	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	4C	511	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	14	414	CL7	CAC-C3C-C2C	2.64	132.05	127.53
21	13	512	CL7	C4C-C3C-C2C	-2.64	103.68	107.13
21	21	414	CL7	CMB-C2B-C1B	2.64	129.40	125.37
32	24	418	ZEX	C27-C26-C25	-2.64	118.57	122.84
32	42	524	ZEX	C11-C12-C13	-2.64	118.99	126.42
23	2C	518	8CT	C01-C02-C07	2.64	118.69	113.62
21	2B	612	CL7	C1C-C2C-C3C	-2.64	103.08	106.94
21	31	407	CL7	CMA-C3A-C2A	-2.64	109.94	116.10
21	22	510	CL7	CHB-C1B-NB	-2.64	121.46	124.26
21	42	507	CL7	CMB-C2B-C1B	2.64	129.39	125.37
21	21	407	CL7	CMA-C3A-C2A	-2.64	109.94	116.10
21	22	518	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
23	3C	514	8CT	C18-C19-C20	-2.64	118.06	123.47
21	13	513	CL7	CMB-C2B-C1B	2.64	129.39	125.37
21	14	413	CL7	CHD-C1D-ND	-2.64	121.46	124.26
21	33	516	CL7	CHC-C1C-NC	-2.64	122.03	124.45
21	41	405	CL7	C3B-C2B-C1B	-2.64	103.97	107.16
21	1C	511	CL7	C1C-C2C-C3C	-2.64	103.09	106.94
32	12	524	ZEX	C11-C12-C13	-2.64	119.00	126.42
21	12	516	CL7	CMB-C2B-C1B	2.64	129.39	125.37
21	43	406	CL7	CHB-C1B-NB	-2.64	121.46	124.26
32	12	522	ZEX	C7-C6-C5	2.64	127.86	121.46
21	12	504	CL7	CHD-C4C-C3C	-2.64	120.66	124.94
32	12	524	ZEX	C27-C26-C25	-2.64	118.58	122.84
32	42	524	ZEX	C27-C26-C25	-2.64	118.58	122.84
21	1D	405	CL7	O2D-CGD-O1D	-2.64	118.68	123.84
21	31	413	CL7	C3B-C2B-C1B	-2.64	103.98	107.16
21	2C	511	CL7	C1C-C2C-C3C	-2.64	103.09	106.94
21	3B	611	CL7	C1C-C2C-C3C	-2.64	103.09	106.94
21	12	507	CL7	CMB-C2B-C1B	2.64	129.38	125.37
21	23	414	CL7	CMB-C2B-C1B	2.64	129.38	125.37
21	32	503	CL7	C4C-C3C-C2C	-2.64	103.69	107.13
21	1A	403	CL7	C3B-C2B-C1B	-2.64	103.98	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	513	CL7	C3B-C2B-C1B	-2.64	103.98	107.16
21	42	506	CL7	CHC-C1C-NC	-2.64	122.03	124.45
21	13	511	CL7	CHC-C1C-NC	-2.63	122.03	124.45
21	11	420	CL7	C4C-C3C-C2C	-2.63	103.69	107.13
21	31	406	CL7	CMB-C2B-C1B	2.63	129.38	125.37
21	1C	512	CL7	CHB-C1B-NB	-2.63	121.47	124.26
21	4B	609	CL7	CHD-C1D-ND	-2.63	121.47	124.26
21	4C	512	CL7	CHB-C1B-NB	-2.63	121.47	124.26
21	34	412	CL7	C3B-C2B-C1B	-2.63	103.98	107.16
21	42	510	CL7	C3B-C2B-C1B	-2.63	103.98	107.16
21	3A	403	CL7	C1-C2-C3	2.63	130.60	126.04
23	2B	601	8CT	C28-C26-C25	2.63	122.98	118.94
21	11	412	CL7	CHB-C1B-NB	-2.63	121.47	124.26
21	2B	609	CL7	CHB-C1B-NB	-2.63	121.47	124.26
21	3C	513	CL7	C3B-C2B-C1B	-2.63	103.98	107.16
21	4C	511	CL7	C1C-C2C-C3C	-2.63	103.10	106.94
21	1A	401	CL7	CMB-C2B-C1B	2.63	129.38	125.37
21	41	406	CL7	CMB-C2B-C1B	2.63	129.38	125.37
21	22	510	CL7	C3B-C2B-C1B	-2.63	103.98	107.16
21	32	510	CL7	C3B-C2B-C1B	-2.63	103.98	107.16
21	41	408	CL7	CHC-C1C-NC	-2.63	122.04	124.45
32	22	524	ZEX	C27-C26-C25	-2.63	118.59	122.84
27	4C	516	DGD	C3G-C2G-C1G	-2.63	105.57	111.79
23	1C	518	8CT	C01-C02-C07	2.63	118.67	113.62
21	42	516	CL7	CMB-C2B-C1B	2.63	129.38	125.37
27	2C	516	DGD	C3G-C2G-C1G	-2.63	105.57	111.79
32	44	418	ZEX	C11-C12-C13	-2.63	119.03	126.42
21	41	410	CL7	CHB-C1B-NB	-2.63	121.47	124.26
21	43	414	CL7	CMB-C2B-C1B	2.63	129.37	125.37
21	11	407	CL7	CMA-C3A-C2A	-2.63	109.96	116.10
21	3C	511	CL7	C1C-C2C-C3C	-2.63	103.10	106.94
21	22	505	CL7	C7-C6-C5	-2.63	106.22	113.36
21	33	513	CL7	C4C-C3C-C2C	-2.63	103.70	107.13
21	4B	603	CL7	C3B-C2B-C1B	-2.63	103.99	107.16
21	3B	610	CL7	CHB-C1B-NB	-2.63	121.48	124.26
21	2D	404	CL7	C7-C6-C5	-2.63	106.22	113.36
21	42	505	CL7	C7-C6-C5	-2.63	106.22	113.36
21	11	415	CL7	C3B-C2B-C1B	-2.63	103.99	107.16
21	21	413	CL7	C3B-C2B-C1B	-2.63	103.99	107.16
21	33	505	CL7	CHB-C1B-NB	-2.63	121.48	124.26
21	1C	503	CL7	C3B-C2B-C1B	-2.63	103.99	107.16
21	4C	503	CL7	C3B-C2B-C1B	-2.63	103.99	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	41	420	CL7	C3B-C2B-C1B	-2.63	103.99	107.16
21	1A	403	CL7	C1-C2-C3	2.62	130.58	126.04
32	44	419	ZEX	C30-C31-C32	-2.62	115.03	123.22
21	1B	602	CL7	C3B-C2B-C1B	-2.62	103.99	107.16
21	11	405	CL7	C3B-C2B-C1B	-2.62	103.99	107.16
23	1C	514	8CT	C18-C19-C20	-2.62	118.10	123.47
32	34	418	ZEX	C11-C12-C13	-2.62	119.05	126.42
21	3D	404	CL7	C7-C6-C5	-2.62	106.23	113.36
21	33	509	CL7	C4-C3-C5	2.62	119.68	115.27
21	2B	603	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	21	407	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	24	414	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	3C	512	CL7	CHB-C1B-NB	-2.62	121.48	124.26
32	12	519	ZEX	C10-C11-C12	-2.62	115.03	123.22
27	1C	516	DGD	C3G-C2G-C1G	-2.62	105.59	111.79
32	14	419	ZEX	C30-C31-C32	-2.62	115.03	123.22
21	1D	404	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	31	408	CL7	C4C-C3C-C2C	-2.62	103.71	107.13
21	1C	509	CL7	CHB-C1B-NB	-2.62	121.48	124.26
21	14	410	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	21	407	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	41	417	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	12	505	CL7	C7-C6-C5	-2.62	106.24	113.36
21	44	409	CL7	C7-C6-C5	-2.62	106.24	113.36
21	31	415	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
32	34	419	ZEX	C30-C31-C32	-2.62	115.04	123.22
21	24	410	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	32	505	CL7	C7-C6-C5	-2.62	106.25	113.36
21	4B	611	CL7	CHB-C1B-NB	-2.62	121.48	124.26
23	3C	514	8CT	C40-C12-C11	2.62	122.20	118.08
32	24	418	ZEX	C11-C12-C13	-2.62	119.06	126.42
32	32	519	ZEX	C10-C11-C12	-2.62	115.05	123.22
21	24	407	CL7	CHB-C1B-NB	-2.62	121.48	124.26
21	13	501	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	13	504	CL7	CHC-C1C-NC	-2.62	122.05	124.45
21	23	412	CL7	CHC-C1C-NC	-2.62	122.05	124.45
21	2A	401	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	33	513	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	44	410	CL7	CMB-C2B-C1B	2.62	129.36	125.37
21	23	403	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	42	511	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	22	507	CL7	CMB-C2B-C1B	2.62	129.35	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	420	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	21	405	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	12	508	CL7	CHC-C1C-NC	-2.62	122.05	124.45
21	23	405	CL7	CHC-C1C-NC	-2.62	122.05	124.45
21	22	504	CL7	CHD-C4C-C3C	-2.62	120.70	124.94
21	41	407	CL7	CMA-C3A-C2A	-2.62	109.99	116.10
21	12	511	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	42	509	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	41	415	CL7	C3B-C2B-C1B	-2.62	104.00	107.16
21	2A	403	CL7	C1-C2-C3	2.62	130.57	126.04
32	32	524	ZEX	C27-C26-C25	-2.62	118.61	122.84
21	4C	509	CL7	CMB-C2B-C1B	2.62	129.35	125.37
21	2C	503	CL7	C3B-C2B-C1B	-2.61	104.00	107.16
21	3C	503	CL7	C3B-C2B-C1B	-2.61	104.00	107.16
21	4B	606	CL7	CHC-C1C-NC	-2.61	122.05	124.45
21	1C	511	CL7	CHB-C1B-NB	-2.61	121.49	124.26
23	4C	514	8CT	C18-C19-C20	-2.61	118.12	123.47
23	4C	514	8CT	C40-C12-C11	2.61	122.20	118.08
23	2C	514	8CT	C18-C19-C20	-2.61	118.12	123.47
21	32	518	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	11	403	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	11	407	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	13	506	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	33	506	CL7	CMB-C2B-C1B	2.61	129.35	125.37
31	1F	101	HEM	CHD-C4C-NC	2.61	127.27	124.44
21	1C	513	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	23	407	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	1B	609	CL7	CAA-CBA-CGA	-2.61	105.62	113.25
21	44	414	CL7	CAC-C3C-C2C	2.61	132.00	127.53
32	42	519	ZEX	C8-C7-C6	-2.61	119.86	127.20
21	24	410	CL7	CHC-C1C-NC	-2.61	122.05	124.45
21	34	410	CL7	CHC-C1C-NC	-2.61	122.05	124.45
32	24	419	ZEX	C30-C31-C32	-2.61	115.06	123.22
21	12	509	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	2B	623	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	2C	513	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	3B	622	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	2B	610	CL7	CAA-CBA-CGA	-2.61	105.62	113.25
21	1D	404	CL7	C7-C6-C5	-2.61	106.27	113.36
21	32	516	CL7	CMB-C2B-C1B	2.61	129.35	125.37
21	4A	403	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	14	409	CL7	C7-C6-C5	-2.61	106.27	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	34	409	CL7	C7-C6-C5	-2.61	106.27	113.36
21	43	404	CL7	C4C-C3C-C2C	-2.61	103.72	107.13
21	34	407	CL7	O2D-CGD-CBD	2.61	115.91	111.27
32	22	519	ZEX	C10-C11-C12	-2.61	115.07	123.22
21	21	406	CL7	CMB-C2B-C1B	2.61	129.34	125.37
32	14	418	ZEX	C11-C12-C13	-2.61	119.08	126.42
21	4A	403	CL7	C1-C2-C3	2.61	130.56	126.04
21	4B	610	CL7	CAA-CBA-CGA	-2.61	105.63	113.25
21	21	420	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	3B	602	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	41	413	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	44	412	CL7	C3B-C2B-C1B	-2.61	104.01	107.16
21	22	506	CL7	CHC-C1C-NC	-2.61	122.06	124.45
21	13	511	CL7	CHB-C1B-NB	-2.61	121.50	124.26
21	42	510	CL7	CAA-CBA-CGA	-2.61	105.63	113.25
21	2C	509	CL7	CMB-C2B-C1B	2.61	129.34	125.37
21	13	517	CL7	CHB-C1B-NB	-2.61	121.50	124.26
21	21	410	CL7	CHB-C1B-NB	-2.61	121.50	124.26
21	34	407	CL7	CHB-C1B-NB	-2.61	121.50	124.26
21	32	511	CL7	C3B-C2B-C1B	-2.61	104.02	107.16
32	12	519	ZEX	C8-C7-C6	-2.61	119.88	127.20
21	24	412	CL7	CHB-C1B-NB	-2.61	121.50	124.26
27	3C	516	DGD	C3G-C2G-C1G	-2.61	105.62	111.79
21	13	509	CL7	C4-C3-C5	2.61	119.66	115.27
21	12	518	CL7	C3B-C2B-C1B	-2.61	104.02	107.16
23	1K	101	8CT	C40-C12-C13	-2.61	119.27	122.92
21	32	510	CL7	CAA-CBA-CGA	-2.61	105.64	113.25
21	43	405	CL7	CHC-C1C-NC	-2.61	122.06	124.45
21	42	501	CL7	C1C-C2C-C3C	-2.60	103.14	106.94
23	24	402	8CT	C35-C30-C29	-2.60	109.41	112.70
32	32	519	ZEX	C8-C7-C6	-2.60	119.89	127.20
21	31	407	CL7	CMB-C2B-C1B	2.60	129.33	125.37
21	33	511	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	34	412	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	21	417	CL7	CMB-C2B-C1B	2.60	129.33	125.37
32	42	519	ZEX	C10-C11-C12	-2.60	115.09	123.22
21	11	413	CL7	C3B-C2B-C1B	-2.60	104.02	107.16
21	42	511	CL7	O2D-CGD-CBD	2.60	115.89	111.27
21	33	506	CL7	CHC-C1C-NC	-2.60	122.06	124.45
21	43	407	CL7	CMB-C2B-C1B	2.60	129.33	125.37
21	1B	610	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	3C	509	CL7	CHB-C1B-NB	-2.60	121.50	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	412	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	21	408	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	2C	509	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	2C	512	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	43	417	CL7	C4-C3-C5	2.60	119.64	115.27
21	11	412	CL7	CAA-CBA-CGA	-2.60	105.61	112.51
21	21	412	CL7	CAA-CBA-CGA	-2.60	105.61	112.51
21	3B	609	CL7	CAA-CBA-CGA	-2.60	105.66	113.25
21	31	410	CL7	CHB-C1B-NB	-2.60	121.50	124.26
21	31	417	CL7	CMB-C2B-C1B	2.60	129.33	125.37
21	24	407	CL7	O2D-CGD-CBD	2.60	115.89	111.27
21	32	511	CL7	O2D-CGD-CBD	2.60	115.89	111.27
21	11	407	CL7	C3B-C2B-C1B	-2.60	104.02	107.16
21	14	408	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	14	407	CL7	O2D-CGD-CBD	2.60	115.89	111.27
21	11	403	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
21	33	502	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
21	44	407	CL7	O2D-CGD-CBD	2.60	115.89	111.27
21	43	410	CL7	C4-C3-C5	2.60	119.64	115.27
23	2C	514	8CT	C40-C12-C11	2.60	122.17	118.08
21	24	409	CL7	C7-C6-C5	-2.60	106.30	113.36
21	23	415	CL7	CHB-C1B-NB	-2.60	121.51	124.26
21	21	415	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
21	21	416	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
21	11	408	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	41	408	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	4C	512	CL7	CMB-C2B-C1B	2.60	129.32	125.37
21	41	403	CL7	CMB-C2B-C1B	2.60	129.32	125.37
21	22	510	CL7	CAA-CBA-CGA	-2.60	105.66	113.25
21	3C	509	CL7	CMB-C2B-C1B	2.60	129.32	125.37
21	34	410	CL7	CMB-C2B-C1B	2.60	129.32	125.37
21	3B	613	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	23	417	CL7	C4-C3-C5	2.60	119.64	115.27
21	33	510	CL7	CAA-C2A-C3A	-2.60	105.67	112.78
21	3B	616	CL7	CHC-C1C-NC	-2.60	122.07	124.45
21	2C	504	CL7	C3B-C2B-C1B	-2.60	104.03	107.16
32	22	524	ZEX	C39-C29-C30	-2.59	119.29	122.92
21	44	410	CL7	CHB-C1B-NB	-2.59	121.51	124.26
21	4D	404	CL7	C7-C6-C5	-2.59	106.31	113.36
21	12	501	CL7	C1C-C2C-C3C	-2.59	103.15	106.94
21	42	518	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
21	23	404	CL7	C4C-C3C-C2C	-2.59	103.75	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	615	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	32	504	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	42	508	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	2B	610	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	14	414	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
21	31	412	CL7	CAA-CBA-CGA	-2.59	105.63	112.51
21	31	403	CL7	CMB-C2B-C1B	2.59	129.32	125.37
21	23	410	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	44	408	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	43	412	CL7	CHC-C1C-NC	-2.59	122.07	124.45
23	34	402	8CT	C35-C30-C29	-2.59	109.42	112.70
21	11	413	CL7	C3B-C4B-NB	2.59	112.92	110.52
21	44	412	CL7	CHB-C1B-NB	-2.59	121.51	124.26
21	32	508	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	22	511	CL7	C3B-C2B-C1B	-2.59	104.03	107.16
23	44	402	8CT	C35-C30-C29	-2.59	109.43	112.70
21	12	504	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	41	407	CL7	CMB-C2B-C1B	2.59	129.31	125.37
32	22	519	ZEX	C8-C7-C6	-2.59	119.93	127.20
23	1C	514	8CT	C40-C12-C11	2.59	122.16	118.08
21	11	417	CL7	CHB-C1B-NB	-2.59	121.52	124.26
21	23	412	CL7	CHB-C1B-NB	-2.59	121.52	124.26
21	33	503	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	2A	403	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	3A	403	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	3B	606	CL7	C7-C6-C5	-2.59	106.33	113.36
21	1B	606	CL7	C7-C6-C5	-2.59	106.33	113.36
21	4B	607	CL7	C7-C6-C5	-2.59	106.33	113.36
21	3C	512	CL7	CMB-C2B-C1B	2.59	129.31	125.37
21	13	511	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	31	419	CL7	C3B-C2B-C1B	-2.59	104.04	107.16
21	41	402	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	1C	509	CL7	CMB-C2B-C1B	2.59	129.31	125.37
21	13	510	CL7	CAA-C2A-C3A	-2.59	105.70	112.78
21	43	411	CL7	CAA-C2A-C3A	-2.59	105.70	112.78
21	2B	604	CL7	O2A-C1-C2	-2.58	101.84	108.64
21	3B	603	CL7	O2A-C1-C2	-2.58	101.84	108.64
21	13	503	CL7	C4C-C3C-C2C	-2.58	103.76	107.13
21	31	411	CL7	C4C-C3C-C2C	-2.58	103.76	107.13
21	2B	611	CL7	CHB-C1B-NB	-2.58	121.52	124.26
21	11	417	CL7	CMB-C2B-C1B	2.58	129.31	125.37
21	23	410	CL7	C4-C3-C5	2.58	119.62	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	413	CL7	C3B-C4B-NB	2.58	112.91	110.52
21	2C	502	CL7	C3B-C2B-C1B	-2.58	104.04	107.16
21	3C	502	CL7	C3B-C2B-C1B	-2.58	104.04	107.16
21	13	513	CL7	C4C-C3C-C2C	-2.58	103.76	107.13
21	42	503	CL7	C4C-C3C-C2C	-2.58	103.76	107.13
21	44	407	CL7	C4C-C3C-C2C	-2.58	103.76	107.13
21	13	515	CL7	CHB-C1B-NB	-2.58	121.52	124.26
21	41	412	CL7	CAA-CBA-CGA	-2.58	105.65	112.51
21	2C	503	CL7	CAA-CBA-CGA	-2.58	105.71	113.25
21	2D	404	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	3D	404	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	31	407	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	31	403	CL7	C1C-C2C-C3C	-2.58	103.17	106.94
21	33	509	CL7	C4C-C3C-C2C	-2.58	103.76	107.13
32	12	524	ZEX	C39-C29-C30	-2.58	119.31	122.92
32	42	524	ZEX	C39-C29-C30	-2.58	119.31	122.92
21	13	502	CL7	C4-C3-C5	2.58	119.61	115.27
21	4C	503	CL7	CAA-CBA-CGA	-2.58	105.71	113.25
23	14	402	8CT	C35-C30-C29	-2.58	109.44	112.70
21	21	413	CL7	C3B-C4B-NB	2.58	112.91	110.52
21	11	415	CL7	CMB-C2B-C1B	2.58	129.30	125.37
21	1B	603	CL7	O2A-C1-C2	-2.58	101.86	108.64
21	4B	604	CL7	O2A-C1-C2	-2.58	101.86	108.64
21	31	408	CL7	CHC-C1C-NC	-2.58	122.08	124.45
21	41	413	CL7	C3B-C4B-NB	2.58	112.91	110.52
21	12	503	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	11	402	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	23	411	CL7	CAA-C2A-C3A	-2.58	105.72	112.78
21	43	415	CL7	CHB-C1B-NB	-2.58	121.53	124.26
21	43	418	CL7	CHB-C1B-NB	-2.58	121.53	124.26
21	2B	607	CL7	C7-C6-C5	-2.58	106.36	113.36
21	41	407	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	44	406	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	12	510	CL7	CAA-CBA-CGA	-2.58	105.72	113.25
21	22	501	CL7	C1C-C2C-C3C	-2.58	103.18	106.94
21	43	403	CL7	C3B-C2B-C1B	-2.58	104.05	107.16
21	11	410	CL7	CHB-C1B-NB	-2.58	121.53	124.26
23	4K	101	8CT	C40-C12-C13	-2.58	119.31	122.92
21	11	403	CL7	C1C-C2C-C3C	-2.58	103.18	106.94
21	24	408	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	12	506	CL7	CHC-C1C-NC	-2.57	122.09	124.45
21	43	407	CL7	CHC-C1C-NC	-2.57	122.09	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	402	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	21	403	CL7	CMB-C2B-C1B	2.57	129.29	125.37
21	3B	608	CL7	CHB-C1B-NB	-2.57	121.53	124.26
21	1C	512	CL7	CMB-C2B-C1B	2.57	129.29	125.37
21	1B	609	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	31	403	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	3B	609	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	3B	610	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	34	408	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	4B	616	CL7	CHC-C1C-NC	-2.57	122.09	124.45
21	1B	608	CL7	CHB-C1B-NB	-2.57	121.53	124.26
21	4B	609	CL7	CHB-C1B-NB	-2.57	121.53	124.26
21	3C	504	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	4D	404	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	23	410	CL7	CHB-C1B-NB	-2.57	121.53	124.26
21	43	403	CL7	C4-C3-C5	2.57	119.60	115.27
21	13	509	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	21	402	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	41	415	CL7	CMB-C2B-C1B	2.57	129.28	125.37
21	13	514	CL7	CHB-C1B-NB	-2.57	121.54	124.26
21	1C	502	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	4C	502	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	23	407	CL7	CHC-C1C-NC	-2.57	122.09	124.45
21	1B	613	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	3C	503	CL7	CAA-CBA-CGA	-2.57	105.74	113.25
21	22	511	CL7	O2D-CGD-CBD	2.57	115.83	111.27
21	32	506	CL7	CHC-C1C-NC	-2.57	122.09	124.45
21	44	410	CL7	CHC-C1C-NC	-2.57	122.09	124.45
21	22	503	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	1C	503	CL7	CAA-CBA-CGA	-2.57	105.75	113.25
21	13	516	CL7	C4-C3-C5	2.57	119.59	115.27
21	1B	611	CL7	CMB-C2B-C1B	2.57	129.28	125.37
21	14	412	CL7	CHB-C1B-NB	-2.57	121.54	124.26
21	21	408	CL7	CHC-C1C-NC	-2.57	122.09	124.45
21	13	502	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	4B	612	CL7	CMB-C2B-C1B	2.57	129.28	125.37
21	12	511	CL7	O2D-CGD-CBD	2.57	115.83	111.27
21	12	505	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	33	502	CL7	C4-C3-C5	2.57	119.59	115.27
21	11	416	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
21	41	416	CL7	C3B-C2B-C1B	-2.57	104.06	107.16
32	32	524	ZEX	C39-C29-C30	-2.57	119.33	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	13	509	CL7	CHB-C1B-NB	-2.57	121.54	124.26
21	43	410	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	32	501	CL7	C1C-C2C-C3C	-2.56	103.20	106.94
21	2B	612	CL7	CMB-C2B-C1B	2.56	129.27	125.37
21	2C	512	CL7	CMB-C2B-C1B	2.56	129.27	125.37
21	2B	614	CL7	C4C-C3C-C2C	-2.56	103.78	107.13
21	22	517	CL7	C4C-C3C-C2C	-2.56	103.78	107.13
21	11	419	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
21	41	419	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
21	34	414	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
21	24	410	CL7	CHB-C1B-NB	-2.56	121.54	124.26
21	34	410	CL7	CHB-C1B-NB	-2.56	121.54	124.26
21	11	411	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	23	412	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
21	44	414	CL7	C3B-C2B-C1B	-2.56	104.07	107.16
21	31	417	CL7	CHB-C1B-NB	-2.56	121.55	124.26
21	33	516	CL7	C4-C3-C5	2.56	119.58	115.27
21	23	418	CL7	CHB-C1B-NB	-2.56	121.55	124.26
21	33	517	CL7	CHB-C1B-NB	-2.56	121.55	124.26
21	4C	501	CL7	CAA-CBA-CGA	-2.56	105.78	113.25
21	33	514	CL7	CHB-C1B-NB	-2.56	121.55	124.26
31	4F	101	HEM	CHD-C4C-NC	2.56	127.21	124.44
21	12	514	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	14	407	CL7	CHB-C1B-NB	-2.56	121.55	124.26
31	3F	101	HEM	CHD-C4C-NC	2.56	127.20	124.44
32	43	420	ZEX	C11-C12-C13	-2.56	119.23	126.42
21	2C	501	CL7	CAA-CBA-CGA	-2.56	105.78	113.25
21	11	410	CL7	CHC-C1C-NC	-2.56	122.11	124.45
21	42	504	CL7	CHC-C1C-NC	-2.56	122.11	124.45
32	23	420	ZEX	C11-C12-C13	-2.56	119.24	126.42
21	14	409	CL7	C1-C2-C3	-2.56	121.62	126.04
21	21	419	CL7	C3B-C2B-C1B	-2.56	104.08	107.16
21	13	506	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	4B	610	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	2C	501	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
21	42	517	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
21	3B	611	CL7	CMB-C2B-C1B	2.55	129.26	125.37
21	33	509	CL7	CHB-C1B-NB	-2.55	121.55	124.26
21	13	505	CL7	C4-C3-C5	2.55	119.57	115.27
21	43	406	CL7	C4-C3-C5	2.55	119.57	115.27
21	33	509	CL7	CMB-C2B-C1B	2.55	129.26	125.37
21	1C	502	CL7	CHC-C1C-NC	-2.55	122.11	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	502	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	34	409	CL7	C1-C2-C3	-2.55	121.63	126.04
21	32	511	CL7	C7-C6-C5	-2.55	106.43	113.36
21	41	403	CL7	C1C-C2C-C3C	-2.55	103.21	106.94
21	33	511	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
21	3C	505	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	32	514	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	23	411	CL7	CHB-C1B-NB	-2.55	121.56	124.26
27	3C	516	DGD	C4E-C3E-C2E	-2.55	106.37	110.82
21	1B	616	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	4B	617	CL7	CHC-C1C-NC	-2.55	122.11	124.45
25	3B	620	SQD	O8-S-C6	-2.55	101.68	105.74
21	23	403	CL7	C4-C3-C5	2.55	119.56	115.27
21	1C	501	CL7	C7-C6-C5	-2.55	106.43	113.36
21	12	507	CL7	CED-O2D-CGD	-2.55	110.17	115.94
21	3C	501	CL7	CAA-CBA-CGA	-2.55	105.80	113.25
21	44	411	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	22	508	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	11	413	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
23	2C	514	8CT	C35-C30-C31	2.55	115.98	111.42
21	1C	501	CL7	CAA-CBA-CGA	-2.55	105.81	113.25
21	1C	504	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
21	4C	504	CL7	C3B-C2B-C1B	-2.55	104.08	107.16
21	43	410	CL7	CHB-C1B-NB	-2.55	121.56	124.26
21	21	410	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	3C	501	CL7	C4C-C3C-C2C	-2.55	103.81	107.13
21	24	405	CL7	O2A-CGA-CBA	2.55	119.91	111.91
32	13	519	ZEX	C11-C12-C13	-2.55	119.26	126.42
32	14	420	ZEX	C15-C35-C34	-2.55	118.25	123.47
32	23	401	ZEX	C7-C8-C9	-2.55	122.39	126.23
31	2F	101	HEM	CHD-C4C-NC	2.55	127.19	124.44
25	4B	621	SQD	O8-S-C6	-2.55	101.68	105.74
21	1C	505	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	31	415	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	4C	505	CL7	CMB-C2B-C1B	2.55	129.25	125.37
21	12	517	CL7	C4C-C3C-C2C	-2.55	103.81	107.13
21	21	411	CL7	C4C-C3C-C2C	-2.55	103.81	107.13
21	14	410	CL7	CHB-C1B-NB	-2.55	121.56	124.26
21	32	517	CL7	CHB-C1B-NB	-2.55	121.56	124.26
21	31	420	CL7	C3B-C2B-C1B	-2.55	104.09	107.16
21	41	403	CL7	C3B-C2B-C1B	-2.55	104.09	107.16
21	12	511	CL7	C7-C6-C5	-2.55	106.44	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4C	509	CL7	CHB-C1B-NB	-2.55	121.56	124.26
21	42	511	CL7	C7-C6-C5	-2.55	106.45	113.36
21	24	407	CL7	C4C-C3C-C2C	-2.55	103.81	107.13
21	3C	502	CL7	CHC-C1C-NC	-2.55	122.11	124.45
23	1C	514	8CT	C35-C30-C31	2.55	115.98	111.42
32	21	421	ZEX	C7-C8-C9	-2.54	122.39	126.23
21	14	407	CL7	C4C-C3C-C2C	-2.54	103.81	107.13
32	24	420	ZEX	C15-C35-C34	-2.54	118.26	123.47
23	1D	406	8CT	C13-C14-C15	-2.54	115.28	123.22
23	3C	514	8CT	C35-C30-C31	2.54	115.97	111.42
21	32	505	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
21	23	407	CL7	O2D-CGD-CBD	2.54	115.79	111.27
21	43	407	CL7	O2D-CGD-CBD	2.54	115.79	111.27
21	14	411	CL7	CMB-C2B-C1B	2.54	129.24	125.37
21	21	415	CL7	CMB-C2B-C1B	2.54	129.24	125.37
21	23	409	CL7	O2A-C1-C2	-2.54	101.95	108.64
21	33	508	CL7	O2A-C1-C2	-2.54	101.95	108.64
21	34	405	CL7	O2A-CGA-CBA	2.54	119.89	111.91
32	33	519	ZEX	C11-C12-C13	-2.54	119.27	126.42
21	32	517	CL7	C4C-C3C-C2C	-2.54	103.81	107.13
21	22	507	CL7	CED-O2D-CGD	-2.54	110.19	115.94
21	32	507	CL7	CED-O2D-CGD	-2.54	110.19	115.94
21	1B	615	CL7	CHC-C1C-NC	-2.54	122.12	124.45
21	43	409	CL7	C1C-C2C-C3C	-2.54	103.23	106.94
32	34	420	ZEX	C15-C35-C34	-2.54	118.27	123.47
21	4B	611	CL7	C4C-C3C-C2C	-2.54	103.81	107.13
23	2K	101	8CT	C40-C12-C13	-2.54	119.36	122.92
23	3K	101	8CT	C40-C12-C13	-2.54	119.36	122.92
21	22	505	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
21	4C	501	CL7	C4C-C3C-C2C	-2.54	103.81	107.13
21	43	412	CL7	C3B-C2B-C1B	-2.54	104.09	107.16
21	23	406	CL7	C4-C3-C5	2.54	119.54	115.27
21	31	404	CL7	CHB-C1B-NB	-2.54	121.57	124.26
21	22	504	CL7	CHC-C1C-NC	-2.54	122.12	124.45
21	2C	508	CL7	CHC-C1C-NC	-2.54	122.12	124.45
21	4B	614	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	41	413	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	24	409	CL7	C1-C2-C3	-2.54	121.65	126.04
21	3C	501	CL7	C7-C6-C5	-2.54	106.47	113.36
32	31	421	ZEX	C7-C8-C9	-2.54	122.40	126.23
21	3C	508	CL7	CHC-C1C-NC	-2.54	122.12	124.45
21	14	405	CL7	O2A-CGA-CBA	2.54	119.87	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	41	421	ZEX	C7-C8-C9	-2.54	122.40	126.23
21	22	511	CL7	C7-C6-C5	-2.54	106.47	113.36
21	12	511	CL7	CHB-C1B-NB	-2.54	121.57	124.26
21	44	409	CL7	C1-C2-C3	-2.54	121.66	126.04
21	22	501	CL7	C3B-C2B-C1B	-2.54	104.10	107.16
21	22	506	CL7	CMB-C2B-C1B	2.54	129.23	125.37
23	1B	618	8CT	C01-C02-C07	2.54	118.49	113.62
23	4B	619	8CT	C01-C02-C07	2.54	118.49	113.62
27	1C	516	DGD	C4E-C3E-C2E	-2.54	106.39	110.82
27	4C	516	DGD	C4E-C3E-C2E	-2.54	106.39	110.82
21	21	403	CL7	C1C-C2C-C3C	-2.54	103.24	106.94
21	24	411	CL7	CMB-C2B-C1B	2.54	129.23	125.37
21	1C	512	CL7	CMA-C3A-C2A	-2.54	110.18	116.10
21	4C	512	CL7	CMA-C3A-C2A	-2.54	110.18	116.10
21	42	501	CL7	C3B-C2B-C1B	-2.54	104.10	107.16
21	42	505	CL7	C3B-C2B-C1B	-2.54	104.10	107.16
21	34	411	CL7	CMB-C2B-C1B	2.54	129.23	125.37
21	4B	610	CL7	C4C-C3C-C2C	-2.53	103.82	107.13
21	44	405	CL7	O2A-CGA-CBA	2.53	119.86	111.91
21	14	410	CL7	CHC-C1C-NC	-2.53	122.12	124.45
21	1B	610	CL7	C4C-C3C-C2C	-2.53	103.82	107.13
21	43	409	CL7	O2A-C1-C2	-2.53	101.98	108.64
32	11	421	ZEX	C7-C8-C9	-2.53	122.41	126.23
21	12	517	CL7	CHB-C1B-NB	-2.53	121.58	124.26
21	41	411	CL7	CHB-C1B-NB	-2.53	121.58	124.26
21	3B	606	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	32	514	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	23	410	CL7	CMB-C2B-C1B	2.53	129.22	125.37
21	12	517	CL7	CAA-CBA-CGA	-2.53	105.86	113.25
21	34	407	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	21	407	CL7	CHB-C1B-NB	-2.53	121.58	124.26
21	31	407	CL7	CHB-C1B-NB	-2.53	121.58	124.26
21	42	517	CL7	CAA-CBA-CGA	-2.53	105.86	113.25
21	11	408	CL7	CHC-C1C-NC	-2.53	122.13	124.45
23	4C	514	8CT	C35-C30-C31	2.53	115.95	111.42
23	3D	406	8CT	C13-C14-C15	-2.53	115.32	123.22
21	13	509	CL7	CMB-C2B-C1B	2.53	129.22	125.37
21	33	512	CL7	CMB-C2B-C1B	2.53	129.22	125.37
21	43	410	CL7	CMB-C2B-C1B	2.53	129.22	125.37
21	42	507	CL7	CED-O2D-CGD	-2.53	110.22	115.94
21	22	513	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	2C	512	CL7	CMA-C3A-C2A	-2.53	110.20	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	501	CL7	C3B-C2B-C1B	-2.53	104.11	107.16
21	42	517	CL7	CHB-C1B-NB	-2.53	121.58	124.26
21	1C	504	CL7	C1C-C2C-C3C	-2.53	103.25	106.94
32	44	420	ZEX	C15-C35-C34	-2.53	118.30	123.47
21	1C	508	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	41	410	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	12	514	CL7	CMB-C2B-C1B	2.53	129.22	125.37
21	3C	512	CL7	CMA-C3A-C2A	-2.53	110.20	116.10
21	2B	610	CL7	CHC-C1C-NC	-2.53	122.13	124.45
23	2B	619	8CT	C01-C02-C07	2.53	118.47	113.62
23	3B	618	8CT	C01-C02-C07	2.53	118.47	113.62
21	4C	504	CL7	C1C-C2C-C3C	-2.52	103.25	106.94
21	22	516	CL7	C3B-C2B-C1B	-2.52	104.11	107.16
21	2C	501	CL7	C7-C6-C5	-2.52	106.50	113.36
21	21	413	CL7	C4C-C3C-C2C	-2.52	103.84	107.13
21	2C	502	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	3B	609	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	22	517	CL7	CAA-CBA-CGA	-2.52	105.88	113.25
21	2C	505	CL7	CMB-C2B-C1B	2.52	129.21	125.37
23	3C	514	8CT	C13-C14-C15	-2.52	115.34	123.22
21	31	413	CL7	C4C-C3C-C2C	-2.52	103.84	107.13
21	1B	609	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	4C	508	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	42	506	CL7	CMB-C2B-C1B	2.52	129.21	125.37
23	4C	514	8CT	C13-C14-C15	-2.52	115.35	123.22
21	42	512	CL7	C4C-C3C-C2C	-2.52	103.84	107.13
23	4D	406	8CT	C13-C14-C15	-2.52	115.35	123.22
21	21	403	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	31	410	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	4C	501	CL7	C7-C6-C5	-2.52	106.51	113.36
23	2D	406	8CT	C13-C14-C15	-2.52	115.35	123.22
21	4B	609	CL7	C4C-C3C-C2C	-2.52	103.84	107.13
21	12	501	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	33	510	CL7	CHB-C1B-NB	-2.52	121.59	124.26
21	42	514	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	13	508	CL7	O2A-C1-C2	-2.52	102.01	108.64
21	4B	602	CL7	C3B-C4B-NB	2.52	112.85	110.52
21	32	517	CL7	CAA-CBA-CGA	-2.52	105.89	113.25
21	2D	405	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	33	505	CL7	C4-C3-C5	2.52	119.51	115.27
21	3B	606	CL7	CHB-C1B-NB	-2.52	121.59	124.26
21	3C	504	CL7	C1C-C2C-C3C	-2.52	103.27	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1C	501	CL7	C4C-C3C-C2C	-2.52	103.85	107.13
21	14	413	CL7	C4C-C3C-C2C	-2.52	103.85	107.13
21	2B	607	CL7	C4C-C3C-C2C	-2.52	103.85	107.13
21	41	411	CL7	C4C-C3C-C2C	-2.52	103.85	107.13
21	44	413	CL7	C4C-C3C-C2C	-2.52	103.85	107.13
21	13	506	CL7	O2D-CGD-CBD	2.52	115.74	111.27
27	2C	516	DGD	C4E-C3E-C2E	-2.52	106.43	110.82
21	12	516	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	21	404	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	31	404	CL7	C3B-C2B-C1B	-2.52	104.12	107.16
21	32	506	CL7	CMB-C2B-C1B	2.52	129.20	125.37
23	1C	515	8CT	C11-C10-C03	-2.52	120.14	127.20
23	4C	515	8CT	C11-C10-C03	-2.52	120.14	127.20
23	1C	514	8CT	C13-C14-C15	-2.52	115.37	123.22
21	1B	605	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
21	4B	606	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
21	21	411	CL7	CHB-C1B-NB	-2.51	121.59	124.26
32	43	401	ZEX	C7-C8-C9	-2.51	122.44	126.23
21	13	504	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
21	24	413	CL7	C4C-C3C-C2C	-2.51	103.85	107.13
21	1A	403	CL7	CHB-C1B-NB	-2.51	121.60	124.26
21	21	404	CL7	CHB-C1B-NB	-2.51	121.60	124.26
21	13	502	CL7	C7-C6-C5	-2.51	106.53	113.36
25	1B	620	SQD	O8-S-C6	-2.51	101.74	105.74
23	2C	515	8CT	C11-C10-C03	-2.51	120.15	127.20
23	2C	514	8CT	C13-C14-C15	-2.51	115.38	123.22
21	32	506	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
21	34	406	CL7	C3B-C2B-C1B	-2.51	104.13	107.16
21	1D	405	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	4D	405	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	21	417	CL7	CHB-C1B-NB	-2.51	121.60	124.26
21	32	507	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	41	417	CL7	CHB-C1B-NB	-2.51	121.60	124.26
21	13	508	CL7	C1C-C2C-C3C	-2.51	103.28	106.94
21	33	504	CL7	C3B-C2B-C1B	-2.51	104.14	107.16
21	22	514	CL7	CHC-C1C-NC	-2.51	122.15	124.45
21	2B	609	CL7	C7-C6-C5	-2.51	106.55	113.36
21	3B	608	CL7	C7-C6-C5	-2.51	106.55	113.36
21	2D	405	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	3C	505	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	12	507	CL7	C7-C6-C5	-2.51	106.55	113.36
21	23	403	CL7	C7-C6-C5	-2.51	106.55	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	24	406	CL7	C3B-C2B-C1B	-2.51	104.14	107.16
21	41	404	CL7	CHB-C1B-NB	-2.51	121.61	124.26
21	3B	610	CL7	C4-C3-C5	2.51	119.48	115.27
23	3B	618	8CT	C19-C20-C21	-2.50	123.73	127.31
21	2B	616	CL7	CHC-C1C-NC	-2.50	122.15	124.45
21	22	507	CL7	C7-C6-C5	-2.50	106.56	113.36
21	34	404	CL7	C3B-C2B-C1B	-2.50	104.14	107.16
21	2B	611	CL7	C4C-C3C-C2C	-2.50	103.86	107.13
23	3C	515	8CT	C11-C10-C03	-2.50	120.17	127.20
21	2B	617	CL7	CHC-C1C-NC	-2.50	122.15	124.45
21	1B	608	CL7	C7-C6-C5	-2.50	106.56	113.36
21	33	502	CL7	C7-C6-C5	-2.50	106.56	113.36
21	1B	610	CL7	C4-C3-C5	2.50	119.48	115.27
21	2B	606	CL7	C3B-C2B-C1B	-2.50	104.14	107.16
25	2B	621	SQD	O8-S-C6	-2.50	101.75	105.74
32	33	525	ZEX	C7-C8-C9	-2.50	122.45	126.23
21	2B	607	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	4B	607	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	43	403	CL7	C7-C6-C5	-2.50	106.57	113.36
21	22	506	CL7	C3B-C2B-C1B	-2.50	104.14	107.16
21	13	512	CL7	CMB-C2B-C1B	2.50	129.18	125.37
21	11	418	CL7	C1C-C2C-C3C	-2.50	103.29	106.94
21	1B	603	CL7	C1-C2-C3	2.50	130.37	126.04
21	4B	604	CL7	C1-C2-C3	2.50	130.37	126.04
23	3C	514	8CT	C27-C26-C28	2.50	122.02	118.08
21	41	403	CL7	C4-C3-C5	2.50	119.47	115.27
21	3D	405	CL7	CHC-C1C-NC	-2.50	122.16	124.45
21	2B	604	CL7	C1-C2-C3	2.50	130.36	126.04
21	12	506	CL7	CMB-C2B-C1B	2.50	129.17	125.37
32	13	525	ZEX	C7-C8-C9	-2.50	122.46	126.23
21	14	406	CL7	C3B-C2B-C1B	-2.50	104.15	107.16
21	22	514	CL7	CMB-C2B-C1B	2.50	129.17	125.37
21	13	510	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	43	411	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	12	512	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
21	22	511	CL7	CHB-C1B-NB	-2.50	121.61	124.26
21	12	506	CL7	C3B-C2B-C1B	-2.50	104.15	107.16
21	41	404	CL7	C3B-C2B-C1B	-2.49	104.15	107.16
21	22	507	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	2C	504	CL7	C1C-C2C-C3C	-2.49	103.30	106.94
21	41	407	CL7	CHB-C1B-NB	-2.49	121.62	124.26
23	2B	619	8CT	C19-C20-C21	-2.49	123.75	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3A	401	CL7	C6-C5-C3	-2.49	106.92	113.45
21	31	414	CL7	CMA-C3A-C2A	-2.49	110.28	116.10
21	1B	606	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	24	414	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
23	1D	406	8CT	C05-C04-C03	2.49	114.32	110.48
21	4A	401	CL7	C6-C5-C3	-2.49	106.92	113.45
21	23	409	CL7	C1C-C2C-C3C	-2.49	103.30	106.94
21	14	404	CL7	C3B-C2B-C1B	-2.49	104.15	107.16
21	2B	609	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	3B	608	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	1C	501	CL7	C3B-C2B-C1B	-2.49	104.15	107.16
21	33	506	CL7	O2D-CGD-CBD	2.49	115.70	111.27
21	4B	609	CL7	C7-C6-C5	-2.49	106.59	113.36
21	32	511	CL7	CHB-C1B-NB	-2.49	121.62	124.26
21	4C	506	CL7	C1C-C2C-C3C	-2.49	103.30	106.94
21	11	414	CL7	CMA-C3A-C2A	-2.49	110.29	116.10
21	41	414	CL7	CMA-C3A-C2A	-2.49	110.29	116.10
21	34	413	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	33	508	CL7	C1C-C2C-C3C	-2.49	103.31	106.94
21	1B	601	CL7	C1C-C2C-C3C	-2.49	103.31	106.94
21	4B	602	CL7	C1C-C2C-C3C	-2.49	103.31	106.94
21	32	507	CL7	C7-C6-C5	-2.49	106.60	113.36
21	4A	403	CL7	CAA-CBA-CGA	-2.49	105.98	113.25
24	21	401	LMG	O1-C7-C8	-2.49	104.90	110.90
21	42	507	CL7	C7-C6-C5	-2.49	106.60	113.36
23	1B	626	8CT	C22-C21-C20	-2.49	119.44	122.92
24	31	401	LMG	O1-C7-C8	-2.49	104.90	110.90
21	3B	605	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
21	4C	501	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
21	42	516	CL7	C3B-C2B-C1B	-2.49	104.16	107.16
32	24	419	ZEX	C38-C24-C25	-2.49	106.91	110.87
21	4C	503	CL7	C1C-C2C-C3C	-2.49	103.31	106.94
21	2C	506	CL7	C1C-C2C-C3C	-2.49	103.31	106.94
21	1B	608	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	11	411	CL7	CHB-C1B-NB	-2.49	121.63	124.26
21	1C	503	CL7	C1C-C2C-C3C	-2.49	103.31	106.94
21	23	413	CL7	CMB-C2B-C1B	2.48	129.15	125.37
21	1B	606	CL7	CHB-C1B-NB	-2.48	121.63	124.26
23	4K	101	8CT	C22-C21-C20	-2.48	119.44	122.92
21	2B	611	CL7	C4-C3-C5	2.48	119.45	115.27
21	4B	611	CL7	C4-C3-C5	2.48	119.45	115.27
21	43	410	CL7	O2A-CGA-O1A	-2.48	117.32	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	603	CL7	C1-C2-C3	2.48	130.34	126.04
23	1K	101	8CT	C22-C21-C20	-2.48	119.44	122.92
21	4C	501	CL7	CMB-C2B-C1B	2.48	129.15	125.37
21	2A	403	CL7	CAA-CBA-CGA	-2.48	106.00	113.25
21	4B	610	CL7	CMB-C2B-C1B	2.48	129.15	125.37
21	44	407	CL7	CMB-C2B-C1B	2.48	129.15	125.37
21	41	408	CL7	C4-C3-C5	2.48	119.45	115.27
21	11	404	CL7	CHB-C1B-NB	-2.48	121.63	124.26
21	31	411	CL7	CHB-C1B-NB	-2.48	121.63	124.26
23	2K	101	8CT	C22-C21-C20	-2.48	119.45	122.92
21	11	403	CL7	C4-C3-C5	2.48	119.44	115.27
21	12	513	CL7	C4C-C3C-C2C	-2.48	103.89	107.13
21	31	418	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	4B	607	CL7	C4C-C3C-C2C	-2.48	103.89	107.13
21	31	409	CL7	CMB-C2B-C1B	2.48	129.15	125.37
21	43	418	CL7	C4-C3-C5	2.48	120.08	114.60
21	1A	401	CL7	C6-C5-C3	-2.48	106.95	113.45
21	12	515	CL7	C4C-C3C-C2C	-2.48	103.89	107.13
21	42	514	CL7	CMB-C2B-C1B	2.48	129.14	125.37
21	22	512	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	32	512	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	42	513	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
23	3B	626	8CT	C22-C21-C20	-2.48	119.45	122.92
23	4C	514	8CT	C27-C26-C28	2.48	121.98	118.08
21	3B	602	CL7	O2A-CGA-O1A	-2.48	117.34	123.59
21	42	506	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
21	1B	602	CL7	O2A-CGA-O1A	-2.48	117.34	123.59
21	3A	401	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	42	507	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	1C	517	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	4C	517	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	23	405	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
21	1B	601	CL7	C3B-C4B-NB	2.48	112.81	110.52
21	1C	509	CL7	C1-C2-C3	2.48	130.33	126.04
21	3B	613	CL7	C7-C6-C5	-2.48	106.63	113.36
21	43	413	CL7	CMB-C2B-C1B	2.48	129.14	125.37
21	44	404	CL7	C3B-C2B-C1B	-2.48	104.17	107.16
21	24	409	CL7	CAA-CBA-CGA	-2.48	106.02	113.25
21	2A	401	CL7	C6-C5-C3	-2.48	106.96	113.45
21	24	407	CL7	CMB-C2B-C1B	2.48	129.14	125.37
21	3B	601	CL7	C3B-C4B-NB	2.48	112.81	110.52
21	44	409	CL7	CAA-CBA-CGA	-2.48	106.02	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	511	CL7	CHB-C1B-NB	-2.48	121.64	124.26
21	11	408	CL7	C4-C3-C5	2.48	119.44	115.27
23	1C	514	8CT	C27-C26-C28	2.48	121.98	118.08
21	2B	603	CL7	O2A-CGA-O1A	-2.48	117.34	123.59
32	13	520	ZEX	C2-C3-C4	-2.47	106.92	110.30
21	2C	501	CL7	C3B-C2B-C1B	-2.47	104.17	107.16
21	3C	501	CL7	C3B-C2B-C1B	-2.47	104.17	107.16
21	3C	506	CL7	C1C-C2C-C3C	-2.47	103.33	106.94
24	41	401	LMG	O1-C7-C8	-2.47	104.93	110.90
21	4B	603	CL7	O2A-CGA-O1A	-2.47	117.35	123.59
21	21	414	CL7	CMA-C3A-C2A	-2.47	110.33	116.10
21	31	403	CL7	C4-C3-C5	2.47	119.43	115.27
21	42	502	CL7	C4-C3-C5	2.47	119.43	115.27
21	1A	403	CL7	CAA-CBA-CGA	-2.47	106.03	113.25
21	12	507	CL7	C4C-C3C-C2C	-2.47	103.90	107.13
21	33	506	CL7	C4C-C3C-C2C	-2.47	103.90	107.13
21	14	404	CL7	CHB-C1B-NB	-2.47	121.64	124.26
21	22	517	CL7	CHB-C1B-NB	-2.47	121.64	124.26
21	44	404	CL7	CHB-C1B-NB	-2.47	121.64	124.26
21	3C	509	CL7	C1-C2-C3	2.47	130.32	126.04
21	41	418	CL7	C1C-C2C-C3C	-2.47	103.33	106.94
21	32	502	CL7	C4-C3-C5	2.47	119.43	115.27
21	11	409	CL7	CMB-C2B-C1B	2.47	129.13	125.37
21	41	409	CL7	CMB-C2B-C1B	2.47	129.13	125.37
21	3A	403	CL7	CHB-C1B-NB	-2.47	121.64	124.26
21	3B	614	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	21	403	CL7	C4-C3-C5	2.47	119.43	115.27
21	3C	510	CL7	O2D-CGD-CBD	2.47	115.66	111.27
21	11	407	CL7	CHB-C1B-NB	-2.47	121.64	124.26
32	24	419	ZEX	C11-C12-C13	-2.47	119.48	126.42
21	2C	505	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	33	509	CL7	O2A-CGA-O1A	-2.47	117.36	123.59
21	13	509	CL7	O2A-CGA-O1A	-2.47	117.36	123.59
21	2B	602	CL7	C1C-C2C-C3C	-2.47	103.34	106.94
23	3K	101	8CT	C22-C21-C20	-2.47	119.47	122.92
21	33	501	CL7	C3B-C4B-NB	2.47	112.81	110.52
23	2C	514	8CT	C27-C26-C28	2.47	121.97	118.08
21	2B	610	CL7	CMB-C2B-C1B	2.47	129.13	125.37
21	3A	403	CL7	CAA-CBA-CGA	-2.47	106.04	113.25
21	23	418	CL7	C4-C3-C5	2.47	120.05	114.60
23	4B	619	8CT	C19-C20-C21	-2.47	123.79	127.31
21	11	404	CL7	C3B-C2B-C1B	-2.47	104.18	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	43	405	CL7	C3B-C2B-C1B	-2.47	104.18	107.16
21	34	404	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	24	404	CL7	C3B-C2B-C1B	-2.47	104.18	107.16
21	32	516	CL7	C3B-C2B-C1B	-2.47	104.18	107.16
21	2C	506	CL7	CHB-C1B-NB	-2.47	121.65	124.26
21	1C	501	CL7	CMB-C2B-C1B	2.47	129.12	125.37
21	21	409	CL7	CMB-C2B-C1B	2.47	129.12	125.37
32	43	421	ZEX	C35-C15-C14	-2.47	118.42	123.47
32	14	419	ZEX	C38-C24-C25	-2.47	106.95	110.87
32	13	522	ZEX	C31-C30-C29	-2.47	123.79	127.31
21	2C	501	CL7	CMB-C2B-C1B	2.46	129.12	125.37
21	3C	501	CL7	CMB-C2B-C1B	2.46	129.12	125.37
24	11	401	LMG	O1-C7-C8	-2.46	104.95	110.90
21	2B	602	CL7	C3B-C4B-NB	2.46	112.80	110.52
21	21	408	CL7	C4-C3-C5	2.46	119.42	115.27
21	33	517	CL7	C4-C3-C5	2.46	120.05	114.60
21	31	411	CL7	C3B-C2B-C1B	-2.46	104.19	107.16
32	44	419	ZEX	C11-C12-C13	-2.46	119.50	126.42
21	3C	517	CL7	C1C-C2C-C3C	-2.46	103.34	106.94
21	2C	502	CL7	CMB-C2B-C1B	2.46	129.12	125.37
21	3C	502	CL7	CMB-C2B-C1B	2.46	129.12	125.37
21	14	414	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	31	408	CL7	C4-C3-C5	2.46	119.41	115.27
21	1B	609	CL7	CMB-C2B-C1B	2.46	129.12	125.37
32	44	419	ZEX	C38-C24-C25	-2.46	106.95	110.87
21	34	409	CL7	CAA-CBA-CGA	-2.46	106.06	113.25
21	3D	405	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	31	408	CL7	O2D-CGD-O1D	-2.46	119.03	123.84
32	34	419	ZEX	C11-C12-C13	-2.46	119.50	126.42
21	14	409	CL7	CAA-CBA-CGA	-2.46	106.06	113.25
21	44	411	CL7	C4-C3-C5	2.46	119.41	115.27
21	23	410	CL7	O2A-CGA-O1A	-2.46	117.38	123.59
21	2B	614	CL7	C7-C6-C5	-2.46	106.68	113.36
21	1C	506	CL7	CHB-C1B-NB	-2.46	121.65	124.26
21	12	509	CL7	CHB-C1B-NB	-2.46	121.65	124.26
21	2B	610	CL7	CHB-C1B-NB	-2.46	121.65	124.26
21	1C	510	CL7	O2D-CGD-CBD	2.46	115.64	111.27
21	32	513	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	4C	510	CL7	O2D-CGD-CBD	2.46	115.64	111.27
21	3B	615	CL7	C1C-C2C-C3C	-2.46	103.35	106.94
21	2A	407	CL7	CHB-C1B-NB	-2.46	121.65	124.26
21	1B	613	CL7	C7-C6-C5	-2.46	106.68	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2C	504	CL7	CHC-C1C-NC	-2.46	122.19	124.45
21	42	517	CL7	C7-C6-C5	-2.46	106.68	113.36
21	13	517	CL7	C4-C3-C5	2.46	120.03	114.60
23	1B	618	8CT	C19-C20-C21	-2.46	123.80	127.31
21	3B	609	CL7	CMB-C2B-C1B	2.46	129.11	125.37
23	2D	406	8CT	C05-C04-C03	2.46	114.27	110.48
21	4B	614	CL7	C7-C6-C5	-2.46	106.68	113.36
21	3B	601	CL7	C1C-C2C-C3C	-2.46	103.35	106.94
21	34	411	CL7	C4-C3-C5	2.46	119.41	115.27
21	1C	504	CL7	CHC-C1C-NC	-2.46	122.20	124.45
32	14	419	ZEX	C11-C12-C13	-2.46	119.51	126.42
23	3C	514	8CT	C14-C13-C12	-2.46	123.80	127.31
21	4C	509	CL7	C1-C2-C3	2.46	130.29	126.04
21	21	405	CL7	C1C-C2C-C3C	-2.46	103.36	106.94
21	23	412	CL7	CMB-C2B-C1B	2.46	129.11	125.37
21	2B	616	CL7	C4-C3-C5	2.46	120.03	114.60
21	14	411	CL7	C7-C6-C5	-2.46	106.69	113.36
21	22	512	CL7	O2D-CGD-O1D	-2.46	119.04	123.84
32	33	520	ZEX	C2-C3-C4	-2.45	106.94	110.30
32	34	419	ZEX	C38-C24-C25	-2.45	106.96	110.87
21	1C	506	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
23	2B	601	8CT	C22-C21-C20	-2.45	119.48	122.92
21	34	414	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	41	405	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
32	23	421	ZEX	C2-C3-C4	-2.45	106.95	110.30
32	43	421	ZEX	C2-C3-C4	-2.45	106.95	110.30
21	34	407	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	3C	508	CL7	CHB-C1B-NB	-2.45	121.66	124.26
21	32	515	CL7	C3B-C2B-C1B	-2.45	104.20	107.16
21	13	506	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	3B	615	CL7	C4-C3-C5	2.45	120.02	114.60
32	23	421	ZEX	C35-C15-C14	-2.45	118.45	123.47
21	4A	401	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	33	511	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	33	501	CL7	C4-C3-C5	2.45	119.39	115.27
21	21	404	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	31	404	CL7	CMB-C2B-C1B	2.45	129.10	125.37
23	1C	514	8CT	C14-C13-C12	-2.45	123.81	127.31
21	43	402	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	1C	512	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	43	407	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	24	404	CL7	CHB-C1B-NB	-2.45	121.66	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	515	CL7	C3B-C2B-C1B	-2.45	104.20	107.16
21	24	411	CL7	C7-C6-C5	-2.45	106.71	113.36
21	34	411	CL7	C7-C6-C5	-2.45	106.71	113.36
21	32	517	CL7	C7-C6-C5	-2.45	106.71	113.36
21	21	418	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	23	407	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	12	517	CL7	C7-C6-C5	-2.45	106.71	113.36
21	14	407	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	41	404	CL7	CMB-C2B-C1B	2.45	129.10	125.37
21	2D	405	CL7	CAA-CBA-CGA	-2.45	106.01	112.51
21	4B	616	CL7	C1C-C2C-C3C	-2.45	103.37	106.94
21	2A	403	CL7	CHB-C1B-NB	-2.45	121.67	124.26
21	13	515	CL7	C3B-C2B-C1B	-2.45	104.21	107.16
21	14	411	CL7	CHB-C1B-NB	-2.45	121.67	124.26
23	3A	404	8CT	C22-C21-C20	-2.45	119.50	122.92
21	12	512	CL7	O2D-CGD-O1D	-2.45	119.06	123.84
21	3C	504	CL7	CHC-C1C-NC	-2.45	122.21	124.45
21	4C	504	CL7	CHC-C1C-NC	-2.45	122.21	124.45
21	2C	510	CL7	O2D-CGD-CBD	2.45	115.61	111.27
23	4D	406	8CT	C05-C04-C03	2.45	114.25	110.48
21	12	510	CL7	C4C-C3C-C2C	-2.44	103.94	107.13
21	4B	612	CL7	C4-C3-C5	2.44	119.38	115.27
23	4A	404	8CT	C22-C21-C20	-2.44	119.50	122.92
21	44	405	CL7	C3B-C2B-C1B	-2.44	104.21	107.16
21	2B	605	CL7	C1C-C2C-C3C	-2.44	103.37	106.94
21	43	402	CL7	C4-C3-C5	2.44	119.38	115.27
21	3D	405	CL7	CAA-CBA-CGA	-2.44	106.02	112.51
21	4A	403	CL7	CHB-C1B-NB	-2.44	121.67	124.26
21	22	502	CL7	C4-C3-C5	2.44	119.38	115.27
21	1D	405	CL7	CAA-CBA-CGA	-2.44	106.03	112.51
21	2C	508	CL7	C1C-C2C-C3C	-2.44	103.38	106.94
21	31	409	CL7	C3B-C2B-C1B	-2.44	104.21	107.16
21	33	515	CL7	C3B-C2B-C1B	-2.44	104.21	107.16
21	44	414	CL7	C4C-C3C-C2C	-2.44	103.94	107.13
21	4B	606	CL7	C1C-C2C-C3C	-2.44	103.38	106.94
21	41	402	CL7	C3B-C2B-C1B	-2.44	104.22	107.16
21	12	502	CL7	C4-C3-C5	2.44	119.38	115.27
21	22	517	CL7	C7-C6-C5	-2.44	106.73	113.36
21	32	512	CL7	O2D-CGD-O1D	-2.44	119.07	123.84
21	1C	502	CL7	CMB-C2B-C1B	2.44	129.09	125.37
21	4C	502	CL7	CMB-C2B-C1B	2.44	129.09	125.37
21	1C	505	CL7	C4C-C3C-C2C	-2.44	103.95	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	408	CL7	O2D-CGD-O1D	-2.44	119.07	123.84
21	42	515	CL7	C3B-C2B-C1B	-2.44	104.22	107.16
32	43	401	ZEX	C31-C32-C33	-2.44	119.56	126.42
21	34	413	CL7	C7-C6-C5	-2.44	106.73	113.36
21	4C	511	CL7	C3B-C2B-C1B	-2.44	104.22	107.16
21	24	409	CL7	O2A-C1-C2	2.44	115.05	108.64
21	24	413	CL7	C7-C6-C5	-2.44	106.73	113.36
21	44	409	CL7	O2A-C1-C2	2.44	115.05	108.64
23	3D	406	8CT	C05-C04-C03	2.44	114.23	110.48
21	3C	506	CL7	CHB-C1B-NB	-2.44	121.68	124.26
21	1B	615	CL7	C4-C3-C5	2.44	119.99	114.60
21	13	511	CL7	CMB-C2B-C1B	2.44	129.08	125.37
23	4A	404	8CT	C11-C10-C03	-2.44	120.36	127.20
23	1A	404	8CT	C22-C21-C20	-2.44	119.51	122.92
21	2C	503	CL7	C1C-C2C-C3C	-2.44	103.38	106.94
21	3C	503	CL7	C1C-C2C-C3C	-2.44	103.38	106.94
21	24	411	CL7	C4-C3-C5	2.44	119.37	115.27
21	3A	407	CL7	CHB-C1B-NB	-2.44	121.68	124.26
32	13	520	ZEX	C35-C15-C14	-2.44	118.48	123.47
21	4D	405	CL7	CAA-CBA-CGA	-2.44	106.04	112.51
21	44	410	CL7	C1C-C2C-C3C	-2.44	103.38	106.94
21	1B	614	CL7	C4C-C3C-C2C	-2.44	103.95	107.13
21	13	501	CL7	C4-C3-C5	2.44	119.37	115.27
21	11	405	CL7	C1C-C2C-C3C	-2.44	103.38	106.94
21	44	411	CL7	C7-C6-C5	-2.44	106.75	113.36
32	11	421	ZEX	C31-C32-C33	-2.44	119.58	126.42
21	14	413	CL7	C7-C6-C5	-2.43	106.75	113.36
21	24	404	CL7	C7-C6-C5	-2.43	106.75	113.36
21	21	419	CL7	C4C-C3C-C2C	-2.43	103.95	107.13
21	4C	512	CL7	C3B-C2B-C1B	-2.43	104.22	107.16
21	22	510	CL7	C4C-C3C-C2C	-2.43	103.95	107.13
32	13	519	ZEX	C39-C29-C30	-2.43	119.51	122.92
32	23	420	ZEX	C39-C29-C30	-2.43	119.51	122.92
21	42	512	CL7	O2D-CGD-O1D	-2.43	119.08	123.84
21	11	411	CL7	C3B-C2B-C1B	-2.43	104.22	107.16
21	41	411	CL7	C3B-C2B-C1B	-2.43	104.22	107.16
21	11	412	CL7	CMB-C2B-C1B	2.43	129.07	125.37
21	41	412	CL7	CMB-C2B-C1B	2.43	129.07	125.37
21	1D	405	CL7	CHC-C1C-NC	-2.43	122.22	124.45
21	31	405	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
32	33	522	ZEX	C31-C30-C29	-2.43	123.84	127.31
21	32	510	CL7	C4C-C3C-C2C	-2.43	103.96	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	512	CL7	C4-C3-C5	2.43	119.36	115.27
21	1C	508	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	4C	508	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	1A	407	CL7	CHB-C1B-NB	-2.43	121.68	124.26
32	22	519	ZEX	C28-C27-C26	-2.43	122.93	127.09
21	21	416	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	4C	506	CL7	CHB-C1B-NB	-2.43	121.68	124.26
23	2A	404	8CT	C11-C10-C03	-2.43	120.37	127.20
23	3A	404	8CT	C11-C10-C03	-2.43	120.37	127.20
21	22	515	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
23	1B	618	8CT	C28-C26-C25	-2.43	115.21	118.94
21	2C	509	CL7	C1-C2-C3	2.43	130.25	126.04
32	23	401	ZEX	C31-C32-C33	-2.43	119.59	126.42
21	14	406	CL7	CHB-C1B-NB	-2.43	121.68	124.26
21	44	413	CL7	C7-C6-C5	-2.43	106.76	113.36
21	3C	508	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
23	1A	404	8CT	C11-C10-C03	-2.43	120.38	127.20
32	41	421	ZEX	C31-C32-C33	-2.43	119.59	126.42
21	4C	513	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	32	505	CL7	CGD-CBD-CAD	2.43	118.60	110.73
21	11	409	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	21	411	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	23	402	CL7	C3B-C4B-NB	2.43	112.77	110.52
21	3B	609	CL7	CHB-C1B-NB	-2.43	121.69	124.26
21	3B	605	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	41	408	CL7	CMB-C2B-C1B	2.43	129.07	125.37
21	4C	509	CL7	CAA-CBA-CGA	-2.43	106.16	113.25
21	2B	615	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	4C	505	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	1B	606	CL7	CHC-C1C-NC	-2.43	122.22	124.45
32	33	525	ZEX	C31-C32-C33	-2.43	119.60	126.42
21	44	404	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	22	510	CL7	C4-C3-C5	2.43	119.35	115.27
21	23	402	CL7	C4-C3-C5	2.43	119.35	115.27
21	24	405	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	1B	609	CL7	CHB-C1B-NB	-2.43	121.69	124.26
21	4C	508	CL7	CHB-C1B-NB	-2.43	121.69	124.26
23	4B	601	8CT	C22-C21-C20	-2.43	119.53	122.92
32	24	419	ZEX	C1-C6-C5	-2.43	119.20	122.61
32	43	421	ZEX	C1-C6-C5	-2.43	119.20	122.61
21	2C	517	CL7	C1C-C2C-C3C	-2.43	103.40	106.94
21	34	410	CL7	C1C-C2C-C3C	-2.43	103.40	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	32	510	CL7	C4-C3-C5	2.43	119.35	115.27
21	44	404	CL7	C7-C6-C5	-2.43	106.77	113.36
21	14	405	CL7	C3B-C2B-C1B	-2.43	104.23	107.16
21	21	412	CL7	CMB-C2B-C1B	2.42	129.06	125.37
21	44	406	CL7	CHB-C1B-NB	-2.42	121.69	124.26
21	14	404	CL7	C7-C6-C5	-2.42	106.78	113.36
32	23	423	ZEX	C31-C30-C29	-2.42	123.85	127.31
21	13	503	CL7	C4-C3-C5	2.42	119.35	115.27
21	33	501	CL7	C1C-C2C-C3C	-2.42	103.40	106.94
21	43	412	CL7	CMB-C2B-C1B	2.42	129.06	125.37
21	4C	512	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	13	501	CL7	C1C-C2C-C3C	-2.42	103.40	106.94
21	14	410	CL7	C1C-C2C-C3C	-2.42	103.40	106.94
21	11	402	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
21	41	409	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
32	33	520	ZEX	C35-C15-C14	-2.42	118.51	123.47
21	31	413	CL7	O2D-CGD-CBD	2.42	115.57	111.27
21	4B	616	CL7	C4-C3-C5	2.42	119.95	114.60
21	12	510	CL7	C4-C3-C5	2.42	119.35	115.27
21	42	510	CL7	C4-C3-C5	2.42	119.35	115.27
21	34	404	CL7	C7-C6-C5	-2.42	106.78	113.36
23	2B	601	8CT	C40-C12-C13	-2.42	119.53	122.92
21	11	404	CL7	CMB-C2B-C1B	2.42	129.06	125.37
21	12	502	CL7	C1C-C2C-C3C	-2.42	103.40	106.94
21	12	516	CL7	CAA-CBA-CGA	-2.42	106.17	113.25
32	14	419	ZEX	C1-C6-C5	-2.42	119.20	122.61
21	43	416	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
21	12	505	CL7	CGD-CBD-CAD	2.42	118.58	110.73
21	42	505	CL7	CGD-CBD-CAD	2.42	118.58	110.73
21	12	503	CL7	C4-C3-C5	2.42	119.34	115.27
32	11	421	ZEX	C8-C7-C6	-2.42	120.40	127.20
21	21	418	CL7	CAC-C3C-C2C	2.42	131.67	127.53
21	24	406	CL7	CHB-C1B-NB	-2.42	121.69	124.26
21	34	406	CL7	CHB-C1B-NB	-2.42	121.69	124.26
21	4A	407	CL7	CHB-C1B-NB	-2.42	121.69	124.26
32	31	421	ZEX	C31-C32-C33	-2.42	119.62	126.42
32	21	421	ZEX	C8-C7-C6	-2.42	120.41	127.20
21	3C	509	CL7	CAA-CBA-CGA	-2.42	106.18	113.25
32	34	403	ZEX	C39-C29-C30	-2.42	119.53	122.92
21	2A	401	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	23	416	CL7	C3B-C2B-C1B	-2.42	104.24	107.16
21	2B	616	CL7	C1C-C2C-C3C	-2.42	103.41	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	502	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	2C	508	CL7	CHB-C1B-NB	-2.42	121.70	124.26
32	44	419	ZEX	C1-C6-C5	-2.42	119.21	122.61
32	13	525	ZEX	C31-C32-C33	-2.42	119.62	126.42
21	1B	604	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	2B	606	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
32	43	423	ZEX	C31-C30-C29	-2.42	123.86	127.31
21	2C	513	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	2C	509	CL7	CAA-CBA-CGA	-2.42	106.19	113.25
21	22	509	CL7	CHB-C1B-NB	-2.42	121.70	124.26
21	32	503	CL7	C4-C3-C5	2.42	119.34	115.27
32	31	421	ZEX	C8-C7-C6	-2.42	120.42	127.20
21	3C	512	CL7	C4C-C3C-C2C	-2.42	103.98	107.13
21	4B	615	CL7	C4C-C3C-C2C	-2.42	103.98	107.13
21	41	408	CL7	O2D-CGD-O1D	-2.42	119.11	123.84
32	23	421	ZEX	C1-C6-C5	-2.42	119.21	122.61
32	41	421	ZEX	C8-C7-C6	-2.42	120.42	127.20
21	3C	513	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
32	21	421	ZEX	C31-C32-C33	-2.42	119.63	126.42
23	4C	518	8CT	C18-C19-C20	-2.41	118.53	123.47
21	4D	405	CL7	CHC-C1C-NC	-2.41	122.23	124.45
23	4C	514	8CT	C14-C13-C12	-2.41	123.86	127.31
21	32	509	CL7	CHB-C1B-NB	-2.41	121.70	124.26
32	24	403	ZEX	C39-C29-C30	-2.41	119.54	122.92
21	31	412	CL7	CMB-C2B-C1B	2.41	129.05	125.37
32	13	520	ZEX	C1-C6-C5	-2.41	119.21	122.61
21	22	516	CL7	CAA-CBA-CGA	-2.41	106.20	113.25
21	32	516	CL7	CAA-CBA-CGA	-2.41	106.20	113.25
21	3A	403	CL7	O2A-CGA-CBA	2.41	119.48	111.91
21	14	409	CL7	O2A-C1-C2	2.41	114.98	108.64
21	22	503	CL7	O2D-CGD-CBD	2.41	115.56	111.27
21	1A	401	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	21	406	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	42	515	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	42	509	CL7	CHB-C1B-NB	-2.41	121.70	124.26
21	44	407	CL7	CHD-C1D-ND	-2.41	121.70	124.26
21	4B	605	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
32	12	519	ZEX	C28-C27-C26	-2.41	122.97	127.09
32	42	519	ZEX	C28-C27-C26	-2.41	122.97	127.09
21	22	505	CL7	CGD-CBD-CAD	2.41	118.55	110.73
32	14	403	ZEX	C39-C29-C30	-2.41	119.54	122.92
21	1C	513	CL7	C1C-C2C-C3C	-2.41	103.42	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	408	CL7	CMB-C2B-C1B	2.41	129.04	125.37
21	32	512	CL7	C4-C3-C5	2.41	119.33	115.27
21	12	515	CL7	C3B-C2B-C1B	-2.41	104.25	107.16
21	23	402	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	3B	604	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	33	518	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	14	411	CL7	C4-C3-C5	2.41	119.33	115.27
21	1C	508	CL7	CHB-C1B-NB	-2.41	121.70	124.26
21	2B	612	CL7	C4-C3-C5	2.41	119.33	115.27
21	42	512	CL7	C4-C3-C5	2.41	119.33	115.27
21	11	406	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	32	515	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	1B	615	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	24	411	CL7	CHB-C1B-NB	-2.41	121.71	124.26
21	2C	511	CL7	C3B-C2B-C1B	-2.41	104.25	107.16
21	3C	511	CL7	C3B-C2B-C1B	-2.41	104.25	107.16
21	11	416	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
21	42	510	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
23	4C	515	8CT	C27-C26-C25	-2.41	119.55	122.92
21	34	409	CL7	O2A-C1-C2	2.41	114.97	108.64
21	13	501	CL7	C3B-C4B-NB	2.41	112.75	110.52
32	32	519	ZEX	C28-C27-C26	-2.41	122.97	127.09
23	2C	514	8CT	C14-C13-C12	-2.41	123.87	127.31
21	1B	602	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
21	41	416	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
21	2A	403	CL7	O2A-CGA-CBA	2.41	119.47	111.91
21	1C	509	CL7	CAA-CBA-CGA	-2.41	106.22	113.25
21	21	408	CL7	O2D-CGD-O1D	-2.41	119.13	123.84
21	31	416	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
21	21	409	CL7	C3B-C2B-C1B	-2.41	104.25	107.16
21	4A	403	CL7	O2A-CGA-CBA	2.41	119.46	111.91
21	1B	611	CL7	C4-C3-C5	2.41	119.32	115.27
21	4B	610	CL7	CHB-C1B-NB	-2.41	121.71	124.26
21	4B	612	CL7	CHB-C1B-NB	-2.41	121.71	124.26
21	44	411	CL7	CHB-C1B-NB	-2.41	121.71	124.26
23	1C	515	8CT	C27-C26-C25	-2.41	119.55	122.92
21	13	518	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
21	2C	512	CL7	C4C-C3C-C2C	-2.41	103.99	107.13
21	43	417	CL7	CAA-C2A-C1A	-2.41	104.27	112.19
21	34	404	CL7	CHB-C1B-NB	-2.40	121.71	124.26
21	33	515	CL7	C4C-C3C-C2C	-2.40	103.99	107.13
23	2B	619	8CT	C28-C26-C25	-2.40	115.25	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	503	CL7	C4-C3-C5	2.40	119.32	115.27
32	34	419	ZEX	C1-C6-C5	-2.40	119.23	122.61
21	11	413	CL7	O2D-CGD-CBD	2.40	115.54	111.27
21	4B	607	CL7	CHC-C1C-NC	-2.40	122.25	124.45
21	1B	605	CL7	C1C-C2C-C3C	-2.40	103.43	106.94
23	3C	515	8CT	C27-C26-C25	-2.40	119.56	122.92
23	4B	619	8CT	C28-C26-C25	-2.40	115.25	118.94
21	24	405	CL7	C1C-C2C-C3C	-2.40	103.43	106.94
21	32	503	CL7	O2D-CGD-CBD	2.40	115.54	111.27
21	22	503	CL7	C4-C3-C5	2.40	119.31	115.27
23	3B	618	8CT	C28-C26-C25	-2.40	115.25	118.94
21	33	516	CL7	CAA-C2A-C1A	-2.40	104.28	112.19
23	2C	518	8CT	C18-C19-C20	-2.40	118.55	123.47
21	1A	403	CL7	O2A-CGA-CBA	2.40	119.45	111.91
21	4C	510	CL7	C1C-C2C-C3C	-2.40	103.43	106.94
21	13	508	CL7	CHC-C1C-NC	-2.40	122.25	124.45
21	21	416	CL7	CMA-C3A-C2A	-2.40	110.50	116.10
21	43	402	CL7	C3B-C4B-NB	2.40	112.74	110.52
21	31	418	CL7	CAC-C3C-C2C	2.40	131.63	127.53
21	41	418	CL7	CAC-C3C-C2C	2.40	131.63	127.53
21	11	416	CL7	CMA-C3A-C2A	-2.40	110.50	116.10
21	3C	507	CL7	CHB-C1B-NB	-2.40	121.72	124.26
21	1B	604	CL7	C7-C6-C5	-2.40	106.84	113.36
21	2C	512	CL7	C3B-C2B-C1B	-2.40	104.27	107.16
23	4B	601	8CT	C40-C12-C13	-2.40	119.56	122.92
23	1B	626	8CT	C40-C12-C13	-2.40	119.56	122.92
21	12	503	CL7	O2D-CGD-CBD	2.40	115.53	111.27
21	42	503	CL7	O2D-CGD-CBD	2.40	115.53	111.27
21	2B	605	CL7	C7-C6-C5	-2.40	106.85	113.36
23	2C	515	8CT	C27-C26-C25	-2.40	119.57	122.92
21	24	404	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
21	43	419	CL7	C4C-C3C-C2C	-2.40	104.00	107.13
21	3C	512	CL7	C3B-C2B-C1B	-2.40	104.27	107.16
21	42	516	CL7	CAA-CBA-CGA	-2.40	106.25	113.25
21	32	502	CL7	C1C-C2C-C3C	-2.39	103.44	106.94
21	1C	511	CL7	C3B-C2B-C1B	-2.39	104.27	107.16
23	3B	626	8CT	C40-C12-C13	-2.39	119.57	122.92
31	2F	101	HEM	C4D-ND-C1D	2.39	107.55	105.07
21	31	406	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	4B	604	CL7	C1C-C2C-C3C	-2.39	103.44	106.94
21	14	404	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	43	402	CL7	CMB-C2B-C1B	2.39	129.01	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	402	CL7	C3B-C2B-C1B	-2.39	104.27	107.16
21	34	407	CL7	CHD-C1D-ND	-2.39	121.72	124.26
21	44	417	CL7	CAA-C2A-C3A	2.39	120.23	114.26
21	32	513	CL7	CHC-C1C-NC	-2.39	122.26	124.45
21	21	408	CL7	CMB-C2B-C1B	2.39	129.01	125.37
21	43	409	CL7	CBA-CAA-C2A	-2.39	106.81	113.86
23	3C	518	8CT	C18-C19-C20	-2.39	118.58	123.47
21	22	512	CL7	C4-C3-C5	2.39	119.29	115.27
21	1B	611	CL7	CHB-C1B-NB	-2.39	121.73	124.26
21	1C	510	CL7	C1C-C2C-C3C	-2.39	103.45	106.94
21	24	417	CL7	CAA-C2A-C3A	2.39	120.23	114.26
21	23	419	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	23	402	CL7	CAA-C2A-C1A	-2.39	104.33	112.19
21	34	414	CL7	CAA-CBA-CGA	-2.39	106.27	113.25
21	2B	603	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
32	33	519	ZEX	C39-C29-C30	-2.39	119.58	122.92
21	3B	603	CL7	C1C-C2C-C3C	-2.39	103.45	106.94
21	43	402	CL7	CAA-C2A-C1A	-2.39	104.33	112.19
21	33	503	CL7	C4-C3-C5	2.39	119.29	115.27
21	21	413	CL7	O2D-CGD-CBD	2.39	115.51	111.27
21	13	515	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
32	43	401	ZEX	C1-C6-C5	-2.39	119.25	122.61
32	44	403	ZEX	C39-C29-C30	-2.39	119.58	122.92
21	3C	502	CL7	C7-C6-C5	-2.39	106.87	113.36
21	4B	605	CL7	C7-C6-C5	-2.39	106.87	113.36
21	4B	603	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	11	418	CL7	CAC-C3C-C2C	2.39	131.61	127.53
21	24	405	CL7	O2A-CGA-O1A	-2.39	117.57	123.59
23	1A	404	8CT	C18-C19-C20	-2.39	118.59	123.47
21	2B	612	CL7	CHB-C1B-NB	-2.39	121.73	124.26
21	3B	611	CL7	C4-C3-C5	2.39	119.28	115.27
32	33	520	ZEX	C1-C6-C5	-2.39	119.25	122.61
21	3B	612	CL7	C4C-C3C-C2C	-2.38	104.02	107.13
21	34	405	CL7	C3B-C2B-C1B	-2.38	104.28	107.16
21	2B	604	CL7	C1C-C2C-C3C	-2.38	103.46	106.94
21	13	516	CL7	CAA-C2A-C1A	-2.38	104.35	112.19
23	4A	404	8CT	C18-C19-C20	-2.38	118.59	123.47
21	13	508	CL7	CBA-CAA-C2A	-2.38	106.83	113.86
21	3C	506	CL7	C4C-C3C-C2C	-2.38	104.02	107.13
21	41	406	CL7	C4C-C3C-C2C	-2.38	104.02	107.13
21	14	417	CL7	CAA-C2A-C3A	2.38	120.21	114.26
21	24	410	CL7	C1C-C2C-C3C	-2.38	103.46	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	34	405	CL7	C1C-C2C-C3C	-2.38	103.46	106.94
32	23	401	ZEX	C1-C6-C5	-2.38	119.26	122.61
32	43	420	ZEX	C39-C29-C30	-2.38	119.59	122.92
21	1C	502	CL7	C7-C6-C5	-2.38	106.89	113.36
21	2C	506	CL7	C7-C6-C5	-2.38	106.89	113.36
21	4C	502	CL7	C7-C6-C5	-2.38	106.89	113.36
21	44	414	CL7	CAA-CBA-CGA	-2.38	106.29	113.25
31	1F	101	HEM	C4D-ND-C1D	2.38	107.53	105.07
32	13	525	ZEX	C1-C6-C5	-2.38	119.26	122.61
21	2B	608	CL7	C4-C3-C5	2.38	119.28	115.27
21	2A	403	CL7	O2A-CGA-O1A	-2.38	117.58	123.59
21	31	419	CL7	C4C-C3C-C2C	-2.38	104.02	107.13
21	23	409	CL7	CHC-C1C-NC	-2.38	122.27	124.45
21	23	404	CL7	C4-C3-C5	2.38	119.28	115.27
21	1A	403	CL7	O2A-CGA-O1A	-2.38	117.58	123.59
21	41	413	CL7	O2D-CGD-CBD	2.38	115.50	111.27
21	34	411	CL7	CHB-C1B-NB	-2.38	121.74	124.26
21	43	404	CL7	C4-C3-C5	2.38	119.28	115.27
21	23	417	CL7	CAA-C2A-C1A	-2.38	104.36	112.19
32	12	522	ZEX	C21-C26-C27	2.38	122.51	115.78
21	21	402	CL7	C3B-C2B-C1B	-2.38	104.29	107.16
23	3B	617	8CT	C04-C03-C10	2.38	122.51	115.78
23	2A	404	8CT	C22-C21-C20	-2.38	119.59	122.92
21	3A	403	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
21	3B	607	CL7	C4-C3-C5	2.38	119.27	115.27
21	11	419	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
21	41	419	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
21	42	513	CL7	CHC-C1C-NC	-2.38	122.27	124.45
21	14	405	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
32	32	522	ZEX	C21-C26-C27	2.38	122.51	115.78
23	1C	518	8CT	C18-C19-C20	-2.38	118.60	123.47
21	13	504	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	42	502	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	43	405	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	14	414	CL7	CAA-CBA-CGA	-2.38	106.30	113.25
21	12	518	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
21	33	501	CL7	CAA-C2A-C1A	-2.38	104.37	112.19
21	12	513	CL7	CHC-C1C-NC	-2.38	122.27	124.45
21	2C	502	CL7	C7-C6-C5	-2.38	106.90	113.36
21	3B	604	CL7	C7-C6-C5	-2.38	106.90	113.36
21	3C	506	CL7	C7-C6-C5	-2.38	106.90	113.36
21	21	409	CL7	C4C-C3C-C2C	-2.38	104.03	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	409	CL7	C4C-C3C-C2C	-2.38	104.03	107.13
21	1B	603	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	41	416	CL7	CMA-C3A-C2A	-2.38	110.55	116.10
21	14	407	CL7	CHD-C1D-ND	-2.38	121.74	124.26
21	34	417	CL7	CAA-C2A-C3A	2.38	120.20	114.26
21	34	405	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
21	1C	512	CL7	C3B-C2B-C1B	-2.38	104.29	107.16
21	13	518	CL7	CMB-C2B-C1B	2.38	128.99	125.37
21	23	409	CL7	CBA-CAA-C2A	-2.38	106.85	113.86
21	33	508	CL7	CBA-CAA-C2A	-2.38	106.85	113.86
21	2C	513	CL7	CAA-CBA-CGA	-2.38	106.20	112.51
21	3C	513	CL7	CAA-CBA-CGA	-2.38	106.20	112.51
23	4B	618	8CT	C04-C03-C10	2.38	122.50	115.78
23	3A	404	8CT	C18-C19-C20	-2.37	118.61	123.47
21	11	408	CL7	CMB-C2B-C1B	2.37	128.99	125.37
32	11	421	ZEX	C1-C6-C5	-2.37	119.27	122.61
21	1B	612	CL7	C4C-C3C-C2C	-2.37	104.03	107.13
21	1C	513	CL7	CAA-CBA-CGA	-2.37	106.21	112.51
21	3C	510	CL7	C1C-C2C-C3C	-2.37	103.48	106.94
32	21	421	ZEX	C1-C6-C5	-2.37	119.27	122.61
21	24	414	CL7	CAA-CBA-CGA	-2.37	106.33	113.25
21	21	418	CL7	C4-C3-C5	2.37	119.26	115.27
21	1C	506	CL7	C7-C6-C5	-2.37	106.92	113.36
21	4C	506	CL7	C7-C6-C5	-2.37	106.92	113.36
23	2B	618	8CT	C04-C03-C10	2.37	122.48	115.78
32	42	522	ZEX	C21-C26-C27	2.37	122.48	115.78
21	31	416	CL7	CMA-C3A-C2A	-2.37	110.57	116.10
21	41	409	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
32	33	525	ZEX	C1-C6-C5	-2.37	119.28	122.61
21	13	501	CL7	CAA-C2A-C1A	-2.37	104.39	112.19
21	44	405	CL7	O2A-CGA-O1A	-2.37	117.61	123.59
21	33	501	CL7	CMB-C2B-C1B	2.37	128.98	125.37
23	1B	617	8CT	C04-C03-C10	2.37	122.48	115.78
32	22	522	ZEX	C21-C26-C27	2.37	122.48	115.78
21	2C	507	CL7	CHB-C1B-NB	-2.37	121.75	124.26
21	2C	509	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	4B	610	CL7	C4-C3-C5	2.37	119.25	115.27
21	1C	509	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	11	412	CL7	C3B-C2B-C1B	-2.37	104.31	107.16
21	41	412	CL7	C3B-C2B-C1B	-2.37	104.31	107.16
21	4C	509	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	11	418	CL7	C4-C3-C5	2.37	119.25	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	24	405	CL7	C7-C6-C5	-2.37	106.94	113.36
21	3B	602	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	4A	403	CL7	O2A-CGA-O1A	-2.36	117.62	123.59
21	33	517	CL7	C4C-C3C-C2C	-2.36	104.05	107.13
21	4B	608	CL7	C4-C3-C5	2.36	119.25	115.27
21	43	408	CL7	CHD-C1D-ND	-2.36	121.75	124.26
23	2A	404	8CT	C18-C19-C20	-2.36	118.63	123.47
21	41	418	CL7	C4-C3-C5	2.36	119.25	115.27
21	22	518	CL7	C4C-C3C-C2C	-2.36	104.05	107.13
21	23	408	CL7	CHD-C1D-ND	-2.36	121.76	124.26
21	33	507	CL7	CHD-C1D-ND	-2.36	121.76	124.26
21	3C	509	CL7	C4C-C3C-C2C	-2.36	104.05	107.13
21	2C	510	CL7	C1C-C2C-C3C	-2.36	103.49	106.94
21	4C	513	CL7	CAA-CBA-CGA	-2.36	106.24	112.51
21	2B	613	CL7	O2D-CGD-O1D	-2.36	119.22	123.84
21	3B	612	CL7	O2D-CGD-O1D	-2.36	119.22	123.84
21	23	416	CL7	C4C-C3C-C2C	-2.36	104.05	107.13
21	12	502	CL7	C3B-C4B-NB	2.36	112.70	110.52
21	14	405	CL7	C7-C6-C5	-2.36	106.95	113.36
21	14	405	CL7	C1C-C2C-C3C	-2.36	103.50	106.94
21	2A	407	CL7	C1C-C2C-C3C	-2.36	103.50	106.94
21	23	405	CL7	C1C-C2C-C3C	-2.36	103.50	106.94
21	33	504	CL7	C1C-C2C-C3C	-2.36	103.50	106.94
21	2B	617	CL7	C4C-C3C-C2C	-2.36	104.05	107.13
31	4F	101	HEM	C4D-ND-C1D	2.36	107.51	105.07
21	22	516	CL7	C1C-C2C-C3C	-2.36	103.50	106.94
32	31	421	ZEX	C1-C6-C5	-2.36	119.29	122.61
21	12	506	CL7	C1C-C2C-C3C	-2.36	103.50	106.94
21	43	409	CL7	CHC-C1C-NC	-2.36	122.29	124.45
21	24	407	CL7	CHD-C1D-ND	-2.36	121.76	124.26
21	2B	613	CL7	C4C-C3C-C2C	-2.36	104.06	107.13
21	3B	610	CL7	CMB-C2B-C1B	2.35	128.96	125.37
21	23	418	CL7	C1C-C2C-C3C	-2.35	103.50	106.94
21	4B	613	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	1D	405	CL7	C3B-C4B-NB	2.35	112.70	110.52
21	32	516	CL7	C1C-C2C-C3C	-2.35	103.50	106.94
21	1B	607	CL7	C4-C3-C5	2.35	119.23	115.27
21	44	405	CL7	C7-C6-C5	-2.35	106.97	113.36
21	14	413	CL7	C4-C3-C5	2.35	119.23	115.27
21	4B	617	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	12	508	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	3A	407	CL7	C1C-C2C-C3C	-2.35	103.51	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	611	CL7	CHB-C1B-NB	-2.35	121.77	124.26
32	41	421	ZEX	C1-C6-C5	-2.35	119.30	122.61
21	11	407	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	13	510	CL7	C4-C3-C5	2.35	119.23	115.27
21	34	405	CL7	C7-C6-C5	-2.35	106.97	113.36
21	3B	616	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	42	518	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	43	416	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	31	418	CL7	C4-C3-C5	2.35	119.22	115.27
21	1C	506	CL7	C4-C3-C5	2.35	119.22	115.27
21	4C	506	CL7	C4-C3-C5	2.35	119.22	115.27
23	2A	404	8CT	C19-C18-C17	-2.35	118.66	123.47
21	43	418	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	24	411	CL7	CAA-CBA-CGA	-2.35	106.39	113.25
21	34	413	CL7	CAA-CBA-CGA	-2.35	106.39	113.25
21	3B	606	CL7	CHC-C1C-NC	-2.35	122.30	124.45
21	41	407	CL7	C4C-C3C-C2C	-2.35	104.07	107.13
21	1B	609	CL7	C4-C3-C5	2.35	119.22	115.27
21	43	419	CL7	CMB-C2B-C1B	2.35	128.94	125.37
32	12	520	ZEX	C17-C1-C6	-2.35	106.49	110.30
32	42	520	ZEX	C17-C1-C6	-2.35	106.49	110.30
21	14	411	CL7	CAA-CBA-CGA	-2.35	106.39	113.25
31	3F	101	HEM	C4D-ND-C1D	2.35	107.50	105.07
21	1B	616	CL7	C4C-C3C-C2C	-2.35	104.07	107.13
21	32	518	CL7	C4C-C3C-C2C	-2.35	104.07	107.13
21	2C	506	CL7	C4-C3-C5	2.35	119.22	115.27
32	33	522	ZEX	C21-C22-C23	-2.35	108.61	113.69
23	2B	620	8CT	C14-C15-C16	-2.35	119.83	126.42
21	41	413	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	1B	612	CL7	O2D-CGD-O1D	-2.34	119.25	123.84
21	4B	613	CL7	O2D-CGD-O1D	-2.34	119.25	123.84
23	4K	101	8CT	C27-C26-C25	-2.34	119.64	122.92
21	12	516	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	3C	512	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	42	516	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
23	2K	101	8CT	C27-C26-C25	-2.34	119.64	122.92
32	43	423	ZEX	C21-C22-C23	-2.34	108.61	113.69
21	12	509	CL7	C4C-C3C-C2C	-2.34	104.07	107.13
21	32	516	CL7	C4C-C3C-C2C	-2.34	104.07	107.13
21	42	509	CL7	C4C-C3C-C2C	-2.34	104.07	107.13
21	2B	611	CL7	CMB-C2B-C1B	2.34	128.94	125.37
23	4B	620	8CT	C14-C15-C16	-2.34	119.83	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1C	515	8CT	C35-C30-C31	2.34	115.61	111.42
21	1C	512	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
23	4A	404	8CT	C19-C18-C17	-2.34	118.68	123.47
21	33	508	CL7	CHC-C1C-NC	-2.34	122.30	124.45
21	2D	402	CL7	C3B-C4B-NB	2.34	112.69	110.52
21	2B	610	CL7	C4-C3-C5	2.34	119.21	115.27
21	3B	609	CL7	C4-C3-C5	2.34	119.21	115.27
21	14	410	CL7	C3B-C2B-C1B	-2.34	104.34	107.16
21	44	411	CL7	CAA-CBA-CGA	-2.34	106.41	113.25
21	1C	506	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	4C	506	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	13	516	CL7	C3B-C4B-NB	2.34	112.69	110.52
21	31	406	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
23	1A	404	8CT	C19-C18-C17	-2.34	118.68	123.47
21	13	517	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	23	419	CL7	CMB-C2B-C1B	2.34	128.93	125.37
23	3K	101	8CT	C27-C26-C25	-2.34	119.65	122.92
21	14	413	CL7	CAA-CBA-CGA	-2.34	106.42	113.25
21	4D	402	CL7	C3B-C4B-NB	2.34	112.68	110.52
23	3C	515	8CT	C35-C30-C31	2.34	115.61	111.42
23	1K	101	8CT	C27-C26-C25	-2.34	119.65	122.92
21	24	413	CL7	CAA-CBA-CGA	-2.34	106.42	113.25
21	34	411	CL7	CAA-CBA-CGA	-2.34	106.42	113.25
21	44	410	CL7	C3B-C2B-C1B	-2.34	104.34	107.16
21	43	408	CL7	C4-C3-C5	2.34	119.20	115.27
21	32	502	CL7	C3B-C4B-NB	2.34	112.68	110.52
21	4C	507	CL7	CHB-C1B-NB	-2.34	121.78	124.26
32	21	422	ZEX	C15-C35-C34	-2.34	118.69	123.47
21	1C	507	CL7	CMB-C2B-C1B	2.34	128.93	125.37
21	23	402	CL7	CMB-C2B-C1B	2.34	128.93	125.37
21	1B	610	CL7	CMB-C2B-C1B	2.34	128.93	125.37
21	44	405	CL7	C1C-C2C-C3C	-2.33	103.53	106.94
21	32	506	CL7	C1C-C2C-C3C	-2.33	103.53	106.94
21	44	413	CL7	CAA-CBA-CGA	-2.33	106.43	113.25
21	34	411	CL7	C4C-C3C-C2C	-2.33	104.08	107.13
21	4B	611	CL7	CMB-C2B-C1B	2.33	128.92	125.37
21	24	408	CL7	C3B-C2B-C1B	-2.33	104.34	107.16
21	24	408	CL7	CHB-C1B-NB	-2.33	121.79	124.26
21	34	408	CL7	CHB-C1B-NB	-2.33	121.79	124.26
32	32	519	ZEX	C15-C35-C34	-2.33	118.69	123.47
21	13	501	CL7	CMB-C2B-C1B	2.33	128.92	125.37
21	2B	607	CL7	C3B-C4B-NB	2.33	112.68	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3B	602	CL7	C1C-C2C-C3C	-2.33	103.53	106.94
32	24	420	ZEX	C20-C13-C12	2.33	121.75	118.08
32	32	522	ZEX	C39-C29-C28	2.33	121.75	118.08
23	1B	619	8CT	C14-C15-C16	-2.33	119.86	126.42
21	44	413	CL7	C4-C3-C5	2.33	119.19	115.27
21	21	407	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	22	513	CL7	CHC-C1C-NC	-2.33	122.31	124.45
21	2C	512	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	13	507	CL7	C4-C3-C5	2.33	119.19	115.27
23	2C	515	8CT	C35-C30-C31	2.33	115.59	111.42
21	13	507	CL7	CHD-C1D-ND	-2.33	121.79	124.26
32	22	524	ZEX	C1-C6-C7	2.33	122.37	115.78
32	23	423	ZEX	C21-C22-C23	-2.33	108.64	113.69
21	11	413	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	31	407	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	43	418	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	44	414	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
32	42	519	ZEX	C15-C35-C34	-2.33	118.70	123.47
21	11	409	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
32	12	519	ZEX	C15-C35-C34	-2.33	118.70	123.47
21	1C	506	CL7	O2A-CGA-CBA	2.33	119.22	111.91
21	4C	506	CL7	O2A-CGA-CBA	2.33	119.22	111.91
21	23	411	CL7	C4-C3-C5	2.33	119.19	115.27
21	1A	407	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	34	408	CL7	C3B-C2B-C1B	-2.33	104.35	107.16
21	23	417	CL7	C3B-C4B-NB	2.33	112.67	110.52
21	33	516	CL7	C3B-C4B-NB	2.33	112.67	110.52
21	12	511	CL7	CMB-C2B-C1B	2.33	128.91	125.37
21	23	416	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	31	407	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	33	507	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
23	3B	619	8CT	C14-C15-C16	-2.33	119.88	126.42
21	21	412	CL7	C3B-C2B-C1B	-2.33	104.35	107.16
21	31	412	CL7	C3B-C2B-C1B	-2.33	104.35	107.16
23	3A	404	8CT	C19-C18-C17	-2.33	118.71	123.47
21	24	413	CL7	C4-C3-C5	2.33	119.18	115.27
21	34	413	CL7	C4-C3-C5	2.33	119.18	115.27
27	4C	516	DGD	O3G-C3G-C2G	-2.33	105.29	110.90
21	43	416	CL7	C1C-C2C-C3C	-2.33	103.55	106.94
32	14	419	ZEX	C1-C6-C7	2.33	122.36	115.78
32	44	419	ZEX	C1-C6-C7	2.33	122.36	115.78
23	2C	518	8CT	C27-C26-C25	-2.33	119.67	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	413	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	4C	512	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
32	22	522	ZEX	C39-C29-C28	2.32	121.74	118.08
32	12	524	ZEX	C1-C6-C7	2.32	122.35	115.78
32	42	524	ZEX	C1-C6-C7	2.32	122.35	115.78
32	33	520	ZEX	C39-C29-C30	-2.32	119.67	122.92
21	11	406	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	23	408	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	32	510	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
32	34	419	ZEX	C1-C6-C7	2.32	122.35	115.78
32	13	522	ZEX	C21-C22-C23	-2.32	108.66	113.69
27	1C	516	DGD	O3G-C3G-C2G	-2.32	105.29	110.90
21	23	418	CL7	C4C-C3C-C2C	-2.32	104.10	107.13
23	34	402	8CT	C25-C24-C23	-2.32	115.97	123.22
32	32	524	ZEX	C1-C6-C7	2.32	122.35	115.78
21	22	502	CL7	C3B-C4B-NB	2.32	112.67	110.52
21	42	506	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	2C	506	CL7	O2A-CGA-CBA	2.32	119.19	111.91
21	4A	407	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	12	517	CL7	C1-C2-C3	2.32	130.06	126.04
32	42	524	ZEX	C15-C35-C34	-2.32	118.72	123.47
21	22	506	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	44	406	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	3C	506	CL7	O2A-CGA-CBA	2.32	119.19	111.91
21	43	408	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	23	408	CL7	C4-C3-C5	2.32	119.17	115.27
23	2B	620	8CT	C05-C04-C03	2.32	114.05	110.48
21	13	507	CL7	CAA-CBA-CGA	-2.32	106.47	113.25
21	1C	507	CL7	CHB-C1B-NB	-2.32	121.80	124.26
21	2C	507	CL7	CMB-C2B-C1B	2.32	128.90	125.37
32	22	519	ZEX	C15-C35-C34	-2.32	118.72	123.47
32	32	524	ZEX	C15-C35-C34	-2.32	118.72	123.47
21	12	504	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
21	32	508	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
32	31	422	ZEX	C15-C35-C34	-2.32	118.73	123.47
21	32	511	CL7	CMB-C2B-C1B	2.32	128.90	125.37
21	21	407	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
23	44	402	8CT	C25-C24-C23	-2.32	115.99	123.22
32	44	419	ZEX	C40-C33-C32	2.32	121.73	118.08
21	3B	606	CL7	C3B-C4B-NB	2.32	112.66	110.52
21	41	406	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
23	4C	515	8CT	C35-C30-C31	2.32	115.56	111.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	21	413	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
32	32	520	ZEX	C17-C1-C6	-2.31	106.55	110.30
23	4C	518	8CT	C27-C26-C25	-2.31	119.68	122.92
32	13	520	ZEX	C39-C29-C30	-2.31	119.68	122.92
21	22	505	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	33	507	CL7	CAA-CBA-CGA	-2.31	106.49	113.25
21	13	507	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	14	408	CL7	C3B-C2B-C1B	-2.31	104.37	107.16
21	33	515	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
21	11	409	CL7	CAA-CBA-CGA	-2.31	106.37	112.51
21	41	409	CL7	CAA-CBA-CGA	-2.31	106.37	112.51
21	3C	506	CL7	C4-C3-C5	2.31	119.16	115.27
21	42	510	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
23	14	402	8CT	C25-C24-C23	-2.31	116.00	123.22
23	3D	406	8CT	C24-C25-C26	-2.31	124.01	127.31
23	3C	518	8CT	C27-C26-C25	-2.31	119.68	122.92
21	12	505	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
32	24	419	ZEX	C1-C6-C7	2.31	122.32	115.78
27	2C	516	DGD	O3G-C3G-C2G	-2.31	105.32	110.90
21	12	516	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	33	504	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	42	516	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	13	507	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	43	403	CL7	CHB-C1B-NB	-2.31	121.81	124.26
21	21	410	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	42	508	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	2C	506	CL7	C4C-C3C-C2C	-2.31	104.12	107.13
21	23	405	CL7	C4C-C3C-C2C	-2.31	104.12	107.13
32	24	419	ZEX	C40-C33-C32	2.31	121.72	118.08
21	43	408	CL7	CAA-CBA-CGA	-2.31	106.50	113.25
32	22	524	ZEX	C15-C35-C34	-2.31	118.74	123.47
23	1B	619	8CT	C05-C04-C03	2.31	114.04	110.48
21	33	518	CL7	CMB-C2B-C1B	2.31	128.89	125.37
21	2B	607	CL7	CHC-C1C-NC	-2.31	122.33	124.45
32	34	420	ZEX	C20-C13-C12	2.31	121.72	118.08
21	13	515	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	44	408	CL7	C3B-C2B-C1B	-2.31	104.38	107.16
21	4C	510	CL7	C4-C3-C5	2.31	119.15	115.27
21	22	508	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	3D	402	CL7	C3B-C4B-NB	2.31	112.66	110.52
21	13	517	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
32	11	422	ZEX	C15-C35-C34	-2.31	118.75	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3C	510	CL7	C4-C3-C5	2.31	119.15	115.27
21	24	410	CL7	C3B-C2B-C1B	-2.31	104.38	107.16
21	44	408	CL7	CHB-C1B-NB	-2.31	121.81	124.26
21	14	414	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	31	409	CL7	CAA-CBA-CGA	-2.31	106.39	112.51
23	24	402	8CT	C25-C24-C23	-2.31	116.02	123.22
21	2C	505	CL7	C7-C6-C5	-2.31	107.10	113.36
21	22	511	CL7	CMB-C2B-C1B	2.31	128.88	125.37
21	42	506	CL7	C4C-C3C-C2C	-2.31	104.12	107.13
32	44	420	ZEX	C20-C13-C12	2.31	121.71	118.08
21	2C	505	CL7	C3B-C4B-NB	2.31	112.65	110.52
21	4D	405	CL7	C3B-C4B-NB	2.31	112.65	110.52
21	23	408	CL7	CAA-CBA-CGA	-2.31	106.52	113.25
32	12	522	ZEX	C39-C29-C28	2.31	121.71	118.08
21	2B	603	CL7	C1C-C2C-C3C	-2.31	103.58	106.94
21	22	504	CL7	C1C-C2C-C3C	-2.31	103.58	106.94
21	1C	510	CL7	C4-C3-C5	2.30	119.15	115.27
21	33	510	CL7	C4-C3-C5	2.30	119.15	115.27
21	4C	504	CL7	C4-C3-C5	2.30	119.15	115.27
21	22	517	CL7	C1-C2-C3	2.30	130.03	126.04
22	3D	408	PHO	C1C-C2C-C3C	-2.30	106.69	108.61
27	3C	516	DGD	O3G-C3G-C2G	-2.30	105.34	110.90
21	1B	602	CL7	C1C-C2C-C3C	-2.30	103.58	106.94
21	12	508	CL7	C3B-C4B-NB	2.30	112.65	110.52
21	24	416	CL7	C3B-C2B-C1B	-2.30	104.38	107.16
21	34	416	CL7	C3B-C2B-C1B	-2.30	104.38	107.16
21	44	416	CL7	C3B-C2B-C1B	-2.30	104.38	107.16
21	3B	608	CL7	O2D-CGD-O1D	-2.30	119.34	123.84
32	14	420	ZEX	C20-C13-C12	2.30	121.70	118.08
21	42	508	CL7	C3B-C4B-NB	2.30	112.65	110.52
32	43	421	ZEX	C39-C29-C30	-2.30	119.70	122.92
21	24	412	CL7	C4C-C3C-C2C	-2.30	104.13	107.13
21	13	514	CL7	C3B-C2B-C1B	-2.30	104.38	107.16
21	3B	604	CL7	C3B-C2B-C1B	-2.30	104.38	107.16
32	33	519	ZEX	C2-C3-C4	-2.30	107.15	110.30
22	1D	408	PHO	C1C-C2C-C3C	-2.30	106.70	108.61
22	4D	408	PHO	C1C-C2C-C3C	-2.30	106.70	108.61
21	4C	507	CL7	CMB-C2B-C1B	2.30	128.87	125.37
21	24	412	CL7	CAC-C3C-C2C	2.30	131.46	127.53
21	1B	615	CL7	C4C-C3C-C2C	-2.30	104.13	107.13
21	33	507	CL7	C4-C3-C5	2.30	119.14	115.27
21	4B	603	CL7	C1C-C2C-C3C	-2.30	103.58	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	505	CL7	C4C-C3C-C2C	-2.30	104.13	107.13
21	24	414	CL7	C1C-C2C-C3C	-2.30	103.58	106.94
21	1C	504	CL7	C4-C3-C5	2.30	119.14	115.27
21	12	510	CL7	C1C-C2C-C3C	-2.30	103.58	106.94
32	42	522	ZEX	C39-C29-C28	2.30	121.70	118.08
21	33	517	CL7	C1C-C2C-C3C	-2.30	103.58	106.94
21	2C	510	CL7	C4-C3-C5	2.30	119.14	115.27
32	12	524	ZEX	C15-C35-C34	-2.30	118.77	123.47
21	21	406	CL7	C1C-C2C-C3C	-2.30	103.59	106.94
21	43	411	CL7	C4-C3-C5	2.30	119.14	115.27
32	14	419	ZEX	C40-C33-C32	2.30	121.70	118.08
21	1B	612	CL7	CAC-C3C-C2C	2.30	131.46	127.53
21	2D	405	CL7	C3B-C4B-NB	2.30	112.65	110.52
21	3D	405	CL7	C3B-C4B-NB	2.30	112.65	110.52
32	41	422	ZEX	C15-C35-C34	-2.30	118.77	123.47
21	3C	507	CL7	CMB-C2B-C1B	2.30	128.87	125.37
32	22	520	ZEX	C17-C1-C6	-2.30	106.57	110.30
32	34	419	ZEX	C40-C33-C32	2.30	121.69	118.08
21	14	416	CL7	C3B-C2B-C1B	-2.30	104.39	107.16
21	42	517	CL7	C1-C2-C3	2.30	130.01	126.04
21	1D	402	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	21	409	CL7	CAA-CBA-CGA	-2.29	106.42	112.51
21	24	405	CL7	O2A-C1-C2	-2.29	102.61	108.64
21	1D	402	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
21	11	410	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
21	34	414	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
21	34	412	CL7	CAC-C3C-C2C	2.29	131.45	127.53
21	13	504	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	43	405	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	44	412	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	14	406	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
21	44	412	CL7	CAC-C3C-C2C	2.29	131.45	127.53
21	42	511	CL7	CMB-C2B-C1B	2.29	128.86	125.37
21	42	502	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	11	420	CL7	CMB-C2B-C1B	2.29	128.86	125.37
21	43	419	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
32	43	420	ZEX	C2-C3-C4	-2.29	107.17	110.30
21	42	508	CL7	CHB-C1B-NB	-2.29	121.83	124.26
21	12	506	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	41	410	CL7	C1C-C2C-C3C	-2.29	103.60	106.94
21	2B	609	CL7	O2D-CGD-O1D	-2.29	119.36	123.84
21	4B	609	CL7	O2D-CGD-O1D	-2.29	119.36	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	509	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	22	510	CL7	C1C-C2C-C3C	-2.29	103.60	106.94
21	32	508	CL7	CHB-C1B-NB	-2.29	121.83	124.26
32	23	421	ZEX	C39-C29-C30	-2.29	119.72	122.92
21	22	503	CL7	C4D-C3D-C2D	2.29	110.28	107.30
21	2C	504	CL7	C4-C3-C5	2.29	119.12	115.27
21	3C	504	CL7	C4-C3-C5	2.29	119.12	115.27
21	1B	606	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	4B	607	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	14	405	CL7	O2A-C1-C2	-2.29	102.62	108.64
23	2B	620	8CT	C04-C03-C02	-2.29	119.39	122.61
23	3B	619	8CT	C05-C04-C03	2.29	114.00	110.48
21	1C	505	CL7	C7-C6-C5	-2.29	107.15	113.36
21	4C	505	CL7	C7-C6-C5	-2.29	107.15	113.36
21	32	505	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	42	511	CL7	C1C-C2C-C3C	-2.29	103.60	106.94
21	41	407	CL7	C1C-C2C-C3C	-2.29	103.60	106.94
21	1B	608	CL7	O2D-CGD-O1D	-2.29	119.37	123.84
21	32	517	CL7	C1-C2-C3	2.29	130.00	126.04
21	33	507	CL7	C4C-C3C-C2C	-2.29	104.15	107.13
21	21	403	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	31	403	CL7	C3B-C4B-NB	2.29	112.64	110.52
21	2B	616	CL7	C4C-C3C-C2C	-2.29	104.15	107.13
21	33	502	CL7	CHB-C1B-NB	-2.29	121.84	124.26
21	3C	505	CL7	C7-C6-C5	-2.29	107.15	113.36
21	43	415	CL7	C3B-C2B-C1B	-2.29	104.40	107.16
21	32	505	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	22	516	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	14	412	CL7	CAC-C3C-C2C	2.28	131.44	127.53
21	43	417	CL7	C3B-C4B-NB	2.28	112.63	110.52
21	42	504	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	11	415	CL7	CMA-C3A-C2A	-2.28	110.77	116.10
23	4D	406	8CT	C24-C25-C26	-2.28	124.05	127.31
21	13	513	CL7	CAA-CBA-CGA	-2.28	106.45	112.51
21	13	518	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	41	415	CL7	CMA-C3A-C2A	-2.28	110.77	116.10
21	33	513	CL7	CAA-CBA-CGA	-2.28	106.45	112.51
32	14	418	ZEX	C20-C13-C14	-2.28	119.72	122.92
23	2D	406	8CT	C24-C25-C26	-2.28	124.05	127.31
23	4B	620	8CT	C05-C04-C03	2.28	114.00	110.48
21	44	405	CL7	O2A-C1-C2	-2.28	102.64	108.64
21	1B	607	CL7	C4C-C3C-C2C	-2.28	104.15	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	510	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
23	1D	406	8CT	C18-C19-C20	2.28	128.15	123.47
21	14	408	CL7	CHB-C1B-NB	-2.28	121.84	124.26
21	11	407	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	34	410	CL7	C3B-C2B-C1B	-2.28	104.41	107.16
21	34	405	CL7	O2A-C1-C2	-2.28	102.64	108.64
21	23	414	CL7	CAA-CBA-CGA	-2.28	106.46	112.51
21	33	518	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
23	2D	406	8CT	C18-C19-C20	2.28	128.14	123.47
23	4D	406	8CT	C18-C19-C20	2.28	128.14	123.47
21	41	420	CL7	CMB-C2B-C1B	2.28	128.84	125.37
21	2B	613	CL7	CAC-C3C-C2C	2.28	131.43	127.53
21	3B	612	CL7	CAC-C3C-C2C	2.28	131.43	127.53
21	12	508	CL7	CHB-C1B-NB	-2.28	121.84	124.26
23	2A	404	8CT	C27-C26-C25	-2.28	119.73	122.92
21	43	414	CL7	CAA-CBA-CGA	-2.28	106.46	112.51
32	24	418	ZEX	C20-C13-C14	-2.28	119.73	122.92
21	13	501	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
23	1B	619	8CT	C04-C03-C02	-2.28	119.41	122.61
32	23	420	ZEX	C2-C3-C4	-2.28	107.19	110.30
21	33	514	CL7	C3B-C2B-C1B	-2.28	104.41	107.16
21	14	412	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
23	44	402	8CT	C10-C11-C12	-2.28	122.80	126.23
21	23	411	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
21	24	411	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
21	32	509	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
21	31	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	1B	604	CL7	C3B-C2B-C1B	-2.27	104.42	107.16
21	2B	605	CL7	C3B-C2B-C1B	-2.27	104.42	107.16
32	44	418	ZEX	C20-C13-C14	-2.27	119.74	122.92
21	11	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	41	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	13	510	CL7	C4C-C3C-C2C	-2.27	104.16	107.13
23	1C	518	8CT	C27-C26-C25	-2.27	119.74	122.92
21	22	508	CL7	CHB-C1B-NB	-2.27	121.85	124.26
21	2C	509	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
21	32	511	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
21	22	506	CL7	C3B-C4B-NB	2.27	112.62	110.52
21	32	506	CL7	C3B-C4B-NB	2.27	112.62	110.52
21	31	410	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
21	4C	509	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
21	4B	605	CL7	C3B-C2B-C1B	-2.27	104.42	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	419	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
23	24	402	8CT	C01-C02-C07	2.27	117.98	113.62
23	34	402	8CT	C01-C02-C07	2.27	117.98	113.62
21	23	402	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
22	3A	402	PHO	CMA-C3A-C4A	-2.27	109.40	114.38
23	4C	518	8CT	C40-C12-C13	-2.27	119.74	122.92
21	2B	608	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	3B	607	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	22	506	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
32	44	403	ZEX	C35-C15-C14	-2.27	118.82	123.47
21	4B	623	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	2B	613	CL7	CMB-C2B-C1B	2.27	128.83	125.37
21	3B	612	CL7	CMB-C2B-C1B	2.27	128.83	125.37
21	2D	402	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	43	411	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	44	409	CL7	C4-C3-C5	2.27	119.09	115.27
21	32	506	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	24	406	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	4B	616	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	31	402	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
22	1A	402	PHO	CMA-C3A-C4A	-2.27	109.41	114.38
22	4A	402	PHO	CMA-C3A-C4A	-2.27	109.41	114.38
23	4B	620	8CT	C04-C03-C02	-2.27	119.42	122.61
21	31	415	CL7	CMA-C3A-C2A	-2.27	110.81	116.10
23	3C	518	8CT	C40-C12-C13	-2.27	119.75	122.92
21	34	406	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
23	1A	404	8CT	C27-C26-C25	-2.27	119.75	122.92
21	42	503	CL7	CAA-C2A-C1A	2.27	119.64	112.19
21	4B	613	CL7	CAC-C3C-C2C	2.27	131.41	127.53
21	22	509	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	23	403	CL7	CHB-C1B-NB	-2.27	121.86	124.26
21	14	411	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	44	411	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
23	2C	515	8CT	C22-C21-C20	-2.27	119.75	122.92
23	14	402	8CT	C01-C02-C07	2.27	117.97	113.62
21	24	406	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	34	406	CL7	C4C-C3C-C2C	-2.27	104.17	107.13
21	3B	604	CL7	CAA-CBA-CGA	-2.27	106.63	113.25
21	13	510	CL7	C1C-C2C-C3C	-2.26	103.63	106.94
21	11	403	CL7	C3B-C4B-NB	2.26	112.62	110.52
23	3D	406	8CT	C18-C19-C20	2.26	128.11	123.47
21	23	403	CL7	CGD-CBD-CAD	2.26	118.06	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	623	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
32	23	401	ZEX	C19-C9-C8	2.26	121.64	118.08
32	34	418	ZEX	C20-C13-C14	-2.26	119.75	122.92
21	3B	604	CL7	C3B-C4B-NB	2.26	112.61	110.52
21	4B	608	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
21	1D	405	CL7	CMB-C2B-C1B	2.26	128.81	125.37
21	24	408	CL7	CMB-C2B-C1B	2.26	128.81	125.37
31	1F	101	HEM	C1A-CHA-C4D	-2.26	120.97	126.34
21	31	420	CL7	CMB-C2B-C1B	2.26	128.81	125.37
21	4D	402	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
21	42	506	CL7	CAA-CBA-CGA	-2.26	106.65	113.25
32	41	422	ZEX	C18-C5-C6	-2.26	121.99	124.53
31	1F	101	HEM	C4C-CHD-C1D	-2.26	121.18	126.06
21	4B	605	CL7	CAA-CBA-CGA	-2.26	106.65	113.25
21	13	516	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
31	1F	101	HEM	CHA-C4D-C3D	-2.26	121.09	125.33
21	12	503	CL7	CAA-C2A-C1A	2.26	119.61	112.19
23	1C	518	8CT	C40-C12-C13	-2.26	119.76	122.92
21	43	403	CL7	CGD-CBD-CAD	2.26	118.05	110.73
21	24	410	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
21	34	412	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
32	44	419	ZEX	C35-C15-C14	-2.26	118.85	123.47
21	32	506	CL7	CAA-CBA-CGA	-2.26	106.65	113.25
31	2F	101	HEM	C4C-CHD-C1D	-2.26	121.19	126.06
32	21	421	ZEX	C3-C4-C5	-2.26	107.36	111.85
32	43	421	ZEX	C3-C4-C5	-2.26	107.36	111.85
21	12	506	CL7	CAA-CBA-CGA	-2.26	106.66	113.25
21	23	408	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
23	4A	404	8CT	C27-C26-C25	-2.26	119.76	122.92
21	23	415	CL7	C3B-C2B-C1B	-2.26	104.44	107.16
21	1B	606	CL7	O2D-CGD-O1D	-2.26	119.42	123.84
21	4B	607	CL7	O2D-CGD-O1D	-2.26	119.42	123.84
21	21	415	CL7	CMA-C3A-C2A	-2.26	110.83	116.10
21	42	501	CL7	C1-C2-C3	2.26	129.95	126.04
21	32	504	CL7	C1C-C2C-C3C	-2.26	103.65	106.94
31	3F	101	HEM	CHA-C4D-C3D	-2.26	121.09	125.33
21	3C	505	CL7	C3B-C4B-NB	2.26	112.61	110.52
21	21	420	CL7	CMB-C2B-C1B	2.26	128.81	125.37
21	43	408	CL7	C4C-C3C-C2C	-2.26	104.19	107.13
23	3B	619	8CT	C04-C03-C02	-2.26	119.44	122.61
21	22	511	CL7	C1C-C2C-C3C	-2.26	103.65	106.94
21	32	503	CL7	CAA-C2A-C1A	2.26	119.60	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	44	402	8CT	C01-C02-C07	2.26	117.95	113.62
21	43	412	CL7	C1-C2-C3	2.26	129.94	126.04
23	1B	618	8CT	C24-C25-C26	-2.26	124.09	127.31
23	4B	619	8CT	C24-C25-C26	-2.26	124.09	127.31
32	24	419	ZEX	C35-C15-C14	-2.26	118.85	123.47
21	3B	615	CL7	C4C-C3C-C2C	-2.26	104.19	107.13
21	32	502	CL7	C4C-C3C-C2C	-2.26	104.19	107.13
21	21	417	CL7	CAC-C3C-C4C	-2.25	121.13	124.68
21	13	515	CL7	CAC-C3C-C2C	2.25	131.38	127.53
22	2A	402	PHO	CMA-C3A-C4A	-2.25	109.44	114.38
31	4F	101	HEM	C4C-CHD-C1D	-2.25	121.19	126.06
31	4F	101	HEM	CHA-C4D-C3D	-2.25	121.10	125.33
21	41	403	CL7	C3B-C4B-NB	2.25	112.61	110.52
21	14	404	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	1C	507	CL7	C4C-C3C-C2C	-2.25	104.19	107.13
21	2B	613	CL7	O2A-CGA-O1A	-2.25	117.90	123.59
32	13	519	ZEX	C2-C3-C4	-2.25	107.22	110.30
21	33	501	CL7	C4C-C3C-C2C	-2.25	104.19	107.13
32	41	421	ZEX	C3-C4-C5	-2.25	107.37	111.85
22	2D	408	PHO	C1C-C2C-C3C	-2.25	106.74	108.61
23	4B	620	8CT	C18-C19-C20	-2.25	118.86	123.47
21	12	505	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	4B	613	CL7	CMB-C2B-C1B	2.25	128.80	125.37
21	2B	607	CL7	O2D-CGD-O1D	-2.25	119.44	123.84
21	34	409	CL7	C4-C3-C5	2.25	119.06	115.27
21	1B	604	CL7	C3B-C4B-NB	2.25	112.60	110.52
21	11	402	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
23	3A	404	8CT	C27-C26-C25	-2.25	119.77	122.92
21	33	510	CL7	C4C-C3C-C2C	-2.25	104.19	107.13
32	34	403	ZEX	C35-C15-C14	-2.25	118.86	123.47
27	4C	516	DGD	O1G-C1A-C2A	2.25	118.97	111.91
21	22	506	CL7	CAA-CBA-CGA	-2.25	106.67	113.25
21	2C	513	CL7	C4C-C3C-C2C	-2.25	104.19	107.13
31	3F	101	HEM	C1A-CHA-C4D	-2.25	121.00	126.34
21	4B	613	CL7	C1C-C2C-C3C	-2.25	103.66	106.94
21	3B	606	CL7	O2D-CGD-O1D	-2.25	119.44	123.84
21	3D	402	CL7	C1C-C2C-C3C	-2.25	103.66	106.94
21	42	505	CL7	C1C-C2C-C3C	-2.25	103.66	106.94
21	4C	505	CL7	C3B-C4B-NB	2.25	112.60	110.52
21	12	503	CL7	C4D-C3D-C2D	2.25	110.23	107.30
21	42	503	CL7	C4D-C3D-C2D	2.25	110.23	107.30
23	3C	515	8CT	C22-C21-C20	-2.25	119.77	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	406	CL7	C4C-C3C-C2C	-2.25	104.19	107.13
21	1B	604	CL7	CAA-CBA-CGA	-2.25	106.68	113.25
21	1B	612	CL7	CMB-C2B-C1B	2.25	128.79	125.37
32	13	525	ZEX	C19-C9-C8	2.25	121.62	118.08
32	43	401	ZEX	C19-C9-C8	2.25	121.62	118.08
21	1C	505	CL7	C3B-C4B-NB	2.25	112.60	110.52
21	34	408	CL7	CMB-C2B-C1B	2.25	128.79	125.37
32	24	403	ZEX	C35-C15-C14	-2.25	118.87	123.47
21	42	506	CL7	C3B-C4B-NB	2.25	112.60	110.52
21	23	416	CL7	CAC-C3C-C2C	2.25	131.37	127.53
32	22	519	ZEX	C39-C29-C30	-2.25	119.78	122.92
32	32	519	ZEX	C39-C29-C30	-2.25	119.78	122.92
23	2B	620	8CT	C18-C19-C20	-2.25	118.87	123.47
21	13	502	CL7	CGD-CBD-CAD	2.25	118.01	110.73
21	14	408	CL7	CMB-C2B-C1B	2.25	128.79	125.37
22	3A	402	PHO	C1C-C2C-C3C	-2.25	106.74	108.61
21	22	503	CL7	CAA-C2A-C1A	2.25	119.57	112.19
21	3C	502	CL7	CHB-C1B-NB	-2.25	121.88	124.26
21	12	511	CL7	C1C-C2C-C3C	-2.25	103.66	106.94
21	3B	622	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
32	14	419	ZEX	C35-C15-C14	-2.25	118.87	123.47
32	33	520	ZEX	C3-C4-C5	-2.25	107.38	111.85
32	14	403	ZEX	C35-C15-C14	-2.25	118.87	123.47
22	2A	402	PHO	C1C-C2C-C3C	-2.25	106.74	108.61
32	23	421	ZEX	C3-C4-C5	-2.25	107.38	111.85
21	1B	605	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
21	4C	513	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
21	24	409	CL7	C4-C3-C5	2.25	119.05	115.27
21	43	412	CL7	C4-C3-C5	2.24	119.05	115.27
23	1D	406	8CT	C24-C25-C26	-2.24	124.11	127.31
23	3B	618	8CT	C24-C25-C26	-2.24	124.11	127.31
21	31	410	CL7	C3B-C4B-NB	2.24	112.60	110.52
21	44	408	CL7	CMB-C2B-C1B	2.24	128.79	125.37
21	3B	612	CL7	O2A-CGA-O1A	-2.24	117.93	123.59
21	23	411	CL7	C1C-C2C-C3C	-2.24	103.66	106.94
21	22	516	CL7	C1-C2-C3	2.24	129.92	126.04
32	12	519	ZEX	C39-C29-C30	-2.24	119.78	122.92
32	42	519	ZEX	C39-C29-C30	-2.24	119.78	122.92
32	24	403	ZEX	C10-C11-C12	-2.24	116.22	123.22
21	12	507	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	42	507	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	2B	605	CL7	CAA-CBA-CGA	-2.24	106.70	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3C	516	DGD	O1G-C1A-C2A	2.24	118.94	111.91
31	3F	101	HEM	C4C-CHD-C1D	-2.24	121.22	126.06
27	2C	516	DGD	O1G-C1A-C2A	2.24	118.94	111.91
21	11	403	CL7	CAA-CBA-CGA	-2.24	106.70	113.25
21	41	403	CL7	CAA-CBA-CGA	-2.24	106.70	113.25
21	3D	402	CL7	C4C-C3C-C2C	-2.24	104.20	107.13
21	1C	509	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	22	505	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	1B	612	CL7	O2A-CGA-O1A	-2.24	117.94	123.59
32	11	421	ZEX	C3-C4-C5	-2.24	107.39	111.85
21	3D	405	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	4C	507	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	31	410	CL7	C4C-C3C-C2C	-2.24	104.21	107.13
21	32	501	CL7	C1-C2-C3	2.24	129.92	126.04
21	2B	613	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	3B	612	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	43	411	CL7	C4C-C3C-C2C	-2.24	104.21	107.13
21	22	508	CL7	C3B-C4B-NB	2.24	112.59	110.52
21	32	508	CL7	C3B-C4B-NB	2.24	112.59	110.52
21	32	509	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	31	419	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
23	2C	518	8CT	C40-C12-C13	-2.24	119.79	122.92
21	3D	405	CL7	CMB-C2B-C1B	2.24	128.78	125.37
23	1B	619	8CT	C18-C19-C20	-2.24	118.89	123.47
21	33	502	CL7	CGD-CBD-CAD	2.24	117.98	110.73
21	2D	405	CL7	CMB-C2B-C1B	2.24	128.78	125.37
31	2F	101	HEM	CHA-C4D-C3D	-2.24	121.13	125.33
21	3C	507	CL7	C4C-C3C-C2C	-2.24	104.21	107.13
32	42	524	ZEX	C35-C15-C14	-2.24	118.89	123.47
21	1B	622	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	32	511	CL7	C4D-C3D-C2D	2.24	110.21	107.30
21	14	409	CL7	C4-C3-C5	2.24	119.03	115.27
32	34	419	ZEX	C35-C15-C14	-2.24	118.89	123.47
31	2F	101	HEM	C1A-CHA-C4D	-2.24	121.03	126.34
21	43	417	CL7	C1C-C2C-C3C	-2.24	103.68	106.94
21	12	516	CL7	C1-C2-C3	2.24	129.91	126.04
21	32	516	CL7	C1-C2-C3	2.24	129.91	126.04
21	44	412	CL7	C3B-C4B-NB	2.24	112.59	110.52
21	43	416	CL7	CAC-C3C-C2C	2.24	131.35	127.53
32	34	403	ZEX	C10-C11-C12	-2.24	116.24	123.22
21	13	502	CL7	CHB-C1B-NB	-2.23	121.89	124.26
23	34	402	8CT	C10-C11-C12	-2.23	122.86	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	509	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	42	509	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	44	410	CL7	C4C-C3C-C2C	-2.23	104.21	107.13
32	13	520	ZEX	C3-C4-C5	-2.23	107.40	111.85
21	31	403	CL7	CAA-CBA-CGA	-2.23	106.72	113.25
21	2B	623	CL7	CHB-C1B-NB	-2.23	121.89	124.26
21	3B	622	CL7	CHB-C1B-NB	-2.23	121.89	124.26
21	33	515	CL7	CAC-C3C-C2C	2.23	131.35	127.53
21	13	504	CL7	CAA-CBA-CGA	-2.23	106.72	113.25
21	41	410	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
31	4F	101	HEM	C1A-CHA-C4D	-2.23	121.04	126.34
32	22	524	ZEX	C35-C15-C14	-2.23	118.90	123.47
21	33	503	CL7	CED-O2D-CGD	-2.23	110.89	115.94
32	33	525	ZEX	C19-C9-C8	2.23	121.59	118.08
21	13	517	CL7	CMB-C2B-C1B	2.23	128.77	125.37
21	2B	605	CL7	C3B-C4B-NB	2.23	112.59	110.52
21	4B	613	CL7	O2A-CGA-O1A	-2.23	117.96	123.59
21	43	402	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
32	31	421	ZEX	C3-C4-C5	-2.23	107.41	111.85
21	21	402	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	21	403	CL7	CAA-CBA-CGA	-2.23	106.73	113.25
27	1C	516	DGD	O1G-C1A-C2A	2.23	118.91	111.91
21	23	412	CL7	C1-C2-C3	2.23	129.90	126.04
21	1D	405	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	2D	405	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	3C	509	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	4D	405	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
32	31	422	ZEX	C18-C5-C6	-2.23	122.02	124.53
21	12	501	CL7	C1-C2-C3	2.23	129.90	126.04
21	33	511	CL7	C1-C2-C3	2.23	129.90	126.04
21	13	506	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	32	515	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	43	407	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
32	12	524	ZEX	C35-C15-C14	-2.23	118.91	123.47
23	2B	619	8CT	C24-C25-C26	-2.23	124.13	127.31
22	4A	402	PHO	C1C-C2C-C3C	-2.23	106.76	108.61
21	22	518	CL7	CMB-C2B-C1B	2.23	128.76	125.37
21	12	506	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	33	511	CL7	C4-C3-C5	2.23	119.02	115.27
32	22	519	ZEX	C31-C32-C33	-2.23	120.16	126.42
21	13	511	CL7	C1-C2-C3	2.23	129.90	126.04
23	4C	515	8CT	C22-C21-C20	-2.23	119.80	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	518	CL7	CMB-C2B-C1B	2.23	128.76	125.37
21	42	518	CL7	CMB-C2B-C1B	2.23	128.76	125.37
21	22	511	CL7	C4D-C3D-C2D	2.23	110.20	107.30
21	1B	622	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	11	410	CL7	C3B-C4B-NB	2.23	112.58	110.52
21	1C	507	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	42	516	CL7	C1-C2-C3	2.23	129.89	126.04
32	44	403	ZEX	C10-C11-C12	-2.23	116.27	123.22
23	2B	619	8CT	C40-C12-C11	2.23	121.58	118.08
32	32	520	ZEX	C40-C33-C32	2.23	121.58	118.08
21	41	402	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	23	405	CL7	CAA-CBA-CGA	-2.22	106.75	113.25
21	22	502	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	12	503	CL7	CAA-C2A-C3A	2.22	118.87	112.78
21	23	418	CL7	CMB-C2B-C1B	2.22	128.76	125.37
21	2B	608	CL7	CHB-C1B-NB	-2.22	121.90	124.26
21	3B	607	CL7	CHB-C1B-NB	-2.22	121.90	124.26
32	12	519	ZEX	C31-C32-C33	-2.22	120.17	126.42
23	1C	515	8CT	C22-C21-C20	-2.22	119.81	122.92
21	31	410	CL7	O2A-CGA-O1A	-2.22	117.98	123.59
21	23	404	CL7	CED-O2D-CGD	-2.22	110.91	115.94
32	32	524	ZEX	C35-C15-C14	-2.22	118.92	123.47
21	23	407	CL7	C3B-C2B-C1B	-2.22	104.48	107.16
21	12	511	CL7	C4D-C3D-C2D	2.22	110.20	107.30
21	42	511	CL7	C4D-C3D-C2D	2.22	110.20	107.30
21	13	503	CL7	CED-O2D-CGD	-2.22	110.91	115.94
21	43	404	CL7	CED-O2D-CGD	-2.22	110.91	115.94
21	43	405	CL7	CAA-CBA-CGA	-2.22	106.76	113.25
21	21	419	CL7	C1C-C2C-C3C	-2.22	103.69	106.94
21	33	504	CL7	CAA-CBA-CGA	-2.22	106.76	113.25
21	24	412	CL7	C3B-C4B-NB	2.22	112.58	110.52
21	42	502	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	34	404	CL7	CAC-C3C-C2C	2.22	131.33	127.53
21	2D	404	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
32	32	519	ZEX	C31-C32-C33	-2.22	120.17	126.42
21	1B	605	CL7	CAA-CBA-CGA	-2.22	106.76	113.25
21	4B	606	CL7	CAA-CBA-CGA	-2.22	106.76	113.25
32	33	520	ZEX	C40-C33-C34	-2.22	119.81	122.92
21	3C	510	CL7	CHB-C1B-NB	-2.22	121.91	124.26
32	42	519	ZEX	C31-C32-C33	-2.22	120.18	126.42
21	41	410	CL7	C3B-C4B-NB	2.22	112.58	110.52
21	33	506	CL7	C1C-C2C-C3C	-2.22	103.70	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1C	513	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	1D	402	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	2C	507	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	32	507	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
21	32	518	CL7	CMB-C2B-C1B	2.22	128.75	125.37
21	22	501	CL7	C1-C2-C3	2.22	129.88	126.04
21	44	404	CL7	CAC-C3C-C2C	2.22	131.32	127.53
21	3B	605	CL7	CAA-CBA-CGA	-2.22	106.77	113.25
21	32	504	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	21	405	CL7	C3B-C4B-NB	2.22	112.57	110.52
21	4B	605	CL7	C3B-C4B-NB	2.22	112.57	110.52
23	3B	619	8CT	C18-C19-C20	-2.22	118.93	123.47
23	2C	515	8CT	C24-C23-C21	-2.22	120.19	126.42
21	44	406	CL7	C4C-C3C-C2C	-2.22	104.24	107.13
32	21	422	ZEX	C18-C5-C6	-2.22	122.04	124.53
21	2B	617	CL7	CHB-C1B-NB	-2.22	121.91	124.26
21	2B	606	CL7	C4C-C3C-C2C	-2.22	104.24	107.13
21	24	404	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
21	1C	505	CL7	CBA-CAA-C2A	-2.22	107.32	113.86
22	1A	402	PHO	C1C-C2C-C3C	-2.22	106.77	108.61
21	13	506	CL7	C3B-C2B-C1B	-2.22	104.49	107.16
32	14	403	ZEX	C10-C11-C12	-2.22	116.30	123.22
21	14	412	CL7	C3B-C4B-NB	2.22	112.57	110.52
21	4C	507	CL7	C4C-C3C-C2C	-2.22	104.24	107.13
21	11	419	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
23	2A	404	8CT	C14-C15-C16	-2.22	120.19	126.42
21	33	506	CL7	C3B-C2B-C1B	-2.22	104.49	107.16
21	23	412	CL7	C4-C3-C5	2.22	119.00	115.27
21	33	510	CL7	C4D-C3D-C2D	2.21	110.19	107.30
23	4K	101	8CT	C25-C24-C23	-2.21	116.31	123.22
21	2D	402	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	3B	605	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	34	410	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	42	503	CL7	CAA-C2A-C3A	2.21	118.84	112.78
21	4D	405	CL7	CMB-C2B-C1B	2.21	128.74	125.37
21	3D	402	CL7	C4-C3-C5	2.21	119.49	114.60
21	11	410	CL7	C4-C3-C5	2.21	119.00	115.27
21	22	503	CL7	CAA-C2A-C3A	2.21	118.84	112.78
21	44	416	CL7	C1C-C2C-C3C	-2.21	103.71	106.94
23	2C	518	8CT	C13-C14-C15	-2.21	116.31	123.22
21	13	511	CL7	C4-C3-C5	2.21	118.99	115.27
32	12	520	ZEX	C40-C33-C32	2.21	121.56	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	502	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	22	508	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	21	410	CL7	C3B-C4B-NB	2.21	112.57	110.52
21	4B	617	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	2C	505	CL7	CBA-CAA-C2A	-2.21	107.33	113.86
21	34	412	CL7	C3B-C4B-NB	2.21	112.57	110.52
21	23	417	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	31	403	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
21	41	419	CL7	C1C-C2C-C3C	-2.21	103.71	106.94
21	32	503	CL7	C4D-C3D-C2D	2.21	110.18	107.30
32	12	524	ZEX	C30-C31-C32	-2.21	116.32	123.22
21	41	403	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
23	1K	101	8CT	C25-C24-C23	-2.21	116.32	123.22
23	4C	518	8CT	C13-C14-C15	-2.21	116.32	123.22
21	4B	623	CL7	C1C-C2C-C3C	-2.21	103.71	106.94
32	13	520	ZEX	C27-C26-C25	-2.21	119.27	122.84
21	22	507	CL7	C1C-C2C-C3C	-2.21	103.71	106.94
21	11	410	CL7	O2A-CGA-O1A	-2.21	118.02	123.59
23	3A	404	8CT	C14-C15-C16	-2.21	120.21	126.42
21	23	417	CL7	CMB-C2B-C1B	2.21	128.73	125.37
21	1B	607	CL7	CHB-C1B-NB	-2.21	121.92	124.26
23	1B	618	8CT	C40-C12-C11	2.21	121.56	118.08
21	23	407	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	21	418	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
23	4B	619	8CT	C40-C12-C11	2.21	121.56	118.08
21	34	413	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	4B	607	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	3C	513	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	4D	402	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
23	1A	404	8CT	C14-C15-C16	-2.21	120.21	126.42
29	2D	403	BCT	O2-C-O1	2.21	125.27	119.55
32	41	421	ZEX	C10-C11-C12	-2.21	116.33	123.22
32	13	520	ZEX	C40-C33-C34	-2.21	119.83	122.92
21	14	413	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	44	414	CL7	C4-C3-C5	2.21	118.98	115.27
32	43	421	ZEX	C27-C26-C25	-2.21	119.27	122.84
23	24	402	8CT	C10-C11-C12	-2.21	122.90	126.23
23	2K	101	8CT	C25-C24-C23	-2.21	116.33	123.22
23	3K	101	8CT	C25-C24-C23	-2.21	116.33	123.22
23	3C	514	8CT	C22-C21-C23	2.21	121.55	118.08
21	4D	402	CL7	C4-C3-C5	2.21	119.48	114.60
21	1D	404	CL7	C1C-C2C-C3C	-2.21	103.72	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2C	507	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
23	34	402	8CT	C18-C19-C20	-2.21	118.95	123.47
32	11	422	ZEX	C18-C5-C6	-2.21	122.05	124.53
21	1B	622	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	4B	623	CL7	CHB-C1B-NB	-2.21	121.92	124.26
21	31	418	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	32	503	CL7	CAA-C2A-C3A	2.21	118.81	112.78
23	1C	515	8CT	C24-C23-C21	-2.21	120.22	126.42
21	4C	502	CL7	CHB-C1B-NB	-2.20	121.92	124.26
32	23	401	ZEX	C8-C9-C10	-2.20	115.56	118.94
21	2D	402	CL7	C4-C3-C5	2.20	119.47	114.60
21	3C	511	CL7	CAC-C3C-C2C	2.20	131.30	127.53
21	4C	505	CL7	CBA-CAA-C2A	-2.20	107.36	113.86
21	1A	407	CL7	C4C-C3C-C2C	-2.20	104.25	107.13
21	21	410	CL7	C4C-C3C-C2C	-2.20	104.25	107.13
21	4B	606	CL7	C4C-C3C-C2C	-2.20	104.25	107.13
21	22	512	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	3B	622	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	33	516	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
23	24	402	8CT	C18-C19-C20	-2.20	118.96	123.47
32	23	401	ZEX	C23-C24-C25	-2.20	106.19	109.33
21	2B	607	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
23	4A	404	8CT	C14-C15-C16	-2.20	120.23	126.42
32	31	421	ZEX	C10-C11-C12	-2.20	116.34	123.22
21	41	410	CL7	C4-C3-C5	2.20	118.98	115.27
21	11	409	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	23	417	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	42	515	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	4C	511	CL7	CAC-C3C-C2C	2.20	131.30	127.53
21	11	410	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	43	417	CL7	CMB-C2B-C1B	2.20	128.72	125.37
23	1C	518	8CT	C13-C14-C15	-2.20	116.34	123.22
21	1B	606	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
21	3A	401	CL7	C4D-C3D-CAD	-2.20	105.94	107.42
23	3C	518	8CT	C13-C14-C15	-2.20	116.35	123.22
32	42	520	ZEX	C40-C33-C32	2.20	121.55	118.08
21	3B	616	CL7	CHB-C1B-NB	-2.20	121.93	124.26
21	43	407	CL7	C3B-C2B-C1B	-2.20	104.50	107.16
21	14	414	CL7	C4-C3-C5	2.20	118.97	115.27
21	2C	511	CL7	CAC-C3C-C2C	2.20	131.29	127.53
21	24	413	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
21	21	410	CL7	O2A-CGA-O1A	-2.20	118.04	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	517	CL7	CMB-C2B-C1B	2.20	128.72	125.37
21	43	406	CL7	CMB-C2B-C1B	2.20	128.72	125.37
32	22	524	ZEX	C30-C31-C32	-2.20	116.35	123.22
21	42	508	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	43	417	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	1C	507	CL7	CED-O2D-CGD	-2.20	110.96	115.94
21	4C	507	CL7	O2D-CGD-O1D	-2.20	119.54	123.84
29	4D	403	BCT	O2-C-O1	2.20	125.25	119.55
21	2C	505	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
21	2B	606	CL7	CAA-CBA-CGA	-2.20	106.83	113.25
23	3B	618	8CT	C40-C12-C11	2.20	121.54	118.08
21	21	403	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	1D	402	CL7	C4-C3-C5	2.20	119.46	114.60
32	13	520	ZEX	C1-C6-C7	2.20	122.00	115.78
32	11	421	ZEX	C10-C11-C12	-2.20	116.36	123.22
21	13	516	CL7	CMB-C2B-C1B	2.20	128.72	125.37
23	14	402	8CT	C10-C11-C12	-2.20	122.92	126.23
21	11	418	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	41	418	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
32	32	524	ZEX	C30-C31-C32	-2.20	116.36	123.22
21	3C	504	CL7	C3B-C4B-NB	2.20	112.55	110.52
32	21	421	ZEX	C10-C11-C12	-2.20	116.36	123.22
21	33	516	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
29	3D	403	BCT	O2-C-O1	2.20	125.24	119.55
21	4D	402	CL7	CMB-C2B-C1B	2.20	128.71	125.37
21	2C	503	CL7	C4C-C3C-C2C	-2.20	104.27	107.13
21	43	418	CL7	CMB-C2B-C1B	2.19	128.71	125.37
21	14	410	CL7	C4C-C3C-C2C	-2.19	104.27	107.13
21	4A	407	CL7	C4C-C3C-C2C	-2.19	104.27	107.13
23	44	402	8CT	C18-C19-C20	-2.19	118.98	123.47
21	2C	517	CL7	C3B-C4B-NB	2.19	112.55	110.52
21	3A	407	CL7	C4C-C3C-C2C	-2.19	104.27	107.13
23	4C	515	8CT	C24-C23-C21	-2.19	120.25	126.42
21	1C	511	CL7	CAC-C3C-C2C	2.19	131.28	127.53
21	3C	505	CL7	CBA-CAA-C2A	-2.19	107.39	113.86
21	1B	611	CL7	O2A-CGA-O1A	-2.19	118.06	123.59
29	1D	403	BCT	O2-C-O1	2.19	125.23	119.55
21	1B	612	CL7	C1C-C2C-C3C	-2.19	103.74	106.94
21	3D	404	CL7	C1C-C2C-C3C	-2.19	103.74	106.94
32	42	524	ZEX	C30-C31-C32	-2.19	116.38	123.22
21	14	404	CL7	CAC-C3C-C2C	2.19	131.28	127.53
23	14	402	8CT	C18-C19-C20	-2.19	118.99	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	33	505	CL7	CMB-C2B-C1B	2.19	128.71	125.37
21	22	514	CL7	C3B-C4B-NB	2.19	112.55	110.52
23	4C	514	8CT	C22-C21-C23	2.19	121.53	118.08
32	22	520	ZEX	C40-C33-C32	2.19	121.53	118.08
21	32	512	CL7	C1C-C2C-C3C	-2.19	103.74	106.94
21	1C	510	CL7	CHB-C1B-NB	-2.19	121.94	124.26
21	4C	510	CL7	CHB-C1B-NB	-2.19	121.94	124.26
21	43	403	CL7	C4C-C3C-C2C	-2.19	104.27	107.13
21	2B	623	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	11	403	CL7	C4C-C3C-C2C	-2.19	104.27	107.13
21	33	516	CL7	CMB-C2B-C1B	2.19	128.70	125.37
21	24	416	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	41	410	CL7	O2A-CGA-O1A	-2.19	118.07	123.59
21	34	416	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
32	43	421	ZEX	C40-C33-C34	-2.19	119.86	122.92
21	34	414	CL7	C4-C3-C5	2.19	118.95	115.27
32	13	525	ZEX	C23-C24-C25	-2.19	106.22	109.33
21	23	411	CL7	C4D-C3D-C2D	2.19	110.15	107.30
21	3C	503	CL7	C4C-C3C-C2C	-2.19	104.28	107.13
21	3C	507	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	31	412	CL7	C3B-C4B-NB	2.18	112.54	110.52
23	3C	515	8CT	C24-C23-C21	-2.18	120.28	126.42
21	1C	505	CL7	C1C-C2C-C3C	-2.18	103.75	106.94
21	4C	505	CL7	C1C-C2C-C3C	-2.18	103.75	106.94
23	1B	617	8CT	C39-C16-C17	-2.18	119.86	122.92
23	4B	618	8CT	C39-C16-C17	-2.18	119.86	122.92
21	22	505	CL7	CAC-C3C-C2C	2.18	131.26	127.53
32	33	520	ZEX	C1-C6-C7	2.18	121.96	115.78
21	1C	502	CL7	C4-C3-C5	2.18	118.94	115.27
21	43	411	CL7	C4D-C3D-C2D	2.18	110.14	107.30
21	4C	507	CL7	CED-O2D-CGD	-2.18	111.00	115.94
21	2C	502	CL7	CHB-C1B-NB	-2.18	121.95	124.26
21	33	515	CL7	C4D-C3D-C2D	2.18	110.14	107.30
21	44	413	CL7	C1C-C2C-C3C	-2.18	103.75	106.94
21	34	415	CL7	C3B-C4B-NB	2.18	112.54	110.52
21	32	511	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	4A	401	CL7	O2A-CGA-CBA	2.18	118.75	111.91
32	23	421	ZEX	C40-C33-C34	-2.18	119.87	122.92
21	2A	407	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	42	504	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
23	4B	619	8CT	C08-C04-C03	-2.18	106.76	110.30
21	3A	407	CL7	CMB-C2B-C1B	2.18	128.69	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	409	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	31	410	CL7	C4-C3-C5	2.18	118.94	115.27
21	24	404	CL7	CAC-C3C-C2C	2.18	131.26	127.53
21	13	505	CL7	CHD-C1D-ND	-2.18	121.95	124.26
21	4C	504	CL7	C3B-C4B-NB	2.18	112.54	110.52
32	44	403	ZEX	C20-C13-C12	2.18	121.51	118.08
21	2A	401	CL7	C4D-C3D-CAD	-2.18	105.95	107.42
21	22	515	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	34	404	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	4D	404	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
32	23	421	ZEX	C1-C6-C7	2.18	121.94	115.78
23	2C	514	8CT	C22-C21-C23	2.18	121.51	118.08
21	44	407	CL7	CAC-C3C-C2C	2.18	131.25	127.53
21	23	403	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
21	23	410	CL7	C4D-C3D-C2D	2.18	110.14	107.30
32	43	421	ZEX	C1-C6-C7	2.18	121.94	115.78
21	2C	507	CL7	O2D-CGD-O1D	-2.18	119.58	123.84
21	3C	507	CL7	O2D-CGD-O1D	-2.18	119.58	123.84
21	1B	616	CL7	CHB-C1B-NB	-2.18	121.95	124.26
21	33	502	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
21	13	509	CL7	C4D-C3D-C2D	2.18	110.14	107.30
21	12	515	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	14	412	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	44	404	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	4D	404	CL7	C3B-C4B-NB	2.18	112.53	110.52
21	21	410	CL7	C4-C3-C5	2.18	118.93	115.27
23	44	402	8CT	C40-C12-C11	2.18	121.50	118.08
21	1A	401	CL7	O2A-CGA-CBA	2.18	118.73	111.91
21	2D	404	CL7	O2A-CGA-O1A	-2.17	118.10	123.59
21	4B	608	CL7	CHB-C1B-NB	-2.17	121.95	124.26
23	24	402	8CT	C22-C21-C23	2.17	121.50	118.08
21	2C	507	CL7	CED-O2D-CGD	-2.17	111.02	115.94
21	3C	507	CL7	CED-O2D-CGD	-2.17	111.02	115.94
21	14	415	CL7	C3B-C4B-NB	2.17	112.53	110.52
32	33	520	ZEX	C27-C26-C25	-2.17	119.33	122.84
23	3B	617	8CT	C39-C16-C17	-2.17	119.88	122.92
21	3A	401	CL7	O2A-CGA-CBA	2.17	118.73	111.91
23	4C	514	8CT	C15-C16-C17	-2.17	115.61	118.94
23	1A	404	8CT	C01-C02-C07	2.17	117.79	113.62
21	24	407	CL7	CAC-C3C-C2C	2.17	131.25	127.53
21	1A	401	CL7	C4D-C3D-CAD	-2.17	105.96	107.42
31	4F	101	HEM	C4A-NA-C1A	2.17	107.47	105.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	608	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
21	1C	503	CL7	C4C-C3C-C2C	-2.17	104.30	107.13
23	1C	514	8CT	C22-C21-C23	2.17	121.50	118.08
21	2C	502	CL7	C4-C3-C5	2.17	118.92	115.27
21	3C	502	CL7	C4-C3-C5	2.17	118.92	115.27
21	3B	606	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
21	22	511	CL7	C4C-C3C-C2C	-2.17	104.30	107.13
21	32	508	CL7	C4C-C3C-C2C	-2.17	104.30	107.13
23	2B	618	8CT	C36-C35-C30	2.17	112.83	109.55
21	2C	510	CL7	CHB-C1B-NB	-2.17	121.96	124.26
32	23	421	ZEX	C27-C26-C25	-2.17	119.34	122.84
21	41	420	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
21	1C	517	CL7	C3B-C4B-NB	2.17	112.53	110.52
21	4C	517	CL7	C3B-C4B-NB	2.17	112.53	110.52
32	44	403	ZEX	C20-C13-C14	-2.17	119.89	122.92
21	2A	401	CL7	O2A-CGA-CBA	2.17	118.71	111.91
21	4C	502	CL7	C4-C3-C5	2.17	118.92	115.27
21	14	416	CL7	C1C-C2C-C3C	-2.17	103.78	106.94
21	13	510	CL7	C4D-C3D-C2D	2.17	110.12	107.30
21	33	515	CL7	CMA-C3A-C2A	-2.17	111.04	116.10
21	12	504	CL7	C4C-C3C-C2C	-2.17	104.30	107.13
21	42	511	CL7	C4C-C3C-C2C	-2.17	104.30	107.13
21	42	508	CL7	C3B-C2B-C1B	-2.17	104.55	107.16
32	24	403	ZEX	C1-C6-C7	2.17	121.91	115.78
32	33	525	ZEX	C8-C9-C10	-2.17	115.61	118.94
23	2B	618	8CT	C39-C16-C17	-2.17	119.89	122.92
23	3B	617	8CT	C36-C35-C30	2.17	112.83	109.55
21	41	409	CL7	C1C-C2C-C3C	-2.17	103.78	106.94
21	3C	505	CL7	C1C-C2C-C3C	-2.17	103.78	106.94
32	34	403	ZEX	C1-C6-C7	2.17	121.91	115.78
23	3A	404	8CT	C01-C02-C07	2.17	117.78	113.62
21	24	416	CL7	CHB-C1B-NB	-2.17	121.96	124.26
23	3C	514	8CT	C15-C16-C17	-2.17	115.62	118.94
21	4B	612	CL7	O2A-CGA-O1A	-2.17	118.13	123.59
23	3B	618	8CT	C08-C04-C03	-2.17	106.79	110.30
21	21	409	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	34	412	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	4C	501	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	42	512	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	12	511	CL7	C4C-C3C-C2C	-2.16	104.31	107.13
21	23	406	CL7	CMB-C2B-C1B	2.16	128.66	125.37
21	14	416	CL7	CHB-C1B-NB	-2.16	121.97	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4B	618	8CT	C36-C35-C30	2.16	112.82	109.55
21	13	505	CL7	CMB-C2B-C1B	2.16	128.66	125.37
21	1B	607	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	32	518	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
32	34	403	ZEX	C20-C13-C14	-2.16	119.89	122.92
21	44	412	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
32	43	401	ZEX	C23-C24-C25	-2.16	106.25	109.33
21	43	410	CL7	C4D-C3D-C2D	2.16	110.12	107.30
23	1C	514	8CT	C15-C16-C17	-2.16	115.62	118.94
32	14	403	ZEX	C1-C6-C7	2.16	121.89	115.78
21	13	507	CL7	CAC-C3C-C2C	2.16	131.23	127.53
21	22	503	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	31	409	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	4B	612	CL7	C3B-C2B-C1B	-2.16	104.55	107.16
23	2B	619	8CT	C08-C04-C03	-2.16	106.79	110.30
21	44	416	CL7	CHB-C1B-NB	-2.16	121.97	124.26
21	44	408	CL7	C3B-C4B-NB	2.16	112.52	110.52
21	13	502	CL7	C4C-C3C-C2C	-2.16	104.31	107.13
21	12	503	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
21	21	409	CL7	CHC-C1C-NC	-2.16	122.47	124.45
21	3D	404	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
23	4A	404	8CT	C01-C02-C07	2.16	117.77	113.62
21	1D	402	CL7	CMB-C2B-C1B	2.16	128.66	125.37
21	3B	611	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
32	44	403	ZEX	C1-C6-C7	2.16	121.89	115.78
21	41	417	CL7	C4-C3-C5	2.16	118.90	115.27
21	34	404	CL7	CMB-C2B-C1B	2.16	128.66	125.37
32	24	403	ZEX	C20-C13-C14	-2.16	119.90	122.92
21	4A	401	CL7	C4D-C3D-CAD	-2.16	105.97	107.42
21	2B	608	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
21	3B	607	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
32	33	525	ZEX	C23-C24-C25	-2.16	106.26	109.33
23	2C	514	8CT	C15-C16-C17	-2.16	115.63	118.94
21	2B	612	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
23	2A	404	8CT	C01-C02-C07	2.16	117.76	113.62
21	2D	402	CL7	CMB-C2B-C1B	2.16	128.66	125.37
21	2B	615	CL7	C4D-C3D-C2D	2.16	110.11	107.30
21	3B	614	CL7	C4D-C3D-C2D	2.16	110.11	107.30
21	42	505	CL7	CAC-C3C-C2C	2.16	131.22	127.53
21	11	405	CL7	C3B-C4B-NB	2.16	112.52	110.52
31	2F	101	HEM	C4A-NA-C1A	2.16	107.46	105.35
32	24	419	ZEX	C21-C26-C27	2.16	121.88	115.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	34	403	ZEX	C20-C13-C12	2.16	121.47	118.08
32	14	403	ZEX	C20-C13-C14	-2.16	119.90	122.92
21	34	407	CL7	CAC-C3C-C2C	2.16	131.22	127.53
21	24	414	CL7	C4-C3-C5	2.15	118.90	115.27
21	1C	504	CL7	C3B-C4B-NB	2.15	112.51	110.52
21	2C	504	CL7	C3B-C4B-NB	2.15	112.51	110.52
23	1B	618	8CT	C08-C04-C03	-2.15	106.80	110.30
23	34	402	8CT	C40-C12-C11	2.15	121.47	118.08
21	34	417	CL7	C3B-C2B-C1B	-2.15	104.56	107.16
21	14	407	CL7	CAC-C3C-C2C	2.15	131.21	127.53
21	31	417	CL7	C4-C3-C5	2.15	118.89	115.27
21	1D	404	CL7	O2A-CGA-O1A	-2.15	118.16	123.59
21	4D	404	CL7	O2A-CGA-O1A	-2.15	118.16	123.59
32	43	420	ZEX	C20-C13-C14	-2.15	119.91	122.92
21	23	406	CL7	CHD-C1D-ND	-2.15	121.98	124.26
21	33	507	CL7	CAC-C3C-C2C	2.15	131.21	127.53
32	31	422	ZEX	C27-C26-C25	-2.15	119.36	122.84
21	42	514	CL7	C3B-C4B-NB	2.15	112.51	110.52
21	41	412	CL7	C3B-C4B-NB	2.15	112.51	110.52
21	11	404	CL7	C3D-C4D-ND	2.15	113.25	110.17
21	41	404	CL7	C3D-C4D-ND	2.15	113.25	110.17
21	12	512	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
23	1C	518	8CT	C39-C16-C15	2.15	121.47	118.08
21	11	417	CL7	C4-C3-C5	2.15	118.89	115.27
21	14	406	CL7	C4-C3-C5	2.15	118.89	115.27
21	1C	507	CL7	O2D-CGD-O1D	-2.15	119.63	123.84
21	22	504	CL7	C4C-C3C-C2C	-2.15	104.32	107.13
21	3C	517	CL7	C3B-C4B-NB	2.15	112.51	110.52
21	41	405	CL7	C3B-C4B-NB	2.15	112.51	110.52
21	43	416	CL7	C4D-C3D-C2D	2.15	110.10	107.30
21	34	416	CL7	CHB-C1B-NB	-2.15	121.98	124.26
23	1B	617	8CT	C36-C35-C30	2.15	112.80	109.55
21	13	515	CL7	CMA-C3A-C2A	-2.15	111.08	116.10
23	44	402	8CT	C22-C21-C23	2.15	121.46	118.08
21	43	403	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
21	24	415	CL7	CMB-C2B-C1B	2.15	128.64	125.37
31	2F	101	HEM	CBD-CAD-C3D	-2.15	106.66	112.63
31	3F	101	HEM	CBD-CAD-C3D	-2.15	106.66	112.63
21	33	509	CL7	C4D-C3D-C2D	2.15	110.10	107.30
32	43	401	ZEX	C8-C9-C10	-2.15	115.65	118.94
21	1C	502	CL7	CHB-C1B-NB	-2.15	121.98	124.26
21	14	417	CL7	C3B-C2B-C1B	-2.15	104.57	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2B	612	CL7	C3B-C2B-C1B	-2.15	104.57	107.16
21	3B	611	CL7	C3B-C2B-C1B	-2.15	104.57	107.16
21	43	408	CL7	CAC-C3C-C2C	2.15	131.20	127.53
32	44	419	ZEX	C21-C26-C27	2.15	121.85	115.78
21	23	413	CL7	CED-O2D-CGD	-2.15	111.08	115.94
32	44	419	ZEX	C10-C11-C12	-2.15	116.52	123.22
21	32	514	CL7	C3B-C4B-NB	2.15	112.50	110.52
21	41	402	CL7	CAA-C2A-C3A	-2.14	106.90	112.78
21	32	505	CL7	CAC-C3C-C2C	2.14	131.20	127.53
31	1F	101	HEM	CBD-CAD-C3D	-2.14	106.67	112.63
21	21	417	CL7	C4-C3-C5	2.14	118.88	115.27
32	24	419	ZEX	C10-C11-C12	-2.14	116.53	123.22
32	34	419	ZEX	C10-C11-C12	-2.14	116.53	123.22
21	31	411	CL7	CAA-CBA-CGA	-2.14	106.82	112.51
21	12	505	CL7	CAC-C3C-C2C	2.14	131.20	127.53
23	2C	518	8CT	C22-C21-C20	-2.14	119.92	122.92
21	1B	611	CL7	C3B-C2B-C1B	-2.14	104.57	107.16
21	42	503	CL7	C1C-C2C-C3C	-2.14	103.81	106.94
21	31	402	CL7	CAA-C2A-C3A	-2.14	106.91	112.78
21	23	416	CL7	CMA-C3A-C2A	-2.14	111.10	116.10
21	43	416	CL7	CMA-C3A-C2A	-2.14	111.10	116.10
31	4F	101	HEM	CBD-CAD-C3D	-2.14	106.67	112.63
32	24	403	ZEX	C20-C13-C12	2.14	121.45	118.08
21	31	404	CL7	C3D-C4D-ND	2.14	113.24	110.17
21	24	415	CL7	C3B-C4B-NB	2.14	112.50	110.52
21	31	405	CL7	C3B-C4B-NB	2.14	112.50	110.52
21	23	416	CL7	C4D-C3D-C2D	2.14	110.09	107.30
21	21	402	CL7	CAA-C2A-C3A	-2.14	106.91	112.78
21	24	404	CL7	CMB-C2B-C1B	2.14	128.63	125.37
21	3D	402	CL7	CMB-C2B-C1B	2.14	128.63	125.37
21	4A	407	CL7	CMB-C2B-C1B	2.14	128.63	125.37
32	33	519	ZEX	C21-C26-C27	2.14	121.84	115.78
21	21	404	CL7	C3D-C4D-ND	2.14	113.24	110.17
21	2B	602	CL7	C4C-C3C-C2C	-2.14	104.34	107.13
23	14	402	8CT	C40-C12-C11	2.14	121.45	118.08
23	24	402	8CT	C39-C16-C15	2.14	121.45	118.08
21	43	413	CL7	CED-O2D-CGD	-2.14	111.09	115.94
21	12	508	CL7	C4C-C3C-C2C	-2.14	104.34	107.13
21	4C	503	CL7	C4C-C3C-C2C	-2.14	104.34	107.13
21	42	501	CL7	C4-C3-C5	2.14	118.87	115.27
32	14	419	ZEX	C21-C26-C27	2.14	121.83	115.78
21	43	406	CL7	CHD-C1D-ND	-2.14	121.99	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	13	525	ZEX	C8-C9-C10	-2.14	115.66	118.94
23	14	402	8CT	C39-C16-C15	2.14	121.45	118.08
21	11	419	CL7	CMB-C2B-C1B	2.14	128.63	125.37
21	41	419	CL7	CMB-C2B-C1B	2.14	128.63	125.37
32	14	419	ZEX	C10-C11-C12	-2.14	116.54	123.22
32	11	422	ZEX	C27-C26-C25	-2.14	119.39	122.84
32	41	422	ZEX	C27-C26-C25	-2.14	119.39	122.84
21	13	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	2B	604	CL7	C4C-C3C-C2C	-2.14	104.34	107.13
21	24	417	CL7	C3B-C2B-C1B	-2.14	104.58	107.16
21	42	515	CL7	CAA-CBA-CGA	-2.14	106.83	112.51
23	3C	518	8CT	C22-C21-C20	-2.14	119.93	122.92
21	12	508	CL7	C3B-C2B-C1B	-2.14	104.58	107.16
21	23	408	CL7	CAC-C3C-C2C	2.14	131.18	127.53
21	32	508	CL7	C3B-C2B-C1B	-2.14	104.58	107.16
21	12	518	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	32	518	CL7	C3B-C4B-NB	2.14	112.50	110.52
21	13	516	CL7	C4C-C3C-C2C	-2.13	104.34	107.13
21	14	404	CL7	CMB-C2B-C1B	2.13	128.62	125.37
21	44	404	CL7	CMB-C2B-C1B	2.13	128.62	125.37
23	14	402	8CT	C22-C21-C23	2.13	121.44	118.08
31	1F	101	HEM	C4A-NA-C1A	2.13	107.44	105.35
32	34	419	ZEX	C21-C26-C27	2.13	121.81	115.78
21	11	402	CL7	CAA-C2A-C3A	-2.13	106.94	112.78
21	24	412	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	34	408	CL7	C3B-C4B-NB	2.13	112.49	110.52
21	42	518	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	12	515	CL7	CAA-CBA-CGA	-2.13	106.85	112.51
21	22	515	CL7	CAA-CBA-CGA	-2.13	106.85	112.51
25	32	523	SQD	O8-S-C6	-2.13	102.34	105.74
21	3D	404	CL7	C3B-C4B-NB	2.13	112.49	110.52
21	1B	614	CL7	C4D-C3D-C2D	2.13	110.08	107.30
21	1A	407	CL7	CMB-C2B-C1B	2.13	128.62	125.37
23	24	402	8CT	C40-C12-C11	2.13	121.44	118.08
21	1B	601	CL7	C4C-C3C-C2C	-2.13	104.35	107.13
21	33	514	CL7	O2D-CGD-O1D	-2.13	119.67	123.84
21	11	420	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	24	411	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
23	34	402	8CT	C39-C16-C15	2.13	121.44	118.08
21	44	415	CL7	C3B-C4B-NB	2.13	112.49	110.52
21	4B	615	CL7	C4D-C3D-C2D	2.13	110.08	107.30
21	1D	404	CL7	C3B-C4B-NB	2.13	112.49	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	12	501	CL7	C4-C3-C5	2.13	118.85	115.27
21	1C	501	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	2B	615	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	3C	501	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	32	503	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	12	511	CL7	CAC-C3C-C2C	2.13	131.17	127.53
21	2C	501	CL7	CAC-C3C-C2C	2.13	131.17	127.53
21	32	511	CL7	CAC-C3C-C2C	2.13	131.17	127.53
21	31	420	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	33	502	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	24	406	CL7	C4-C3-C5	2.13	118.85	115.27
21	3C	501	CL7	CAC-C3C-C2C	2.13	131.17	127.53
21	21	413	CL7	CMB-C2B-C1B	2.13	128.61	125.37
21	24	408	CL7	C3B-C4B-NB	2.13	112.49	110.52
21	13	512	CL7	C4-C3-C5	2.13	118.85	115.27
21	31	413	CL7	CMB-C2B-C1B	2.13	128.61	125.37
21	33	508	CL7	CHB-C1B-NB	-2.13	122.00	124.26
21	13	514	CL7	O2D-CGD-O1D	-2.13	119.68	123.84
21	3B	614	CL7	CBA-CAA-C2A	2.13	120.14	113.86
21	3D	404	CL7	C4C-C3C-C2C	-2.13	104.36	107.13
21	32	501	CL7	C4-C3-C5	2.13	118.85	115.27
23	2C	518	8CT	C39-C16-C15	2.13	121.43	118.08
21	13	515	CL7	C4D-C3D-C2D	2.13	110.07	107.30
32	21	422	ZEX	C27-C26-C25	-2.13	119.41	122.84
23	34	402	8CT	C22-C21-C23	2.13	121.43	118.08
32	14	403	ZEX	C20-C13-C12	2.13	121.43	118.08
21	13	508	CL7	CHB-C1B-NB	-2.13	122.01	124.26
32	44	418	ZEX	C31-C32-C33	-2.13	120.45	126.42
21	14	411	CL7	C1C-C2C-C3C	-2.13	103.84	106.94
21	44	411	CL7	C1C-C2C-C3C	-2.13	103.84	106.94
32	13	525	ZEX	C18-C5-C4	2.13	118.29	114.36
21	1B	608	CL7	CAA-CBA-CGA	-2.12	107.04	113.25
21	3C	512	CL7	C3B-C4B-NB	2.12	112.49	110.52
32	43	420	ZEX	C21-C26-C27	2.12	121.79	115.78
21	41	411	CL7	CAA-CBA-CGA	-2.12	106.87	112.51
21	21	412	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	11	411	CL7	CAA-CBA-CGA	-2.12	106.87	112.51
21	2D	404	CL7	C4C-C3C-C2C	-2.12	104.36	107.13
21	22	518	CL7	C1C-C2C-C3C	-2.12	103.84	106.94
21	21	420	CL7	C1C-C2C-C3C	-2.12	103.84	106.94
21	1C	503	CL7	C4-C3-C5	2.12	118.84	115.27
21	33	512	CL7	C4-C3-C5	2.12	118.84	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	34	415	CL7	CMB-C2B-C1B	2.12	128.60	125.37
21	1B	603	CL7	C4C-C3C-C2C	-2.12	104.36	107.13
21	22	508	CL7	C3B-C2B-C1B	-2.12	104.60	107.16
21	2A	407	CL7	CMB-C2B-C1B	2.12	128.60	125.37
21	3B	601	CL7	C4C-C3C-C2C	-2.12	104.36	107.13
21	43	413	CL7	C4-C3-C5	2.12	118.84	115.27
21	14	415	CL7	CMB-C2B-C1B	2.12	128.60	125.37
21	11	412	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	44	405	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	31	420	CL7	C4D-C3D-C2D	2.12	110.06	107.30
21	41	420	CL7	C4D-C3D-C2D	2.12	110.06	107.30
21	2B	615	CL7	CBA-CAA-C2A	2.12	120.12	113.86
21	4D	404	CL7	C4C-C3C-C2C	-2.12	104.36	107.13
23	4C	518	8CT	C22-C21-C20	-2.12	119.95	122.92
21	31	419	CL7	CMB-C2B-C1B	2.12	128.60	125.37
21	2B	605	CL7	O2D-CGD-O1D	-2.12	119.69	123.84
21	23	415	CL7	O2D-CGD-O1D	-2.12	119.69	123.84
32	23	420	ZEX	C21-C26-C27	2.12	121.78	115.78
21	2B	609	CL7	CAA-CBA-CGA	-2.12	107.06	113.25
21	2D	404	CL7	C3B-C4B-NB	2.12	112.48	110.52
32	33	525	ZEX	C20-C13-C12	2.12	121.42	118.08
21	32	515	CL7	CAA-CBA-CGA	-2.12	106.89	112.51
21	42	513	CL7	C1C-C2C-C3C	-2.12	103.85	106.94
21	12	518	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	14	408	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	44	406	CL7	C4-C3-C5	2.12	118.83	115.27
21	11	409	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	3D	404	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	41	409	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	4B	609	CL7	CAA-CBA-CGA	-2.12	107.07	113.25
21	1C	501	CL7	CAC-C3C-C2C	2.12	131.15	127.53
32	14	418	ZEX	C31-C32-C33	-2.12	120.47	126.42
21	34	406	CL7	C4-C3-C5	2.12	118.83	115.27
21	42	511	CL7	CAC-C3C-C2C	2.12	131.15	127.53
21	33	512	CL7	CED-O2D-CGD	-2.12	111.15	115.94
23	1C	514	8CT	C05-C04-C03	2.12	113.74	110.48
21	23	413	CL7	C4-C3-C5	2.12	118.83	115.27
32	24	418	ZEX	C31-C32-C33	-2.12	120.47	126.42
21	34	410	CL7	C3B-C4B-NB	2.12	112.48	110.52
21	3B	604	CL7	O2D-CGD-O1D	-2.12	119.70	123.84
23	4C	518	8CT	C39-C16-C15	2.12	121.41	118.08
21	4B	604	CL7	C4-C3-C5	2.12	118.83	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	14	403	ZEX	C7-C6-C5	-2.11	116.34	121.46
32	13	525	ZEX	C20-C13-C12	2.11	121.41	118.08
23	1C	515	8CT	C11-C12-C13	2.11	122.19	118.94
23	2C	515	8CT	C11-C12-C13	2.11	122.19	118.94
21	23	403	CL7	C1C-C2C-C3C	-2.11	103.85	106.94
21	4B	615	CL7	C1C-C2C-C3C	-2.11	103.85	106.94
21	2B	604	CL7	C4-C3-C5	2.11	118.83	115.27
21	3B	603	CL7	C4-C3-C5	2.11	118.83	115.27
21	11	418	CL7	CAA-CBA-CGA	-2.11	107.08	113.25
21	11	420	CL7	C4D-C3D-C2D	2.11	110.05	107.30
21	1B	614	CL7	CBA-CAA-C2A	2.11	120.10	113.86
21	4B	615	CL7	CBA-CAA-C2A	2.11	120.10	113.86
21	23	411	CL7	CAC-C3C-C2C	2.11	131.14	127.53
21	1B	604	CL7	O2D-CGD-O1D	-2.11	119.71	123.84
21	33	512	CL7	O2D-CGD-O1D	-2.11	119.71	123.84
21	43	415	CL7	O2D-CGD-O1D	-2.11	119.71	123.84
21	2C	508	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
21	2C	510	CL7	C2A-C1A-CHA	-2.11	122.14	126.36
21	32	513	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	22	511	CL7	CAC-C3C-C2C	2.11	131.14	127.53
32	13	519	ZEX	C21-C26-C27	2.11	121.75	115.78
21	1D	404	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
21	21	409	CL7	C3B-C4B-NB	2.11	112.47	110.52
25	22	523	SQD	O8-S-C6	-2.11	102.38	105.74
21	22	501	CL7	C4-C3-C5	2.11	118.82	115.27
21	1B	610	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
32	34	420	ZEX	C18-C5-C4	2.11	118.27	114.36
32	44	420	ZEX	C18-C5-C4	2.11	118.27	114.36
23	3C	518	8CT	C39-C16-C15	2.11	121.40	118.08
23	44	402	8CT	C39-C16-C15	2.11	121.40	118.08
32	34	418	ZEX	C31-C32-C33	-2.11	120.49	126.42
25	12	523	SQD	O8-S-C6	-2.11	102.38	105.74
32	23	401	ZEX	C20-C13-C12	2.11	121.40	118.08
21	3C	508	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
23	1C	518	8CT	C22-C21-C20	-2.11	119.97	122.92
32	24	418	ZEX	C19-C9-C10	-2.11	119.97	122.92
21	13	512	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	41	418	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	33	505	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	1C	508	CL7	O2D-CGD-O1D	-2.11	119.71	123.84
21	41	413	CL7	CMB-C2B-C1B	2.11	128.58	125.37
32	23	420	ZEX	C20-C13-C14	-2.11	119.97	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	418	CL7	CAA-CBA-CGA	-2.11	107.09	113.25
32	24	403	ZEX	C40-C33-C34	-2.11	119.97	122.92
21	2B	611	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	3B	603	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	12	508	CL7	CMB-C2B-C1B	2.11	128.58	125.37
32	21	421	ZEX	C15-C35-C34	-2.11	119.16	123.47
21	22	518	CL7	C3B-C4B-NB	2.11	112.47	110.52
21	32	513	CL7	C3B-C4B-NB	2.11	112.47	110.52
21	34	405	CL7	C3B-C4B-NB	2.11	112.47	110.52
21	2C	501	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	4B	602	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	4C	501	CL7	CAC-C3C-C2C	2.11	131.13	127.53
21	22	513	CL7	O2D-CGD-O1D	-2.11	119.72	123.84
21	32	513	CL7	O2D-CGD-O1D	-2.11	119.72	123.84
21	21	411	CL7	CAA-CBA-CGA	-2.11	106.92	112.51
21	44	405	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	3B	608	CL7	CAA-CBA-CGA	-2.11	107.10	113.25
21	12	514	CL7	C3B-C4B-NB	2.11	112.47	110.52
32	24	403	ZEX	C7-C6-C5	-2.11	116.36	121.46
21	4A	401	CL7	CAC-C3C-C2C	2.11	131.13	127.53
32	14	420	ZEX	C18-C5-C4	2.11	118.26	114.36
32	13	522	ZEX	C8-C9-C10	2.11	122.17	118.94
21	43	406	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	24	405	CL7	C3B-C4B-NB	2.11	112.47	110.52
32	23	401	ZEX	C18-C5-C4	2.11	118.25	114.36
32	33	525	ZEX	C18-C5-C4	2.11	118.25	114.36
32	41	421	ZEX	C37-C21-C26	-2.10	106.89	110.30
21	13	510	CL7	CAC-C3C-C2C	2.10	131.13	127.53
21	33	505	CL7	CHD-C1D-ND	-2.10	122.03	124.26
21	11	413	CL7	CMB-C2B-C1B	2.10	128.57	125.37
23	3C	515	8CT	C11-C12-C13	2.10	122.17	118.94
21	1B	603	CL7	C4-C3-C5	2.10	118.81	115.27
32	41	421	ZEX	C15-C35-C34	-2.10	119.17	123.47
21	22	501	CL7	C4C-C3C-C2C	-2.10	104.39	107.13
21	4C	508	CL7	C4C-C3C-C2C	-2.10	104.39	107.13
32	33	519	ZEX	C20-C13-C14	-2.10	119.98	122.92
21	1C	510	CL7	C2A-C1A-CHA	-2.10	122.16	126.36
23	3C	514	8CT	C05-C04-C03	2.10	113.72	110.48
21	4C	503	CL7	C4-C3-C5	2.10	118.81	115.27
21	12	513	CL7	C1C-C2C-C3C	-2.10	103.87	106.94
21	41	411	CL7	C1C-C2C-C3C	-2.10	103.87	106.94
21	4B	604	CL7	C4C-C3C-C2C	-2.10	104.39	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	508	CL7	CMB-C2B-C1B	2.10	128.57	125.37
32	13	519	ZEX	C20-C13-C14	-2.10	119.98	122.92
23	2D	406	8CT	C27-C26-C28	2.10	121.39	118.08
21	32	501	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	34	413	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	11	410	CL7	CAA-CBA-CGA	-2.10	107.11	113.25
21	21	418	CL7	CAA-CBA-CGA	-2.10	107.11	113.25
23	3D	406	8CT	C27-C26-C28	2.10	121.39	118.08
32	43	401	ZEX	C18-C5-C4	2.10	118.25	114.36
21	3A	401	CL7	CAC-C3C-C2C	2.10	131.12	127.53
21	3C	503	CL7	C4-C3-C5	2.10	118.80	115.27
21	31	409	CL7	CHC-C1C-NC	-2.10	122.52	124.45
21	21	418	CL7	CED-O2D-CGD	-2.10	111.19	115.94
21	33	510	CL7	CAC-C3C-C2C	2.10	131.12	127.53
21	1C	508	CL7	C4C-C3C-C2C	-2.10	104.39	107.13
21	32	505	CL7	CMB-C2B-C1B	2.10	128.56	125.37
21	1B	614	CL7	C1C-C2C-C3C	-2.10	103.88	106.94
21	23	417	CL7	CBC-CAC-C3C	-2.10	106.65	112.43
21	33	516	CL7	CBC-CAC-C3C	-2.10	106.65	112.43
21	1B	607	CL7	CED-O2D-CGD	-2.10	111.19	115.94
32	43	401	ZEX	C20-C13-C12	2.10	121.38	118.08
32	14	403	ZEX	C40-C33-C34	-2.10	119.98	122.92
21	13	508	CL7	C4C-C3C-C2C	-2.10	104.39	107.13
25	42	523	SQD	O8-S-C6	-2.10	102.40	105.74
21	43	411	CL7	CAC-C3C-C2C	2.10	131.12	127.53
21	11	409	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	14	413	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	24	410	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	23	411	CL7	CMB-C2B-C1B	2.10	128.56	125.37
32	12	522	ZEX	C4-C5-C6	-2.10	116.17	120.85
21	31	410	CL7	CAA-CBA-CGA	-2.10	107.12	113.25
21	2D	404	CL7	CHC-C1C-NC	-2.10	122.53	124.45
21	3C	510	CL7	C2A-C1A-CHA	-2.10	122.17	126.36
32	43	423	ZEX	C8-C9-C10	2.10	122.16	118.94
21	13	516	CL7	CBC-CAC-C3C	-2.10	106.65	112.43
32	11	421	ZEX	C37-C21-C26	-2.10	106.90	110.30
21	14	405	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	34	404	CL7	C3B-C4B-NB	2.10	112.46	110.52
21	34	411	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
21	24	412	CL7	C4-C3-C5	2.09	118.80	115.27
21	3C	508	CL7	CAC-C3C-C2C	2.09	131.11	127.53
32	23	423	ZEX	C8-C9-C10	2.09	122.16	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3F	101	HEM	C4A-NA-C1A	2.09	107.40	105.35
32	32	522	ZEX	C4-C5-C6	-2.09	116.18	120.85
21	31	418	CL7	CED-O2D-CGD	-2.09	111.20	115.94
21	34	408	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
32	24	420	ZEX	C18-C5-C4	2.09	118.23	114.36
21	44	417	CL7	C3B-C2B-C1B	-2.09	104.63	107.16
23	3B	618	8CT	C18-C19-C20	2.09	127.76	123.47
32	22	522	ZEX	C4-C5-C6	-2.09	116.18	120.85
21	11	418	CL7	CED-O2D-CGD	-2.09	111.20	115.94
21	13	517	CL7	C3B-C4B-NB	2.09	112.46	110.52
23	4C	515	8CT	C11-C12-C13	2.09	122.15	118.94
32	33	522	ZEX	C8-C9-C10	2.09	122.15	118.94
21	13	512	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	4B	605	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	13	514	CL7	CAC-C3C-C4C	-2.09	121.39	124.68
21	34	407	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	4B	608	CL7	CED-O2D-CGD	-2.09	111.20	115.94
21	12	513	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	3C	506	CL7	C1-C2-C3	2.09	129.66	126.04
23	4C	514	8CT	C05-C04-C03	2.09	113.70	110.48
21	3B	607	CL7	CED-O2D-CGD	-2.09	111.21	115.94
32	44	419	ZEX	C20-C13-C14	-2.09	119.99	122.92
21	21	410	CL7	CAA-CBA-CGA	-2.09	107.14	113.25
21	41	410	CL7	CAA-CBA-CGA	-2.09	107.14	113.25
21	42	513	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	23	409	CL7	CHB-C1B-NB	-2.09	122.04	124.26
23	4D	406	8CT	C27-C26-C28	2.09	121.37	118.08
21	41	418	CL7	CAA-CBA-CGA	-2.09	107.14	113.25
21	23	409	CL7	C4C-C3C-C2C	-2.09	104.40	107.13
21	32	517	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	14	412	CL7	C4-C3-C5	2.09	118.79	115.27
21	42	518	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	32	502	CL7	C3B-C2B-C1B	-2.09	104.64	107.16
23	2C	514	8CT	C05-C04-C03	2.09	113.70	110.48
21	44	415	CL7	CMB-C2B-C1B	2.09	128.55	125.37
21	4C	510	CL7	C2A-C1A-CHA	-2.09	122.18	126.36
21	14	410	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	44	410	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	33	503	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	14	405	CL7	C4C-C3C-C2C	-2.09	104.40	107.13
21	43	409	CL7	CHB-C1B-NB	-2.09	122.05	124.26
21	1A	401	CL7	CAC-C3C-C2C	2.09	131.10	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	420	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	42	518	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	3B	616	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
32	44	403	ZEX	C40-C33-C34	-2.09	120.00	122.92
21	31	408	CL7	C1-O2A-CGA	-2.09	110.97	116.44
32	34	403	ZEX	C7-C6-C5	-2.09	116.41	121.46
21	11	411	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	12	513	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	14	409	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	24	404	CL7	C3B-C4B-NB	2.09	112.45	110.52
21	44	409	CL7	C3B-C4B-NB	2.09	112.45	110.52
32	42	522	ZEX	C4-C5-C6	-2.09	116.20	120.85
21	21	408	CL7	C1-O2A-CGA	-2.09	110.97	116.44
21	14	408	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	44	408	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	2C	508	CL7	O2D-CGD-O1D	-2.09	119.76	123.84
21	2B	608	CL7	CED-O2D-CGD	-2.09	111.22	115.94
32	34	418	ZEX	C19-C9-C10	-2.09	120.00	122.92
21	24	405	CL7	C4C-C3C-C2C	-2.08	104.41	107.13
21	33	508	CL7	C4C-C3C-C2C	-2.08	104.41	107.13
21	11	416	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	21	419	CL7	CMB-C2B-C1B	2.08	128.54	125.37
21	23	406	CL7	CED-O2D-CGD	-2.08	111.22	115.94
21	21	411	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	41	420	CL7	O2D-CGD-O1D	-2.08	119.76	123.84
21	42	513	CL7	C3B-C4B-NB	2.08	112.45	110.52
23	2B	619	8CT	C18-C19-C20	2.08	127.74	123.47
21	4B	611	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	23	415	CL7	CAC-C3C-C4C	-2.08	121.40	124.68
32	21	421	ZEX	C1-C2-C3	-2.08	108.94	113.64
32	21	422	ZEX	C1-C2-C3	-2.08	108.94	113.64
32	24	420	ZEX	C38-C24-C23	-2.08	108.98	112.20
21	13	512	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	34	415	CL7	O1D-CGD-CBD	-2.08	120.22	124.48
21	34	405	CL7	C4C-C3C-C2C	-2.08	104.41	107.13
21	11	408	CL7	C1-O2A-CGA	-2.08	110.98	116.44
21	43	417	CL7	CBC-CAC-C3C	-2.08	106.69	112.43
21	41	409	CL7	C3B-C4B-NB	2.08	112.45	110.52
21	13	516	CL7	CBA-CAA-C2A	-2.08	107.72	113.86
23	1D	406	8CT	C27-C26-C28	2.08	121.36	118.08
32	11	421	ZEX	C15-C35-C34	-2.08	119.21	123.47
21	22	502	CL7	C3B-C2B-C1B	-2.08	104.65	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	420	CL7	O2D-CGD-O1D	-2.08	119.77	123.84
21	43	413	CL7	O2D-CGD-O1D	-2.08	119.77	123.84
21	13	505	CL7	CED-O2D-CGD	-2.08	111.23	115.94
21	2B	617	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	3B	610	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
32	24	420	ZEX	C39-C29-C28	2.08	121.35	118.08
32	44	403	ZEX	C7-C6-C5	-2.08	116.42	121.46
21	33	516	CL7	CBA-CAA-C2A	-2.08	107.72	113.86
21	12	505	CL7	CMB-C2B-C1B	2.08	128.54	125.37
21	4A	403	CL7	C3B-C4B-NB	2.08	112.44	110.52
21	4C	506	CL7	C3B-C2B-C1B	-2.08	104.65	107.16
21	33	514	CL7	CAC-C3C-C4C	-2.08	121.41	124.68
32	14	420	ZEX	C38-C24-C23	-2.08	108.99	112.20
21	43	417	CL7	CBA-CAA-C2A	-2.08	107.73	113.86
32	41	421	ZEX	C1-C2-C3	-2.08	108.95	113.64
21	11	404	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
21	32	518	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	32	508	CL7	CMB-C2B-C1B	2.08	128.53	125.37
21	31	404	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
21	21	413	CL7	C4D-C3D-C2D	2.08	110.00	107.30
21	1C	508	CL7	C3B-C2B-C1B	-2.08	104.66	107.16
21	4C	508	CL7	C3B-C2B-C1B	-2.08	104.66	107.16
21	32	513	CL7	C3D-C4D-ND	2.08	113.15	110.17
21	42	513	CL7	C3D-C4D-ND	2.08	113.15	110.17
21	1D	404	CL7	CHC-C1C-NC	-2.08	122.55	124.45
21	4D	404	CL7	CHC-C1C-NC	-2.08	122.55	124.45
21	21	420	CL7	C4D-C3D-C2D	2.08	110.00	107.30
32	44	420	ZEX	C40-C33-C32	2.08	121.35	118.08
21	12	517	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	42	517	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	24	408	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	42	514	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	14	404	CL7	C3B-C4B-NB	2.08	112.44	110.52
32	44	420	ZEX	C38-C24-C23	-2.07	109.00	112.20
21	2C	503	CL7	C4-C3-C5	2.07	118.76	115.27
21	2C	505	CL7	C1-O2A-CGA	-2.07	111.00	116.44
21	43	415	CL7	CAC-C3C-C4C	-2.07	121.41	124.68
21	22	513	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
21	4B	617	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
32	32	524	ZEX	C21-C26-C27	2.07	121.65	115.78
21	34	412	CL7	C4-C3-C5	2.07	118.76	115.27
25	42	521	SQD	O8-S-C6	-2.07	102.44	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	415	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
21	44	407	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
32	44	418	ZEX	C19-C9-C10	-2.07	120.02	122.92
32	22	524	ZEX	C21-C26-C27	2.07	121.64	115.78
21	3C	508	CL7	CED-O2D-CGD	-2.07	111.25	115.94
21	23	417	CL7	CBA-CAA-C2A	-2.07	107.75	113.86
32	34	418	ZEX	C1-C2-C3	-2.07	108.96	113.64
21	1C	508	CL7	CAC-C3C-C2C	2.07	131.07	127.53
21	4C	508	CL7	CAC-C3C-C2C	2.07	131.07	127.53
21	41	404	CL7	CAA-CBA-CGA	-2.07	107.20	113.25
32	21	421	ZEX	C37-C21-C26	-2.07	106.94	110.30
21	41	415	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	14	415	CL7	O1D-CGD-CBD	-2.07	120.25	124.48
32	11	421	ZEX	C1-C2-C3	-2.07	108.97	113.64
21	3B	614	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	21	404	CL7	CAA-CBA-CGA	-2.07	107.20	113.25
21	2A	401	CL7	CAC-C3C-C2C	2.07	131.07	127.53
21	44	413	CL7	C3B-C4B-NB	2.07	112.44	110.52
21	11	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
21	41	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
32	14	418	ZEX	C19-C9-C10	-2.07	120.02	122.92
32	14	420	ZEX	C39-C29-C28	2.07	121.34	118.08
21	23	413	CL7	O2D-CGD-O1D	-2.07	119.79	123.84
21	22	518	CL7	C4-C3-C5	2.07	118.75	115.27
21	3B	614	CL7	C3B-C4B-NB	2.07	112.43	110.52
21	21	420	CL7	O2D-CGD-O1D	-2.07	119.79	123.84
21	22	513	CL7	C3D-C4D-ND	2.07	113.13	110.17
21	43	404	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	33	501	CL7	C2A-C1A-CHA	-2.07	122.23	126.36
32	31	421	ZEX	C15-C35-C34	-2.07	119.24	123.47
21	12	518	CL7	O2D-CGD-O1D	-2.07	119.80	123.84
21	14	406	CL7	CED-O2D-CGD	-2.07	111.26	115.94
21	3C	505	CL7	C1-O2A-CGA	-2.07	111.02	116.44
32	44	418	ZEX	C1-C2-C3	-2.07	108.97	113.64
23	44	402	8CT	C08-C04-C03	-2.07	106.95	110.30
21	43	409	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
21	13	516	CL7	CED-O2D-CGD	-2.07	111.26	115.94
21	4C	508	CL7	O2D-CGD-O1D	-2.07	119.80	123.84
21	1B	616	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	1C	506	CL7	C1-C2-C3	2.07	129.62	126.04
21	4C	506	CL7	C1-C2-C3	2.07	129.62	126.04
25	21	423	SQD	O8-S-C6	-2.07	102.45	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	31	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
21	44	412	CL7	C4-C3-C5	2.07	118.75	115.27
21	23	403	CL7	CMB-C2B-C1B	2.07	128.51	125.37
21	21	415	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
32	11	422	ZEX	C1-C2-C3	-2.07	108.98	113.64
32	41	422	ZEX	C1-C2-C3	-2.07	108.98	113.64
21	1B	614	CL7	C4-C3-C5	2.07	118.75	115.27
21	41	408	CL7	C1-O2A-CGA	-2.06	111.03	116.44
21	24	409	CL7	C3B-C4B-NB	2.06	112.43	110.52
21	24	413	CL7	C3B-C4B-NB	2.06	112.43	110.52
21	14	407	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
32	34	420	ZEX	C39-C29-C28	2.06	121.33	118.08
21	44	406	CL7	CED-O2D-CGD	-2.06	111.27	115.94
21	11	405	CL7	C4C-C3C-C2C	-2.06	104.44	107.13
32	31	421	ZEX	C1-C2-C3	-2.06	108.98	113.64
25	22	521	SQD	O8-S-C6	-2.06	102.45	105.74
25	32	521	SQD	O8-S-C6	-2.06	102.45	105.74
21	22	505	CL7	O2D-CGD-O1D	-2.06	119.80	123.84
32	12	524	ZEX	C21-C26-C27	2.06	121.61	115.78
32	42	524	ZEX	C21-C26-C27	2.06	121.61	115.78
23	4K	101	8CT	C05-C04-C03	2.06	113.66	110.48
21	12	514	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
21	24	406	CL7	CED-O2D-CGD	-2.06	111.27	115.94
21	3B	614	CL7	C4-C3-C5	2.06	118.74	115.27
21	2C	506	CL7	C1-C2-C3	2.06	129.61	126.04
21	2D	405	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	3D	405	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	22	508	CL7	CMB-C2B-C1B	2.06	128.51	125.37
21	4B	606	CL7	C3B-C4B-NB	2.06	112.43	110.52
32	34	420	ZEX	C38-C24-C23	-2.06	109.02	112.20
21	24	407	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
23	1B	618	8CT	C18-C19-C20	2.06	127.69	123.47
21	43	413	CL7	C4D-C3D-C2D	2.06	109.98	107.30
21	4D	405	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	42	518	CL7	C4-C3-C5	2.06	118.74	115.27
23	2C	518	8CT	C35-C30-C31	2.06	115.11	111.42
21	32	514	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
32	42	520	ZEX	C11-C12-C13	-2.06	120.63	126.42
21	3C	508	CL7	C3B-C2B-C1B	-2.06	104.68	107.16
21	42	502	CL7	C3B-C2B-C1B	-2.06	104.68	107.16
32	14	420	ZEX	C40-C33-C32	2.06	121.32	118.08
21	12	501	CL7	C4C-C3C-C2C	-2.06	104.44	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	23	418	CL7	C3B-C4B-NB	2.06	112.42	110.52
21	11	415	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
21	22	505	CL7	CMB-C2B-C1B	2.06	128.50	125.37
23	4B	619	8CT	C18-C19-C20	2.06	127.69	123.47
21	1C	512	CL7	C3B-C4B-NB	2.06	112.42	110.52
21	1D	405	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	43	417	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	41	405	CL7	C4C-C3C-C2C	-2.06	104.44	107.13
21	43	403	CL7	CMB-C2B-C1B	2.06	128.50	125.37
21	31	416	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
21	1C	505	CL7	C1-O2A-CGA	-2.06	111.05	116.44
21	4C	505	CL7	C1-O2A-CGA	-2.06	111.05	116.44
21	22	518	CL7	O2D-CGD-O1D	-2.06	119.82	123.84
21	2C	508	CL7	CED-O2D-CGD	-2.06	111.29	115.94
21	13	501	CL7	C2A-C1A-CHA	-2.06	122.25	126.36
21	22	517	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
21	1C	505	CL7	C9-C8-C7	-2.06	103.85	111.29
21	4C	505	CL7	C9-C8-C7	-2.06	103.85	111.29
23	2C	514	8CT	C24-C25-C26	-2.06	124.38	127.31
32	24	418	ZEX	C1-C2-C3	-2.06	109.00	113.64
21	33	517	CL7	C3B-C4B-NB	2.06	112.42	110.52
21	4C	512	CL7	C3B-C4B-NB	2.06	112.42	110.52
32	14	418	ZEX	C1-C2-C3	-2.06	109.00	113.64
21	13	503	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
32	24	420	ZEX	C40-C33-C32	2.06	121.31	118.08
32	34	420	ZEX	C40-C33-C32	2.06	121.31	118.08
21	2C	505	CL7	C9-C8-C7	-2.05	103.85	111.29
21	32	518	CL7	C4-C3-C5	2.05	118.73	115.27
21	32	501	CL7	C4C-C3C-C2C	-2.05	104.45	107.13
21	2B	614	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
25	12	521	SQD	O8-S-C6	-2.05	102.47	105.74
21	33	516	CL7	CED-O2D-CGD	-2.05	111.29	115.94
32	31	422	ZEX	C1-C2-C3	-2.05	109.00	113.64
21	12	501	CL7	C3B-C4B-NB	2.05	112.42	110.52
21	2C	512	CL7	C3B-C4B-NB	2.05	112.42	110.52
23	2B	619	8CT	C11-C10-C03	-2.05	121.44	127.20
21	1C	506	CL7	C3B-C2B-C1B	-2.05	104.68	107.16
25	11	423	SQD	O8-S-C6	-2.05	102.47	105.74
23	3C	514	8CT	C11-C12-C13	-2.05	115.79	118.94
21	21	412	CL7	C4C-C3C-C2C	-2.05	104.45	107.13
23	1K	101	8CT	C05-C04-C03	2.05	113.64	110.48
21	42	505	CL7	O2D-CGD-O1D	-2.05	119.83	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	42	505	CL7	CMB-C2B-C1B	2.05	128.50	125.37
21	1B	613	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
21	23	404	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
21	4B	614	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
32	24	419	ZEX	C20-C13-C14	-2.05	120.05	122.92
21	22	515	CL7	C3B-C4B-NB	2.05	112.42	110.52
21	42	501	CL7	C3B-C4B-NB	2.05	112.42	110.52
21	24	415	CL7	O1D-CGD-CBD	-2.05	120.29	124.48
32	31	421	ZEX	C37-C21-C26	-2.05	106.97	110.30
21	41	408	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
21	43	411	CL7	CMB-C2B-C1B	2.05	128.49	125.37
21	3C	505	CL7	C9-C8-C7	-2.05	103.87	111.29
21	33	510	CL7	CMB-C2B-C1B	2.05	128.49	125.37
21	12	518	CL7	C4-C3-C5	2.05	118.72	115.27
25	41	423	SQD	O8-S-C6	-2.05	102.47	105.74
21	14	409	CL7	CBC-CAC-C3C	-2.05	106.78	112.43
21	44	409	CL7	CBC-CAC-C3C	-2.05	106.78	112.43
21	3C	508	CL7	O2D-CGD-O1D	-2.05	119.83	123.84
21	44	404	CL7	C3B-C4B-NB	2.05	112.42	110.52
21	31	410	CL7	CMB-C2B-C1B	2.05	128.49	125.37
23	1C	518	8CT	C35-C30-C31	2.05	115.08	111.42
21	31	411	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
21	44	415	CL7	O1D-CGD-CBD	-2.05	120.29	124.48
21	2C	508	CL7	CAC-C3C-C2C	2.05	131.03	127.53
23	3C	518	8CT	C35-C30-C31	2.05	115.08	111.42
21	34	406	CL7	CED-O2D-CGD	-2.05	111.31	115.94
21	4C	508	CL7	CED-O2D-CGD	-2.05	111.31	115.94
32	34	403	ZEX	C40-C33-C34	-2.05	120.06	122.92
23	4C	518	8CT	C35-C30-C31	2.05	115.08	111.42
21	44	412	CL7	C4D-C3D-C2D	2.05	109.97	107.30
21	33	502	CL7	CMB-C2B-C1B	2.05	128.49	125.37
21	2C	508	CL7	C3B-C2B-C1B	-2.05	104.69	107.16
21	2A	403	CL7	C3B-C4B-NB	2.05	112.41	110.52
21	22	501	CL7	C3B-C4B-NB	2.05	112.41	110.52
21	3A	403	CL7	C3B-C4B-NB	2.05	112.41	110.52
21	1B	614	CL7	CMB-C2B-C1B	2.05	128.48	125.37
25	31	423	SQD	O8-S-C6	-2.05	102.48	105.74
21	2D	404	CL7	C4-C3-C5	2.04	118.71	115.27
23	1B	618	8CT	C11-C10-C03	-2.04	121.46	127.20
21	33	502	CL7	C1-C2-C3	2.04	129.58	126.04
21	22	514	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
32	24	419	ZEX	C1-C2-C3	-2.04	109.03	113.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	11	408	CL7	O2A-CGA-O1A	-2.04	118.43	123.59
21	21	416	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
21	41	416	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
21	43	402	CL7	C2A-C1A-CHA	-2.04	122.27	126.36
21	1C	508	CL7	CED-O2D-CGD	-2.04	111.31	115.94
21	2C	506	CL7	C3B-C2B-C1B	-2.04	104.69	107.16
21	21	408	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
21	23	413	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
21	33	512	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
32	14	419	ZEX	C1-C2-C3	-2.04	109.03	113.64
21	13	502	CL7	C1-C2-C3	2.04	129.58	126.04
21	4B	615	CL7	CMB-C2B-C1B	2.04	128.48	125.37
21	12	502	CL7	C3B-C2B-C1B	-2.04	104.70	107.16
21	23	417	CL7	CED-O2D-CGD	-2.04	111.32	115.94
21	3D	404	CL7	C4-C3-C5	2.04	118.71	115.27
32	34	419	ZEX	C1-C2-C3	-2.04	109.03	113.64
21	41	418	CL7	CMB-C2B-C1B	2.04	128.48	125.37
21	43	413	CL7	C1C-C2C-C3C	-2.04	103.96	106.94
23	4B	619	8CT	C11-C10-C03	-2.04	121.47	127.20
21	22	503	CL7	C3B-C4B-NB	2.04	112.41	110.52
21	4B	615	CL7	C3B-C4B-NB	2.04	112.41	110.52
21	43	419	CL7	C3B-C4B-NB	2.04	112.41	110.52
21	24	409	CL7	CBC-CAC-C3C	-2.04	106.81	112.43
21	33	507	CL7	O2D-CGD-O1D	-2.04	119.85	123.84
21	2B	615	CL7	C3B-C4B-NB	2.04	112.41	110.52
21	32	516	CL7	CAC-C3C-C2C	2.04	131.02	127.53
21	24	408	CL7	C4D-C3D-C2D	2.04	109.96	107.30
21	11	413	CL7	O2D-CGD-O1D	-2.04	119.85	123.84
21	33	504	CL7	CBA-CAA-C2A	2.04	119.88	113.86
21	12	505	CL7	O2D-CGD-O1D	-2.04	119.85	123.84
21	2B	615	CL7	C4-C3-C5	2.04	118.70	115.27
23	3C	514	8CT	C24-C25-C26	-2.04	124.40	127.31
32	34	419	ZEX	C20-C13-C14	-2.04	120.07	122.92
21	23	404	CL7	CAC-C3C-C2C	2.04	131.01	127.53
21	23	402	CL7	C2A-C1A-CHA	-2.04	122.28	126.36
32	44	420	ZEX	C39-C29-C28	2.04	121.29	118.08
21	42	516	CL7	O2A-C1-C2	-2.04	103.28	108.64
21	34	409	CL7	CBC-CAC-C3C	-2.04	106.81	112.43
21	14	408	CL7	C4D-C3D-C2D	2.04	109.95	107.30
21	13	507	CL7	O2D-CGD-O1D	-2.04	119.86	123.84
21	3B	605	CL7	C3B-C4B-NB	2.04	112.40	110.52
21	21	418	CL7	CMB-C2B-C1B	2.04	128.47	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4B	615	CL7	C4-C3-C5	2.04	118.70	115.27
21	12	516	CL7	CAC-C3C-C2C	2.04	131.01	127.53
21	42	516	CL7	CAC-C3C-C2C	2.04	131.01	127.53
23	1C	514	8CT	C24-C25-C26	-2.04	124.41	127.31
23	4C	514	8CT	C24-C25-C26	-2.04	124.41	127.31
21	13	518	CL7	C3B-C4B-NB	2.04	112.40	110.52
32	24	419	ZEX	C19-C9-C8	2.03	121.28	118.08
21	4C	501	CL7	C4D-C3D-C2D	2.03	109.95	107.30
21	34	412	CL7	O2D-CGD-O1D	-2.03	119.86	123.84
32	44	420	ZEX	C1-C2-C3	-2.03	109.05	113.64
32	12	520	ZEX	C11-C12-C13	-2.03	120.70	126.42
21	32	505	CL7	O2D-CGD-O1D	-2.03	119.86	123.84
21	13	509	CL7	C1C-C2C-C3C	-2.03	103.97	106.94
21	42	515	CL7	C3B-C4B-NB	2.03	112.40	110.52
21	31	405	CL7	CMB-C2B-C1B	2.03	128.47	125.37
21	31	408	CL7	O2A-CGA-O1A	-2.03	118.46	123.59
21	11	415	CL7	C3B-C4B-NB	2.03	112.40	110.52
21	11	420	CL7	C3B-C4B-NB	2.03	112.40	110.52
21	23	419	CL7	C3B-C4B-NB	2.03	112.40	110.52
21	13	510	CL7	CMB-C2B-C1B	2.03	128.47	125.37
32	44	419	ZEX	C1-C2-C3	-2.03	109.05	113.64
23	24	402	8CT	C08-C04-C03	-2.03	107.00	110.30
23	34	402	8CT	C08-C04-C03	-2.03	107.00	110.30
21	31	413	CL7	C4D-C3D-C2D	2.03	109.95	107.30
21	13	502	CL7	CMB-C2B-C1B	2.03	128.46	125.37
32	22	520	ZEX	C11-C12-C13	-2.03	120.71	126.42
32	32	520	ZEX	C11-C12-C13	-2.03	120.71	126.42
32	31	422	ZEX	C1-C6-C7	2.03	121.53	115.78
21	13	503	CL7	CAC-C3C-C2C	2.03	131.00	127.53
21	22	518	CL7	CAC-C3C-C2C	2.03	131.00	127.53
23	3B	618	8CT	C11-C10-C03	-2.03	121.50	127.20
32	32	519	ZEX	C18-C5-C4	2.03	118.12	114.36
21	4B	611	CL7	C4D-C3D-C2D	2.03	109.95	107.30
21	11	410	CL7	CMB-C2B-C1B	2.03	128.46	125.37
21	11	413	CL7	C4D-C3D-C2D	2.03	109.94	107.30
21	3C	501	CL7	C4D-C3D-C2D	2.03	109.94	107.30
21	4C	507	CL7	C4-C3-C5	2.03	118.69	115.27
21	43	411	CL7	O2A-CGA-CBA	2.03	118.28	111.91
23	14	402	8CT	C08-C04-C03	-2.03	107.01	110.30
21	41	420	CL7	CAA-CBA-CGA	-2.03	107.12	112.51
32	42	520	ZEX	C10-C11-C12	-2.03	116.88	123.22
22	3D	408	PHO	C4A-C3A-C2A	-2.03	100.91	102.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	41	422	ZEX	C1-C6-C7	2.03	121.52	115.78
21	13	504	CL7	CBA-CAA-C2A	2.03	119.85	113.86
21	44	412	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
32	43	401	ZEX	C21-C26-C27	2.03	121.52	115.78
23	4C	514	8CT	C11-C12-C13	-2.03	115.83	118.94
21	21	407	CL7	C3B-C4B-NB	2.03	112.40	110.52
21	14	415	CL7	C1C-C2C-C3C	-2.03	103.98	106.94
21	43	410	CL7	C1C-C2C-C3C	-2.03	103.98	106.94
21	33	503	CL7	C4D-C3D-C2D	2.03	109.94	107.30
32	33	519	ZEX	C31-C32-C33	-2.03	120.72	126.42
32	43	420	ZEX	C31-C32-C33	-2.03	120.72	126.42
21	14	412	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
32	14	419	ZEX	C19-C9-C8	2.03	121.27	118.08
32	44	419	ZEX	C19-C9-C8	2.03	121.27	118.08
21	12	518	CL7	CAC-C3C-C2C	2.03	131.00	127.53
21	24	412	CL7	CMB-C2B-C1B	2.03	128.46	125.37
32	11	421	ZEX	C40-C33-C34	-2.03	120.08	122.92
32	24	420	ZEX	C1-C2-C3	-2.03	109.07	113.64
21	24	410	CL7	CAC-C3C-C2C	2.03	131.00	127.53
21	24	412	CL7	C4D-C3D-C2D	2.03	109.94	107.30
32	14	419	ZEX	C20-C13-C14	-2.03	120.08	122.92
21	32	516	CL7	O2A-C1-C2	-2.03	103.31	108.64
21	14	412	CL7	C4D-C3D-C2D	2.03	109.94	107.30
21	12	513	CL7	C3D-C4D-ND	2.03	113.07	110.17
21	3B	613	CL7	C1C-C2C-C3C	-2.03	103.98	106.94
21	42	501	CL7	C4C-C3C-C2C	-2.03	104.49	107.13
21	22	505	CL7	C4-C3-C2	-2.02	118.48	123.68
21	32	505	CL7	C4-C3-C2	-2.02	118.48	123.68
32	41	421	ZEX	C40-C33-C34	-2.02	120.09	122.92
21	43	403	CL7	C1-C2-C3	2.02	129.54	126.04
21	22	516	CL7	CAC-C3C-C2C	2.02	130.99	127.53
32	22	522	ZEX	C40-C33-C34	-2.02	120.09	122.92
21	31	420	CL7	CAA-CBA-CGA	-2.02	107.14	112.51
21	23	403	CL7	C1-C2-C3	2.02	129.54	126.04
21	21	413	CL7	O2D-CGD-O1D	-2.02	119.88	123.84
32	21	422	ZEX	C10-C11-C12	-2.02	116.90	123.22
21	3C	507	CL7	C4-C3-C5	2.02	118.67	115.27
21	21	405	CL7	C4C-C3C-C2C	-2.02	104.49	107.13
21	31	405	CL7	C4C-C3C-C2C	-2.02	104.49	107.13
32	34	419	ZEX	C19-C9-C8	2.02	121.26	118.08
32	32	520	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	31	413	CL7	O2D-CGD-O1D	-2.02	119.88	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	22	516	CL7	O2A-C1-C2	-2.02	103.32	108.64
21	2B	615	CL7	CMB-C2B-C1B	2.02	128.45	125.37
21	3B	614	CL7	CMB-C2B-C1B	2.02	128.45	125.37
21	43	404	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	23	405	CL7	CBA-CAA-C2A	2.02	119.83	113.86
21	1B	613	CL7	CHB-C1B-NB	-2.02	122.12	124.26
21	43	404	CL7	CAC-C3C-C2C	2.02	130.99	127.53
21	4D	404	CL7	C4-C3-C5	2.02	118.67	115.27
21	13	510	CL7	O2A-CGA-CBA	2.02	118.25	111.91
32	11	422	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	41	410	CL7	CMB-C2B-C1B	2.02	128.45	125.37
21	23	408	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
21	11	420	CL7	CAA-CBA-CGA	-2.02	107.15	112.51
21	1B	610	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	14	415	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	1A	403	CL7	C3B-C4B-NB	2.02	112.39	110.52
21	12	505	CL7	C3B-C4B-NB	2.02	112.39	110.52
21	34	409	CL7	C3B-C4B-NB	2.02	112.39	110.52
21	41	420	CL7	C3B-C4B-NB	2.02	112.39	110.52
21	41	405	CL7	CMB-C2B-C1B	2.02	128.44	125.37
21	12	516	CL7	O2A-C1-C2	-2.02	103.33	108.64
32	23	420	ZEX	C31-C32-C33	-2.02	120.74	126.42
32	31	422	ZEX	C10-C11-C12	-2.02	116.92	123.22
21	33	512	CL7	C4D-C3D-C2D	2.02	109.93	107.30
32	12	519	ZEX	C18-C5-C4	2.02	118.10	114.36
32	12	520	ZEX	C10-C11-C12	-2.02	116.92	123.22
32	22	520	ZEX	C10-C11-C12	-2.02	116.92	123.22
32	21	421	ZEX	C40-C33-C34	-2.02	120.09	122.92
21	42	518	CL7	CAC-C3C-C2C	2.02	130.98	127.53
32	33	525	ZEX	C21-C26-C27	2.02	121.49	115.78
21	41	413	CL7	C4D-C3D-C2D	2.02	109.93	107.30
32	41	422	ZEX	C10-C11-C12	-2.02	116.92	123.22
21	24	412	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
21	41	413	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
21	1B	605	CL7	C3B-C4B-NB	2.02	112.39	110.52
21	2B	609	CL7	C1C-C2C-C3C	-2.02	104.00	106.94
21	23	411	CL7	O2A-CGA-CBA	2.02	118.24	111.91
32	24	420	ZEX	C37-C21-C26	-2.02	107.03	110.30
21	44	405	CL7	C4-C3-C5	2.02	118.66	115.27
21	1B	614	CL7	C3B-C4B-NB	2.02	112.39	110.52
22	4D	408	PHO	C4A-C3A-C2A	-2.02	100.92	102.84
32	21	422	ZEX	C1-C6-C7	2.02	121.48	115.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	42	522	ZEX	C10-C11-C12	-2.02	116.92	123.22
21	42	502	CL7	CAC-C3C-C2C	2.02	130.98	127.53
23	1C	514	8CT	C11-C12-C13	-2.02	115.85	118.94
21	1C	501	CL7	C4D-C3D-C2D	2.02	109.93	107.30
21	24	409	CL7	C1C-C2C-C3C	-2.02	104.00	106.94
21	21	420	CL7	CAA-CBA-CGA	-2.02	107.16	112.51
27	2B	625	DGD	O1G-C1A-O1A	-2.02	118.51	123.59
21	1B	608	CL7	C1C-C2C-C3C	-2.01	104.00	106.94
21	3B	605	CL7	C4D-C3D-C2D	2.01	109.92	107.30
21	12	503	CL7	C3B-C4B-NB	2.01	112.38	110.52
21	43	418	CL7	C3B-C4B-NB	2.01	112.38	110.52
21	4B	603	CL7	O2D-CGD-O1D	-2.01	119.90	123.84
21	43	409	CL7	CHC-C1C-C2C	-2.01	121.26	125.48
21	33	510	CL7	O2A-CGA-CBA	2.01	118.23	111.91
21	21	420	CL7	C3B-C4B-NB	2.01	112.38	110.52
21	32	503	CL7	C3B-C4B-NB	2.01	112.38	110.52
32	22	522	ZEX	C10-C11-C12	-2.01	116.93	123.22
32	32	522	ZEX	C10-C11-C12	-2.01	116.93	123.22
32	14	420	ZEX	C1-C2-C3	-2.01	109.10	113.64
21	24	415	CL7	C4D-C3D-C2D	2.01	109.92	107.30
21	41	407	CL7	CAC-C3C-C2C	2.01	130.97	127.53
21	1B	615	CL7	O2A-CGA-O1A	-2.01	118.51	123.59
21	22	513	CL7	C3B-C4B-NB	2.01	112.38	110.52
23	3C	518	8CT	C35-C30-C29	-2.01	110.16	112.70
21	44	415	CL7	C4D-C3D-C2D	2.01	109.92	107.30
21	43	405	CL7	CBA-CAA-C2A	2.01	119.80	113.86
21	2C	510	CL7	C4C-C3C-C2C	-2.01	104.50	107.13
21	24	405	CL7	C4-C3-C5	2.01	118.66	115.27
32	34	420	ZEX	C1-C2-C3	-2.01	109.10	113.64
21	14	417	CL7	C1C-C2C-C3C	-2.01	104.00	106.94
21	31	402	CL7	C3B-C4B-NB	2.01	112.38	110.52
32	13	525	ZEX	C21-C26-C27	2.01	121.47	115.78
21	3C	506	CL7	C3B-C2B-C1B	-2.01	104.73	107.16
32	12	522	ZEX	C28-C29-C30	-2.01	115.86	118.94
21	12	505	CL7	C4-C3-C2	-2.01	118.52	123.68
21	42	505	CL7	C4-C3-C2	-2.01	118.52	123.68
21	4B	607	CL7	CAC-C3C-C4C	-2.01	121.51	124.68
21	22	502	CL7	CAC-C3C-C2C	2.01	130.97	127.53
21	1C	507	CL7	C4-C3-C5	2.01	118.65	115.27
23	3K	101	8CT	C05-C04-C03	2.01	113.58	110.48
23	2C	514	8CT	C11-C12-C13	-2.01	115.86	118.94
21	3B	602	CL7	O2D-CGD-O1D	-2.01	119.91	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	14	409	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
21	13	503	CL7	C4D-C3D-C2D	2.01	109.92	107.30
21	2B	616	CL7	O2A-CGA-O1A	-2.01	118.52	123.59
21	12	515	CL7	C3B-C4B-NB	2.01	112.38	110.52
21	4B	608	CL7	CAA-CBA-CGA	-2.01	107.38	113.25
21	31	418	CL7	O2D-CGD-O1D	-2.01	119.91	123.84
32	23	401	ZEX	C21-C26-C27	2.01	121.46	115.78
32	13	519	ZEX	C31-C32-C33	-2.01	120.77	126.42
32	42	519	ZEX	C18-C5-C4	2.01	118.08	114.36
21	2B	605	CL7	CED-O2D-CGD	-2.01	111.39	115.94
21	3B	604	CL7	CED-O2D-CGD	-2.01	111.39	115.94
21	23	410	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
21	33	509	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
21	22	515	CL7	O2D-CGD-O1D	-2.01	119.91	123.84
32	22	519	ZEX	C18-C5-C4	2.01	118.07	114.36
21	13	512	CL7	C4D-C3D-C2D	2.01	109.91	107.30
32	12	522	ZEX	C10-C11-C12	-2.01	116.95	123.22
21	11	405	CL7	CMB-C2B-C1B	2.01	128.43	125.37
21	3B	613	CL7	CHB-C1B-NB	-2.01	122.13	124.26
32	32	522	ZEX	C40-C33-C34	-2.01	120.11	122.92
32	32	522	ZEX	C28-C29-C30	-2.01	115.86	118.94
27	3B	624	DGD	O1G-C1A-O1A	-2.01	118.53	123.59
32	23	423	ZEX	C39-C29-C28	2.01	121.24	118.08
32	11	422	ZEX	C1-C6-C7	2.01	121.45	115.78
21	11	414	CL7	CGD-CBD-CAD	2.01	117.23	110.73
21	2B	606	CL7	C4D-C3D-C2D	2.01	109.91	107.30
21	41	407	CL7	C3B-C4B-NB	2.00	112.38	110.52
27	4B	625	DGD	O1G-C1A-O1A	-2.00	118.53	123.59
21	3B	607	CL7	CAA-CBA-CGA	-2.00	107.39	113.25
21	1D	404	CL7	C4-C3-C5	2.00	118.64	115.27
21	33	503	CL7	CAC-C3C-C2C	2.00	130.96	127.53
21	31	414	CL7	CGD-CBD-CAD	2.00	117.22	110.73
21	3B	608	CL7	C1C-C2C-C3C	-2.00	104.02	106.94
21	2B	611	CL7	C4D-C3D-C2D	2.00	109.91	107.30
32	22	522	ZEX	C28-C29-C30	-2.00	115.87	118.94
21	3B	615	CL7	O2A-CGA-O1A	-2.00	118.53	123.59
21	1B	614	CL7	O2A-C1-C2	2.00	113.90	108.64
21	2B	615	CL7	O2A-C1-C2	2.00	113.90	108.64
21	4B	615	CL7	O2A-C1-C2	2.00	113.90	108.64
21	2B	603	CL7	O2D-CGD-O1D	-2.00	119.92	123.84
21	1B	604	CL7	CED-O2D-CGD	-2.00	111.41	115.94
21	14	412	CL7	CMB-C2B-C1B	2.00	128.42	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	44	406	CL7	CMB-C2B-C1B	2.00	128.42	125.37
32	14	420	ZEX	C37-C21-C26	-2.00	107.05	110.30
21	34	408	CL7	C4D-C3D-C2D	2.00	109.91	107.30
21	1C	510	CL7	C4C-C3C-C2C	-2.00	104.52	107.13
21	31	418	CL7	CMB-C2B-C1B	2.00	128.42	125.37
21	11	407	CL7	C3B-C4B-NB	2.00	112.37	110.52
21	33	518	CL7	C3B-C4B-NB	2.00	112.37	110.52
21	2B	612	CL7	C4C-C3C-C2C	-2.00	104.52	107.13
21	3C	510	CL7	C4C-C3C-C2C	-2.00	104.52	107.13
23	3C	515	8CT	C39-C16-C17	-2.00	120.12	122.92
32	31	421	ZEX	C40-C33-C34	-2.00	120.12	122.92
21	12	516	CL7	C3B-C4B-NB	2.00	112.37	110.52
21	13	501	CL7	C3D-C4D-ND	2.00	113.04	110.17
32	12	522	ZEX	C40-C33-C34	-2.00	120.12	122.92
21	23	404	CL7	C4D-C3D-C2D	2.00	109.91	107.30

All (860) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1A	401	CL7	NA
21	1A	401	CL7	NC
21	1A	403	CL7	NA
21	1A	403	CL7	NC
21	1A	407	CL7	NA
21	1A	407	CL7	NC
21	1B	601	CL7	NA
21	1B	601	CL7	NC
21	1B	602	CL7	NA
21	1B	602	CL7	NC
21	1B	603	CL7	NA
21	1B	603	CL7	NC
21	1B	604	CL7	NA
21	1B	604	CL7	NC
21	1B	605	CL7	NA
21	1B	605	CL7	NC
21	1B	606	CL7	NA
21	1B	606	CL7	NC
21	1B	607	CL7	NA
21	1B	607	CL7	NC
21	1B	608	CL7	NA
21	1B	608	CL7	NC
21	1B	609	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	1B	609	CL7	NC
21	1B	610	CL7	NA
21	1B	610	CL7	NC
21	1B	611	CL7	NA
21	1B	611	CL7	NC
21	1B	612	CL7	NA
21	1B	612	CL7	NC
21	1B	613	CL7	NA
21	1B	613	CL7	NC
21	1B	614	CL7	NA
21	1B	614	CL7	NC
21	1B	615	CL7	NA
21	1B	615	CL7	NC
21	1B	616	CL7	NA
21	1B	616	CL7	NC
21	1B	622	CL7	NA
21	1B	622	CL7	NC
21	1C	501	CL7	NA
21	1C	501	CL7	NC
21	1C	502	CL7	NA
21	1C	502	CL7	NC
21	1C	503	CL7	NA
21	1C	503	CL7	NC
21	1C	504	CL7	NA
21	1C	504	CL7	NC
21	1C	505	CL7	NA
21	1C	505	CL7	NC
21	1C	506	CL7	NA
21	1C	506	CL7	NC
21	1C	507	CL7	NA
21	1C	507	CL7	NC
21	1C	508	CL7	NA
21	1C	508	CL7	NC
21	1C	509	CL7	NA
21	1C	509	CL7	NC
21	1C	510	CL7	NA
21	1C	510	CL7	NC
21	1C	511	CL7	NA
21	1C	511	CL7	NC
21	1C	512	CL7	NA
21	1C	512	CL7	NC
21	1C	513	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	1C	513	CL7	NC
21	1C	517	CL7	NA
21	1C	517	CL7	NC
21	1D	402	CL7	NA
21	1D	402	CL7	NC
21	1D	404	CL7	NA
21	1D	404	CL7	NC
21	1D	405	CL7	NA
21	1D	405	CL7	NC
21	12	501	CL7	NA
21	12	501	CL7	NC
21	12	502	CL7	NA
21	12	502	CL7	NC
21	12	503	CL7	NA
21	12	503	CL7	NC
21	12	504	CL7	NA
21	12	504	CL7	NC
21	12	505	CL7	NA
21	12	505	CL7	NC
21	12	506	CL7	NA
21	12	506	CL7	NC
21	12	507	CL7	NA
21	12	507	CL7	NC
21	12	508	CL7	NA
21	12	508	CL7	NC
21	12	509	CL7	NA
21	12	509	CL7	NC
21	12	510	CL7	NA
21	12	510	CL7	NC
21	12	511	CL7	NA
21	12	511	CL7	NC
21	12	512	CL7	NA
21	12	512	CL7	NC
21	12	513	CL7	NA
21	12	513	CL7	NC
21	12	514	CL7	NA
21	12	514	CL7	NC
21	12	515	CL7	NA
21	12	515	CL7	NC
21	12	516	CL7	NA
21	12	516	CL7	NC
21	12	517	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	12	517	CL7	NC
21	12	518	CL7	NA
21	12	518	CL7	NC
21	11	402	CL7	NA
21	11	402	CL7	NC
21	11	403	CL7	NA
21	11	403	CL7	NC
21	11	404	CL7	NA
21	11	404	CL7	NC
21	11	405	CL7	NA
21	11	405	CL7	NC
21	11	406	CL7	NA
21	11	406	CL7	NC
21	11	407	CL7	NA
21	11	407	CL7	NC
21	11	408	CL7	NA
21	11	408	CL7	NC
21	11	409	CL7	NA
21	11	409	CL7	NC
21	11	410	CL7	NA
21	11	410	CL7	NC
21	11	411	CL7	NA
21	11	411	CL7	NC
21	11	412	CL7	NA
21	11	412	CL7	NC
21	11	413	CL7	NA
21	11	413	CL7	NC
21	11	414	CL7	NA
21	11	414	CL7	NC
21	11	415	CL7	NA
21	11	415	CL7	NC
21	11	416	CL7	NA
21	11	416	CL7	NC
21	11	417	CL7	NA
21	11	417	CL7	NC
21	11	418	CL7	NA
21	11	418	CL7	NC
21	11	419	CL7	NA
21	11	419	CL7	NC
21	11	420	CL7	NA
21	11	420	CL7	NC
21	13	501	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	13	501	CL7	NC
21	13	502	CL7	NA
21	13	502	CL7	NC
21	13	503	CL7	NA
21	13	503	CL7	NC
21	13	504	CL7	NA
21	13	504	CL7	NC
21	13	505	CL7	NA
21	13	505	CL7	NC
21	13	506	CL7	NA
21	13	506	CL7	NC
21	13	507	CL7	NA
21	13	507	CL7	NC
21	13	508	CL7	NA
21	13	508	CL7	NC
21	13	509	CL7	NA
21	13	509	CL7	NC
21	13	510	CL7	NA
21	13	510	CL7	NC
21	13	511	CL7	NA
21	13	511	CL7	NC
21	13	512	CL7	NA
21	13	512	CL7	NC
21	13	513	CL7	NA
21	13	513	CL7	NC
21	13	514	CL7	NA
21	13	514	CL7	NC
21	13	515	CL7	NA
21	13	515	CL7	NC
21	13	516	CL7	NA
21	13	516	CL7	NC
21	13	517	CL7	NA
21	13	517	CL7	NC
21	13	518	CL7	NA
21	13	518	CL7	NC
21	14	404	CL7	NA
21	14	404	CL7	NC
21	14	405	CL7	NA
21	14	405	CL7	NC
21	14	406	CL7	NA
21	14	406	CL7	NC
21	14	407	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	14	407	CL7	NC
21	14	408	CL7	NA
21	14	408	CL7	NC
21	14	409	CL7	NA
21	14	409	CL7	NC
21	14	410	CL7	NA
21	14	410	CL7	NC
21	14	411	CL7	NA
21	14	411	CL7	NC
21	14	412	CL7	NA
21	14	412	CL7	NC
21	14	413	CL7	NA
21	14	413	CL7	NC
21	14	414	CL7	NA
21	14	414	CL7	NC
21	14	415	CL7	NA
21	14	415	CL7	NC
21	14	416	CL7	NA
21	14	416	CL7	NC
21	14	417	CL7	NA
21	14	417	CL7	NC
21	2A	401	CL7	NA
21	2A	401	CL7	NC
21	2A	403	CL7	NA
21	2A	403	CL7	NC
21	2A	407	CL7	NA
21	2A	407	CL7	NC
21	2B	602	CL7	NA
21	2B	602	CL7	NC
21	2B	603	CL7	NA
21	2B	603	CL7	NC
21	2B	604	CL7	NA
21	2B	604	CL7	NC
21	2B	605	CL7	NA
21	2B	605	CL7	NC
21	2B	606	CL7	NA
21	2B	606	CL7	NC
21	2B	607	CL7	NA
21	2B	607	CL7	NC
21	2B	608	CL7	NA
21	2B	608	CL7	NC
21	2B	609	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	2B	609	CL7	NC
21	2B	610	CL7	NA
21	2B	610	CL7	NC
21	2B	611	CL7	NA
21	2B	611	CL7	NC
21	2B	612	CL7	NA
21	2B	612	CL7	NC
21	2B	613	CL7	NA
21	2B	613	CL7	NC
21	2B	614	CL7	NA
21	2B	614	CL7	NC
21	2B	615	CL7	NA
21	2B	615	CL7	NC
21	2B	616	CL7	NA
21	2B	616	CL7	NC
21	2B	617	CL7	NA
21	2B	617	CL7	NC
21	2B	623	CL7	NA
21	2B	623	CL7	NC
21	2C	501	CL7	NA
21	2C	501	CL7	NC
21	2C	502	CL7	NA
21	2C	502	CL7	NC
21	2C	503	CL7	NA
21	2C	503	CL7	NC
21	2C	504	CL7	NA
21	2C	504	CL7	NC
21	2C	505	CL7	NA
21	2C	505	CL7	NC
21	2C	506	CL7	NA
21	2C	506	CL7	NC
21	2C	507	CL7	NA
21	2C	507	CL7	NC
21	2C	508	CL7	NA
21	2C	508	CL7	NC
21	2C	509	CL7	NA
21	2C	509	CL7	NC
21	2C	510	CL7	NA
21	2C	510	CL7	NC
21	2C	511	CL7	NA
21	2C	511	CL7	NC
21	2C	512	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	2C	512	CL7	NC
21	2C	513	CL7	NA
21	2C	513	CL7	NC
21	2C	517	CL7	NA
21	2C	517	CL7	NC
21	2D	402	CL7	NA
21	2D	402	CL7	NC
21	2D	404	CL7	NA
21	2D	404	CL7	NC
21	2D	405	CL7	NA
21	2D	405	CL7	NC
21	22	501	CL7	NA
21	22	501	CL7	NC
21	22	502	CL7	NA
21	22	502	CL7	NC
21	22	503	CL7	NA
21	22	503	CL7	NC
21	22	504	CL7	NA
21	22	504	CL7	NC
21	22	505	CL7	NA
21	22	505	CL7	NC
21	22	506	CL7	NA
21	22	506	CL7	NC
21	22	507	CL7	NA
21	22	507	CL7	NC
21	22	508	CL7	NA
21	22	508	CL7	NC
21	22	509	CL7	NA
21	22	509	CL7	NC
21	22	510	CL7	NA
21	22	510	CL7	NC
21	22	511	CL7	NA
21	22	511	CL7	NC
21	22	512	CL7	NA
21	22	512	CL7	NC
21	22	513	CL7	NA
21	22	513	CL7	NC
21	22	514	CL7	NA
21	22	514	CL7	NC
21	22	515	CL7	NA
21	22	515	CL7	NC
21	22	516	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	22	516	CL7	NC
21	22	517	CL7	NA
21	22	517	CL7	NC
21	22	518	CL7	NA
21	22	518	CL7	NC
21	21	402	CL7	NA
21	21	402	CL7	NC
21	21	403	CL7	NA
21	21	403	CL7	NC
21	21	404	CL7	NA
21	21	404	CL7	NC
21	21	405	CL7	NA
21	21	405	CL7	NC
21	21	406	CL7	NA
21	21	406	CL7	NC
21	21	407	CL7	NA
21	21	407	CL7	NC
21	21	408	CL7	NA
21	21	408	CL7	NC
21	21	409	CL7	NA
21	21	409	CL7	NC
21	21	410	CL7	NA
21	21	410	CL7	NC
21	21	411	CL7	NA
21	21	411	CL7	NC
21	21	412	CL7	NA
21	21	412	CL7	NC
21	21	413	CL7	NA
21	21	413	CL7	NC
21	21	414	CL7	NA
21	21	414	CL7	NC
21	21	415	CL7	NA
21	21	415	CL7	NC
21	21	416	CL7	NA
21	21	416	CL7	NC
21	21	417	CL7	NA
21	21	417	CL7	NC
21	21	418	CL7	NA
21	21	418	CL7	NC
21	21	419	CL7	NA
21	21	419	CL7	NC
21	21	420	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	21	420	CL7	NC
21	23	402	CL7	NA
21	23	402	CL7	NC
21	23	403	CL7	NA
21	23	403	CL7	NC
21	23	404	CL7	NA
21	23	404	CL7	NC
21	23	405	CL7	NA
21	23	405	CL7	NC
21	23	406	CL7	NA
21	23	406	CL7	NC
21	23	407	CL7	NA
21	23	407	CL7	NC
21	23	408	CL7	NA
21	23	408	CL7	NC
21	23	409	CL7	NA
21	23	409	CL7	NC
21	23	410	CL7	NA
21	23	410	CL7	NC
21	23	411	CL7	NA
21	23	411	CL7	NC
21	23	412	CL7	NA
21	23	412	CL7	NC
21	23	413	CL7	NA
21	23	413	CL7	NC
21	23	414	CL7	NA
21	23	414	CL7	NC
21	23	415	CL7	NA
21	23	415	CL7	NC
21	23	416	CL7	NA
21	23	416	CL7	NC
21	23	417	CL7	NA
21	23	417	CL7	NC
21	23	418	CL7	NA
21	23	418	CL7	NC
21	23	419	CL7	NA
21	23	419	CL7	NC
21	24	404	CL7	NA
21	24	404	CL7	NC
21	24	405	CL7	NA
21	24	405	CL7	NC
21	24	406	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	24	406	CL7	NC
21	24	407	CL7	NA
21	24	407	CL7	NC
21	24	408	CL7	NA
21	24	408	CL7	NC
21	24	409	CL7	NA
21	24	409	CL7	NC
21	24	410	CL7	NA
21	24	410	CL7	NC
21	24	411	CL7	NA
21	24	411	CL7	NC
21	24	412	CL7	NA
21	24	412	CL7	NC
21	24	413	CL7	NA
21	24	413	CL7	NC
21	24	414	CL7	NA
21	24	414	CL7	NC
21	24	415	CL7	NA
21	24	415	CL7	NC
21	24	416	CL7	NA
21	24	416	CL7	NC
21	24	417	CL7	NA
21	24	417	CL7	NC
21	3A	401	CL7	NA
21	3A	401	CL7	NC
21	3A	403	CL7	NA
21	3A	403	CL7	NC
21	3A	407	CL7	NA
21	3A	407	CL7	NC
21	3B	601	CL7	NA
21	3B	601	CL7	NC
21	3B	602	CL7	NA
21	3B	602	CL7	NC
21	3B	603	CL7	NA
21	3B	603	CL7	NC
21	3B	604	CL7	NA
21	3B	604	CL7	NC
21	3B	605	CL7	NA
21	3B	605	CL7	NC
21	3B	606	CL7	NA
21	3B	606	CL7	NC
21	3B	607	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	3B	607	CL7	NC
21	3B	608	CL7	NA
21	3B	608	CL7	NC
21	3B	609	CL7	NA
21	3B	609	CL7	NC
21	3B	610	CL7	NA
21	3B	610	CL7	NC
21	3B	611	CL7	NA
21	3B	611	CL7	NC
21	3B	612	CL7	NA
21	3B	612	CL7	NC
21	3B	613	CL7	NA
21	3B	613	CL7	NC
21	3B	614	CL7	NA
21	3B	614	CL7	NC
21	3B	615	CL7	NA
21	3B	615	CL7	NC
21	3B	616	CL7	NA
21	3B	616	CL7	NC
21	3B	622	CL7	NA
21	3B	622	CL7	NC
21	3C	501	CL7	NA
21	3C	501	CL7	NC
21	3C	502	CL7	NA
21	3C	502	CL7	NC
21	3C	503	CL7	NA
21	3C	503	CL7	NC
21	3C	504	CL7	NA
21	3C	504	CL7	NC
21	3C	505	CL7	NA
21	3C	505	CL7	NC
21	3C	506	CL7	NA
21	3C	506	CL7	NC
21	3C	507	CL7	NA
21	3C	507	CL7	NC
21	3C	508	CL7	NA
21	3C	508	CL7	NC
21	3C	509	CL7	NA
21	3C	509	CL7	NC
21	3C	510	CL7	NA
21	3C	510	CL7	NC
21	3C	511	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	3C	511	CL7	NC
21	3C	512	CL7	NA
21	3C	512	CL7	NC
21	3C	513	CL7	NA
21	3C	513	CL7	NC
21	3C	517	CL7	NA
21	3C	517	CL7	NC
21	3D	402	CL7	NA
21	3D	402	CL7	NC
21	3D	404	CL7	NA
21	3D	404	CL7	NC
21	3D	405	CL7	NA
21	3D	405	CL7	NC
21	32	501	CL7	NA
21	32	501	CL7	NC
21	32	502	CL7	NA
21	32	502	CL7	NC
21	32	503	CL7	NA
21	32	503	CL7	NC
21	32	504	CL7	NA
21	32	504	CL7	NC
21	32	505	CL7	NA
21	32	505	CL7	NC
21	32	506	CL7	NA
21	32	506	CL7	NC
21	32	507	CL7	NA
21	32	507	CL7	NC
21	32	508	CL7	NA
21	32	508	CL7	NC
21	32	509	CL7	NA
21	32	509	CL7	NC
21	32	510	CL7	NA
21	32	510	CL7	NC
21	32	511	CL7	NA
21	32	511	CL7	NC
21	32	512	CL7	NA
21	32	512	CL7	NC
21	32	513	CL7	NA
21	32	513	CL7	NC
21	32	514	CL7	NA
21	32	514	CL7	NC
21	32	515	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	32	515	CL7	NC
21	32	516	CL7	NA
21	32	516	CL7	NC
21	32	517	CL7	NA
21	32	517	CL7	NC
21	32	518	CL7	NA
21	32	518	CL7	NC
21	31	402	CL7	NA
21	31	402	CL7	NC
21	31	403	CL7	NA
21	31	403	CL7	NC
21	31	404	CL7	NA
21	31	404	CL7	NC
21	31	405	CL7	NA
21	31	405	CL7	NC
21	31	406	CL7	NA
21	31	406	CL7	NC
21	31	407	CL7	NA
21	31	407	CL7	NC
21	31	408	CL7	NA
21	31	408	CL7	NC
21	31	409	CL7	NA
21	31	409	CL7	NC
21	31	410	CL7	NA
21	31	410	CL7	NC
21	31	411	CL7	NA
21	31	411	CL7	NC
21	31	412	CL7	NA
21	31	412	CL7	NC
21	31	413	CL7	NA
21	31	413	CL7	NC
21	31	414	CL7	NA
21	31	414	CL7	NC
21	31	415	CL7	NA
21	31	415	CL7	NC
21	31	416	CL7	NA
21	31	416	CL7	NC
21	31	417	CL7	NA
21	31	417	CL7	NC
21	31	418	CL7	NA
21	31	418	CL7	NC
21	31	419	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	31	419	CL7	NC
21	31	420	CL7	NA
21	31	420	CL7	NC
21	33	501	CL7	NA
21	33	501	CL7	NC
21	33	502	CL7	NA
21	33	502	CL7	NC
21	33	503	CL7	NA
21	33	503	CL7	NC
21	33	504	CL7	NA
21	33	504	CL7	NC
21	33	505	CL7	NA
21	33	505	CL7	NC
21	33	506	CL7	NA
21	33	506	CL7	NC
21	33	507	CL7	NA
21	33	507	CL7	NC
21	33	508	CL7	NA
21	33	508	CL7	NC
21	33	509	CL7	NA
21	33	509	CL7	NC
21	33	510	CL7	NA
21	33	510	CL7	NC
21	33	511	CL7	NA
21	33	511	CL7	NC
21	33	512	CL7	NA
21	33	512	CL7	NC
21	33	513	CL7	NA
21	33	513	CL7	NC
21	33	514	CL7	NA
21	33	514	CL7	NC
21	33	515	CL7	NA
21	33	515	CL7	NC
21	33	516	CL7	NA
21	33	516	CL7	NC
21	33	517	CL7	NA
21	33	517	CL7	NC
21	33	518	CL7	NA
21	33	518	CL7	NC
21	34	404	CL7	NA
21	34	404	CL7	NC
21	34	405	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	34	405	CL7	NC
21	34	406	CL7	NA
21	34	406	CL7	NC
21	34	407	CL7	NA
21	34	407	CL7	NC
21	34	408	CL7	NA
21	34	408	CL7	NC
21	34	409	CL7	NA
21	34	409	CL7	NC
21	34	410	CL7	NA
21	34	410	CL7	NC
21	34	411	CL7	NA
21	34	411	CL7	NC
21	34	412	CL7	NA
21	34	412	CL7	NC
21	34	413	CL7	NA
21	34	413	CL7	NC
21	34	414	CL7	NA
21	34	414	CL7	NC
21	34	415	CL7	NA
21	34	415	CL7	NC
21	34	416	CL7	NA
21	34	416	CL7	NC
21	34	417	CL7	NA
21	34	417	CL7	NC
21	4A	401	CL7	NA
21	4A	401	CL7	NC
21	4A	403	CL7	NA
21	4A	403	CL7	NC
21	4A	407	CL7	NA
21	4A	407	CL7	NC
21	4B	602	CL7	NA
21	4B	602	CL7	NC
21	4B	603	CL7	NA
21	4B	603	CL7	NC
21	4B	604	CL7	NA
21	4B	604	CL7	NC
21	4B	605	CL7	NA
21	4B	605	CL7	NC
21	4B	606	CL7	NA
21	4B	606	CL7	NC
21	4B	607	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	4B	607	CL7	NC
21	4B	608	CL7	NA
21	4B	608	CL7	NC
21	4B	609	CL7	NA
21	4B	609	CL7	NC
21	4B	610	CL7	NA
21	4B	610	CL7	NC
21	4B	611	CL7	NA
21	4B	611	CL7	NC
21	4B	612	CL7	NA
21	4B	612	CL7	NC
21	4B	613	CL7	NA
21	4B	613	CL7	NC
21	4B	614	CL7	NA
21	4B	614	CL7	NC
21	4B	615	CL7	NA
21	4B	615	CL7	NC
21	4B	616	CL7	NA
21	4B	616	CL7	NC
21	4B	617	CL7	NA
21	4B	617	CL7	NC
21	4B	623	CL7	NA
21	4B	623	CL7	NC
21	4C	501	CL7	NA
21	4C	501	CL7	NC
21	4C	502	CL7	NA
21	4C	502	CL7	NC
21	4C	503	CL7	NA
21	4C	503	CL7	NC
21	4C	504	CL7	NA
21	4C	504	CL7	NC
21	4C	505	CL7	NA
21	4C	505	CL7	NC
21	4C	506	CL7	NA
21	4C	506	CL7	NC
21	4C	507	CL7	NA
21	4C	507	CL7	NC
21	4C	508	CL7	NA
21	4C	508	CL7	NC
21	4C	509	CL7	NA
21	4C	509	CL7	NC
21	4C	510	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	4C	510	CL7	NC
21	4C	511	CL7	NA
21	4C	511	CL7	NC
21	4C	512	CL7	NA
21	4C	512	CL7	NC
21	4C	513	CL7	NA
21	4C	513	CL7	NC
21	4C	517	CL7	NA
21	4C	517	CL7	NC
21	4D	402	CL7	NA
21	4D	402	CL7	NC
21	4D	404	CL7	NA
21	4D	404	CL7	NC
21	4D	405	CL7	NA
21	4D	405	CL7	NC
21	42	501	CL7	NA
21	42	501	CL7	NC
21	42	502	CL7	NA
21	42	502	CL7	NC
21	42	503	CL7	NA
21	42	503	CL7	NC
21	42	504	CL7	NA
21	42	504	CL7	NC
21	42	505	CL7	NA
21	42	505	CL7	NC
21	42	506	CL7	NA
21	42	506	CL7	NC
21	42	507	CL7	NA
21	42	507	CL7	NC
21	42	508	CL7	NA
21	42	508	CL7	NC
21	42	509	CL7	NA
21	42	509	CL7	NC
21	42	510	CL7	NA
21	42	510	CL7	NC
21	42	511	CL7	NA
21	42	511	CL7	NC
21	42	512	CL7	NA
21	42	512	CL7	NC
21	42	513	CL7	NA
21	42	513	CL7	NC
21	42	514	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	42	514	CL7	NC
21	42	515	CL7	NA
21	42	515	CL7	NC
21	42	516	CL7	NA
21	42	516	CL7	NC
21	42	517	CL7	NA
21	42	517	CL7	NC
21	42	518	CL7	NA
21	42	518	CL7	NC
21	41	402	CL7	NA
21	41	402	CL7	NC
21	41	403	CL7	NA
21	41	403	CL7	NC
21	41	404	CL7	NA
21	41	404	CL7	NC
21	41	405	CL7	NA
21	41	405	CL7	NC
21	41	406	CL7	NA
21	41	406	CL7	NC
21	41	407	CL7	NA
21	41	407	CL7	NC
21	41	408	CL7	NA
21	41	408	CL7	NC
21	41	409	CL7	NA
21	41	409	CL7	NC
21	41	410	CL7	NA
21	41	410	CL7	NC
21	41	411	CL7	NA
21	41	411	CL7	NC
21	41	412	CL7	NA
21	41	412	CL7	NC
21	41	413	CL7	NA
21	41	413	CL7	NC
21	41	414	CL7	NA
21	41	414	CL7	NC
21	41	415	CL7	NA
21	41	415	CL7	NC
21	41	416	CL7	NA
21	41	416	CL7	NC
21	41	417	CL7	NA
21	41	417	CL7	NC
21	41	418	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	41	418	CL7	NC
21	41	419	CL7	NA
21	41	419	CL7	NC
21	41	420	CL7	NA
21	41	420	CL7	NC
21	43	402	CL7	NA
21	43	402	CL7	NC
21	43	403	CL7	NA
21	43	403	CL7	NC
21	43	404	CL7	NA
21	43	404	CL7	NC
21	43	405	CL7	NA
21	43	405	CL7	NC
21	43	406	CL7	NA
21	43	406	CL7	NC
21	43	407	CL7	NA
21	43	407	CL7	NC
21	43	408	CL7	NA
21	43	408	CL7	NC
21	43	409	CL7	NA
21	43	409	CL7	NC
21	43	410	CL7	NA
21	43	410	CL7	NC
21	43	411	CL7	NA
21	43	411	CL7	NC
21	43	412	CL7	NA
21	43	412	CL7	NC
21	43	413	CL7	NA
21	43	413	CL7	NC
21	43	414	CL7	NA
21	43	414	CL7	NC
21	43	415	CL7	NA
21	43	415	CL7	NC
21	43	416	CL7	NA
21	43	416	CL7	NC
21	43	417	CL7	NA
21	43	417	CL7	NC
21	43	418	CL7	NA
21	43	418	CL7	NC
21	43	419	CL7	NA
21	43	419	CL7	NC
21	44	404	CL7	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	44	404	CL7	NC
21	44	405	CL7	NA
21	44	405	CL7	NC
21	44	406	CL7	NA
21	44	406	CL7	NC
21	44	407	CL7	NA
21	44	407	CL7	NC
21	44	408	CL7	NA
21	44	408	CL7	NC
21	44	409	CL7	NA
21	44	409	CL7	NC
21	44	410	CL7	NA
21	44	410	CL7	NC
21	44	411	CL7	NA
21	44	411	CL7	NC
21	44	412	CL7	NA
21	44	412	CL7	NC
21	44	413	CL7	NA
21	44	413	CL7	NC
21	44	414	CL7	NA
21	44	414	CL7	NC
21	44	415	CL7	NA
21	44	415	CL7	NC
21	44	416	CL7	NA
21	44	416	CL7	NC
21	44	417	CL7	NA
21	44	417	CL7	NC
22	1D	408	PHO	C2A
22	2D	408	PHO	C2A
22	3D	408	PHO	C2A
22	4D	408	PHO	C2A
24	1A	405	LMG	C1
24	1A	405	LMG	C4
24	2A	405	LMG	C1
24	2A	405	LMG	C4
24	3A	405	LMG	C1
24	3A	405	LMG	C4
24	4A	405	LMG	C1
24	4A	405	LMG	C4

All (6574) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1A	401	CL7	C2B-C3B-CAB-OBB
21	1A	401	CL7	C4B-C3B-CAB-OBB
21	1A	403	CL7	O1A-CGA-O2A-C1
21	1A	403	CL7	CBA-CGA-O2A-C1
21	1A	403	CL7	C1A-C2A-CAA-CBA
21	1A	403	CL7	C3A-C2A-CAA-CBA
21	1A	407	CL7	C1A-C2A-CAA-CBA
21	1A	407	CL7	C3A-C2A-CAA-CBA
21	1A	407	CL7	C2B-C3B-CAB-OBB
21	1A	407	CL7	C4B-C3B-CAB-OBB
21	1B	602	CL7	O1A-CGA-O2A-C1
21	1B	602	CL7	CBA-CGA-O2A-C1
21	1B	602	CL7	C2-C3-C5-C6
21	1B	602	CL7	C4-C3-C5-C6
21	1B	602	CL7	C2B-C3B-CAB-OBB
21	1B	602	CL7	C4B-C3B-CAB-OBB
21	1B	604	CL7	C1A-C2A-CAA-CBA
21	1B	604	CL7	C3A-C2A-CAA-CBA
21	1B	604	CL7	C2B-C3B-CAB-OBB
21	1B	604	CL7	C4B-C3B-CAB-OBB
21	1B	605	CL7	C1A-C2A-CAA-CBA
21	1B	605	CL7	C3A-C2A-CAA-CBA
21	1B	607	CL7	C1A-C2A-CAA-CBA
21	1B	607	CL7	C3A-C2A-CAA-CBA
21	1B	607	CL7	CBD-CGD-O2D-CED
21	1B	607	CL7	C2B-C3B-CAB-OBB
21	1B	607	CL7	C4B-C3B-CAB-OBB
21	1B	608	CL7	C4-C3-C5-C6
21	1B	608	CL7	C1A-C2A-CAA-CBA
21	1B	608	CL7	C3A-C2A-CAA-CBA
21	1B	609	CL7	C3A-C2A-CAA-CBA
21	1B	609	CL7	C2B-C3B-CAB-OBB
21	1B	609	CL7	C4B-C3B-CAB-OBB
21	1B	610	CL7	O1A-CGA-O2A-C1
21	1B	610	CL7	CBA-CGA-O2A-C1
21	1B	611	CL7	C2B-C3B-CAB-OBB
21	1B	611	CL7	C4B-C3B-CAB-OBB
21	1B	612	CL7	C6-C7-C8-C10
21	1B	612	CL7	C3A-C2A-CAA-CBA
21	1B	612	CL7	C2B-C3B-CAB-OBB
21	1B	612	CL7	C4B-C3B-CAB-OBB
21	1B	614	CL7	C4-C3-C5-C6
21	1B	614	CL7	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	614	CL7	CHA-CBD-CGD-O1D
21	1B	614	CL7	CAD-CBD-CGD-O1D
21	1B	614	CL7	C4B-C3B-CAB-OBB
21	1B	615	CL7	O1A-CGA-O2A-C1
21	1B	615	CL7	CBA-CGA-O2A-C1
21	1B	615	CL7	C1A-C2A-CAA-CBA
21	1B	615	CL7	C3A-C2A-CAA-CBA
21	1B	622	CL7	CBD-CGD-O2D-CED
21	1B	622	CL7	C2B-C3B-CAB-OBB
21	1B	622	CL7	C4B-C3B-CAB-OBB
21	1C	501	CL7	C1A-C2A-CAA-CBA
21	1C	501	CL7	C3A-C2A-CAA-CBA
21	1C	501	CL7	C4B-C3B-CAB-OBB
21	1C	502	CL7	C2-C3-C5-C6
21	1C	502	CL7	C4-C3-C5-C6
21	1C	502	CL7	CBD-CGD-O2D-CED
21	1C	502	CL7	C2B-C3B-CAB-OBB
21	1C	502	CL7	C4B-C3B-CAB-OBB
21	1C	503	CL7	C2-C3-C5-C6
21	1C	503	CL7	C4-C3-C5-C6
21	1C	503	CL7	C1A-C2A-CAA-CBA
21	1C	504	CL7	C1A-C2A-CAA-CBA
21	1C	504	CL7	C2B-C3B-CAB-OBB
21	1C	504	CL7	C4B-C3B-CAB-OBB
21	1C	505	CL7	C14-C13-C15-C16
21	1C	505	CL7	C2B-C3B-CAB-OBB
21	1C	505	CL7	C4B-C3B-CAB-OBB
21	1C	506	CL7	O1A-CGA-O2A-C1
21	1C	506	CL7	CBA-CGA-O2A-C1
21	1C	506	CL7	C1A-C2A-CAA-CBA
21	1C	506	CL7	C3A-C2A-CAA-CBA
21	1C	506	CL7	CHA-CBD-CGD-O2D
21	1C	506	CL7	CHA-CBD-CGD-O1D
21	1C	506	CL7	C2B-C3B-CAB-OBB
21	1C	506	CL7	C4B-C3B-CAB-OBB
21	1C	507	CL7	C2-C3-C5-C6
21	1C	507	CL7	C4-C3-C5-C6
21	1C	507	CL7	C2B-C3B-CAB-OBB
21	1C	507	CL7	C4B-C3B-CAB-OBB
21	1C	508	CL7	O1A-CGA-O2A-C1
21	1C	508	CL7	CBA-CGA-O2A-C1
21	1C	508	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1C	508	CL7	C4B-C3B-CAB-OBB
21	1C	509	CL7	O2A-C1-C2-C3
21	1C	509	CL7	C2-C3-C5-C6
21	1C	509	CL7	C4-C3-C5-C6
21	1C	509	CL7	C14-C13-C15-C16
21	1C	509	CL7	C1A-C2A-CAA-CBA
21	1C	509	CL7	C2B-C3B-CAB-OBB
21	1C	509	CL7	C4B-C3B-CAB-OBB
21	1C	510	CL7	C3A-C2A-CAA-CBA
21	1C	510	CL7	C4B-C3B-CAB-OBB
21	1C	511	CL7	C1A-C2A-CAA-CBA
21	1C	511	CL7	C2B-C3B-CAB-OBB
21	1C	511	CL7	C4B-C3B-CAB-OBB
21	1C	512	CL7	CBD-CGD-O2D-CED
21	1C	513	CL7	CHA-CBD-CGD-O2D
21	1C	513	CL7	CHA-CBD-CGD-O1D
21	1C	513	CL7	CBD-CGD-O2D-CED
21	1C	513	CL7	C2B-C3B-CAB-OBB
21	1C	513	CL7	C4B-C3B-CAB-OBB
21	1C	517	CL7	C2B-C3B-CAB-OBB
21	1C	517	CL7	C4B-C3B-CAB-OBB
21	1D	402	CL7	CHA-CBD-CGD-O2D
21	1D	402	CL7	CHA-CBD-CGD-O1D
21	1D	402	CL7	C2B-C3B-CAB-OBB
21	1D	402	CL7	C4B-C3B-CAB-OBB
21	1D	404	CL7	C2-C3-C5-C6
21	1D	404	CL7	C4-C3-C5-C6
21	1D	404	CL7	C4B-C3B-CAB-OBB
21	1D	405	CL7	C1A-C2A-CAA-CBA
21	1D	405	CL7	C3A-C2A-CAA-CBA
21	1D	405	CL7	CAD-CBD-CGD-O2D
21	1D	405	CL7	CAD-CBD-CGD-O1D
21	1D	405	CL7	C2B-C3B-CAB-OBB
21	1D	405	CL7	C4B-C3B-CAB-OBB
21	12	501	CL7	C2B-C3B-CAB-OBB
21	12	501	CL7	C4B-C3B-CAB-OBB
21	12	502	CL7	C1A-C2A-CAA-CBA
21	12	502	CL7	C3A-C2A-CAA-CBA
21	12	502	CL7	C2B-C3B-CAB-OBB
21	12	502	CL7	C4B-C3B-CAB-OBB
21	12	503	CL7	C1A-C2A-CAA-CBA
21	12	504	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	504	CL7	CBD-CGD-O2D-CED
21	12	504	CL7	C2B-C3B-CAB-OBB
21	12	504	CL7	C4B-C3B-CAB-OBB
21	12	505	CL7	C4B-C3B-CAB-OBB
21	12	506	CL7	C2B-C3B-CAB-OBB
21	12	506	CL7	C4B-C3B-CAB-OBB
21	12	507	CL7	C2B-C3B-CAB-OBB
21	12	507	CL7	C4B-C3B-CAB-OBB
21	12	508	CL7	C4B-C3B-CAB-OBB
21	12	509	CL7	C11-C12-C13-C15
21	12	509	CL7	C2B-C3B-CAB-OBB
21	12	509	CL7	C4B-C3B-CAB-OBB
21	12	510	CL7	C2-C3-C5-C6
21	12	510	CL7	C4-C3-C5-C6
21	12	511	CL7	C2-C3-C5-C6
21	12	511	CL7	C4-C3-C5-C6
21	12	511	CL7	CBD-CGD-O2D-CED
21	12	511	CL7	C4B-C3B-CAB-OBB
21	12	512	CL7	C4B-C3B-CAB-OBB
21	12	513	CL7	C1A-C2A-CAA-CBA
21	12	513	CL7	CHA-CBD-CGD-O1D
21	12	513	CL7	C2B-C3B-CAB-OBB
21	12	513	CL7	C4B-C3B-CAB-OBB
21	12	514	CL7	C1A-C2A-CAA-CBA
21	12	514	CL7	C3A-C2A-CAA-CBA
21	12	514	CL7	CBD-CGD-O2D-CED
21	12	514	CL7	C2B-C3B-CAB-OBB
21	12	514	CL7	C4B-C3B-CAB-OBB
21	12	515	CL7	CHA-CBD-CGD-O2D
21	12	515	CL7	CHA-CBD-CGD-O1D
21	12	515	CL7	CAD-CBD-CGD-O1D
21	12	515	CL7	C2B-C3B-CAB-OBB
21	12	515	CL7	C4B-C3B-CAB-OBB
21	12	516	CL7	O1A-CGA-O2A-C1
21	12	516	CL7	CBA-CGA-O2A-C1
21	12	516	CL7	C3A-C2A-CAA-CBA
21	12	516	CL7	C4B-C3B-CAB-OBB
21	12	517	CL7	C1A-C2A-CAA-CBA
21	12	517	CL7	C3A-C2A-CAA-CBA
21	12	517	CL7	C2B-C3B-CAB-OBB
21	12	517	CL7	C4B-C3B-CAB-OBB
21	12	518	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	518	CL7	C3A-C2A-CAA-CBA
21	12	518	CL7	C4B-C3B-CAB-OBB
21	11	402	CL7	C1A-C2A-CAA-CBA
21	11	402	CL7	C3A-C2A-CAA-CBA
21	11	403	CL7	C2B-C3B-CAB-OBB
21	11	403	CL7	C4B-C3B-CAB-OBB
21	11	404	CL7	O2A-C1-C2-C3
21	11	404	CL7	C2-C3-C5-C6
21	11	404	CL7	C4-C3-C5-C6
21	11	404	CL7	C2B-C3B-CAB-OBB
21	11	404	CL7	C4B-C3B-CAB-OBB
21	11	406	CL7	C2B-C3B-CAB-OBB
21	11	406	CL7	C4B-C3B-CAB-OBB
21	11	407	CL7	C2B-C3B-CAB-OBB
21	11	407	CL7	C4B-C3B-CAB-OBB
21	11	408	CL7	C1A-C2A-CAA-CBA
21	11	408	CL7	C3A-C2A-CAA-CBA
21	11	408	CL7	C2B-C3B-CAB-OBB
21	11	408	CL7	C4B-C3B-CAB-OBB
21	11	409	CL7	CBD-CGD-O2D-CED
21	11	409	CL7	C2B-C3B-CAB-OBB
21	11	409	CL7	C4B-C3B-CAB-OBB
21	11	410	CL7	O1A-CGA-O2A-C1
21	11	410	CL7	CBA-CGA-O2A-C1
21	11	410	CL7	C1A-C2A-CAA-CBA
21	11	410	CL7	C3A-C2A-CAA-CBA
21	11	410	CL7	C2B-C3B-CAB-OBB
21	11	410	CL7	C4B-C3B-CAB-OBB
21	11	411	CL7	CBD-CGD-O2D-CED
21	11	411	CL7	C4B-C3B-CAB-OBB
21	11	412	CL7	C1A-C2A-CAA-CBA
21	11	412	CL7	C2B-C3B-CAB-OBB
21	11	412	CL7	C4B-C3B-CAB-OBB
21	11	413	CL7	CAD-CBD-CGD-O2D
21	11	413	CL7	CAD-CBD-CGD-O1D
21	11	414	CL7	C2B-C3B-CAB-OBB
21	11	414	CL7	C4B-C3B-CAB-OBB
21	11	415	CL7	CHA-CBD-CGD-O2D
21	11	415	CL7	CHA-CBD-CGD-O1D
21	11	415	CL7	C2B-C3B-CAB-OBB
21	11	415	CL7	C4B-C3B-CAB-OBB
21	11	416	CL7	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	11	416	CL7	C2B-C3B-CAB-OBB
21	11	416	CL7	C4B-C3B-CAB-OBB
21	11	417	CL7	O1A-CGA-O2A-C1
21	11	417	CL7	CBA-CGA-O2A-C1
21	11	417	CL7	C3A-C2A-CAA-CBA
21	11	417	CL7	C2B-C3B-CAB-OBB
21	11	417	CL7	C4B-C3B-CAB-OBB
21	11	418	CL7	CHA-CBD-CGD-O2D
21	11	418	CL7	CHA-CBD-CGD-O1D
21	11	418	CL7	C2B-C3B-CAB-OBB
21	11	418	CL7	C4B-C3B-CAB-OBB
21	11	419	CL7	CBD-CGD-O2D-CED
21	11	419	CL7	C2B-C3B-CAB-OBB
21	11	419	CL7	C4B-C3B-CAB-OBB
21	11	420	CL7	C2B-C3B-CAB-OBB
21	11	420	CL7	C4B-C3B-CAB-OBB
21	13	501	CL7	C1A-C2A-CAA-CBA
21	13	501	CL7	C2B-C3B-CAB-OBB
21	13	501	CL7	C4B-C3B-CAB-OBB
21	13	502	CL7	CBD-CGD-O2D-CED
21	13	502	CL7	C2B-C3B-CAB-OBB
21	13	502	CL7	C4B-C3B-CAB-OBB
21	13	503	CL7	CBD-CGD-O2D-CED
21	13	503	CL7	C2B-C3B-CAB-OBB
21	13	503	CL7	C4B-C3B-CAB-OBB
21	13	504	CL7	C1A-C2A-CAA-CBA
21	13	504	CL7	C2B-C3B-CAB-OBB
21	13	504	CL7	C4B-C3B-CAB-OBB
21	13	506	CL7	C1A-C2A-CAA-CBA
21	13	506	CL7	C3A-C2A-CAA-CBA
21	13	506	CL7	CHA-CBD-CGD-O1D
21	13	506	CL7	CAD-CBD-CGD-O2D
21	13	506	CL7	CAD-CBD-CGD-O1D
21	13	506	CL7	C4B-C3B-CAB-OBB
21	13	507	CL7	C2-C3-C5-C6
21	13	507	CL7	C4-C3-C5-C6
21	13	507	CL7	C2B-C3B-CAB-OBB
21	13	507	CL7	C4B-C3B-CAB-OBB
21	13	508	CL7	C2-C3-C5-C6
21	13	508	CL7	C4-C3-C5-C6
21	13	508	CL7	C2B-C3B-CAB-OBB
21	13	508	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	13	509	CL7	O1A-CGA-O2A-C1
21	13	509	CL7	CBA-CGA-O2A-C1
21	13	509	CL7	C2B-C3B-CAB-OBB
21	13	509	CL7	C4B-C3B-CAB-OBB
21	13	510	CL7	C1A-C2A-CAA-CBA
21	13	510	CL7	CBD-CGD-O2D-CED
21	13	510	CL7	C2B-C3B-CAB-OBB
21	13	510	CL7	C4B-C3B-CAB-OBB
21	13	511	CL7	O1A-CGA-O2A-C1
21	13	511	CL7	CBA-CGA-O2A-C1
21	13	511	CL7	C2B-C3B-CAB-OBB
21	13	511	CL7	C4B-C3B-CAB-OBB
21	13	513	CL7	C1A-C2A-CAA-CBA
21	13	513	CL7	C2B-C3B-CAB-OBB
21	13	513	CL7	C4B-C3B-CAB-OBB
21	13	516	CL7	O1A-CGA-O2A-C1
21	13	516	CL7	CBA-CGA-O2A-C1
21	13	516	CL7	C3A-C2A-CAA-CBA
21	13	516	CL7	C2B-C3B-CAB-OBB
21	13	516	CL7	C4B-C3B-CAB-OBB
21	13	517	CL7	C1A-C2A-CAA-CBA
21	13	517	CL7	C3A-C2A-CAA-CBA
21	13	517	CL7	C4B-C3B-CAB-OBB
21	13	518	CL7	C2B-C3B-CAB-OBB
21	13	518	CL7	C4B-C3B-CAB-OBB
21	14	404	CL7	C3A-C2A-CAA-CBA
21	14	405	CL7	O1A-CGA-O2A-C1
21	14	405	CL7	CBA-CGA-O2A-C1
21	14	405	CL7	C2-C3-C5-C6
21	14	405	CL7	C4-C3-C5-C6
21	14	405	CL7	C4B-C3B-CAB-OBB
21	14	406	CL7	C1A-C2A-CAA-CBA
21	14	406	CL7	C3A-C2A-CAA-CBA
21	14	406	CL7	C4B-C3B-CAB-OBB
21	14	407	CL7	C2B-C3B-CAB-OBB
21	14	407	CL7	C4B-C3B-CAB-OBB
21	14	408	CL7	C4B-C3B-CAB-OBB
21	14	409	CL7	C1A-C2A-CAA-CBA
21	14	409	CL7	C3A-C2A-CAA-CBA
21	14	409	CL7	C2B-C3B-CAB-OBB
21	14	409	CL7	C4B-C3B-CAB-OBB
21	14	410	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	14	410	CL7	C2B-C3B-CAB-OBB
21	14	410	CL7	C4B-C3B-CAB-OBB
21	14	411	CL7	C1A-C2A-CAA-CBA
21	14	411	CL7	CBD-CGD-O2D-CED
21	14	411	CL7	C2B-C3B-CAB-OBB
21	14	411	CL7	C4B-C3B-CAB-OBB
21	14	412	CL7	C1A-C2A-CAA-CBA
21	14	414	CL7	C2B-C3B-CAB-OBB
21	14	414	CL7	C4B-C3B-CAB-OBB
21	14	415	CL7	C1A-C2A-CAA-CBA
21	14	415	CL7	C3A-C2A-CAA-CBA
21	14	415	CL7	CAD-CBD-CGD-O2D
21	14	416	CL7	CHA-CBD-CGD-O2D
21	14	416	CL7	CHA-CBD-CGD-O1D
21	14	416	CL7	C2B-C3B-CAB-OBB
21	14	416	CL7	C4B-C3B-CAB-OBB
21	14	417	CL7	C1A-C2A-CAA-CBA
21	14	417	CL7	C2B-C3B-CAB-OBB
21	14	417	CL7	C4B-C3B-CAB-OBB
21	2A	401	CL7	C2B-C3B-CAB-OBB
21	2A	401	CL7	C4B-C3B-CAB-OBB
21	2A	403	CL7	O1A-CGA-O2A-C1
21	2A	403	CL7	CBA-CGA-O2A-C1
21	2A	403	CL7	C1A-C2A-CAA-CBA
21	2A	403	CL7	C3A-C2A-CAA-CBA
21	2A	407	CL7	C1A-C2A-CAA-CBA
21	2A	407	CL7	C3A-C2A-CAA-CBA
21	2A	407	CL7	C2B-C3B-CAB-OBB
21	2A	407	CL7	C4B-C3B-CAB-OBB
21	2B	603	CL7	O1A-CGA-O2A-C1
21	2B	603	CL7	CBA-CGA-O2A-C1
21	2B	603	CL7	C2-C3-C5-C6
21	2B	603	CL7	C4-C3-C5-C6
21	2B	603	CL7	C2B-C3B-CAB-OBB
21	2B	603	CL7	C4B-C3B-CAB-OBB
21	2B	605	CL7	C1A-C2A-CAA-CBA
21	2B	605	CL7	C3A-C2A-CAA-CBA
21	2B	605	CL7	C2B-C3B-CAB-OBB
21	2B	605	CL7	C4B-C3B-CAB-OBB
21	2B	606	CL7	C1A-C2A-CAA-CBA
21	2B	606	CL7	C3A-C2A-CAA-CBA
21	2B	608	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2B	608	CL7	C3A-C2A-CAA-CBA
21	2B	608	CL7	CBD-CGD-O2D-CED
21	2B	608	CL7	C2B-C3B-CAB-OBB
21	2B	608	CL7	C4B-C3B-CAB-OBB
21	2B	609	CL7	C4-C3-C5-C6
21	2B	609	CL7	C1A-C2A-CAA-CBA
21	2B	609	CL7	C3A-C2A-CAA-CBA
21	2B	610	CL7	C3A-C2A-CAA-CBA
21	2B	610	CL7	C2B-C3B-CAB-OBB
21	2B	610	CL7	C4B-C3B-CAB-OBB
21	2B	611	CL7	O1A-CGA-O2A-C1
21	2B	611	CL7	CBA-CGA-O2A-C1
21	2B	612	CL7	C2B-C3B-CAB-OBB
21	2B	612	CL7	C4B-C3B-CAB-OBB
21	2B	613	CL7	C6-C7-C8-C10
21	2B	613	CL7	C3A-C2A-CAA-CBA
21	2B	613	CL7	C2B-C3B-CAB-OBB
21	2B	613	CL7	C4B-C3B-CAB-OBB
21	2B	615	CL7	C4-C3-C5-C6
21	2B	615	CL7	CHA-CBD-CGD-O2D
21	2B	615	CL7	CHA-CBD-CGD-O1D
21	2B	615	CL7	CAD-CBD-CGD-O1D
21	2B	615	CL7	C4B-C3B-CAB-OBB
21	2B	616	CL7	O1A-CGA-O2A-C1
21	2B	616	CL7	CBA-CGA-O2A-C1
21	2B	616	CL7	C1A-C2A-CAA-CBA
21	2B	616	CL7	C3A-C2A-CAA-CBA
21	2B	623	CL7	CBD-CGD-O2D-CED
21	2B	623	CL7	C2B-C3B-CAB-OBB
21	2B	623	CL7	C4B-C3B-CAB-OBB
21	2C	501	CL7	C1A-C2A-CAA-CBA
21	2C	501	CL7	C3A-C2A-CAA-CBA
21	2C	501	CL7	C4B-C3B-CAB-OBB
21	2C	502	CL7	C2-C3-C5-C6
21	2C	502	CL7	C4-C3-C5-C6
21	2C	502	CL7	CBD-CGD-O2D-CED
21	2C	502	CL7	C2B-C3B-CAB-OBB
21	2C	502	CL7	C4B-C3B-CAB-OBB
21	2C	503	CL7	C2-C3-C5-C6
21	2C	503	CL7	C4-C3-C5-C6
21	2C	503	CL7	C1A-C2A-CAA-CBA
21	2C	504	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2C	504	CL7	C2B-C3B-CAB-OBB
21	2C	504	CL7	C4B-C3B-CAB-OBB
21	2C	505	CL7	C14-C13-C15-C16
21	2C	505	CL7	C2B-C3B-CAB-OBB
21	2C	505	CL7	C4B-C3B-CAB-OBB
21	2C	506	CL7	O1A-CGA-O2A-C1
21	2C	506	CL7	CBA-CGA-O2A-C1
21	2C	506	CL7	C1A-C2A-CAA-CBA
21	2C	506	CL7	C3A-C2A-CAA-CBA
21	2C	506	CL7	CHA-CBD-CGD-O2D
21	2C	506	CL7	CHA-CBD-CGD-O1D
21	2C	506	CL7	C2B-C3B-CAB-OBB
21	2C	506	CL7	C4B-C3B-CAB-OBB
21	2C	507	CL7	C2-C3-C5-C6
21	2C	507	CL7	C4-C3-C5-C6
21	2C	507	CL7	C2B-C3B-CAB-OBB
21	2C	507	CL7	C4B-C3B-CAB-OBB
21	2C	508	CL7	O1A-CGA-O2A-C1
21	2C	508	CL7	CBA-CGA-O2A-C1
21	2C	508	CL7	C2B-C3B-CAB-OBB
21	2C	508	CL7	C4B-C3B-CAB-OBB
21	2C	509	CL7	O2A-C1-C2-C3
21	2C	509	CL7	C2-C3-C5-C6
21	2C	509	CL7	C4-C3-C5-C6
21	2C	509	CL7	C14-C13-C15-C16
21	2C	509	CL7	C1A-C2A-CAA-CBA
21	2C	509	CL7	C2B-C3B-CAB-OBB
21	2C	509	CL7	C4B-C3B-CAB-OBB
21	2C	510	CL7	C3A-C2A-CAA-CBA
21	2C	510	CL7	C4B-C3B-CAB-OBB
21	2C	511	CL7	C1A-C2A-CAA-CBA
21	2C	511	CL7	C2B-C3B-CAB-OBB
21	2C	511	CL7	C4B-C3B-CAB-OBB
21	2C	512	CL7	CBD-CGD-O2D-CED
21	2C	513	CL7	CHA-CBD-CGD-O2D
21	2C	513	CL7	CHA-CBD-CGD-O1D
21	2C	513	CL7	CBD-CGD-O2D-CED
21	2C	513	CL7	C2B-C3B-CAB-OBB
21	2C	513	CL7	C4B-C3B-CAB-OBB
21	2C	517	CL7	C2B-C3B-CAB-OBB
21	2C	517	CL7	C4B-C3B-CAB-OBB
21	2D	402	CL7	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2D	402	CL7	CHA-CBD-CGD-O1D
21	2D	402	CL7	C2B-C3B-CAB-OBB
21	2D	402	CL7	C4B-C3B-CAB-OBB
21	2D	404	CL7	C2-C3-C5-C6
21	2D	404	CL7	C4-C3-C5-C6
21	2D	404	CL7	C4B-C3B-CAB-OBB
21	2D	405	CL7	C1A-C2A-CAA-CBA
21	2D	405	CL7	C3A-C2A-CAA-CBA
21	2D	405	CL7	CAD-CBD-CGD-O2D
21	2D	405	CL7	CAD-CBD-CGD-O1D
21	2D	405	CL7	C2B-C3B-CAB-OBB
21	2D	405	CL7	C4B-C3B-CAB-OBB
21	22	501	CL7	C2B-C3B-CAB-OBB
21	22	501	CL7	C4B-C3B-CAB-OBB
21	22	502	CL7	C1A-C2A-CAA-CBA
21	22	502	CL7	C3A-C2A-CAA-CBA
21	22	502	CL7	C2B-C3B-CAB-OBB
21	22	502	CL7	C4B-C3B-CAB-OBB
21	22	503	CL7	C1A-C2A-CAA-CBA
21	22	504	CL7	C1A-C2A-CAA-CBA
21	22	504	CL7	CBD-CGD-O2D-CED
21	22	504	CL7	C2B-C3B-CAB-OBB
21	22	504	CL7	C4B-C3B-CAB-OBB
21	22	505	CL7	C4B-C3B-CAB-OBB
21	22	506	CL7	C2B-C3B-CAB-OBB
21	22	506	CL7	C4B-C3B-CAB-OBB
21	22	507	CL7	C2B-C3B-CAB-OBB
21	22	507	CL7	C4B-C3B-CAB-OBB
21	22	508	CL7	C4B-C3B-CAB-OBB
21	22	509	CL7	C11-C12-C13-C15
21	22	509	CL7	C2B-C3B-CAB-OBB
21	22	509	CL7	C4B-C3B-CAB-OBB
21	22	510	CL7	C2-C3-C5-C6
21	22	510	CL7	C4-C3-C5-C6
21	22	511	CL7	C2-C3-C5-C6
21	22	511	CL7	C4-C3-C5-C6
21	22	511	CL7	CBD-CGD-O2D-CED
21	22	511	CL7	C4B-C3B-CAB-OBB
21	22	512	CL7	C4B-C3B-CAB-OBB
21	22	513	CL7	C1A-C2A-CAA-CBA
21	22	513	CL7	CHA-CBD-CGD-O1D
21	22	513	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	22	513	CL7	C4B-C3B-CAB-OBB
21	22	514	CL7	C1A-C2A-CAA-CBA
21	22	514	CL7	C3A-C2A-CAA-CBA
21	22	514	CL7	CBD-CGD-O2D-CED
21	22	514	CL7	C2B-C3B-CAB-OBB
21	22	514	CL7	C4B-C3B-CAB-OBB
21	22	515	CL7	CHA-CBD-CGD-O2D
21	22	515	CL7	CHA-CBD-CGD-O1D
21	22	515	CL7	CAD-CBD-CGD-O1D
21	22	515	CL7	C2B-C3B-CAB-OBB
21	22	515	CL7	C4B-C3B-CAB-OBB
21	22	516	CL7	O1A-CGA-O2A-C1
21	22	516	CL7	CBA-CGA-O2A-C1
21	22	516	CL7	C3A-C2A-CAA-CBA
21	22	516	CL7	C4B-C3B-CAB-OBB
21	22	517	CL7	C1A-C2A-CAA-CBA
21	22	517	CL7	C3A-C2A-CAA-CBA
21	22	517	CL7	C2B-C3B-CAB-OBB
21	22	517	CL7	C4B-C3B-CAB-OBB
21	22	518	CL7	C1A-C2A-CAA-CBA
21	22	518	CL7	C3A-C2A-CAA-CBA
21	22	518	CL7	C4B-C3B-CAB-OBB
21	21	402	CL7	C1A-C2A-CAA-CBA
21	21	402	CL7	C3A-C2A-CAA-CBA
21	21	403	CL7	C2B-C3B-CAB-OBB
21	21	403	CL7	C4B-C3B-CAB-OBB
21	21	404	CL7	O2A-C1-C2-C3
21	21	404	CL7	C2-C3-C5-C6
21	21	404	CL7	C4-C3-C5-C6
21	21	404	CL7	C2B-C3B-CAB-OBB
21	21	404	CL7	C4B-C3B-CAB-OBB
21	21	406	CL7	C2B-C3B-CAB-OBB
21	21	406	CL7	C4B-C3B-CAB-OBB
21	21	407	CL7	C2B-C3B-CAB-OBB
21	21	407	CL7	C4B-C3B-CAB-OBB
21	21	408	CL7	C1A-C2A-CAA-CBA
21	21	408	CL7	C3A-C2A-CAA-CBA
21	21	408	CL7	C2B-C3B-CAB-OBB
21	21	408	CL7	C4B-C3B-CAB-OBB
21	21	409	CL7	CBD-CGD-O2D-CED
21	21	409	CL7	C2B-C3B-CAB-OBB
21	21	409	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	21	410	CL7	O1A-CGA-O2A-C1
21	21	410	CL7	CBA-CGA-O2A-C1
21	21	410	CL7	C1A-C2A-CAA-CBA
21	21	410	CL7	C3A-C2A-CAA-CBA
21	21	410	CL7	C2B-C3B-CAB-OBB
21	21	410	CL7	C4B-C3B-CAB-OBB
21	21	411	CL7	CBD-CGD-O2D-CED
21	21	411	CL7	C4B-C3B-CAB-OBB
21	21	412	CL7	C1A-C2A-CAA-CBA
21	21	412	CL7	C2B-C3B-CAB-OBB
21	21	412	CL7	C4B-C3B-CAB-OBB
21	21	413	CL7	CAD-CBD-CGD-O2D
21	21	413	CL7	CAD-CBD-CGD-O1D
21	21	414	CL7	C2B-C3B-CAB-OBB
21	21	414	CL7	C4B-C3B-CAB-OBB
21	21	415	CL7	CHA-CBD-CGD-O2D
21	21	415	CL7	CHA-CBD-CGD-O1D
21	21	415	CL7	C2B-C3B-CAB-OBB
21	21	415	CL7	C4B-C3B-CAB-OBB
21	21	416	CL7	CBD-CGD-O2D-CED
21	21	416	CL7	C2B-C3B-CAB-OBB
21	21	416	CL7	C4B-C3B-CAB-OBB
21	21	417	CL7	O1A-CGA-O2A-C1
21	21	417	CL7	CBA-CGA-O2A-C1
21	21	417	CL7	C3A-C2A-CAA-CBA
21	21	417	CL7	C2B-C3B-CAB-OBB
21	21	417	CL7	C4B-C3B-CAB-OBB
21	21	418	CL7	CHA-CBD-CGD-O2D
21	21	418	CL7	CHA-CBD-CGD-O1D
21	21	418	CL7	C2B-C3B-CAB-OBB
21	21	418	CL7	C4B-C3B-CAB-OBB
21	21	419	CL7	CBD-CGD-O2D-CED
21	21	419	CL7	C2B-C3B-CAB-OBB
21	21	419	CL7	C4B-C3B-CAB-OBB
21	21	420	CL7	C2B-C3B-CAB-OBB
21	21	420	CL7	C4B-C3B-CAB-OBB
21	23	402	CL7	C1A-C2A-CAA-CBA
21	23	402	CL7	C2B-C3B-CAB-OBB
21	23	402	CL7	C4B-C3B-CAB-OBB
21	23	403	CL7	CBD-CGD-O2D-CED
21	23	403	CL7	C2B-C3B-CAB-OBB
21	23	403	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	23	404	CL7	CBD-CGD-O2D-CED
21	23	404	CL7	C2B-C3B-CAB-OBB
21	23	404	CL7	C4B-C3B-CAB-OBB
21	23	405	CL7	C1A-C2A-CAA-CBA
21	23	405	CL7	C2B-C3B-CAB-OBB
21	23	405	CL7	C4B-C3B-CAB-OBB
21	23	407	CL7	C1A-C2A-CAA-CBA
21	23	407	CL7	C3A-C2A-CAA-CBA
21	23	407	CL7	CHA-CBD-CGD-O1D
21	23	407	CL7	CAD-CBD-CGD-O2D
21	23	407	CL7	CAD-CBD-CGD-O1D
21	23	407	CL7	C4B-C3B-CAB-OBB
21	23	408	CL7	C2-C3-C5-C6
21	23	408	CL7	C4-C3-C5-C6
21	23	408	CL7	C2B-C3B-CAB-OBB
21	23	408	CL7	C4B-C3B-CAB-OBB
21	23	409	CL7	C2-C3-C5-C6
21	23	409	CL7	C4-C3-C5-C6
21	23	409	CL7	C2B-C3B-CAB-OBB
21	23	409	CL7	C4B-C3B-CAB-OBB
21	23	410	CL7	O1A-CGA-O2A-C1
21	23	410	CL7	CBA-CGA-O2A-C1
21	23	410	CL7	C2B-C3B-CAB-OBB
21	23	410	CL7	C4B-C3B-CAB-OBB
21	23	411	CL7	C1A-C2A-CAA-CBA
21	23	411	CL7	CBD-CGD-O2D-CED
21	23	411	CL7	C2B-C3B-CAB-OBB
21	23	411	CL7	C4B-C3B-CAB-OBB
21	23	412	CL7	O1A-CGA-O2A-C1
21	23	412	CL7	CBA-CGA-O2A-C1
21	23	412	CL7	C2B-C3B-CAB-OBB
21	23	412	CL7	C4B-C3B-CAB-OBB
21	23	414	CL7	C1A-C2A-CAA-CBA
21	23	414	CL7	C2B-C3B-CAB-OBB
21	23	414	CL7	C4B-C3B-CAB-OBB
21	23	417	CL7	O1A-CGA-O2A-C1
21	23	417	CL7	CBA-CGA-O2A-C1
21	23	417	CL7	C3A-C2A-CAA-CBA
21	23	417	CL7	C2B-C3B-CAB-OBB
21	23	417	CL7	C4B-C3B-CAB-OBB
21	23	418	CL7	C1A-C2A-CAA-CBA
21	23	418	CL7	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	23	418	CL7	C4B-C3B-CAB-OBB
21	23	419	CL7	C2B-C3B-CAB-OBB
21	23	419	CL7	C4B-C3B-CAB-OBB
21	24	404	CL7	C3A-C2A-CAA-CBA
21	24	405	CL7	O1A-CGA-O2A-C1
21	24	405	CL7	CBA-CGA-O2A-C1
21	24	405	CL7	C2-C3-C5-C6
21	24	405	CL7	C4-C3-C5-C6
21	24	405	CL7	C4B-C3B-CAB-OBB
21	24	406	CL7	C1A-C2A-CAA-CBA
21	24	406	CL7	C3A-C2A-CAA-CBA
21	24	406	CL7	C4B-C3B-CAB-OBB
21	24	407	CL7	C2B-C3B-CAB-OBB
21	24	407	CL7	C4B-C3B-CAB-OBB
21	24	408	CL7	C4B-C3B-CAB-OBB
21	24	409	CL7	C1A-C2A-CAA-CBA
21	24	409	CL7	C3A-C2A-CAA-CBA
21	24	409	CL7	C2B-C3B-CAB-OBB
21	24	409	CL7	C4B-C3B-CAB-OBB
21	24	410	CL7	C1A-C2A-CAA-CBA
21	24	410	CL7	C2B-C3B-CAB-OBB
21	24	410	CL7	C4B-C3B-CAB-OBB
21	24	411	CL7	C1A-C2A-CAA-CBA
21	24	411	CL7	CBD-CGD-O2D-CED
21	24	411	CL7	C2B-C3B-CAB-OBB
21	24	411	CL7	C4B-C3B-CAB-OBB
21	24	412	CL7	C1A-C2A-CAA-CBA
21	24	414	CL7	C2B-C3B-CAB-OBB
21	24	414	CL7	C4B-C3B-CAB-OBB
21	24	415	CL7	C1A-C2A-CAA-CBA
21	24	415	CL7	C3A-C2A-CAA-CBA
21	24	415	CL7	CAD-CBD-CGD-O2D
21	24	416	CL7	CHA-CBD-CGD-O2D
21	24	416	CL7	CHA-CBD-CGD-O1D
21	24	416	CL7	C2B-C3B-CAB-OBB
21	24	416	CL7	C4B-C3B-CAB-OBB
21	24	417	CL7	C1A-C2A-CAA-CBA
21	24	417	CL7	C2B-C3B-CAB-OBB
21	24	417	CL7	C4B-C3B-CAB-OBB
21	3A	401	CL7	C2B-C3B-CAB-OBB
21	3A	401	CL7	C4B-C3B-CAB-OBB
21	3A	403	CL7	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3A	403	CL7	CBA-CGA-O2A-C1
21	3A	403	CL7	C1A-C2A-CAA-CBA
21	3A	403	CL7	C3A-C2A-CAA-CBA
21	3A	407	CL7	C1A-C2A-CAA-CBA
21	3A	407	CL7	C3A-C2A-CAA-CBA
21	3A	407	CL7	C2B-C3B-CAB-OBB
21	3A	407	CL7	C4B-C3B-CAB-OBB
21	3B	602	CL7	O1A-CGA-O2A-C1
21	3B	602	CL7	CBA-CGA-O2A-C1
21	3B	602	CL7	C2-C3-C5-C6
21	3B	602	CL7	C4-C3-C5-C6
21	3B	602	CL7	C2B-C3B-CAB-OBB
21	3B	602	CL7	C4B-C3B-CAB-OBB
21	3B	604	CL7	C1A-C2A-CAA-CBA
21	3B	604	CL7	C3A-C2A-CAA-CBA
21	3B	604	CL7	C2B-C3B-CAB-OBB
21	3B	604	CL7	C4B-C3B-CAB-OBB
21	3B	605	CL7	C1A-C2A-CAA-CBA
21	3B	605	CL7	C3A-C2A-CAA-CBA
21	3B	607	CL7	C1A-C2A-CAA-CBA
21	3B	607	CL7	C3A-C2A-CAA-CBA
21	3B	607	CL7	CBD-CGD-O2D-CED
21	3B	607	CL7	C2B-C3B-CAB-OBB
21	3B	607	CL7	C4B-C3B-CAB-OBB
21	3B	608	CL7	C4-C3-C5-C6
21	3B	608	CL7	C1A-C2A-CAA-CBA
21	3B	608	CL7	C3A-C2A-CAA-CBA
21	3B	609	CL7	C3A-C2A-CAA-CBA
21	3B	609	CL7	C2B-C3B-CAB-OBB
21	3B	609	CL7	C4B-C3B-CAB-OBB
21	3B	610	CL7	O1A-CGA-O2A-C1
21	3B	610	CL7	CBA-CGA-O2A-C1
21	3B	611	CL7	C2B-C3B-CAB-OBB
21	3B	611	CL7	C4B-C3B-CAB-OBB
21	3B	612	CL7	C6-C7-C8-C10
21	3B	612	CL7	C3A-C2A-CAA-CBA
21	3B	612	CL7	C2B-C3B-CAB-OBB
21	3B	612	CL7	C4B-C3B-CAB-OBB
21	3B	614	CL7	C4-C3-C5-C6
21	3B	614	CL7	CHA-CBD-CGD-O2D
21	3B	614	CL7	CHA-CBD-CGD-O1D
21	3B	614	CL7	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3B	614	CL7	C4B-C3B-CAB-OBB
21	3B	615	CL7	O1A-CGA-O2A-C1
21	3B	615	CL7	CBA-CGA-O2A-C1
21	3B	615	CL7	C1A-C2A-CAA-CBA
21	3B	615	CL7	C3A-C2A-CAA-CBA
21	3B	622	CL7	CBD-CGD-O2D-CED
21	3B	622	CL7	C2B-C3B-CAB-OBB
21	3B	622	CL7	C4B-C3B-CAB-OBB
21	3C	501	CL7	C1A-C2A-CAA-CBA
21	3C	501	CL7	C3A-C2A-CAA-CBA
21	3C	501	CL7	C4B-C3B-CAB-OBB
21	3C	502	CL7	C2-C3-C5-C6
21	3C	502	CL7	C4-C3-C5-C6
21	3C	502	CL7	CBD-CGD-O2D-CED
21	3C	502	CL7	C2B-C3B-CAB-OBB
21	3C	502	CL7	C4B-C3B-CAB-OBB
21	3C	503	CL7	C2-C3-C5-C6
21	3C	503	CL7	C4-C3-C5-C6
21	3C	503	CL7	C1A-C2A-CAA-CBA
21	3C	504	CL7	C1A-C2A-CAA-CBA
21	3C	504	CL7	C2B-C3B-CAB-OBB
21	3C	504	CL7	C4B-C3B-CAB-OBB
21	3C	505	CL7	C14-C13-C15-C16
21	3C	505	CL7	C2B-C3B-CAB-OBB
21	3C	505	CL7	C4B-C3B-CAB-OBB
21	3C	506	CL7	O1A-CGA-O2A-C1
21	3C	506	CL7	CBA-CGA-O2A-C1
21	3C	506	CL7	C1A-C2A-CAA-CBA
21	3C	506	CL7	C3A-C2A-CAA-CBA
21	3C	506	CL7	CHA-CBD-CGD-O2D
21	3C	506	CL7	CHA-CBD-CGD-O1D
21	3C	506	CL7	C2B-C3B-CAB-OBB
21	3C	506	CL7	C4B-C3B-CAB-OBB
21	3C	507	CL7	C2-C3-C5-C6
21	3C	507	CL7	C4-C3-C5-C6
21	3C	507	CL7	C2B-C3B-CAB-OBB
21	3C	507	CL7	C4B-C3B-CAB-OBB
21	3C	508	CL7	O1A-CGA-O2A-C1
21	3C	508	CL7	CBA-CGA-O2A-C1
21	3C	508	CL7	C2B-C3B-CAB-OBB
21	3C	508	CL7	C4B-C3B-CAB-OBB
21	3C	509	CL7	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3C	509	CL7	C2-C3-C5-C6
21	3C	509	CL7	C4-C3-C5-C6
21	3C	509	CL7	C14-C13-C15-C16
21	3C	509	CL7	C1A-C2A-CAA-CBA
21	3C	509	CL7	C2B-C3B-CAB-OBB
21	3C	509	CL7	C4B-C3B-CAB-OBB
21	3C	510	CL7	C3A-C2A-CAA-CBA
21	3C	510	CL7	C4B-C3B-CAB-OBB
21	3C	511	CL7	C1A-C2A-CAA-CBA
21	3C	511	CL7	C2B-C3B-CAB-OBB
21	3C	511	CL7	C4B-C3B-CAB-OBB
21	3C	512	CL7	CBD-CGD-O2D-CED
21	3C	513	CL7	CHA-CBD-CGD-O2D
21	3C	513	CL7	CHA-CBD-CGD-O1D
21	3C	513	CL7	CBD-CGD-O2D-CED
21	3C	513	CL7	C2B-C3B-CAB-OBB
21	3C	513	CL7	C4B-C3B-CAB-OBB
21	3C	517	CL7	C2B-C3B-CAB-OBB
21	3C	517	CL7	C4B-C3B-CAB-OBB
21	3D	402	CL7	CHA-CBD-CGD-O2D
21	3D	402	CL7	CHA-CBD-CGD-O1D
21	3D	402	CL7	C2B-C3B-CAB-OBB
21	3D	402	CL7	C4B-C3B-CAB-OBB
21	3D	404	CL7	C2-C3-C5-C6
21	3D	404	CL7	C4-C3-C5-C6
21	3D	404	CL7	C4B-C3B-CAB-OBB
21	3D	405	CL7	C1A-C2A-CAA-CBA
21	3D	405	CL7	C3A-C2A-CAA-CBA
21	3D	405	CL7	CAD-CBD-CGD-O2D
21	3D	405	CL7	CAD-CBD-CGD-O1D
21	3D	405	CL7	C2B-C3B-CAB-OBB
21	3D	405	CL7	C4B-C3B-CAB-OBB
21	32	501	CL7	C2B-C3B-CAB-OBB
21	32	501	CL7	C4B-C3B-CAB-OBB
21	32	502	CL7	C1A-C2A-CAA-CBA
21	32	502	CL7	C3A-C2A-CAA-CBA
21	32	502	CL7	C2B-C3B-CAB-OBB
21	32	502	CL7	C4B-C3B-CAB-OBB
21	32	503	CL7	C1A-C2A-CAA-CBA
21	32	504	CL7	C1A-C2A-CAA-CBA
21	32	504	CL7	CBD-CGD-O2D-CED
21	32	504	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	32	504	CL7	C4B-C3B-CAB-OBB
21	32	505	CL7	C4B-C3B-CAB-OBB
21	32	506	CL7	C2B-C3B-CAB-OBB
21	32	506	CL7	C4B-C3B-CAB-OBB
21	32	507	CL7	C2B-C3B-CAB-OBB
21	32	507	CL7	C4B-C3B-CAB-OBB
21	32	508	CL7	C4B-C3B-CAB-OBB
21	32	509	CL7	C11-C12-C13-C15
21	32	509	CL7	C2B-C3B-CAB-OBB
21	32	509	CL7	C4B-C3B-CAB-OBB
21	32	510	CL7	C2-C3-C5-C6
21	32	510	CL7	C4-C3-C5-C6
21	32	511	CL7	C2-C3-C5-C6
21	32	511	CL7	C4-C3-C5-C6
21	32	511	CL7	CBD-CGD-O2D-CED
21	32	511	CL7	C4B-C3B-CAB-OBB
21	32	512	CL7	C4B-C3B-CAB-OBB
21	32	513	CL7	C1A-C2A-CAA-CBA
21	32	513	CL7	CHA-CBD-CGD-O1D
21	32	513	CL7	C2B-C3B-CAB-OBB
21	32	513	CL7	C4B-C3B-CAB-OBB
21	32	514	CL7	C1A-C2A-CAA-CBA
21	32	514	CL7	C3A-C2A-CAA-CBA
21	32	514	CL7	CBD-CGD-O2D-CED
21	32	514	CL7	C2B-C3B-CAB-OBB
21	32	514	CL7	C4B-C3B-CAB-OBB
21	32	515	CL7	CHA-CBD-CGD-O2D
21	32	515	CL7	CHA-CBD-CGD-O1D
21	32	515	CL7	CAD-CBD-CGD-O1D
21	32	515	CL7	C2B-C3B-CAB-OBB
21	32	515	CL7	C4B-C3B-CAB-OBB
21	32	516	CL7	O1A-CGA-O2A-C1
21	32	516	CL7	CBA-CGA-O2A-C1
21	32	516	CL7	C3A-C2A-CAA-CBA
21	32	516	CL7	C4B-C3B-CAB-OBB
21	32	517	CL7	C1A-C2A-CAA-CBA
21	32	517	CL7	C3A-C2A-CAA-CBA
21	32	517	CL7	C2B-C3B-CAB-OBB
21	32	517	CL7	C4B-C3B-CAB-OBB
21	32	518	CL7	C1A-C2A-CAA-CBA
21	32	518	CL7	C3A-C2A-CAA-CBA
21	32	518	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	31	402	CL7	C1A-C2A-CAA-CBA
21	31	402	CL7	C3A-C2A-CAA-CBA
21	31	403	CL7	C2B-C3B-CAB-OBB
21	31	403	CL7	C4B-C3B-CAB-OBB
21	31	404	CL7	O2A-C1-C2-C3
21	31	404	CL7	C2-C3-C5-C6
21	31	404	CL7	C4-C3-C5-C6
21	31	404	CL7	C2B-C3B-CAB-OBB
21	31	404	CL7	C4B-C3B-CAB-OBB
21	31	406	CL7	C2B-C3B-CAB-OBB
21	31	406	CL7	C4B-C3B-CAB-OBB
21	31	407	CL7	C2B-C3B-CAB-OBB
21	31	407	CL7	C4B-C3B-CAB-OBB
21	31	408	CL7	C1A-C2A-CAA-CBA
21	31	408	CL7	C3A-C2A-CAA-CBA
21	31	408	CL7	C2B-C3B-CAB-OBB
21	31	408	CL7	C4B-C3B-CAB-OBB
21	31	409	CL7	CBD-CGD-O2D-CED
21	31	409	CL7	C2B-C3B-CAB-OBB
21	31	409	CL7	C4B-C3B-CAB-OBB
21	31	410	CL7	O1A-CGA-O2A-C1
21	31	410	CL7	CBA-CGA-O2A-C1
21	31	410	CL7	C1A-C2A-CAA-CBA
21	31	410	CL7	C3A-C2A-CAA-CBA
21	31	410	CL7	C2B-C3B-CAB-OBB
21	31	410	CL7	C4B-C3B-CAB-OBB
21	31	411	CL7	CBD-CGD-O2D-CED
21	31	411	CL7	C4B-C3B-CAB-OBB
21	31	412	CL7	C1A-C2A-CAA-CBA
21	31	412	CL7	C2B-C3B-CAB-OBB
21	31	412	CL7	C4B-C3B-CAB-OBB
21	31	413	CL7	CAD-CBD-CGD-O2D
21	31	413	CL7	CAD-CBD-CGD-O1D
21	31	414	CL7	C2B-C3B-CAB-OBB
21	31	414	CL7	C4B-C3B-CAB-OBB
21	31	415	CL7	CHA-CBD-CGD-O2D
21	31	415	CL7	CHA-CBD-CGD-O1D
21	31	415	CL7	C2B-C3B-CAB-OBB
21	31	415	CL7	C4B-C3B-CAB-OBB
21	31	416	CL7	CBD-CGD-O2D-CED
21	31	416	CL7	C2B-C3B-CAB-OBB
21	31	416	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	31	417	CL7	O1A-CGA-O2A-C1
21	31	417	CL7	CBA-CGA-O2A-C1
21	31	417	CL7	C3A-C2A-CAA-CBA
21	31	417	CL7	C2B-C3B-CAB-OBB
21	31	417	CL7	C4B-C3B-CAB-OBB
21	31	418	CL7	CHA-CBD-CGD-O2D
21	31	418	CL7	CHA-CBD-CGD-O1D
21	31	418	CL7	C2B-C3B-CAB-OBB
21	31	418	CL7	C4B-C3B-CAB-OBB
21	31	419	CL7	CBD-CGD-O2D-CED
21	31	419	CL7	C2B-C3B-CAB-OBB
21	31	419	CL7	C4B-C3B-CAB-OBB
21	31	420	CL7	C2B-C3B-CAB-OBB
21	31	420	CL7	C4B-C3B-CAB-OBB
21	33	501	CL7	C1A-C2A-CAA-CBA
21	33	501	CL7	C2B-C3B-CAB-OBB
21	33	501	CL7	C4B-C3B-CAB-OBB
21	33	502	CL7	CBD-CGD-O2D-CED
21	33	502	CL7	C2B-C3B-CAB-OBB
21	33	502	CL7	C4B-C3B-CAB-OBB
21	33	503	CL7	CBD-CGD-O2D-CED
21	33	503	CL7	C2B-C3B-CAB-OBB
21	33	503	CL7	C4B-C3B-CAB-OBB
21	33	504	CL7	C1A-C2A-CAA-CBA
21	33	504	CL7	C2B-C3B-CAB-OBB
21	33	504	CL7	C4B-C3B-CAB-OBB
21	33	506	CL7	C1A-C2A-CAA-CBA
21	33	506	CL7	C3A-C2A-CAA-CBA
21	33	506	CL7	CHA-CBD-CGD-O1D
21	33	506	CL7	CAD-CBD-CGD-O2D
21	33	506	CL7	CAD-CBD-CGD-O1D
21	33	506	CL7	C4B-C3B-CAB-OBB
21	33	507	CL7	C2-C3-C5-C6
21	33	507	CL7	C4-C3-C5-C6
21	33	507	CL7	C2B-C3B-CAB-OBB
21	33	507	CL7	C4B-C3B-CAB-OBB
21	33	508	CL7	C2-C3-C5-C6
21	33	508	CL7	C4-C3-C5-C6
21	33	508	CL7	C2B-C3B-CAB-OBB
21	33	508	CL7	C4B-C3B-CAB-OBB
21	33	509	CL7	O1A-CGA-O2A-C1
21	33	509	CL7	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	33	509	CL7	C2B-C3B-CAB-OBB
21	33	509	CL7	C4B-C3B-CAB-OBB
21	33	510	CL7	C1A-C2A-CAA-CBA
21	33	510	CL7	CBD-CGD-O2D-CED
21	33	510	CL7	C2B-C3B-CAB-OBB
21	33	510	CL7	C4B-C3B-CAB-OBB
21	33	511	CL7	O1A-CGA-O2A-C1
21	33	511	CL7	CBA-CGA-O2A-C1
21	33	511	CL7	C2B-C3B-CAB-OBB
21	33	511	CL7	C4B-C3B-CAB-OBB
21	33	513	CL7	C1A-C2A-CAA-CBA
21	33	513	CL7	C2B-C3B-CAB-OBB
21	33	513	CL7	C4B-C3B-CAB-OBB
21	33	516	CL7	O1A-CGA-O2A-C1
21	33	516	CL7	CBA-CGA-O2A-C1
21	33	516	CL7	C3A-C2A-CAA-CBA
21	33	516	CL7	C2B-C3B-CAB-OBB
21	33	516	CL7	C4B-C3B-CAB-OBB
21	33	517	CL7	C1A-C2A-CAA-CBA
21	33	517	CL7	C3A-C2A-CAA-CBA
21	33	517	CL7	C4B-C3B-CAB-OBB
21	33	518	CL7	C2B-C3B-CAB-OBB
21	33	518	CL7	C4B-C3B-CAB-OBB
21	34	404	CL7	C3A-C2A-CAA-CBA
21	34	405	CL7	O1A-CGA-O2A-C1
21	34	405	CL7	CBA-CGA-O2A-C1
21	34	405	CL7	C2-C3-C5-C6
21	34	405	CL7	C4-C3-C5-C6
21	34	405	CL7	C4B-C3B-CAB-OBB
21	34	406	CL7	C1A-C2A-CAA-CBA
21	34	406	CL7	C3A-C2A-CAA-CBA
21	34	406	CL7	C4B-C3B-CAB-OBB
21	34	407	CL7	C2B-C3B-CAB-OBB
21	34	407	CL7	C4B-C3B-CAB-OBB
21	34	408	CL7	C4B-C3B-CAB-OBB
21	34	409	CL7	C1A-C2A-CAA-CBA
21	34	409	CL7	C3A-C2A-CAA-CBA
21	34	409	CL7	C2B-C3B-CAB-OBB
21	34	409	CL7	C4B-C3B-CAB-OBB
21	34	410	CL7	C1A-C2A-CAA-CBA
21	34	410	CL7	C2B-C3B-CAB-OBB
21	34	410	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	34	411	CL7	C1A-C2A-CAA-CBA
21	34	411	CL7	CBD-CGD-O2D-CED
21	34	411	CL7	C2B-C3B-CAB-OBB
21	34	411	CL7	C4B-C3B-CAB-OBB
21	34	412	CL7	C1A-C2A-CAA-CBA
21	34	414	CL7	C2B-C3B-CAB-OBB
21	34	414	CL7	C4B-C3B-CAB-OBB
21	34	415	CL7	C1A-C2A-CAA-CBA
21	34	415	CL7	C3A-C2A-CAA-CBA
21	34	415	CL7	CAD-CBD-CGD-O2D
21	34	416	CL7	CHA-CBD-CGD-O2D
21	34	416	CL7	CHA-CBD-CGD-O1D
21	34	416	CL7	C2B-C3B-CAB-OBB
21	34	416	CL7	C4B-C3B-CAB-OBB
21	34	417	CL7	C1A-C2A-CAA-CBA
21	34	417	CL7	C2B-C3B-CAB-OBB
21	34	417	CL7	C4B-C3B-CAB-OBB
21	4A	401	CL7	C2B-C3B-CAB-OBB
21	4A	401	CL7	C4B-C3B-CAB-OBB
21	4A	403	CL7	O1A-CGA-O2A-C1
21	4A	403	CL7	CBA-CGA-O2A-C1
21	4A	403	CL7	C1A-C2A-CAA-CBA
21	4A	403	CL7	C3A-C2A-CAA-CBA
21	4A	407	CL7	C1A-C2A-CAA-CBA
21	4A	407	CL7	C3A-C2A-CAA-CBA
21	4A	407	CL7	C2B-C3B-CAB-OBB
21	4A	407	CL7	C4B-C3B-CAB-OBB
21	4B	603	CL7	O1A-CGA-O2A-C1
21	4B	603	CL7	CBA-CGA-O2A-C1
21	4B	603	CL7	C2-C3-C5-C6
21	4B	603	CL7	C4-C3-C5-C6
21	4B	603	CL7	C2B-C3B-CAB-OBB
21	4B	603	CL7	C4B-C3B-CAB-OBB
21	4B	605	CL7	C1A-C2A-CAA-CBA
21	4B	605	CL7	C3A-C2A-CAA-CBA
21	4B	605	CL7	C2B-C3B-CAB-OBB
21	4B	605	CL7	C4B-C3B-CAB-OBB
21	4B	606	CL7	C1A-C2A-CAA-CBA
21	4B	606	CL7	C3A-C2A-CAA-CBA
21	4B	608	CL7	C1A-C2A-CAA-CBA
21	4B	608	CL7	C3A-C2A-CAA-CBA
21	4B	608	CL7	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4B	608	CL7	C2B-C3B-CAB-OBB
21	4B	608	CL7	C4B-C3B-CAB-OBB
21	4B	609	CL7	C4-C3-C5-C6
21	4B	609	CL7	C1A-C2A-CAA-CBA
21	4B	609	CL7	C3A-C2A-CAA-CBA
21	4B	610	CL7	C3A-C2A-CAA-CBA
21	4B	610	CL7	C2B-C3B-CAB-OBB
21	4B	610	CL7	C4B-C3B-CAB-OBB
21	4B	611	CL7	O1A-CGA-O2A-C1
21	4B	611	CL7	CBA-CGA-O2A-C1
21	4B	612	CL7	C2B-C3B-CAB-OBB
21	4B	612	CL7	C4B-C3B-CAB-OBB
21	4B	613	CL7	C6-C7-C8-C10
21	4B	613	CL7	C3A-C2A-CAA-CBA
21	4B	613	CL7	C2B-C3B-CAB-OBB
21	4B	613	CL7	C4B-C3B-CAB-OBB
21	4B	615	CL7	C4-C3-C5-C6
21	4B	615	CL7	CHA-CBD-CGD-O2D
21	4B	615	CL7	CHA-CBD-CGD-O1D
21	4B	615	CL7	CAD-CBD-CGD-O1D
21	4B	615	CL7	C4B-C3B-CAB-OBB
21	4B	616	CL7	O1A-CGA-O2A-C1
21	4B	616	CL7	CBA-CGA-O2A-C1
21	4B	616	CL7	C1A-C2A-CAA-CBA
21	4B	616	CL7	C3A-C2A-CAA-CBA
21	4B	623	CL7	CBD-CGD-O2D-CED
21	4B	623	CL7	C2B-C3B-CAB-OBB
21	4B	623	CL7	C4B-C3B-CAB-OBB
21	4C	501	CL7	C1A-C2A-CAA-CBA
21	4C	501	CL7	C3A-C2A-CAA-CBA
21	4C	501	CL7	C4B-C3B-CAB-OBB
21	4C	502	CL7	C2-C3-C5-C6
21	4C	502	CL7	C4-C3-C5-C6
21	4C	502	CL7	CBD-CGD-O2D-CED
21	4C	502	CL7	C2B-C3B-CAB-OBB
21	4C	502	CL7	C4B-C3B-CAB-OBB
21	4C	503	CL7	C2-C3-C5-C6
21	4C	503	CL7	C4-C3-C5-C6
21	4C	503	CL7	C1A-C2A-CAA-CBA
21	4C	504	CL7	C1A-C2A-CAA-CBA
21	4C	504	CL7	C2B-C3B-CAB-OBB
21	4C	504	CL7	C4B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4C	505	CL7	C14-C13-C15-C16
21	4C	505	CL7	C2B-C3B-CAB-OBB
21	4C	505	CL7	C4B-C3B-CAB-OBB
21	4C	506	CL7	O1A-CGA-O2A-C1
21	4C	506	CL7	CBA-CGA-O2A-C1
21	4C	506	CL7	C1A-C2A-CAA-CBA
21	4C	506	CL7	C3A-C2A-CAA-CBA
21	4C	506	CL7	CHA-CBD-CGD-O2D
21	4C	506	CL7	CHA-CBD-CGD-O1D
21	4C	506	CL7	C2B-C3B-CAB-OBB
21	4C	506	CL7	C4B-C3B-CAB-OBB
21	4C	507	CL7	C2-C3-C5-C6
21	4C	507	CL7	C4-C3-C5-C6
21	4C	507	CL7	C2B-C3B-CAB-OBB
21	4C	507	CL7	C4B-C3B-CAB-OBB
21	4C	508	CL7	O1A-CGA-O2A-C1
21	4C	508	CL7	CBA-CGA-O2A-C1
21	4C	508	CL7	C2B-C3B-CAB-OBB
21	4C	508	CL7	C4B-C3B-CAB-OBB
21	4C	509	CL7	O2A-C1-C2-C3
21	4C	509	CL7	C2-C3-C5-C6
21	4C	509	CL7	C4-C3-C5-C6
21	4C	509	CL7	C14-C13-C15-C16
21	4C	509	CL7	C1A-C2A-CAA-CBA
21	4C	509	CL7	C2B-C3B-CAB-OBB
21	4C	509	CL7	C4B-C3B-CAB-OBB
21	4C	510	CL7	C3A-C2A-CAA-CBA
21	4C	510	CL7	C4B-C3B-CAB-OBB
21	4C	511	CL7	C1A-C2A-CAA-CBA
21	4C	511	CL7	C2B-C3B-CAB-OBB
21	4C	511	CL7	C4B-C3B-CAB-OBB
21	4C	512	CL7	CBD-CGD-O2D-CED
21	4C	513	CL7	CHA-CBD-CGD-O2D
21	4C	513	CL7	CHA-CBD-CGD-O1D
21	4C	513	CL7	CBD-CGD-O2D-CED
21	4C	513	CL7	C2B-C3B-CAB-OBB
21	4C	513	CL7	C4B-C3B-CAB-OBB
21	4C	517	CL7	C2B-C3B-CAB-OBB
21	4C	517	CL7	C4B-C3B-CAB-OBB
21	4D	402	CL7	CHA-CBD-CGD-O2D
21	4D	402	CL7	CHA-CBD-CGD-O1D
21	4D	402	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4D	402	CL7	C4B-C3B-CAB-OBB
21	4D	404	CL7	C2-C3-C5-C6
21	4D	404	CL7	C4-C3-C5-C6
21	4D	404	CL7	C4B-C3B-CAB-OBB
21	4D	405	CL7	C1A-C2A-CAA-CBA
21	4D	405	CL7	C3A-C2A-CAA-CBA
21	4D	405	CL7	CAD-CBD-CGD-O2D
21	4D	405	CL7	CAD-CBD-CGD-O1D
21	4D	405	CL7	C2B-C3B-CAB-OBB
21	4D	405	CL7	C4B-C3B-CAB-OBB
21	42	501	CL7	C2B-C3B-CAB-OBB
21	42	501	CL7	C4B-C3B-CAB-OBB
21	42	502	CL7	C1A-C2A-CAA-CBA
21	42	502	CL7	C3A-C2A-CAA-CBA
21	42	502	CL7	C2B-C3B-CAB-OBB
21	42	502	CL7	C4B-C3B-CAB-OBB
21	42	503	CL7	C1A-C2A-CAA-CBA
21	42	504	CL7	C1A-C2A-CAA-CBA
21	42	504	CL7	CBD-CGD-O2D-CED
21	42	504	CL7	C2B-C3B-CAB-OBB
21	42	504	CL7	C4B-C3B-CAB-OBB
21	42	505	CL7	C4B-C3B-CAB-OBB
21	42	506	CL7	C2B-C3B-CAB-OBB
21	42	506	CL7	C4B-C3B-CAB-OBB
21	42	507	CL7	C2B-C3B-CAB-OBB
21	42	507	CL7	C4B-C3B-CAB-OBB
21	42	508	CL7	C4B-C3B-CAB-OBB
21	42	509	CL7	C11-C12-C13-C15
21	42	509	CL7	C2B-C3B-CAB-OBB
21	42	509	CL7	C4B-C3B-CAB-OBB
21	42	510	CL7	C2-C3-C5-C6
21	42	510	CL7	C4-C3-C5-C6
21	42	511	CL7	C2-C3-C5-C6
21	42	511	CL7	C4-C3-C5-C6
21	42	511	CL7	CBD-CGD-O2D-CED
21	42	511	CL7	C4B-C3B-CAB-OBB
21	42	512	CL7	C4B-C3B-CAB-OBB
21	42	513	CL7	C1A-C2A-CAA-CBA
21	42	513	CL7	CHA-CBD-CGD-O1D
21	42	513	CL7	C2B-C3B-CAB-OBB
21	42	513	CL7	C4B-C3B-CAB-OBB
21	42	514	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	514	CL7	C3A-C2A-CAA-CBA
21	42	514	CL7	CBD-CGD-O2D-CED
21	42	514	CL7	C2B-C3B-CAB-OBB
21	42	514	CL7	C4B-C3B-CAB-OBB
21	42	515	CL7	CHA-CBD-CGD-O2D
21	42	515	CL7	CHA-CBD-CGD-O1D
21	42	515	CL7	CAD-CBD-CGD-O1D
21	42	515	CL7	C2B-C3B-CAB-OBB
21	42	515	CL7	C4B-C3B-CAB-OBB
21	42	516	CL7	O1A-CGA-O2A-C1
21	42	516	CL7	CBA-CGA-O2A-C1
21	42	516	CL7	C3A-C2A-CAA-CBA
21	42	516	CL7	C4B-C3B-CAB-OBB
21	42	517	CL7	C1A-C2A-CAA-CBA
21	42	517	CL7	C3A-C2A-CAA-CBA
21	42	517	CL7	C2B-C3B-CAB-OBB
21	42	517	CL7	C4B-C3B-CAB-OBB
21	42	518	CL7	C1A-C2A-CAA-CBA
21	42	518	CL7	C3A-C2A-CAA-CBA
21	42	518	CL7	C4B-C3B-CAB-OBB
21	41	402	CL7	C1A-C2A-CAA-CBA
21	41	402	CL7	C3A-C2A-CAA-CBA
21	41	403	CL7	C2B-C3B-CAB-OBB
21	41	403	CL7	C4B-C3B-CAB-OBB
21	41	404	CL7	O2A-C1-C2-C3
21	41	404	CL7	C2-C3-C5-C6
21	41	404	CL7	C4-C3-C5-C6
21	41	404	CL7	C2B-C3B-CAB-OBB
21	41	404	CL7	C4B-C3B-CAB-OBB
21	41	406	CL7	C2B-C3B-CAB-OBB
21	41	406	CL7	C4B-C3B-CAB-OBB
21	41	407	CL7	C2B-C3B-CAB-OBB
21	41	407	CL7	C4B-C3B-CAB-OBB
21	41	408	CL7	C1A-C2A-CAA-CBA
21	41	408	CL7	C3A-C2A-CAA-CBA
21	41	408	CL7	C2B-C3B-CAB-OBB
21	41	408	CL7	C4B-C3B-CAB-OBB
21	41	409	CL7	CBD-CGD-O2D-CED
21	41	409	CL7	C2B-C3B-CAB-OBB
21	41	409	CL7	C4B-C3B-CAB-OBB
21	41	410	CL7	O1A-CGA-O2A-C1
21	41	410	CL7	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	41	410	CL7	C1A-C2A-CAA-CBA
21	41	410	CL7	C3A-C2A-CAA-CBA
21	41	410	CL7	C2B-C3B-CAB-OBB
21	41	410	CL7	C4B-C3B-CAB-OBB
21	41	411	CL7	CBD-CGD-O2D-CED
21	41	411	CL7	C4B-C3B-CAB-OBB
21	41	412	CL7	C1A-C2A-CAA-CBA
21	41	412	CL7	C2B-C3B-CAB-OBB
21	41	412	CL7	C4B-C3B-CAB-OBB
21	41	413	CL7	CAD-CBD-CGD-O2D
21	41	413	CL7	CAD-CBD-CGD-O1D
21	41	414	CL7	C2B-C3B-CAB-OBB
21	41	414	CL7	C4B-C3B-CAB-OBB
21	41	415	CL7	CHA-CBD-CGD-O2D
21	41	415	CL7	CHA-CBD-CGD-O1D
21	41	415	CL7	C2B-C3B-CAB-OBB
21	41	415	CL7	C4B-C3B-CAB-OBB
21	41	416	CL7	CBD-CGD-O2D-CED
21	41	416	CL7	C2B-C3B-CAB-OBB
21	41	416	CL7	C4B-C3B-CAB-OBB
21	41	417	CL7	O1A-CGA-O2A-C1
21	41	417	CL7	CBA-CGA-O2A-C1
21	41	417	CL7	C3A-C2A-CAA-CBA
21	41	417	CL7	C2B-C3B-CAB-OBB
21	41	417	CL7	C4B-C3B-CAB-OBB
21	41	418	CL7	CHA-CBD-CGD-O2D
21	41	418	CL7	CHA-CBD-CGD-O1D
21	41	418	CL7	C2B-C3B-CAB-OBB
21	41	418	CL7	C4B-C3B-CAB-OBB
21	41	419	CL7	CBD-CGD-O2D-CED
21	41	419	CL7	C2B-C3B-CAB-OBB
21	41	419	CL7	C4B-C3B-CAB-OBB
21	41	420	CL7	C2B-C3B-CAB-OBB
21	41	420	CL7	C4B-C3B-CAB-OBB
21	43	402	CL7	C1A-C2A-CAA-CBA
21	43	402	CL7	C2B-C3B-CAB-OBB
21	43	402	CL7	C4B-C3B-CAB-OBB
21	43	403	CL7	CBD-CGD-O2D-CED
21	43	403	CL7	C2B-C3B-CAB-OBB
21	43	403	CL7	C4B-C3B-CAB-OBB
21	43	404	CL7	CBD-CGD-O2D-CED
21	43	404	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	404	CL7	C4B-C3B-CAB-OBB
21	43	405	CL7	C1A-C2A-CAA-CBA
21	43	405	CL7	C2B-C3B-CAB-OBB
21	43	405	CL7	C4B-C3B-CAB-OBB
21	43	407	CL7	C1A-C2A-CAA-CBA
21	43	407	CL7	C3A-C2A-CAA-CBA
21	43	407	CL7	CHA-CBD-CGD-O1D
21	43	407	CL7	CAD-CBD-CGD-O2D
21	43	407	CL7	CAD-CBD-CGD-O1D
21	43	407	CL7	C4B-C3B-CAB-OBB
21	43	408	CL7	C2-C3-C5-C6
21	43	408	CL7	C4-C3-C5-C6
21	43	408	CL7	C2B-C3B-CAB-OBB
21	43	408	CL7	C4B-C3B-CAB-OBB
21	43	409	CL7	C2-C3-C5-C6
21	43	409	CL7	C4-C3-C5-C6
21	43	409	CL7	C2B-C3B-CAB-OBB
21	43	409	CL7	C4B-C3B-CAB-OBB
21	43	410	CL7	O1A-CGA-O2A-C1
21	43	410	CL7	CBA-CGA-O2A-C1
21	43	410	CL7	C2B-C3B-CAB-OBB
21	43	410	CL7	C4B-C3B-CAB-OBB
21	43	411	CL7	C1A-C2A-CAA-CBA
21	43	411	CL7	CBD-CGD-O2D-CED
21	43	411	CL7	C2B-C3B-CAB-OBB
21	43	411	CL7	C4B-C3B-CAB-OBB
21	43	412	CL7	O1A-CGA-O2A-C1
21	43	412	CL7	CBA-CGA-O2A-C1
21	43	412	CL7	C2B-C3B-CAB-OBB
21	43	412	CL7	C4B-C3B-CAB-OBB
21	43	414	CL7	C1A-C2A-CAA-CBA
21	43	414	CL7	C2B-C3B-CAB-OBB
21	43	414	CL7	C4B-C3B-CAB-OBB
21	43	417	CL7	O1A-CGA-O2A-C1
21	43	417	CL7	CBA-CGA-O2A-C1
21	43	417	CL7	C3A-C2A-CAA-CBA
21	43	417	CL7	C2B-C3B-CAB-OBB
21	43	417	CL7	C4B-C3B-CAB-OBB
21	43	418	CL7	C1A-C2A-CAA-CBA
21	43	418	CL7	C3A-C2A-CAA-CBA
21	43	418	CL7	C4B-C3B-CAB-OBB
21	43	419	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	419	CL7	C4B-C3B-CAB-OBB
21	44	404	CL7	C3A-C2A-CAA-CBA
21	44	405	CL7	O1A-CGA-O2A-C1
21	44	405	CL7	CBA-CGA-O2A-C1
21	44	405	CL7	C2-C3-C5-C6
21	44	405	CL7	C4-C3-C5-C6
21	44	405	CL7	C4B-C3B-CAB-OBB
21	44	406	CL7	C1A-C2A-CAA-CBA
21	44	406	CL7	C3A-C2A-CAA-CBA
21	44	406	CL7	C4B-C3B-CAB-OBB
21	44	407	CL7	C2B-C3B-CAB-OBB
21	44	407	CL7	C4B-C3B-CAB-OBB
21	44	408	CL7	C4B-C3B-CAB-OBB
21	44	409	CL7	C1A-C2A-CAA-CBA
21	44	409	CL7	C3A-C2A-CAA-CBA
21	44	409	CL7	C2B-C3B-CAB-OBB
21	44	409	CL7	C4B-C3B-CAB-OBB
21	44	410	CL7	C1A-C2A-CAA-CBA
21	44	410	CL7	C2B-C3B-CAB-OBB
21	44	410	CL7	C4B-C3B-CAB-OBB
21	44	411	CL7	C1A-C2A-CAA-CBA
21	44	411	CL7	CBD-CGD-O2D-CED
21	44	411	CL7	C2B-C3B-CAB-OBB
21	44	411	CL7	C4B-C3B-CAB-OBB
21	44	412	CL7	C1A-C2A-CAA-CBA
21	44	414	CL7	C2B-C3B-CAB-OBB
21	44	414	CL7	C4B-C3B-CAB-OBB
21	44	415	CL7	C1A-C2A-CAA-CBA
21	44	415	CL7	C3A-C2A-CAA-CBA
21	44	415	CL7	CAD-CBD-CGD-O2D
21	44	416	CL7	CHA-CBD-CGD-O2D
21	44	416	CL7	CHA-CBD-CGD-O1D
21	44	416	CL7	C2B-C3B-CAB-OBB
21	44	416	CL7	C4B-C3B-CAB-OBB
21	44	417	CL7	C1A-C2A-CAA-CBA
21	44	417	CL7	C2B-C3B-CAB-OBB
21	44	417	CL7	C4B-C3B-CAB-OBB
22	1D	408	PHO	C4-C3-C5-C6
22	2D	408	PHO	C4-C3-C5-C6
22	3D	408	PHO	C4-C3-C5-C6
22	4D	408	PHO	C4-C3-C5-C6
23	1A	404	8CT	C25-C26-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1A	404	8CT	C27-C26-C28-C29
23	1B	617	8CT	C14-C15-C16-C17
23	1B	617	8CT	C14-C15-C16-C39
23	1B	618	8CT	C25-C26-C28-C29
23	1B	618	8CT	C27-C26-C28-C29
23	1B	619	8CT	C10-C11-C12-C13
23	1B	619	8CT	C10-C11-C12-C40
23	1B	626	8CT	C14-C15-C16-C17
23	1B	626	8CT	C14-C15-C16-C39
23	1B	626	8CT	C28-C29-C30-C35
23	1C	514	8CT	C02-C03-C10-C11
23	1C	514	8CT	C10-C11-C12-C13
23	1C	514	8CT	C10-C11-C12-C40
23	1C	514	8CT	C16-C17-C18-C19
23	1C	514	8CT	C27-C26-C28-C29
23	1C	514	8CT	C28-C29-C30-C35
23	1C	515	8CT	C02-C03-C10-C11
23	1C	515	8CT	C10-C11-C12-C13
23	1C	515	8CT	C10-C11-C12-C40
23	1C	515	8CT	C14-C15-C16-C17
23	1C	515	8CT	C14-C15-C16-C39
23	1C	515	8CT	C27-C26-C28-C29
23	1C	518	8CT	C25-C26-C28-C29
23	1C	518	8CT	C27-C26-C28-C29
23	1C	518	8CT	C28-C29-C30-C31
23	1C	518	8CT	C28-C29-C30-C35
23	1D	406	8CT	C10-C11-C12-C13
23	1D	406	8CT	C10-C11-C12-C40
23	1D	406	8CT	C16-C17-C18-C19
23	1D	406	8CT	C25-C26-C28-C29
23	1D	406	8CT	C27-C26-C28-C29
23	1K	101	8CT	C20-C21-C23-C24
23	1K	101	8CT	C22-C21-C23-C24
23	1K	101	8CT	C25-C26-C28-C29
23	1K	101	8CT	C27-C26-C28-C29
23	1K	101	8CT	C28-C29-C30-C35
23	2A	404	8CT	C25-C26-C28-C29
23	2A	404	8CT	C27-C26-C28-C29
23	2B	601	8CT	C14-C15-C16-C17
23	2B	601	8CT	C14-C15-C16-C39
23	2B	601	8CT	C28-C29-C30-C35
23	2B	618	8CT	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2B	618	8CT	C14-C15-C16-C39
23	2B	619	8CT	C25-C26-C28-C29
23	2B	619	8CT	C27-C26-C28-C29
23	2B	620	8CT	C10-C11-C12-C13
23	2B	620	8CT	C10-C11-C12-C40
23	2C	514	8CT	C02-C03-C10-C11
23	2C	514	8CT	C10-C11-C12-C13
23	2C	514	8CT	C10-C11-C12-C40
23	2C	514	8CT	C16-C17-C18-C19
23	2C	514	8CT	C27-C26-C28-C29
23	2C	514	8CT	C28-C29-C30-C35
23	2C	515	8CT	C02-C03-C10-C11
23	2C	515	8CT	C10-C11-C12-C13
23	2C	515	8CT	C10-C11-C12-C40
23	2C	515	8CT	C14-C15-C16-C17
23	2C	515	8CT	C14-C15-C16-C39
23	2C	515	8CT	C27-C26-C28-C29
23	2C	518	8CT	C25-C26-C28-C29
23	2C	518	8CT	C27-C26-C28-C29
23	2C	518	8CT	C28-C29-C30-C31
23	2C	518	8CT	C28-C29-C30-C35
23	2D	406	8CT	C10-C11-C12-C13
23	2D	406	8CT	C10-C11-C12-C40
23	2D	406	8CT	C16-C17-C18-C19
23	2D	406	8CT	C25-C26-C28-C29
23	2D	406	8CT	C27-C26-C28-C29
23	2K	101	8CT	C20-C21-C23-C24
23	2K	101	8CT	C22-C21-C23-C24
23	2K	101	8CT	C25-C26-C28-C29
23	2K	101	8CT	C27-C26-C28-C29
23	2K	101	8CT	C28-C29-C30-C35
23	3A	404	8CT	C25-C26-C28-C29
23	3A	404	8CT	C27-C26-C28-C29
23	3B	617	8CT	C14-C15-C16-C17
23	3B	617	8CT	C14-C15-C16-C39
23	3B	618	8CT	C25-C26-C28-C29
23	3B	618	8CT	C27-C26-C28-C29
23	3B	619	8CT	C10-C11-C12-C13
23	3B	619	8CT	C10-C11-C12-C40
23	3B	626	8CT	C14-C15-C16-C17
23	3B	626	8CT	C14-C15-C16-C39
23	3B	626	8CT	C28-C29-C30-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	3C	514	8CT	C02-C03-C10-C11
23	3C	514	8CT	C10-C11-C12-C13
23	3C	514	8CT	C10-C11-C12-C40
23	3C	514	8CT	C16-C17-C18-C19
23	3C	514	8CT	C27-C26-C28-C29
23	3C	514	8CT	C28-C29-C30-C35
23	3C	515	8CT	C02-C03-C10-C11
23	3C	515	8CT	C10-C11-C12-C13
23	3C	515	8CT	C10-C11-C12-C40
23	3C	515	8CT	C14-C15-C16-C17
23	3C	515	8CT	C14-C15-C16-C39
23	3C	515	8CT	C27-C26-C28-C29
23	3C	518	8CT	C25-C26-C28-C29
23	3C	518	8CT	C27-C26-C28-C29
23	3C	518	8CT	C28-C29-C30-C31
23	3C	518	8CT	C28-C29-C30-C35
23	3D	406	8CT	C10-C11-C12-C13
23	3D	406	8CT	C10-C11-C12-C40
23	3D	406	8CT	C16-C17-C18-C19
23	3D	406	8CT	C25-C26-C28-C29
23	3D	406	8CT	C27-C26-C28-C29
23	3K	101	8CT	C20-C21-C23-C24
23	3K	101	8CT	C22-C21-C23-C24
23	3K	101	8CT	C25-C26-C28-C29
23	3K	101	8CT	C27-C26-C28-C29
23	3K	101	8CT	C28-C29-C30-C35
23	4A	404	8CT	C25-C26-C28-C29
23	4A	404	8CT	C27-C26-C28-C29
23	4B	601	8CT	C14-C15-C16-C17
23	4B	601	8CT	C14-C15-C16-C39
23	4B	601	8CT	C28-C29-C30-C35
23	4B	618	8CT	C14-C15-C16-C17
23	4B	618	8CT	C14-C15-C16-C39
23	4B	619	8CT	C25-C26-C28-C29
23	4B	619	8CT	C27-C26-C28-C29
23	4B	620	8CT	C10-C11-C12-C13
23	4B	620	8CT	C10-C11-C12-C40
23	4C	514	8CT	C02-C03-C10-C11
23	4C	514	8CT	C10-C11-C12-C13
23	4C	514	8CT	C10-C11-C12-C40
23	4C	514	8CT	C16-C17-C18-C19
23	4C	514	8CT	C27-C26-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4C	514	8CT	C28-C29-C30-C35
23	4C	515	8CT	C02-C03-C10-C11
23	4C	515	8CT	C10-C11-C12-C13
23	4C	515	8CT	C10-C11-C12-C40
23	4C	515	8CT	C14-C15-C16-C17
23	4C	515	8CT	C14-C15-C16-C39
23	4C	515	8CT	C27-C26-C28-C29
23	4C	518	8CT	C25-C26-C28-C29
23	4C	518	8CT	C27-C26-C28-C29
23	4C	518	8CT	C28-C29-C30-C31
23	4C	518	8CT	C28-C29-C30-C35
23	4D	406	8CT	C10-C11-C12-C13
23	4D	406	8CT	C10-C11-C12-C40
23	4D	406	8CT	C16-C17-C18-C19
23	4D	406	8CT	C25-C26-C28-C29
23	4D	406	8CT	C27-C26-C28-C29
23	4K	101	8CT	C20-C21-C23-C24
23	4K	101	8CT	C22-C21-C23-C24
23	4K	101	8CT	C25-C26-C28-C29
23	4K	101	8CT	C27-C26-C28-C29
23	4K	101	8CT	C28-C29-C30-C35
24	1A	405	LMG	O6-C1-O1-C7
24	1B	621	LMG	C29-C28-O8-C9
24	2A	405	LMG	O6-C1-O1-C7
24	2B	622	LMG	C29-C28-O8-C9
24	3A	405	LMG	O6-C1-O1-C7
24	3B	621	LMG	C29-C28-O8-C9
24	4A	405	LMG	O6-C1-O1-C7
24	4B	622	LMG	C29-C28-O8-C9
25	12	521	SQD	O49-C7-O47-C45
25	12	521	SQD	C8-C7-O47-C45
25	12	521	SQD	O5-C5-C6-S
25	13	521	SQD	O49-C7-O47-C45
25	13	521	SQD	C8-C7-O47-C45
25	13	523	SQD	O5-C5-C6-S
25	22	521	SQD	O49-C7-O47-C45
25	22	521	SQD	C8-C7-O47-C45
25	22	521	SQD	O5-C5-C6-S
25	23	422	SQD	O49-C7-O47-C45
25	23	422	SQD	C8-C7-O47-C45
25	23	424	SQD	O5-C5-C6-S
25	32	521	SQD	O49-C7-O47-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	32	521	SQD	C8-C7-O47-C45
25	32	521	SQD	O5-C5-C6-S
25	33	521	SQD	O49-C7-O47-C45
25	33	521	SQD	C8-C7-O47-C45
25	33	523	SQD	O5-C5-C6-S
25	42	521	SQD	O49-C7-O47-C45
25	42	521	SQD	C8-C7-O47-C45
25	42	521	SQD	O5-C5-C6-S
25	43	422	SQD	O49-C7-O47-C45
25	43	422	SQD	C8-C7-O47-C45
25	43	424	SQD	O5-C5-C6-S
26	1A	408	LHG	C2-C3-O3-P
26	1D	409	LHG	C3-O3-P-O6
26	1D	409	LHG	C4-O6-P-O3
26	14	401	LHG	C2-C3-O3-P
26	14	401	LHG	C4-O6-P-O3
26	2A	408	LHG	C2-C3-O3-P
26	2D	409	LHG	C3-O3-P-O6
26	2D	409	LHG	C4-O6-P-O3
26	24	401	LHG	C2-C3-O3-P
26	24	401	LHG	C4-O6-P-O3
26	3A	408	LHG	C2-C3-O3-P
26	3D	409	LHG	C3-O3-P-O6
26	3D	409	LHG	C4-O6-P-O3
26	34	401	LHG	C2-C3-O3-P
26	34	401	LHG	C4-O6-P-O3
26	4A	408	LHG	C2-C3-O3-P
26	4D	409	LHG	C3-O3-P-O6
26	4D	409	LHG	C4-O6-P-O3
26	44	401	LHG	C2-C3-O3-P
26	44	401	LHG	C4-O6-P-O3
30	1D	407	PL9	C39-C41-C42-C43
30	2D	407	PL9	C39-C41-C42-C43
30	3D	407	PL9	C39-C41-C42-C43
30	4D	407	PL9	C39-C41-C42-C43
31	1F	101	HEM	C2B-C3B-CAB-CBB
31	1F	101	HEM	C2C-C3C-CAC-CBC
31	2F	101	HEM	C2B-C3B-CAB-CBB
31	2F	101	HEM	C2C-C3C-CAC-CBC
31	3F	101	HEM	C2B-C3B-CAB-CBB
31	3F	101	HEM	C2C-C3C-CAC-CBC
31	4F	101	HEM	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	4F	101	HEM	C2C-C3C-CAC-CBC
32	12	519	ZEX	C1-C6-C7-C8
32	12	519	ZEX	C25-C26-C27-C28
32	12	519	ZEX	C7-C8-C9-C19
32	12	519	ZEX	C7-C8-C9-C10
32	12	519	ZEX	C11-C12-C13-C20
32	12	519	ZEX	C11-C12-C13-C14
32	12	519	ZEX	C27-C28-C29-C30
32	12	519	ZEX	C27-C28-C29-C39
32	12	520	ZEX	C25-C26-C27-C28
32	12	522	ZEX	C25-C26-C27-C28
32	12	522	ZEX	C31-C32-C33-C40
32	12	522	ZEX	C27-C28-C29-C30
32	12	522	ZEX	C27-C28-C29-C39
32	12	524	ZEX	C25-C26-C27-C28
32	12	524	ZEX	C31-C32-C33-C34
32	12	524	ZEX	C31-C32-C33-C40
32	12	524	ZEX	C27-C28-C29-C30
32	11	421	ZEX	C25-C26-C27-C28
32	11	421	ZEX	C7-C8-C9-C19
32	11	421	ZEX	C7-C8-C9-C10
32	11	421	ZEX	C11-C12-C13-C20
32	11	421	ZEX	C11-C12-C13-C14
32	11	421	ZEX	C31-C32-C33-C34
32	11	421	ZEX	C31-C32-C33-C40
32	11	421	ZEX	C27-C28-C29-C30
32	11	421	ZEX	C27-C28-C29-C39
32	11	422	ZEX	C25-C26-C27-C28
32	11	422	ZEX	C9-C10-C11-C12
32	13	519	ZEX	C25-C26-C27-C28
32	13	519	ZEX	C31-C32-C33-C34
32	13	519	ZEX	C31-C32-C33-C40
32	13	520	ZEX	C25-C26-C27-C28
32	13	522	ZEX	C1-C6-C7-C8
32	13	522	ZEX	C25-C26-C27-C28
32	13	525	ZEX	C31-C32-C33-C34
32	13	525	ZEX	C31-C32-C33-C40
32	13	525	ZEX	C27-C28-C29-C30
32	13	525	ZEX	C27-C28-C29-C39
32	14	403	ZEX	C5-C6-C7-C8
32	14	403	ZEX	C7-C8-C9-C19
32	14	403	ZEX	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	14	418	ZEX	C7-C8-C9-C19
32	14	418	ZEX	C7-C8-C9-C10
32	14	419	ZEX	C13-C14-C15-C35
32	14	419	ZEX	C27-C28-C29-C30
32	14	419	ZEX	C27-C28-C29-C39
32	14	420	ZEX	C27-C28-C29-C30
32	14	420	ZEX	C27-C28-C29-C39
32	22	519	ZEX	C1-C6-C7-C8
32	22	519	ZEX	C25-C26-C27-C28
32	22	519	ZEX	C7-C8-C9-C19
32	22	519	ZEX	C7-C8-C9-C10
32	22	519	ZEX	C11-C12-C13-C20
32	22	519	ZEX	C11-C12-C13-C14
32	22	519	ZEX	C27-C28-C29-C30
32	22	519	ZEX	C27-C28-C29-C39
32	22	520	ZEX	C25-C26-C27-C28
32	22	522	ZEX	C25-C26-C27-C28
32	22	522	ZEX	C31-C32-C33-C40
32	22	522	ZEX	C27-C28-C29-C30
32	22	522	ZEX	C27-C28-C29-C39
32	22	524	ZEX	C25-C26-C27-C28
32	22	524	ZEX	C31-C32-C33-C34
32	22	524	ZEX	C31-C32-C33-C40
32	22	524	ZEX	C27-C28-C29-C30
32	21	421	ZEX	C25-C26-C27-C28
32	21	421	ZEX	C7-C8-C9-C19
32	21	421	ZEX	C7-C8-C9-C10
32	21	421	ZEX	C11-C12-C13-C20
32	21	421	ZEX	C11-C12-C13-C14
32	21	421	ZEX	C31-C32-C33-C34
32	21	421	ZEX	C31-C32-C33-C40
32	21	421	ZEX	C27-C28-C29-C30
32	21	421	ZEX	C27-C28-C29-C39
32	21	422	ZEX	C25-C26-C27-C28
32	21	422	ZEX	C9-C10-C11-C12
32	23	401	ZEX	C31-C32-C33-C34
32	23	401	ZEX	C31-C32-C33-C40
32	23	401	ZEX	C27-C28-C29-C30
32	23	401	ZEX	C27-C28-C29-C39
32	23	420	ZEX	C25-C26-C27-C28
32	23	420	ZEX	C31-C32-C33-C34
32	23	420	ZEX	C31-C32-C33-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	23	421	ZEX	C25-C26-C27-C28
32	23	423	ZEX	C1-C6-C7-C8
32	23	423	ZEX	C25-C26-C27-C28
32	24	403	ZEX	C5-C6-C7-C8
32	24	403	ZEX	C7-C8-C9-C19
32	24	403	ZEX	C7-C8-C9-C10
32	24	418	ZEX	C7-C8-C9-C19
32	24	418	ZEX	C7-C8-C9-C10
32	24	419	ZEX	C13-C14-C15-C35
32	24	419	ZEX	C27-C28-C29-C30
32	24	419	ZEX	C27-C28-C29-C39
32	24	420	ZEX	C27-C28-C29-C30
32	24	420	ZEX	C27-C28-C29-C39
32	32	519	ZEX	C1-C6-C7-C8
32	32	519	ZEX	C25-C26-C27-C28
32	32	519	ZEX	C7-C8-C9-C19
32	32	519	ZEX	C7-C8-C9-C10
32	32	519	ZEX	C11-C12-C13-C20
32	32	519	ZEX	C11-C12-C13-C14
32	32	519	ZEX	C27-C28-C29-C30
32	32	519	ZEX	C27-C28-C29-C39
32	32	520	ZEX	C25-C26-C27-C28
32	32	522	ZEX	C25-C26-C27-C28
32	32	522	ZEX	C31-C32-C33-C40
32	32	522	ZEX	C27-C28-C29-C30
32	32	522	ZEX	C27-C28-C29-C39
32	32	524	ZEX	C25-C26-C27-C28
32	32	524	ZEX	C31-C32-C33-C34
32	32	524	ZEX	C31-C32-C33-C40
32	32	524	ZEX	C27-C28-C29-C30
32	31	421	ZEX	C25-C26-C27-C28
32	31	421	ZEX	C7-C8-C9-C19
32	31	421	ZEX	C7-C8-C9-C10
32	31	421	ZEX	C11-C12-C13-C20
32	31	421	ZEX	C11-C12-C13-C14
32	31	421	ZEX	C31-C32-C33-C34
32	31	421	ZEX	C31-C32-C33-C40
32	31	421	ZEX	C27-C28-C29-C30
32	31	421	ZEX	C27-C28-C29-C39
32	31	422	ZEX	C25-C26-C27-C28
32	31	422	ZEX	C9-C10-C11-C12
32	33	519	ZEX	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	33	519	ZEX	C31-C32-C33-C34
32	33	519	ZEX	C31-C32-C33-C40
32	33	520	ZEX	C25-C26-C27-C28
32	33	522	ZEX	C1-C6-C7-C8
32	33	522	ZEX	C25-C26-C27-C28
32	33	525	ZEX	C31-C32-C33-C34
32	33	525	ZEX	C31-C32-C33-C40
32	33	525	ZEX	C27-C28-C29-C30
32	33	525	ZEX	C27-C28-C29-C39
32	34	403	ZEX	C5-C6-C7-C8
32	34	403	ZEX	C7-C8-C9-C19
32	34	403	ZEX	C7-C8-C9-C10
32	34	418	ZEX	C7-C8-C9-C19
32	34	418	ZEX	C7-C8-C9-C10
32	34	419	ZEX	C13-C14-C15-C35
32	34	419	ZEX	C27-C28-C29-C30
32	34	419	ZEX	C27-C28-C29-C39
32	34	420	ZEX	C27-C28-C29-C30
32	34	420	ZEX	C27-C28-C29-C39
32	42	519	ZEX	C1-C6-C7-C8
32	42	519	ZEX	C25-C26-C27-C28
32	42	519	ZEX	C7-C8-C9-C19
32	42	519	ZEX	C7-C8-C9-C10
32	42	519	ZEX	C11-C12-C13-C20
32	42	519	ZEX	C11-C12-C13-C14
32	42	519	ZEX	C27-C28-C29-C30
32	42	519	ZEX	C27-C28-C29-C39
32	42	520	ZEX	C25-C26-C27-C28
32	42	522	ZEX	C25-C26-C27-C28
32	42	522	ZEX	C31-C32-C33-C40
32	42	522	ZEX	C27-C28-C29-C30
32	42	522	ZEX	C27-C28-C29-C39
32	42	524	ZEX	C25-C26-C27-C28
32	42	524	ZEX	C31-C32-C33-C34
32	42	524	ZEX	C31-C32-C33-C40
32	42	524	ZEX	C27-C28-C29-C30
32	41	421	ZEX	C25-C26-C27-C28
32	41	421	ZEX	C7-C8-C9-C19
32	41	421	ZEX	C7-C8-C9-C10
32	41	421	ZEX	C11-C12-C13-C20
32	41	421	ZEX	C11-C12-C13-C14
32	41	421	ZEX	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	41	421	ZEX	C31-C32-C33-C40
32	41	421	ZEX	C27-C28-C29-C30
32	41	421	ZEX	C27-C28-C29-C39
32	41	422	ZEX	C25-C26-C27-C28
32	41	422	ZEX	C9-C10-C11-C12
32	43	401	ZEX	C31-C32-C33-C34
32	43	401	ZEX	C31-C32-C33-C40
32	43	401	ZEX	C27-C28-C29-C30
32	43	401	ZEX	C27-C28-C29-C39
32	43	420	ZEX	C25-C26-C27-C28
32	43	420	ZEX	C31-C32-C33-C34
32	43	420	ZEX	C31-C32-C33-C40
32	43	421	ZEX	C25-C26-C27-C28
32	43	423	ZEX	C1-C6-C7-C8
32	43	423	ZEX	C25-C26-C27-C28
32	44	403	ZEX	C5-C6-C7-C8
32	44	403	ZEX	C7-C8-C9-C19
32	44	403	ZEX	C7-C8-C9-C10
32	44	418	ZEX	C7-C8-C9-C19
32	44	418	ZEX	C7-C8-C9-C10
32	44	419	ZEX	C13-C14-C15-C35
32	44	419	ZEX	C27-C28-C29-C30
32	44	419	ZEX	C27-C28-C29-C39
32	44	420	ZEX	C27-C28-C29-C30
32	44	420	ZEX	C27-C28-C29-C39
21	1A	401	CL7	O1D-CGD-O2D-CED
21	1B	601	CL7	O1D-CGD-O2D-CED
21	1B	607	CL7	O1D-CGD-O2D-CED
21	12	502	CL7	O1D-CGD-O2D-CED
21	12	514	CL7	O1D-CGD-O2D-CED
21	13	503	CL7	O1D-CGD-O2D-CED
21	2A	401	CL7	O1D-CGD-O2D-CED
21	2B	602	CL7	O1D-CGD-O2D-CED
21	2B	608	CL7	O1D-CGD-O2D-CED
21	22	502	CL7	O1D-CGD-O2D-CED
21	22	514	CL7	O1D-CGD-O2D-CED
21	23	404	CL7	O1D-CGD-O2D-CED
21	3A	401	CL7	O1D-CGD-O2D-CED
21	3B	601	CL7	O1D-CGD-O2D-CED
21	3B	607	CL7	O1D-CGD-O2D-CED
21	32	502	CL7	O1D-CGD-O2D-CED
21	32	514	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	33	503	CL7	O1D-CGD-O2D-CED
21	4A	401	CL7	O1D-CGD-O2D-CED
21	4B	602	CL7	O1D-CGD-O2D-CED
21	4B	608	CL7	O1D-CGD-O2D-CED
21	42	502	CL7	O1D-CGD-O2D-CED
21	42	514	CL7	O1D-CGD-O2D-CED
21	43	404	CL7	O1D-CGD-O2D-CED
21	1A	403	CL7	C4C-C3C-CAC-CBC
21	2A	403	CL7	C4C-C3C-CAC-CBC
21	3A	403	CL7	C4C-C3C-CAC-CBC
21	4A	403	CL7	C4C-C3C-CAC-CBC
21	1C	502	CL7	O1D-CGD-O2D-CED
21	12	511	CL7	O1D-CGD-O2D-CED
21	11	409	CL7	O1D-CGD-O2D-CED
21	11	416	CL7	O1D-CGD-O2D-CED
21	11	419	CL7	O1D-CGD-O2D-CED
21	13	502	CL7	O1D-CGD-O2D-CED
21	14	417	CL7	O1D-CGD-O2D-CED
21	2C	502	CL7	O1D-CGD-O2D-CED
21	22	511	CL7	O1D-CGD-O2D-CED
21	21	409	CL7	O1D-CGD-O2D-CED
21	21	416	CL7	O1D-CGD-O2D-CED
21	21	419	CL7	O1D-CGD-O2D-CED
21	23	403	CL7	O1D-CGD-O2D-CED
21	24	417	CL7	O1D-CGD-O2D-CED
21	3C	502	CL7	O1D-CGD-O2D-CED
21	32	511	CL7	O1D-CGD-O2D-CED
21	31	409	CL7	O1D-CGD-O2D-CED
21	31	416	CL7	O1D-CGD-O2D-CED
21	31	419	CL7	O1D-CGD-O2D-CED
21	33	502	CL7	O1D-CGD-O2D-CED
21	34	417	CL7	O1D-CGD-O2D-CED
21	4C	502	CL7	O1D-CGD-O2D-CED
21	42	511	CL7	O1D-CGD-O2D-CED
21	41	409	CL7	O1D-CGD-O2D-CED
21	41	416	CL7	O1D-CGD-O2D-CED
21	41	419	CL7	O1D-CGD-O2D-CED
21	43	403	CL7	O1D-CGD-O2D-CED
21	44	417	CL7	O1D-CGD-O2D-CED
21	1A	401	CL7	CBD-CGD-O2D-CED
21	1A	403	CL7	CBD-CGD-O2D-CED
21	1B	601	CL7	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	605	CL7	CBD-CGD-O2D-CED
21	1C	517	CL7	CBD-CGD-O2D-CED
21	12	502	CL7	CBD-CGD-O2D-CED
21	11	405	CL7	CBD-CGD-O2D-CED
21	11	407	CL7	CBD-CGD-O2D-CED
21	11	420	CL7	CBD-CGD-O2D-CED
21	13	506	CL7	CBD-CGD-O2D-CED
21	14	417	CL7	CBD-CGD-O2D-CED
21	2A	401	CL7	CBD-CGD-O2D-CED
21	2A	403	CL7	CBD-CGD-O2D-CED
21	2B	602	CL7	CBD-CGD-O2D-CED
21	2B	606	CL7	CBD-CGD-O2D-CED
21	2C	517	CL7	CBD-CGD-O2D-CED
21	22	502	CL7	CBD-CGD-O2D-CED
21	21	405	CL7	CBD-CGD-O2D-CED
21	21	407	CL7	CBD-CGD-O2D-CED
21	21	420	CL7	CBD-CGD-O2D-CED
21	23	407	CL7	CBD-CGD-O2D-CED
21	24	417	CL7	CBD-CGD-O2D-CED
21	3A	401	CL7	CBD-CGD-O2D-CED
21	3A	403	CL7	CBD-CGD-O2D-CED
21	3B	601	CL7	CBD-CGD-O2D-CED
21	3B	605	CL7	CBD-CGD-O2D-CED
21	3C	517	CL7	CBD-CGD-O2D-CED
21	32	502	CL7	CBD-CGD-O2D-CED
21	31	405	CL7	CBD-CGD-O2D-CED
21	31	407	CL7	CBD-CGD-O2D-CED
21	31	420	CL7	CBD-CGD-O2D-CED
21	33	506	CL7	CBD-CGD-O2D-CED
21	34	417	CL7	CBD-CGD-O2D-CED
21	4A	401	CL7	CBD-CGD-O2D-CED
21	4A	403	CL7	CBD-CGD-O2D-CED
21	4B	602	CL7	CBD-CGD-O2D-CED
21	4B	606	CL7	CBD-CGD-O2D-CED
21	4C	517	CL7	CBD-CGD-O2D-CED
21	42	502	CL7	CBD-CGD-O2D-CED
21	41	405	CL7	CBD-CGD-O2D-CED
21	41	407	CL7	CBD-CGD-O2D-CED
21	41	420	CL7	CBD-CGD-O2D-CED
21	43	407	CL7	CBD-CGD-O2D-CED
21	44	417	CL7	CBD-CGD-O2D-CED
24	1B	621	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2B	622	LMG	O10-C28-O8-C9
24	3B	621	LMG	O10-C28-O8-C9
24	4B	622	LMG	O10-C28-O8-C9
21	1C	513	CL7	O1D-CGD-O2D-CED
21	11	407	CL7	O1D-CGD-O2D-CED
21	13	510	CL7	O1D-CGD-O2D-CED
21	2C	513	CL7	O1D-CGD-O2D-CED
21	21	407	CL7	O1D-CGD-O2D-CED
21	23	411	CL7	O1D-CGD-O2D-CED
21	3C	513	CL7	O1D-CGD-O2D-CED
21	31	407	CL7	O1D-CGD-O2D-CED
21	33	510	CL7	O1D-CGD-O2D-CED
21	4C	513	CL7	O1D-CGD-O2D-CED
21	41	407	CL7	O1D-CGD-O2D-CED
21	43	411	CL7	O1D-CGD-O2D-CED
21	11	414	CL7	C4C-C3C-CAC-CBC
21	14	415	CL7	C4C-C3C-CAC-CBC
21	14	416	CL7	C4C-C3C-CAC-CBC
21	21	414	CL7	C4C-C3C-CAC-CBC
21	24	415	CL7	C4C-C3C-CAC-CBC
21	24	416	CL7	C4C-C3C-CAC-CBC
21	31	414	CL7	C4C-C3C-CAC-CBC
21	34	415	CL7	C4C-C3C-CAC-CBC
21	34	416	CL7	C4C-C3C-CAC-CBC
21	41	414	CL7	C4C-C3C-CAC-CBC
21	44	415	CL7	C4C-C3C-CAC-CBC
21	44	416	CL7	C4C-C3C-CAC-CBC
21	1B	622	CL7	O1D-CGD-O2D-CED
21	14	411	CL7	O1D-CGD-O2D-CED
21	2B	623	CL7	O1D-CGD-O2D-CED
21	24	411	CL7	O1D-CGD-O2D-CED
21	3B	622	CL7	O1D-CGD-O2D-CED
21	34	411	CL7	O1D-CGD-O2D-CED
21	4B	623	CL7	O1D-CGD-O2D-CED
21	44	411	CL7	O1D-CGD-O2D-CED
21	1C	503	CL7	CBD-CGD-O2D-CED
21	1C	509	CL7	CBD-CGD-O2D-CED
21	1C	511	CL7	CBD-CGD-O2D-CED
21	12	510	CL7	CBD-CGD-O2D-CED
21	12	517	CL7	CBD-CGD-O2D-CED
21	11	403	CL7	CBD-CGD-O2D-CED
21	11	410	CL7	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	11	412	CL7	CBD-CGD-O2D-CED
21	11	418	CL7	CBD-CGD-O2D-CED
21	13	508	CL7	CBD-CGD-O2D-CED
21	13	509	CL7	CBD-CGD-O2D-CED
21	13	516	CL7	CBD-CGD-O2D-CED
21	13	518	CL7	CBD-CGD-O2D-CED
21	14	409	CL7	CBD-CGD-O2D-CED
21	14	410	CL7	CBD-CGD-O2D-CED
21	2C	503	CL7	CBD-CGD-O2D-CED
21	2C	509	CL7	CBD-CGD-O2D-CED
21	2C	511	CL7	CBD-CGD-O2D-CED
21	22	510	CL7	CBD-CGD-O2D-CED
21	22	517	CL7	CBD-CGD-O2D-CED
21	21	403	CL7	CBD-CGD-O2D-CED
21	21	410	CL7	CBD-CGD-O2D-CED
21	21	412	CL7	CBD-CGD-O2D-CED
21	21	418	CL7	CBD-CGD-O2D-CED
21	23	409	CL7	CBD-CGD-O2D-CED
21	23	410	CL7	CBD-CGD-O2D-CED
21	23	417	CL7	CBD-CGD-O2D-CED
21	23	419	CL7	CBD-CGD-O2D-CED
21	24	409	CL7	CBD-CGD-O2D-CED
21	24	410	CL7	CBD-CGD-O2D-CED
21	3C	503	CL7	CBD-CGD-O2D-CED
21	3C	509	CL7	CBD-CGD-O2D-CED
21	3C	511	CL7	CBD-CGD-O2D-CED
21	32	510	CL7	CBD-CGD-O2D-CED
21	32	517	CL7	CBD-CGD-O2D-CED
21	31	403	CL7	CBD-CGD-O2D-CED
21	31	410	CL7	CBD-CGD-O2D-CED
21	31	412	CL7	CBD-CGD-O2D-CED
21	31	418	CL7	CBD-CGD-O2D-CED
21	33	508	CL7	CBD-CGD-O2D-CED
21	33	509	CL7	CBD-CGD-O2D-CED
21	33	516	CL7	CBD-CGD-O2D-CED
21	33	518	CL7	CBD-CGD-O2D-CED
21	34	409	CL7	CBD-CGD-O2D-CED
21	34	410	CL7	CBD-CGD-O2D-CED
21	4C	503	CL7	CBD-CGD-O2D-CED
21	4C	509	CL7	CBD-CGD-O2D-CED
21	4C	511	CL7	CBD-CGD-O2D-CED
21	42	510	CL7	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	517	CL7	CBD-CGD-O2D-CED
21	41	403	CL7	CBD-CGD-O2D-CED
21	41	410	CL7	CBD-CGD-O2D-CED
21	41	412	CL7	CBD-CGD-O2D-CED
21	41	418	CL7	CBD-CGD-O2D-CED
21	43	409	CL7	CBD-CGD-O2D-CED
21	43	410	CL7	CBD-CGD-O2D-CED
21	43	417	CL7	CBD-CGD-O2D-CED
21	43	419	CL7	CBD-CGD-O2D-CED
21	44	409	CL7	CBD-CGD-O2D-CED
21	44	410	CL7	CBD-CGD-O2D-CED
21	1C	512	CL7	O1D-CGD-O2D-CED
21	12	504	CL7	O1D-CGD-O2D-CED
21	2C	512	CL7	O1D-CGD-O2D-CED
21	22	504	CL7	O1D-CGD-O2D-CED
21	3C	512	CL7	O1D-CGD-O2D-CED
21	32	504	CL7	O1D-CGD-O2D-CED
21	4C	512	CL7	O1D-CGD-O2D-CED
21	42	504	CL7	O1D-CGD-O2D-CED
21	11	411	CL7	O1D-CGD-O2D-CED
21	21	411	CL7	O1D-CGD-O2D-CED
21	31	411	CL7	O1D-CGD-O2D-CED
21	41	411	CL7	O1D-CGD-O2D-CED
21	1B	611	CL7	CBD-CGD-O2D-CED
21	1C	504	CL7	CBD-CGD-O2D-CED
21	12	509	CL7	CBD-CGD-O2D-CED
21	2B	612	CL7	CBD-CGD-O2D-CED
21	2C	504	CL7	CBD-CGD-O2D-CED
21	22	509	CL7	CBD-CGD-O2D-CED
21	3B	611	CL7	CBD-CGD-O2D-CED
21	3C	504	CL7	CBD-CGD-O2D-CED
21	32	509	CL7	CBD-CGD-O2D-CED
21	4B	612	CL7	CBD-CGD-O2D-CED
21	4C	504	CL7	CBD-CGD-O2D-CED
21	42	509	CL7	CBD-CGD-O2D-CED
21	11	404	CL7	C10-C11-C12-C13
21	21	404	CL7	C10-C11-C12-C13
21	31	404	CL7	C10-C11-C12-C13
21	41	404	CL7	C10-C11-C12-C13
21	1B	602	CL7	C3-C5-C6-C7
21	1B	605	CL7	C3-C5-C6-C7
21	1B	609	CL7	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	613	CL7	C3-C5-C6-C7
21	1B	614	CL7	C3-C5-C6-C7
21	1C	501	CL7	C3-C5-C6-C7
21	1C	507	CL7	C3-C5-C6-C7
21	1C	508	CL7	C3-C5-C6-C7
21	1C	509	CL7	C3-C5-C6-C7
21	12	506	CL7	C3-C5-C6-C7
21	12	507	CL7	C3-C5-C6-C7
21	12	516	CL7	C3-C5-C6-C7
21	11	408	CL7	C3-C5-C6-C7
21	13	501	CL7	C3-C5-C6-C7
21	13	504	CL7	C3-C5-C6-C7
21	13	505	CL7	C3-C5-C6-C7
21	13	508	CL7	C3-C5-C6-C7
21	14	404	CL7	C3-C5-C6-C7
21	14	405	CL7	C3-C5-C6-C7
21	14	413	CL7	C3-C5-C6-C7
21	2B	603	CL7	C3-C5-C6-C7
21	2B	606	CL7	C3-C5-C6-C7
21	2B	610	CL7	C3-C5-C6-C7
21	2B	614	CL7	C3-C5-C6-C7
21	2B	615	CL7	C3-C5-C6-C7
21	2C	501	CL7	C3-C5-C6-C7
21	2C	507	CL7	C3-C5-C6-C7
21	2C	508	CL7	C3-C5-C6-C7
21	2C	509	CL7	C3-C5-C6-C7
21	22	506	CL7	C3-C5-C6-C7
21	22	507	CL7	C3-C5-C6-C7
21	22	516	CL7	C3-C5-C6-C7
21	21	408	CL7	C3-C5-C6-C7
21	23	402	CL7	C3-C5-C6-C7
21	23	405	CL7	C3-C5-C6-C7
21	23	406	CL7	C3-C5-C6-C7
21	23	409	CL7	C3-C5-C6-C7
21	24	404	CL7	C3-C5-C6-C7
21	24	405	CL7	C3-C5-C6-C7
21	24	413	CL7	C3-C5-C6-C7
21	3B	602	CL7	C3-C5-C6-C7
21	3B	605	CL7	C3-C5-C6-C7
21	3B	609	CL7	C3-C5-C6-C7
21	3B	613	CL7	C3-C5-C6-C7
21	3B	614	CL7	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3C	501	CL7	C3-C5-C6-C7
21	3C	507	CL7	C3-C5-C6-C7
21	3C	508	CL7	C3-C5-C6-C7
21	3C	509	CL7	C3-C5-C6-C7
21	32	506	CL7	C3-C5-C6-C7
21	32	507	CL7	C3-C5-C6-C7
21	32	516	CL7	C3-C5-C6-C7
21	31	408	CL7	C3-C5-C6-C7
21	33	501	CL7	C3-C5-C6-C7
21	33	504	CL7	C3-C5-C6-C7
21	33	505	CL7	C3-C5-C6-C7
21	33	508	CL7	C3-C5-C6-C7
21	34	404	CL7	C3-C5-C6-C7
21	34	405	CL7	C3-C5-C6-C7
21	34	413	CL7	C3-C5-C6-C7
21	4B	603	CL7	C3-C5-C6-C7
21	4B	606	CL7	C3-C5-C6-C7
21	4B	610	CL7	C3-C5-C6-C7
21	4B	614	CL7	C3-C5-C6-C7
21	4B	615	CL7	C3-C5-C6-C7
21	4C	501	CL7	C3-C5-C6-C7
21	4C	507	CL7	C3-C5-C6-C7
21	4C	508	CL7	C3-C5-C6-C7
21	4C	509	CL7	C3-C5-C6-C7
21	42	506	CL7	C3-C5-C6-C7
21	42	507	CL7	C3-C5-C6-C7
21	42	516	CL7	C3-C5-C6-C7
21	41	408	CL7	C3-C5-C6-C7
21	43	402	CL7	C3-C5-C6-C7
21	43	405	CL7	C3-C5-C6-C7
21	43	406	CL7	C3-C5-C6-C7
21	43	409	CL7	C3-C5-C6-C7
21	44	404	CL7	C3-C5-C6-C7
21	44	405	CL7	C3-C5-C6-C7
21	44	413	CL7	C3-C5-C6-C7
21	1C	517	CL7	O1D-CGD-O2D-CED
21	11	420	CL7	O1D-CGD-O2D-CED
21	2C	517	CL7	O1D-CGD-O2D-CED
21	21	420	CL7	O1D-CGD-O2D-CED
21	3C	517	CL7	O1D-CGD-O2D-CED
21	31	420	CL7	O1D-CGD-O2D-CED
21	4C	517	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	41	420	CL7	O1D-CGD-O2D-CED
21	1D	402	CL7	C2C-C3C-CAC-CBC
21	12	514	CL7	C4C-C3C-CAC-CBC
21	2D	402	CL7	C2C-C3C-CAC-CBC
21	22	514	CL7	C4C-C3C-CAC-CBC
21	3D	402	CL7	C2C-C3C-CAC-CBC
21	32	514	CL7	C4C-C3C-CAC-CBC
21	4D	402	CL7	C2C-C3C-CAC-CBC
21	42	514	CL7	C4C-C3C-CAC-CBC
21	1B	606	CL7	C4-C3-C5-C6
21	1C	501	CL7	C4-C3-C5-C6
21	11	410	CL7	C4-C3-C5-C6
21	13	512	CL7	C4-C3-C5-C6
21	14	412	CL7	C4-C3-C5-C6
21	2B	607	CL7	C4-C3-C5-C6
21	2C	501	CL7	C4-C3-C5-C6
21	21	410	CL7	C4-C3-C5-C6
21	23	413	CL7	C4-C3-C5-C6
21	24	412	CL7	C4-C3-C5-C6
21	3B	606	CL7	C4-C3-C5-C6
21	3C	501	CL7	C4-C3-C5-C6
21	31	410	CL7	C4-C3-C5-C6
21	33	512	CL7	C4-C3-C5-C6
21	34	412	CL7	C4-C3-C5-C6
21	4B	607	CL7	C4-C3-C5-C6
21	4C	501	CL7	C4-C3-C5-C6
21	41	410	CL7	C4-C3-C5-C6
21	43	413	CL7	C4-C3-C5-C6
21	44	412	CL7	C4-C3-C5-C6
21	1B	606	CL7	C2-C3-C5-C6
21	1C	501	CL7	C2-C3-C5-C6
21	14	412	CL7	C2-C3-C5-C6
21	2B	607	CL7	C2-C3-C5-C6
21	2C	501	CL7	C2-C3-C5-C6
21	24	412	CL7	C2-C3-C5-C6
21	3B	606	CL7	C2-C3-C5-C6
21	3C	501	CL7	C2-C3-C5-C6
21	34	412	CL7	C2-C3-C5-C6
21	4B	607	CL7	C2-C3-C5-C6
21	4C	501	CL7	C2-C3-C5-C6
21	44	412	CL7	C2-C3-C5-C6
22	1D	408	PHO	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	2D	408	PHO	C2-C3-C5-C6
22	3D	408	PHO	C2-C3-C5-C6
22	4D	408	PHO	C2-C3-C5-C6
21	12	506	CL7	CBD-CGD-O2D-CED
21	13	514	CL7	CBD-CGD-O2D-CED
21	22	506	CL7	CBD-CGD-O2D-CED
21	32	506	CL7	CBD-CGD-O2D-CED
21	33	514	CL7	CBD-CGD-O2D-CED
21	42	506	CL7	CBD-CGD-O2D-CED
21	43	415	CL7	CBD-CGD-O2D-CED
21	1B	604	CL7	C2A-CAA-CBA-CGA
21	1B	607	CL7	C2A-CAA-CBA-CGA
21	1B	610	CL7	C2A-CAA-CBA-CGA
21	1C	513	CL7	C2A-CAA-CBA-CGA
21	12	502	CL7	C2A-CAA-CBA-CGA
21	11	409	CL7	C2A-CAA-CBA-CGA
21	13	516	CL7	C2A-CAA-CBA-CGA
21	13	518	CL7	C2A-CAA-CBA-CGA
21	14	409	CL7	C2A-CAA-CBA-CGA
21	2B	605	CL7	C2A-CAA-CBA-CGA
21	2B	608	CL7	C2A-CAA-CBA-CGA
21	2B	611	CL7	C2A-CAA-CBA-CGA
21	2C	513	CL7	C2A-CAA-CBA-CGA
21	22	502	CL7	C2A-CAA-CBA-CGA
21	21	409	CL7	C2A-CAA-CBA-CGA
21	23	417	CL7	C2A-CAA-CBA-CGA
21	23	419	CL7	C2A-CAA-CBA-CGA
21	24	409	CL7	C2A-CAA-CBA-CGA
21	3B	604	CL7	C2A-CAA-CBA-CGA
21	3B	607	CL7	C2A-CAA-CBA-CGA
21	3B	610	CL7	C2A-CAA-CBA-CGA
21	3C	513	CL7	C2A-CAA-CBA-CGA
21	32	502	CL7	C2A-CAA-CBA-CGA
21	31	409	CL7	C2A-CAA-CBA-CGA
21	33	516	CL7	C2A-CAA-CBA-CGA
21	33	518	CL7	C2A-CAA-CBA-CGA
21	34	409	CL7	C2A-CAA-CBA-CGA
21	4B	605	CL7	C2A-CAA-CBA-CGA
21	4B	608	CL7	C2A-CAA-CBA-CGA
21	4B	611	CL7	C2A-CAA-CBA-CGA
21	4C	513	CL7	C2A-CAA-CBA-CGA
21	42	502	CL7	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	41	409	CL7	C2A-CAA-CBA-CGA
21	43	417	CL7	C2A-CAA-CBA-CGA
21	43	419	CL7	C2A-CAA-CBA-CGA
21	44	409	CL7	C2A-CAA-CBA-CGA
21	1C	504	CL7	C3-C5-C6-C7
21	1C	505	CL7	C3-C5-C6-C7
21	12	512	CL7	C3-C5-C6-C7
21	14	406	CL7	C3-C5-C6-C7
21	2C	504	CL7	C3-C5-C6-C7
21	2C	505	CL7	C3-C5-C6-C7
21	22	512	CL7	C3-C5-C6-C7
21	24	406	CL7	C3-C5-C6-C7
21	3C	504	CL7	C3-C5-C6-C7
21	3C	505	CL7	C3-C5-C6-C7
21	32	512	CL7	C3-C5-C6-C7
21	34	406	CL7	C3-C5-C6-C7
21	4C	504	CL7	C3-C5-C6-C7
21	4C	505	CL7	C3-C5-C6-C7
21	42	512	CL7	C3-C5-C6-C7
21	44	406	CL7	C3-C5-C6-C7
21	23	415	CL7	CBD-CGD-O2D-CED
21	1B	605	CL7	O1D-CGD-O2D-CED
21	11	405	CL7	O1D-CGD-O2D-CED
21	13	506	CL7	O1D-CGD-O2D-CED
21	2B	606	CL7	O1D-CGD-O2D-CED
21	21	405	CL7	O1D-CGD-O2D-CED
21	23	407	CL7	O1D-CGD-O2D-CED
21	3B	605	CL7	O1D-CGD-O2D-CED
21	31	405	CL7	O1D-CGD-O2D-CED
21	33	506	CL7	O1D-CGD-O2D-CED
21	4B	606	CL7	O1D-CGD-O2D-CED
21	41	405	CL7	O1D-CGD-O2D-CED
21	43	407	CL7	O1D-CGD-O2D-CED
23	1C	514	8CT	C12-C13-C14-C15
23	2C	514	8CT	C12-C13-C14-C15
23	3C	514	8CT	C12-C13-C14-C15
23	4C	514	8CT	C12-C13-C14-C15
32	12	519	ZEX	C29-C30-C31-C32
32	12	520	ZEX	C9-C10-C11-C12
32	14	418	ZEX	C9-C10-C11-C12
32	22	519	ZEX	C29-C30-C31-C32
32	22	520	ZEX	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	24	418	ZEX	C9-C10-C11-C12
32	32	519	ZEX	C29-C30-C31-C32
32	32	520	ZEX	C9-C10-C11-C12
32	34	418	ZEX	C9-C10-C11-C12
32	42	519	ZEX	C29-C30-C31-C32
32	42	520	ZEX	C9-C10-C11-C12
32	44	418	ZEX	C9-C10-C11-C12
21	1A	407	CL7	CBD-CGD-O2D-CED
21	1C	505	CL7	CBD-CGD-O2D-CED
21	1D	402	CL7	CBD-CGD-O2D-CED
21	12	503	CL7	CBD-CGD-O2D-CED
21	2A	407	CL7	CBD-CGD-O2D-CED
21	2C	505	CL7	CBD-CGD-O2D-CED
21	2D	402	CL7	CBD-CGD-O2D-CED
21	22	503	CL7	CBD-CGD-O2D-CED
21	3A	407	CL7	CBD-CGD-O2D-CED
21	3C	505	CL7	CBD-CGD-O2D-CED
21	3D	402	CL7	CBD-CGD-O2D-CED
21	32	503	CL7	CBD-CGD-O2D-CED
21	4A	407	CL7	CBD-CGD-O2D-CED
21	4C	505	CL7	CBD-CGD-O2D-CED
21	4D	402	CL7	CBD-CGD-O2D-CED
21	42	503	CL7	CBD-CGD-O2D-CED
26	1B	625	LHG	O2-C2-C3-O3
26	2B	626	LHG	O2-C2-C3-O3
26	3B	625	LHG	O2-C2-C3-O3
26	4B	626	LHG	O2-C2-C3-O3
21	1A	401	CL7	C3-C5-C6-C7
21	1C	503	CL7	C3-C5-C6-C7
21	11	406	CL7	C3-C5-C6-C7
21	11	417	CL7	C3-C5-C6-C7
21	11	418	CL7	C3-C5-C6-C7
21	2A	401	CL7	C3-C5-C6-C7
21	2C	503	CL7	C3-C5-C6-C7
21	21	406	CL7	C3-C5-C6-C7
21	21	417	CL7	C3-C5-C6-C7
21	21	418	CL7	C3-C5-C6-C7
21	3A	401	CL7	C3-C5-C6-C7
21	3C	503	CL7	C3-C5-C6-C7
21	31	406	CL7	C3-C5-C6-C7
21	31	417	CL7	C3-C5-C6-C7
21	31	418	CL7	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4A	401	CL7	C3-C5-C6-C7
21	4C	503	CL7	C3-C5-C6-C7
21	41	406	CL7	C3-C5-C6-C7
21	41	417	CL7	C3-C5-C6-C7
21	41	418	CL7	C3-C5-C6-C7
21	23	415	CL7	C4C-C3C-CAC-CBC
21	1C	510	CL7	C13-C15-C16-C17
21	13	509	CL7	C8-C10-C11-C12
21	4C	510	CL7	C13-C15-C16-C17
21	1C	510	CL7	CBD-CGD-O2D-CED
21	12	507	CL7	CBD-CGD-O2D-CED
21	14	412	CL7	CBD-CGD-O2D-CED
21	2C	510	CL7	CBD-CGD-O2D-CED
21	22	507	CL7	CBD-CGD-O2D-CED
21	24	412	CL7	CBD-CGD-O2D-CED
21	3C	510	CL7	CBD-CGD-O2D-CED
21	32	507	CL7	CBD-CGD-O2D-CED
21	34	412	CL7	CBD-CGD-O2D-CED
21	4C	510	CL7	CBD-CGD-O2D-CED
21	42	507	CL7	CBD-CGD-O2D-CED
21	44	412	CL7	CBD-CGD-O2D-CED
21	13	514	CL7	C4C-C3C-CAC-CBC
21	33	514	CL7	C4C-C3C-CAC-CBC
21	43	415	CL7	C4C-C3C-CAC-CBC
21	2C	510	CL7	C13-C15-C16-C17
21	23	410	CL7	C8-C10-C11-C12
21	3C	510	CL7	C13-C15-C16-C17
21	33	509	CL7	C8-C10-C11-C12
21	43	410	CL7	C8-C10-C11-C12
21	1A	403	CL7	O1D-CGD-O2D-CED
21	2A	403	CL7	O1D-CGD-O2D-CED
21	3A	403	CL7	O1D-CGD-O2D-CED
21	4A	403	CL7	O1D-CGD-O2D-CED
21	1C	502	CL7	C3-C5-C6-C7
21	2C	502	CL7	C3-C5-C6-C7
21	3C	502	CL7	C3-C5-C6-C7
21	4C	502	CL7	C3-C5-C6-C7
21	1A	401	CL7	C4-C3-C5-C6
21	1B	603	CL7	C4-C3-C5-C6
21	1C	508	CL7	C4-C3-C5-C6
21	12	505	CL7	C4-C3-C5-C6
21	12	516	CL7	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	517	CL7	C4-C3-C5-C6
21	11	403	CL7	C4-C3-C5-C6
21	13	504	CL7	C4-C3-C5-C6
21	13	510	CL7	C4-C3-C5-C6
21	13	511	CL7	C4-C3-C5-C6
21	14	406	CL7	C4-C3-C5-C6
21	2A	401	CL7	C4-C3-C5-C6
21	2B	604	CL7	C4-C3-C5-C6
21	2C	508	CL7	C4-C3-C5-C6
21	22	505	CL7	C4-C3-C5-C6
21	22	516	CL7	C4-C3-C5-C6
21	22	517	CL7	C4-C3-C5-C6
21	21	403	CL7	C4-C3-C5-C6
21	23	405	CL7	C4-C3-C5-C6
21	23	411	CL7	C4-C3-C5-C6
21	23	412	CL7	C4-C3-C5-C6
21	24	406	CL7	C4-C3-C5-C6
21	3A	401	CL7	C4-C3-C5-C6
21	3B	603	CL7	C4-C3-C5-C6
21	3C	508	CL7	C4-C3-C5-C6
21	32	505	CL7	C4-C3-C5-C6
21	32	516	CL7	C4-C3-C5-C6
21	32	517	CL7	C4-C3-C5-C6
21	31	403	CL7	C4-C3-C5-C6
21	33	504	CL7	C4-C3-C5-C6
21	33	510	CL7	C4-C3-C5-C6
21	33	511	CL7	C4-C3-C5-C6
21	34	406	CL7	C4-C3-C5-C6
21	4A	401	CL7	C4-C3-C5-C6
21	4B	604	CL7	C4-C3-C5-C6
21	4C	508	CL7	C4-C3-C5-C6
21	42	505	CL7	C4-C3-C5-C6
21	42	516	CL7	C4-C3-C5-C6
21	42	517	CL7	C4-C3-C5-C6
21	41	403	CL7	C4-C3-C5-C6
21	43	405	CL7	C4-C3-C5-C6
21	43	411	CL7	C4-C3-C5-C6
21	43	412	CL7	C4-C3-C5-C6
21	44	406	CL7	C4-C3-C5-C6
21	1A	401	CL7	C2-C3-C5-C6
21	1B	603	CL7	C2-C3-C5-C6
21	1B	608	CL7	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	614	CL7	C2-C3-C5-C6
21	1C	508	CL7	C2-C3-C5-C6
21	12	505	CL7	C2-C3-C5-C6
21	12	516	CL7	C2-C3-C5-C6
21	12	517	CL7	C2-C3-C5-C6
21	11	403	CL7	C2-C3-C5-C6
21	13	504	CL7	C2-C3-C5-C6
21	13	510	CL7	C2-C3-C5-C6
21	13	511	CL7	C2-C3-C5-C6
21	14	406	CL7	C2-C3-C5-C6
21	2A	401	CL7	C2-C3-C5-C6
21	2B	604	CL7	C2-C3-C5-C6
21	2B	609	CL7	C2-C3-C5-C6
21	2B	615	CL7	C2-C3-C5-C6
21	2C	508	CL7	C2-C3-C5-C6
21	22	505	CL7	C2-C3-C5-C6
21	22	516	CL7	C2-C3-C5-C6
21	22	517	CL7	C2-C3-C5-C6
21	21	403	CL7	C2-C3-C5-C6
21	23	405	CL7	C2-C3-C5-C6
21	23	411	CL7	C2-C3-C5-C6
21	23	412	CL7	C2-C3-C5-C6
21	24	406	CL7	C2-C3-C5-C6
21	3A	401	CL7	C2-C3-C5-C6
21	3B	603	CL7	C2-C3-C5-C6
21	3B	608	CL7	C2-C3-C5-C6
21	3B	614	CL7	C2-C3-C5-C6
21	3C	508	CL7	C2-C3-C5-C6
21	32	505	CL7	C2-C3-C5-C6
21	32	516	CL7	C2-C3-C5-C6
21	32	517	CL7	C2-C3-C5-C6
21	31	403	CL7	C2-C3-C5-C6
21	33	504	CL7	C2-C3-C5-C6
21	33	510	CL7	C2-C3-C5-C6
21	33	511	CL7	C2-C3-C5-C6
21	34	406	CL7	C2-C3-C5-C6
21	4A	401	CL7	C2-C3-C5-C6
21	4B	604	CL7	C2-C3-C5-C6
21	4B	609	CL7	C2-C3-C5-C6
21	4B	615	CL7	C2-C3-C5-C6
21	4C	508	CL7	C2-C3-C5-C6
21	42	505	CL7	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	516	CL7	C2-C3-C5-C6
21	42	517	CL7	C2-C3-C5-C6
21	41	403	CL7	C2-C3-C5-C6
21	43	405	CL7	C2-C3-C5-C6
21	43	411	CL7	C2-C3-C5-C6
21	43	412	CL7	C2-C3-C5-C6
21	44	406	CL7	C2-C3-C5-C6
21	14	414	CL7	CBD-CGD-O2D-CED
21	34	414	CL7	CBD-CGD-O2D-CED
21	1B	622	CL7	C2A-CAA-CBA-CGA
21	11	405	CL7	C2A-CAA-CBA-CGA
21	13	503	CL7	C2A-CAA-CBA-CGA
21	13	512	CL7	C2A-CAA-CBA-CGA
21	14	404	CL7	C2A-CAA-CBA-CGA
21	2B	623	CL7	C2A-CAA-CBA-CGA
21	21	405	CL7	C2A-CAA-CBA-CGA
21	23	404	CL7	C2A-CAA-CBA-CGA
21	23	413	CL7	C2A-CAA-CBA-CGA
21	24	404	CL7	C2A-CAA-CBA-CGA
21	3B	622	CL7	C2A-CAA-CBA-CGA
21	31	405	CL7	C2A-CAA-CBA-CGA
21	33	503	CL7	C2A-CAA-CBA-CGA
21	33	512	CL7	C2A-CAA-CBA-CGA
21	34	404	CL7	C2A-CAA-CBA-CGA
21	4B	623	CL7	C2A-CAA-CBA-CGA
21	41	405	CL7	C2A-CAA-CBA-CGA
21	43	404	CL7	C2A-CAA-CBA-CGA
21	43	413	CL7	C2A-CAA-CBA-CGA
21	44	404	CL7	C2A-CAA-CBA-CGA
21	1A	407	CL7	C2C-C3C-CAC-CBC
21	24	414	CL7	CBD-CGD-O2D-CED
21	44	414	CL7	CBD-CGD-O2D-CED
21	2A	407	CL7	C2C-C3C-CAC-CBC
21	3A	407	CL7	C2C-C3C-CAC-CBC
21	4A	407	CL7	C2C-C3C-CAC-CBC
21	11	410	CL7	O1D-CGD-O2D-CED
21	13	509	CL7	O1D-CGD-O2D-CED
21	13	516	CL7	O1D-CGD-O2D-CED
21	21	410	CL7	O1D-CGD-O2D-CED
21	23	410	CL7	O1D-CGD-O2D-CED
21	23	417	CL7	O1D-CGD-O2D-CED
21	31	410	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	33	509	CL7	O1D-CGD-O2D-CED
21	33	516	CL7	O1D-CGD-O2D-CED
21	41	410	CL7	O1D-CGD-O2D-CED
21	43	410	CL7	O1D-CGD-O2D-CED
21	43	417	CL7	O1D-CGD-O2D-CED
21	2C	509	CL7	O1D-CGD-O2D-CED
21	3C	509	CL7	O1D-CGD-O2D-CED
21	4C	509	CL7	O1D-CGD-O2D-CED
26	1A	408	LHG	C1-C2-C3-O3
26	4A	408	LHG	C1-C2-C3-O3
21	12	510	CL7	C3-C5-C6-C7
21	22	510	CL7	C3-C5-C6-C7
21	32	510	CL7	C3-C5-C6-C7
21	42	510	CL7	C3-C5-C6-C7
21	1C	503	CL7	O1D-CGD-O2D-CED
21	1C	509	CL7	O1D-CGD-O2D-CED
21	2C	503	CL7	O1D-CGD-O2D-CED
21	3C	503	CL7	O1D-CGD-O2D-CED
21	4C	503	CL7	O1D-CGD-O2D-CED
21	12	510	CL7	C8-C10-C11-C12
21	2C	509	CL7	C13-C15-C16-C17
21	42	510	CL7	C8-C10-C11-C12
21	1A	401	CL7	C2C-C3C-CAC-CBC
21	3A	401	CL7	C2C-C3C-CAC-CBC
21	4A	401	CL7	C2C-C3C-CAC-CBC
21	1C	509	CL7	C13-C15-C16-C17
21	13	503	CL7	C5-C6-C7-C8
21	22	510	CL7	C8-C10-C11-C12
21	23	404	CL7	C5-C6-C7-C8
21	3C	509	CL7	C13-C15-C16-C17
21	32	510	CL7	C8-C10-C11-C12
21	33	503	CL7	C5-C6-C7-C8
21	4C	509	CL7	C13-C15-C16-C17
21	43	404	CL7	C5-C6-C7-C8
21	2A	401	CL7	C2C-C3C-CAC-CBC
27	1C	516	DGD	C4B-C5B-C6B-C7B
21	12	512	CL7	C5-C6-C7-C8
21	13	504	CL7	C8-C10-C11-C12
21	13	504	CL7	C13-C15-C16-C17
21	13	505	CL7	C15-C16-C17-C18
21	13	510	CL7	C5-C6-C7-C8
21	13	510	CL7	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	14	412	CL7	C10-C11-C12-C13
21	22	512	CL7	C5-C6-C7-C8
21	23	405	CL7	C8-C10-C11-C12
21	23	405	CL7	C13-C15-C16-C17
21	23	406	CL7	C15-C16-C17-C18
21	23	411	CL7	C5-C6-C7-C8
21	23	411	CL7	C10-C11-C12-C13
21	24	412	CL7	C10-C11-C12-C13
21	32	512	CL7	C5-C6-C7-C8
21	33	504	CL7	C8-C10-C11-C12
21	33	504	CL7	C13-C15-C16-C17
21	33	505	CL7	C15-C16-C17-C18
21	33	510	CL7	C5-C6-C7-C8
21	33	510	CL7	C10-C11-C12-C13
21	34	412	CL7	C10-C11-C12-C13
21	42	512	CL7	C5-C6-C7-C8
21	43	405	CL7	C8-C10-C11-C12
21	43	405	CL7	C13-C15-C16-C17
21	43	406	CL7	C15-C16-C17-C18
21	43	411	CL7	C5-C6-C7-C8
21	43	411	CL7	C10-C11-C12-C13
21	44	412	CL7	C10-C11-C12-C13
26	1A	408	LHG	O2-C2-C3-O3
26	2A	408	LHG	O2-C2-C3-O3
26	3A	408	LHG	O2-C2-C3-O3
26	4A	408	LHG	O2-C2-C3-O3
27	2C	516	DGD	C4B-C5B-C6B-C7B
27	3C	516	DGD	C4B-C5B-C6B-C7B
27	4C	516	DGD	C4B-C5B-C6B-C7B
21	11	410	CL7	C2-C3-C5-C6
21	21	410	CL7	C2-C3-C5-C6
21	31	410	CL7	C2-C3-C5-C6
21	41	410	CL7	C2-C3-C5-C6
21	1B	603	CL7	C11-C10-C8-C9
21	1B	603	CL7	C14-C13-C15-C16
21	1B	608	CL7	C11-C10-C8-C9
21	1B	611	CL7	C11-C10-C8-C9
21	1B	611	CL7	C11-C12-C13-C14
21	1B	612	CL7	C11-C12-C13-C14
21	1C	506	CL7	C11-C10-C8-C9
21	1C	508	CL7	C11-C10-C8-C9
21	1C	510	CL7	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1D	404	CL7	C11-C10-C8-C9
21	12	505	CL7	C14-C13-C15-C16
21	12	510	CL7	C11-C10-C8-C9
21	12	510	CL7	C11-C12-C13-C14
21	11	408	CL7	C11-C10-C8-C9
21	13	501	CL7	C11-C10-C8-C9
21	13	501	CL7	C11-C12-C13-C14
21	13	504	CL7	C11-C10-C8-C9
21	13	507	CL7	C11-C10-C8-C9
21	13	509	CL7	C14-C13-C15-C16
21	13	511	CL7	C11-C10-C8-C9
21	14	404	CL7	C11-C10-C8-C9
21	14	404	CL7	C14-C13-C15-C16
21	14	406	CL7	C11-C10-C8-C9
21	2B	604	CL7	C11-C10-C8-C9
21	2B	604	CL7	C14-C13-C15-C16
21	2B	609	CL7	C11-C10-C8-C9
21	2B	612	CL7	C11-C10-C8-C9
21	2B	612	CL7	C11-C12-C13-C14
21	2B	613	CL7	C11-C12-C13-C14
21	2C	506	CL7	C11-C10-C8-C9
21	2C	508	CL7	C11-C10-C8-C9
21	2C	510	CL7	C11-C12-C13-C14
21	2D	404	CL7	C11-C10-C8-C9
21	22	505	CL7	C14-C13-C15-C16
21	22	510	CL7	C11-C10-C8-C9
21	22	510	CL7	C11-C12-C13-C14
21	21	408	CL7	C11-C10-C8-C9
21	23	402	CL7	C11-C10-C8-C9
21	23	402	CL7	C11-C12-C13-C14
21	23	405	CL7	C11-C10-C8-C9
21	23	408	CL7	C11-C10-C8-C9
21	23	410	CL7	C14-C13-C15-C16
21	23	412	CL7	C11-C10-C8-C9
21	24	404	CL7	C11-C10-C8-C9
21	24	404	CL7	C14-C13-C15-C16
21	24	406	CL7	C11-C10-C8-C9
21	3B	603	CL7	C11-C10-C8-C9
21	3B	603	CL7	C14-C13-C15-C16
21	3B	608	CL7	C11-C10-C8-C9
21	3B	611	CL7	C11-C10-C8-C9
21	3B	611	CL7	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3B	612	CL7	C11-C12-C13-C14
21	3C	506	CL7	C11-C10-C8-C9
21	3C	508	CL7	C11-C10-C8-C9
21	3C	510	CL7	C11-C12-C13-C14
21	3D	404	CL7	C11-C10-C8-C9
21	32	505	CL7	C14-C13-C15-C16
21	32	510	CL7	C11-C10-C8-C9
21	32	510	CL7	C11-C12-C13-C14
21	31	408	CL7	C11-C10-C8-C9
21	33	501	CL7	C11-C10-C8-C9
21	33	501	CL7	C11-C12-C13-C14
21	33	504	CL7	C11-C10-C8-C9
21	33	507	CL7	C11-C10-C8-C9
21	33	509	CL7	C14-C13-C15-C16
21	33	511	CL7	C11-C10-C8-C9
21	34	404	CL7	C11-C10-C8-C9
21	34	404	CL7	C14-C13-C15-C16
21	34	406	CL7	C11-C10-C8-C9
21	4B	604	CL7	C11-C10-C8-C9
21	4B	604	CL7	C14-C13-C15-C16
21	4B	609	CL7	C11-C10-C8-C9
21	4B	612	CL7	C11-C10-C8-C9
21	4B	612	CL7	C11-C12-C13-C14
21	4B	613	CL7	C11-C12-C13-C14
21	4C	506	CL7	C11-C10-C8-C9
21	4C	508	CL7	C11-C10-C8-C9
21	4C	510	CL7	C11-C12-C13-C14
21	4D	404	CL7	C11-C10-C8-C9
21	42	505	CL7	C14-C13-C15-C16
21	42	510	CL7	C11-C10-C8-C9
21	42	510	CL7	C11-C12-C13-C14
21	41	408	CL7	C11-C10-C8-C9
21	43	402	CL7	C11-C10-C8-C9
21	43	402	CL7	C11-C12-C13-C14
21	43	405	CL7	C11-C10-C8-C9
21	43	408	CL7	C11-C10-C8-C9
21	43	410	CL7	C14-C13-C15-C16
21	43	412	CL7	C11-C10-C8-C9
21	44	404	CL7	C11-C10-C8-C9
21	44	404	CL7	C14-C13-C15-C16
21	44	406	CL7	C11-C10-C8-C9
21	1C	511	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	13	518	CL7	O1D-CGD-O2D-CED
21	2C	511	CL7	O1D-CGD-O2D-CED
21	23	419	CL7	O1D-CGD-O2D-CED
21	3C	511	CL7	O1D-CGD-O2D-CED
21	33	518	CL7	O1D-CGD-O2D-CED
21	4C	511	CL7	O1D-CGD-O2D-CED
21	43	419	CL7	O1D-CGD-O2D-CED
21	1D	404	CL7	CBD-CGD-O2D-CED
21	2D	404	CL7	CBD-CGD-O2D-CED
21	3D	404	CL7	CBD-CGD-O2D-CED
21	4D	404	CL7	CBD-CGD-O2D-CED
21	31	419	CL7	C2A-CAA-CBA-CGA
21	41	419	CL7	C2A-CAA-CBA-CGA
23	1B	618	8CT	C10-C11-C12-C40
23	1C	514	8CT	C14-C15-C16-C39
23	1C	514	8CT	C22-C21-C23-C24
23	1C	518	8CT	C14-C15-C16-C39
23	2B	619	8CT	C10-C11-C12-C40
23	2C	514	8CT	C14-C15-C16-C39
23	2C	514	8CT	C22-C21-C23-C24
23	2C	518	8CT	C14-C15-C16-C39
23	3B	618	8CT	C10-C11-C12-C40
23	3C	514	8CT	C14-C15-C16-C39
23	3C	514	8CT	C22-C21-C23-C24
23	3C	518	8CT	C14-C15-C16-C39
23	4B	619	8CT	C10-C11-C12-C40
23	4C	514	8CT	C14-C15-C16-C39
23	4C	514	8CT	C22-C21-C23-C24
23	4C	518	8CT	C14-C15-C16-C39
32	12	524	ZEX	C27-C28-C29-C39
32	13	519	ZEX	C7-C8-C9-C19
32	13	519	ZEX	C27-C28-C29-C39
32	13	520	ZEX	C27-C28-C29-C39
32	13	522	ZEX	C7-C8-C9-C19
32	14	403	ZEX	C27-C28-C29-C39
32	14	418	ZEX	C27-C28-C29-C39
32	22	524	ZEX	C27-C28-C29-C39
32	23	420	ZEX	C7-C8-C9-C19
32	23	420	ZEX	C27-C28-C29-C39
32	23	421	ZEX	C27-C28-C29-C39
32	23	423	ZEX	C7-C8-C9-C19
32	24	403	ZEX	C27-C28-C29-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	24	418	ZEX	C27-C28-C29-C39
32	32	524	ZEX	C27-C28-C29-C39
32	33	519	ZEX	C7-C8-C9-C19
32	33	519	ZEX	C27-C28-C29-C39
32	33	520	ZEX	C27-C28-C29-C39
32	33	522	ZEX	C7-C8-C9-C19
32	34	403	ZEX	C27-C28-C29-C39
32	34	418	ZEX	C27-C28-C29-C39
32	42	524	ZEX	C27-C28-C29-C39
32	43	420	ZEX	C7-C8-C9-C19
32	43	420	ZEX	C27-C28-C29-C39
32	43	421	ZEX	C27-C28-C29-C39
32	43	423	ZEX	C7-C8-C9-C19
32	44	403	ZEX	C27-C28-C29-C39
32	44	418	ZEX	C27-C28-C29-C39
23	1B	618	8CT	C10-C11-C12-C13
23	1C	514	8CT	C14-C15-C16-C17
23	1C	518	8CT	C14-C15-C16-C17
23	2B	619	8CT	C10-C11-C12-C13
23	2C	514	8CT	C14-C15-C16-C17
23	2C	518	8CT	C14-C15-C16-C17
23	3B	618	8CT	C10-C11-C12-C13
23	3C	514	8CT	C14-C15-C16-C17
23	3C	518	8CT	C14-C15-C16-C17
23	4B	619	8CT	C10-C11-C12-C13
23	4C	514	8CT	C14-C15-C16-C17
23	4C	518	8CT	C14-C15-C16-C17
32	12	520	ZEX	C7-C8-C9-C10
32	12	522	ZEX	C31-C32-C33-C34
32	11	422	ZEX	C7-C8-C9-C10
32	13	519	ZEX	C7-C8-C9-C10
32	13	519	ZEX	C27-C28-C29-C30
32	13	520	ZEX	C27-C28-C29-C30
32	13	522	ZEX	C7-C8-C9-C10
32	14	403	ZEX	C27-C28-C29-C30
32	14	418	ZEX	C27-C28-C29-C30
32	14	419	ZEX	C7-C8-C9-C10
32	22	520	ZEX	C7-C8-C9-C10
32	22	522	ZEX	C31-C32-C33-C34
32	21	422	ZEX	C7-C8-C9-C10
32	23	420	ZEX	C7-C8-C9-C10
32	23	420	ZEX	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	23	421	ZEX	C27-C28-C29-C30
32	23	423	ZEX	C7-C8-C9-C10
32	24	403	ZEX	C27-C28-C29-C30
32	24	418	ZEX	C27-C28-C29-C30
32	24	419	ZEX	C7-C8-C9-C10
32	32	520	ZEX	C7-C8-C9-C10
32	32	522	ZEX	C31-C32-C33-C34
32	31	422	ZEX	C7-C8-C9-C10
32	33	519	ZEX	C7-C8-C9-C10
32	33	519	ZEX	C27-C28-C29-C30
32	33	520	ZEX	C27-C28-C29-C30
32	33	522	ZEX	C7-C8-C9-C10
32	34	403	ZEX	C27-C28-C29-C30
32	34	418	ZEX	C27-C28-C29-C30
32	34	419	ZEX	C7-C8-C9-C10
32	42	520	ZEX	C7-C8-C9-C10
32	42	522	ZEX	C31-C32-C33-C34
32	41	422	ZEX	C7-C8-C9-C10
32	43	420	ZEX	C7-C8-C9-C10
32	43	420	ZEX	C27-C28-C29-C30
32	43	421	ZEX	C27-C28-C29-C30
32	43	423	ZEX	C7-C8-C9-C10
32	44	403	ZEX	C27-C28-C29-C30
32	44	418	ZEX	C27-C28-C29-C30
32	44	419	ZEX	C7-C8-C9-C10
21	12	510	CL7	C13-C15-C16-C17
21	12	511	CL7	C8-C10-C11-C12
21	11	404	CL7	C13-C15-C16-C17
21	11	408	CL7	C15-C16-C17-C18
21	13	501	CL7	C15-C16-C17-C18
21	22	510	CL7	C13-C15-C16-C17
21	22	511	CL7	C8-C10-C11-C12
21	21	404	CL7	C13-C15-C16-C17
21	21	408	CL7	C15-C16-C17-C18
21	23	402	CL7	C15-C16-C17-C18
21	24	409	CL7	C8-C10-C11-C12
21	32	510	CL7	C13-C15-C16-C17
21	32	511	CL7	C8-C10-C11-C12
21	31	408	CL7	C15-C16-C17-C18
21	33	501	CL7	C15-C16-C17-C18
21	42	510	CL7	C13-C15-C16-C17
21	42	511	CL7	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	41	404	CL7	C13-C15-C16-C17
21	41	408	CL7	C15-C16-C17-C18
21	43	402	CL7	C15-C16-C17-C18
21	44	412	CL7	C8-C10-C11-C12
21	11	418	CL7	O1D-CGD-O2D-CED
21	13	508	CL7	O1D-CGD-O2D-CED
21	21	418	CL7	O1D-CGD-O2D-CED
21	23	409	CL7	O1D-CGD-O2D-CED
21	31	418	CL7	O1D-CGD-O2D-CED
21	33	508	CL7	O1D-CGD-O2D-CED
21	41	418	CL7	O1D-CGD-O2D-CED
21	43	409	CL7	O1D-CGD-O2D-CED
21	11	419	CL7	C4C-C3C-CAC-CBC
21	21	419	CL7	C4C-C3C-CAC-CBC
21	31	419	CL7	C4C-C3C-CAC-CBC
21	42	510	CL7	O1D-CGD-O2D-CED
21	1B	604	CL7	C3-C5-C6-C7
21	12	505	CL7	C3-C5-C6-C7
21	2B	605	CL7	C3-C5-C6-C7
21	22	505	CL7	C3-C5-C6-C7
21	3B	604	CL7	C3-C5-C6-C7
21	32	505	CL7	C3-C5-C6-C7
21	4B	605	CL7	C3-C5-C6-C7
21	42	505	CL7	C3-C5-C6-C7
21	1B	604	CL7	C15-C16-C17-C18
21	1B	611	CL7	C5-C6-C7-C8
21	12	517	CL7	C5-C6-C7-C8
21	11	406	CL7	C10-C11-C12-C13
21	13	504	CL7	C5-C6-C7-C8
21	14	406	CL7	C13-C15-C16-C17
21	14	409	CL7	C8-C10-C11-C12
21	14	412	CL7	C8-C10-C11-C12
21	14	412	CL7	C15-C16-C17-C18
21	2B	605	CL7	C15-C16-C17-C18
21	2B	612	CL7	C5-C6-C7-C8
21	2C	509	CL7	C5-C6-C7-C8
21	22	517	CL7	C5-C6-C7-C8
21	21	406	CL7	C10-C11-C12-C13
21	23	405	CL7	C5-C6-C7-C8
21	24	406	CL7	C13-C15-C16-C17
21	24	412	CL7	C8-C10-C11-C12
21	24	412	CL7	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3B	604	CL7	C15-C16-C17-C18
21	3B	611	CL7	C5-C6-C7-C8
21	32	517	CL7	C5-C6-C7-C8
21	31	404	CL7	C13-C15-C16-C17
21	31	406	CL7	C10-C11-C12-C13
21	33	504	CL7	C5-C6-C7-C8
21	34	406	CL7	C13-C15-C16-C17
21	34	409	CL7	C8-C10-C11-C12
21	34	412	CL7	C8-C10-C11-C12
21	34	412	CL7	C15-C16-C17-C18
21	4B	605	CL7	C15-C16-C17-C18
21	4B	612	CL7	C5-C6-C7-C8
21	42	517	CL7	C5-C6-C7-C8
21	41	406	CL7	C10-C11-C12-C13
21	43	405	CL7	C5-C6-C7-C8
21	44	406	CL7	C13-C15-C16-C17
21	44	409	CL7	C8-C10-C11-C12
21	41	419	CL7	C4C-C3C-CAC-CBC
21	12	510	CL7	O1D-CGD-O2D-CED
21	22	510	CL7	O1D-CGD-O2D-CED
21	32	510	CL7	O1D-CGD-O2D-CED
21	1A	401	CL7	C8-C10-C11-C12
21	1B	605	CL7	C5-C6-C7-C8
21	1B	608	CL7	C15-C16-C17-C18
21	1C	501	CL7	C15-C16-C17-C18
21	1C	509	CL7	C5-C6-C7-C8
21	1C	509	CL7	C10-C11-C12-C13
21	12	502	CL7	C8-C10-C11-C12
21	12	510	CL7	C5-C6-C7-C8
21	11	404	CL7	C15-C16-C17-C18
21	13	511	CL7	C10-C11-C12-C13
21	13	512	CL7	C5-C6-C7-C8
21	14	405	CL7	C13-C15-C16-C17
21	14	409	CL7	C10-C11-C12-C13
21	2A	401	CL7	C8-C10-C11-C12
21	2B	604	CL7	C5-C6-C7-C8
21	2B	606	CL7	C5-C6-C7-C8
21	2B	609	CL7	C15-C16-C17-C18
21	2C	501	CL7	C15-C16-C17-C18
21	2C	509	CL7	C10-C11-C12-C13
21	22	502	CL7	C8-C10-C11-C12
21	22	510	CL7	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	21	404	CL7	C15-C16-C17-C18
21	23	412	CL7	C10-C11-C12-C13
21	23	413	CL7	C5-C6-C7-C8
21	24	405	CL7	C13-C15-C16-C17
21	24	409	CL7	C10-C11-C12-C13
21	3A	401	CL7	C8-C10-C11-C12
21	3B	605	CL7	C5-C6-C7-C8
21	3B	608	CL7	C15-C16-C17-C18
21	3C	501	CL7	C15-C16-C17-C18
21	3C	509	CL7	C5-C6-C7-C8
21	3C	509	CL7	C10-C11-C12-C13
21	32	502	CL7	C8-C10-C11-C12
21	32	510	CL7	C5-C6-C7-C8
21	31	404	CL7	C15-C16-C17-C18
21	33	511	CL7	C10-C11-C12-C13
21	33	512	CL7	C5-C6-C7-C8
21	34	405	CL7	C13-C15-C16-C17
21	34	409	CL7	C10-C11-C12-C13
21	4A	401	CL7	C8-C10-C11-C12
21	4B	606	CL7	C5-C6-C7-C8
21	4B	609	CL7	C15-C16-C17-C18
21	4C	501	CL7	C15-C16-C17-C18
21	4C	509	CL7	C5-C6-C7-C8
21	4C	509	CL7	C10-C11-C12-C13
21	42	502	CL7	C8-C10-C11-C12
21	42	510	CL7	C5-C6-C7-C8
21	41	404	CL7	C15-C16-C17-C18
21	43	412	CL7	C10-C11-C12-C13
21	43	413	CL7	C5-C6-C7-C8
21	44	405	CL7	C13-C15-C16-C17
21	44	409	CL7	C10-C11-C12-C13
21	44	412	CL7	C15-C16-C17-C18
21	11	412	CL7	O1D-CGD-O2D-CED
21	14	410	CL7	O1D-CGD-O2D-CED
21	21	412	CL7	O1D-CGD-O2D-CED
21	24	410	CL7	O1D-CGD-O2D-CED
21	31	412	CL7	O1D-CGD-O2D-CED
21	34	410	CL7	O1D-CGD-O2D-CED
21	44	410	CL7	O1D-CGD-O2D-CED
25	12	521	SQD	C7-C8-C9-C10
25	22	521	SQD	C7-C8-C9-C10
25	32	521	SQD	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	42	521	SQD	C7-C8-C9-C10
21	13	517	CL7	CBD-CGD-O2D-CED
21	23	418	CL7	CBD-CGD-O2D-CED
21	33	517	CL7	CBD-CGD-O2D-CED
21	43	418	CL7	CBD-CGD-O2D-CED
21	41	412	CL7	O1D-CGD-O2D-CED
21	1A	407	CL7	C5-C6-C7-C8
21	1B	603	CL7	C5-C6-C7-C8
21	1B	605	CL7	C13-C15-C16-C17
21	12	503	CL7	C8-C10-C11-C12
21	12	512	CL7	C13-C15-C16-C17
21	13	509	CL7	C5-C6-C7-C8
21	13	509	CL7	C10-C11-C12-C13
21	2A	407	CL7	C5-C6-C7-C8
21	2B	606	CL7	C13-C15-C16-C17
21	22	503	CL7	C8-C10-C11-C12
21	22	512	CL7	C13-C15-C16-C17
21	23	410	CL7	C5-C6-C7-C8
21	23	410	CL7	C10-C11-C12-C13
21	3A	407	CL7	C5-C6-C7-C8
21	3B	603	CL7	C5-C6-C7-C8
21	3B	605	CL7	C13-C15-C16-C17
21	32	503	CL7	C8-C10-C11-C12
21	32	512	CL7	C13-C15-C16-C17
21	33	509	CL7	C5-C6-C7-C8
21	33	509	CL7	C10-C11-C12-C13
21	4A	407	CL7	C5-C6-C7-C8
21	4B	604	CL7	C5-C6-C7-C8
21	4B	606	CL7	C13-C15-C16-C17
21	42	503	CL7	C8-C10-C11-C12
21	42	512	CL7	C13-C15-C16-C17
21	43	410	CL7	C5-C6-C7-C8
21	43	410	CL7	C10-C11-C12-C13
21	22	509	CL7	C3-C5-C6-C7
21	1B	608	CL7	C5-C6-C7-C8
21	13	505	CL7	C8-C10-C11-C12
21	14	406	CL7	C15-C16-C17-C18
21	2B	609	CL7	C5-C6-C7-C8
21	23	406	CL7	C8-C10-C11-C12
21	24	406	CL7	C15-C16-C17-C18
21	3B	608	CL7	C5-C6-C7-C8
21	33	505	CL7	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	34	406	CL7	C15-C16-C17-C18
21	4B	609	CL7	C5-C6-C7-C8
21	43	406	CL7	C8-C10-C11-C12
21	44	406	CL7	C15-C16-C17-C18
21	11	415	CL7	CBD-CGD-O2D-CED
21	21	415	CL7	CBD-CGD-O2D-CED
21	31	415	CL7	CBD-CGD-O2D-CED
21	41	415	CL7	CBD-CGD-O2D-CED
21	11	406	CL7	C13-C15-C16-C17
21	21	406	CL7	C13-C15-C16-C17
21	31	406	CL7	C13-C15-C16-C17
21	41	406	CL7	C13-C15-C16-C17
21	12	501	CL7	C15-C16-C17-C18
21	22	501	CL7	C15-C16-C17-C18
21	32	501	CL7	C15-C16-C17-C18
21	42	501	CL7	C15-C16-C17-C18
21	11	403	CL7	O1D-CGD-O2D-CED
21	1B	603	CL7	C12-C13-C15-C16
21	1C	503	CL7	C11-C12-C13-C15
21	1C	507	CL7	C11-C10-C8-C7
21	12	512	CL7	C11-C12-C13-C15
21	11	406	CL7	C12-C13-C15-C16
21	11	408	CL7	C12-C13-C15-C16
21	11	418	CL7	C12-C13-C15-C16
21	13	501	CL7	C11-C10-C8-C7
21	13	503	CL7	C11-C10-C8-C7
21	13	503	CL7	C12-C13-C15-C16
21	13	508	CL7	C6-C7-C8-C10
21	13	510	CL7	C6-C7-C8-C10
21	13	511	CL7	C12-C13-C15-C16
21	14	406	CL7	C6-C7-C8-C10
21	14	406	CL7	C11-C10-C8-C7
21	14	406	CL7	C12-C13-C15-C16
21	2B	604	CL7	C12-C13-C15-C16
21	2C	503	CL7	C11-C12-C13-C15
21	2C	507	CL7	C11-C10-C8-C7
21	22	512	CL7	C11-C12-C13-C15
21	21	406	CL7	C12-C13-C15-C16
21	21	408	CL7	C12-C13-C15-C16
21	21	418	CL7	C12-C13-C15-C16
21	23	402	CL7	C11-C10-C8-C7
21	23	404	CL7	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	23	404	CL7	C12-C13-C15-C16
21	23	409	CL7	C6-C7-C8-C10
21	23	411	CL7	C6-C7-C8-C10
21	23	412	CL7	C12-C13-C15-C16
21	24	406	CL7	C6-C7-C8-C10
21	24	406	CL7	C11-C10-C8-C7
21	24	406	CL7	C12-C13-C15-C16
21	3B	603	CL7	C12-C13-C15-C16
21	3C	503	CL7	C11-C12-C13-C15
21	3C	507	CL7	C11-C10-C8-C7
21	32	512	CL7	C11-C12-C13-C15
21	31	406	CL7	C12-C13-C15-C16
21	31	408	CL7	C12-C13-C15-C16
21	31	418	CL7	C12-C13-C15-C16
21	33	501	CL7	C11-C10-C8-C7
21	33	503	CL7	C11-C10-C8-C7
21	33	503	CL7	C12-C13-C15-C16
21	33	508	CL7	C6-C7-C8-C10
21	33	510	CL7	C6-C7-C8-C10
21	33	511	CL7	C12-C13-C15-C16
21	34	406	CL7	C6-C7-C8-C10
21	34	406	CL7	C11-C10-C8-C7
21	34	406	CL7	C12-C13-C15-C16
21	4B	604	CL7	C12-C13-C15-C16
21	4C	503	CL7	C11-C12-C13-C15
21	4C	507	CL7	C11-C10-C8-C7
21	42	512	CL7	C11-C12-C13-C15
21	41	406	CL7	C12-C13-C15-C16
21	41	408	CL7	C12-C13-C15-C16
21	41	418	CL7	C12-C13-C15-C16
21	43	402	CL7	C11-C10-C8-C7
21	43	404	CL7	C11-C10-C8-C7
21	43	404	CL7	C12-C13-C15-C16
21	43	409	CL7	C6-C7-C8-C10
21	43	411	CL7	C6-C7-C8-C10
21	43	412	CL7	C12-C13-C15-C16
21	44	406	CL7	C6-C7-C8-C10
21	44	406	CL7	C11-C10-C8-C7
21	44	406	CL7	C12-C13-C15-C16
21	1B	610	CL7	C3-C5-C6-C7
21	12	509	CL7	C3-C5-C6-C7
21	13	502	CL7	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2B	611	CL7	C3-C5-C6-C7
21	23	403	CL7	C3-C5-C6-C7
21	3B	610	CL7	C3-C5-C6-C7
21	32	509	CL7	C3-C5-C6-C7
21	33	502	CL7	C3-C5-C6-C7
21	4B	611	CL7	C3-C5-C6-C7
21	42	509	CL7	C3-C5-C6-C7
21	43	403	CL7	C3-C5-C6-C7
23	1B	617	8CT	C12-C13-C14-C15
23	1B	618	8CT	C12-C13-C14-C15
23	1B	618	8CT	C16-C17-C18-C19
23	1B	618	8CT	C18-C19-C20-C21
23	1C	515	8CT	C23-C24-C25-C26
23	1C	518	8CT	C12-C13-C14-C15
23	2B	618	8CT	C12-C13-C14-C15
23	2B	619	8CT	C12-C13-C14-C15
23	2B	619	8CT	C16-C17-C18-C19
23	2B	619	8CT	C18-C19-C20-C21
23	2C	515	8CT	C23-C24-C25-C26
23	2C	518	8CT	C12-C13-C14-C15
23	3B	617	8CT	C12-C13-C14-C15
23	3B	618	8CT	C12-C13-C14-C15
23	3B	618	8CT	C16-C17-C18-C19
23	3B	618	8CT	C18-C19-C20-C21
23	3C	515	8CT	C23-C24-C25-C26
23	3C	518	8CT	C12-C13-C14-C15
23	4B	618	8CT	C12-C13-C14-C15
23	4B	619	8CT	C12-C13-C14-C15
23	4B	619	8CT	C16-C17-C18-C19
23	4B	619	8CT	C18-C19-C20-C21
23	4C	515	8CT	C23-C24-C25-C26
23	4C	518	8CT	C12-C13-C14-C15
32	12	524	ZEX	C9-C10-C11-C12
32	13	519	ZEX	C29-C30-C31-C32
32	13	525	ZEX	C33-C34-C35-C15
32	14	420	ZEX	C29-C30-C31-C32
32	22	524	ZEX	C9-C10-C11-C12
32	23	401	ZEX	C33-C34-C35-C15
32	23	420	ZEX	C29-C30-C31-C32
32	24	420	ZEX	C29-C30-C31-C32
32	32	524	ZEX	C9-C10-C11-C12
32	33	519	ZEX	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	33	525	ZEX	C33-C34-C35-C15
32	34	420	ZEX	C29-C30-C31-C32
32	42	524	ZEX	C9-C10-C11-C12
32	43	401	ZEX	C33-C34-C35-C15
32	43	420	ZEX	C29-C30-C31-C32
32	44	420	ZEX	C29-C30-C31-C32
21	11	419	CL7	C2A-CAA-CBA-CGA
21	14	406	CL7	C2A-CAA-CBA-CGA
21	21	419	CL7	C2A-CAA-CBA-CGA
21	24	406	CL7	C2A-CAA-CBA-CGA
21	34	406	CL7	C2A-CAA-CBA-CGA
21	44	406	CL7	C2A-CAA-CBA-CGA
21	1C	504	CL7	O1D-CGD-O2D-CED
21	12	509	CL7	O1D-CGD-O2D-CED
21	12	517	CL7	O1D-CGD-O2D-CED
21	14	409	CL7	O1D-CGD-O2D-CED
21	2C	504	CL7	O1D-CGD-O2D-CED
21	22	509	CL7	O1D-CGD-O2D-CED
21	22	517	CL7	O1D-CGD-O2D-CED
21	21	403	CL7	O1D-CGD-O2D-CED
21	24	409	CL7	O1D-CGD-O2D-CED
21	3C	504	CL7	O1D-CGD-O2D-CED
21	32	509	CL7	O1D-CGD-O2D-CED
21	32	517	CL7	O1D-CGD-O2D-CED
21	31	403	CL7	O1D-CGD-O2D-CED
21	34	409	CL7	O1D-CGD-O2D-CED
21	4C	504	CL7	O1D-CGD-O2D-CED
21	42	509	CL7	O1D-CGD-O2D-CED
21	42	517	CL7	O1D-CGD-O2D-CED
21	41	403	CL7	O1D-CGD-O2D-CED
21	44	409	CL7	O1D-CGD-O2D-CED
21	1C	505	CL7	C5-C6-C7-C8
21	1C	507	CL7	C5-C6-C7-C8
21	1C	510	CL7	C10-C11-C12-C13
21	11	403	CL7	C5-C6-C7-C8
21	11	404	CL7	C8-C10-C11-C12
21	2C	505	CL7	C5-C6-C7-C8
21	2C	507	CL7	C5-C6-C7-C8
21	2C	510	CL7	C10-C11-C12-C13
21	21	403	CL7	C5-C6-C7-C8
21	21	404	CL7	C8-C10-C11-C12
21	3C	505	CL7	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3C	507	CL7	C5-C6-C7-C8
21	3C	510	CL7	C10-C11-C12-C13
21	31	403	CL7	C5-C6-C7-C8
21	31	404	CL7	C8-C10-C11-C12
21	4C	505	CL7	C5-C6-C7-C8
21	4C	507	CL7	C5-C6-C7-C8
21	4C	510	CL7	C10-C11-C12-C13
21	41	403	CL7	C5-C6-C7-C8
21	41	404	CL7	C8-C10-C11-C12
21	11	410	CL7	C8-C10-C11-C12
21	21	410	CL7	C8-C10-C11-C12
21	24	404	CL7	C5-C6-C7-C8
21	31	410	CL7	C8-C10-C11-C12
21	33	501	CL7	C13-C15-C16-C17
21	34	404	CL7	C5-C6-C7-C8
21	41	410	CL7	C8-C10-C11-C12
21	43	402	CL7	C13-C15-C16-C17
21	44	404	CL7	C5-C6-C7-C8
21	11	402	CL7	C3-C5-C6-C7
21	21	402	CL7	C3-C5-C6-C7
21	31	402	CL7	C3-C5-C6-C7
21	41	402	CL7	C3-C5-C6-C7
21	1B	610	CL7	C8-C10-C11-C12
21	1C	508	CL7	C5-C6-C7-C8
21	12	509	CL7	C13-C15-C16-C17
21	12	511	CL7	C5-C6-C7-C8
21	11	402	CL7	C10-C11-C12-C13
21	11	404	CL7	C5-C6-C7-C8
21	14	404	CL7	C5-C6-C7-C8
21	2B	611	CL7	C8-C10-C11-C12
21	2C	508	CL7	C5-C6-C7-C8
21	22	509	CL7	C5-C6-C7-C8
21	22	509	CL7	C13-C15-C16-C17
21	22	511	CL7	C5-C6-C7-C8
21	21	402	CL7	C10-C11-C12-C13
21	21	404	CL7	C5-C6-C7-C8
21	3B	610	CL7	C8-C10-C11-C12
21	3C	508	CL7	C5-C6-C7-C8
21	32	509	CL7	C13-C15-C16-C17
21	32	511	CL7	C5-C6-C7-C8
21	31	402	CL7	C10-C11-C12-C13
21	31	404	CL7	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4B	611	CL7	C8-C10-C11-C12
21	4C	508	CL7	C5-C6-C7-C8
21	42	509	CL7	C13-C15-C16-C17
21	42	511	CL7	C5-C6-C7-C8
21	41	402	CL7	C10-C11-C12-C13
21	41	404	CL7	C5-C6-C7-C8
21	1B	611	CL7	O1D-CGD-O2D-CED
21	3B	611	CL7	O1D-CGD-O2D-CED
21	4B	612	CL7	O1D-CGD-O2D-CED
21	2B	612	CL7	O1D-CGD-O2D-CED
21	1B	603	CL7	C8-C10-C11-C12
21	1B	614	CL7	C8-C10-C11-C12
21	1C	502	CL7	C8-C10-C11-C12
21	1C	510	CL7	C8-C10-C11-C12
21	12	501	CL7	C8-C10-C11-C12
21	12	509	CL7	C5-C6-C7-C8
21	11	403	CL7	C8-C10-C11-C12
21	11	406	CL7	C8-C10-C11-C12
21	13	501	CL7	C13-C15-C16-C17
21	14	405	CL7	C5-C6-C7-C8
21	2B	604	CL7	C8-C10-C11-C12
21	2B	615	CL7	C8-C10-C11-C12
21	2C	502	CL7	C8-C10-C11-C12
21	2C	510	CL7	C8-C10-C11-C12
21	22	501	CL7	C8-C10-C11-C12
21	21	403	CL7	C8-C10-C11-C12
21	21	406	CL7	C8-C10-C11-C12
21	23	402	CL7	C13-C15-C16-C17
21	24	405	CL7	C5-C6-C7-C8
21	3B	603	CL7	C8-C10-C11-C12
21	3B	614	CL7	C8-C10-C11-C12
21	3C	502	CL7	C8-C10-C11-C12
21	3C	510	CL7	C8-C10-C11-C12
21	32	501	CL7	C8-C10-C11-C12
21	32	509	CL7	C5-C6-C7-C8
21	31	403	CL7	C8-C10-C11-C12
21	31	406	CL7	C8-C10-C11-C12
21	34	405	CL7	C5-C6-C7-C8
21	4B	604	CL7	C8-C10-C11-C12
21	4B	615	CL7	C8-C10-C11-C12
21	4C	502	CL7	C8-C10-C11-C12
21	4C	510	CL7	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	501	CL7	C8-C10-C11-C12
21	42	509	CL7	C5-C6-C7-C8
21	41	403	CL7	C8-C10-C11-C12
21	41	406	CL7	C8-C10-C11-C12
21	44	405	CL7	C5-C6-C7-C8
21	1C	506	CL7	C5-C6-C7-C8
21	1C	508	CL7	C15-C16-C17-C18
21	12	505	CL7	C15-C16-C17-C18
21	12	510	CL7	C15-C16-C17-C18
21	14	404	CL7	C8-C10-C11-C12
21	2C	506	CL7	C5-C6-C7-C8
21	2C	508	CL7	C15-C16-C17-C18
21	22	505	CL7	C15-C16-C17-C18
21	22	510	CL7	C15-C16-C17-C18
21	3C	506	CL7	C5-C6-C7-C8
21	3C	508	CL7	C15-C16-C17-C18
21	32	505	CL7	C15-C16-C17-C18
21	32	510	CL7	C15-C16-C17-C18
21	34	404	CL7	C8-C10-C11-C12
21	4C	506	CL7	C5-C6-C7-C8
21	4C	508	CL7	C15-C16-C17-C18
21	42	505	CL7	C15-C16-C17-C18
21	42	510	CL7	C15-C16-C17-C18
21	44	404	CL7	C8-C10-C11-C12
26	13	524	LHG	C3-O3-P-O6
26	23	425	LHG	C3-O3-P-O6
26	33	524	LHG	C3-O3-P-O6
26	43	425	LHG	C3-O3-P-O6
21	1B	608	CL7	C3-C5-C6-C7
21	2B	609	CL7	C3-C5-C6-C7
21	3B	608	CL7	C3-C5-C6-C7
21	4B	609	CL7	C3-C5-C6-C7
21	1B	616	CL7	CBD-CGD-O2D-CED
21	2B	617	CL7	CBD-CGD-O2D-CED
21	3B	616	CL7	CBD-CGD-O2D-CED
21	4B	617	CL7	CBD-CGD-O2D-CED
21	1B	602	CL7	C5-C6-C7-C8
21	1C	503	CL7	C10-C11-C12-C13
21	12	516	CL7	C15-C16-C17-C18
21	12	517	CL7	C8-C10-C11-C12
21	2B	603	CL7	C5-C6-C7-C8
21	2C	503	CL7	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	22	516	CL7	C15-C16-C17-C18
21	22	517	CL7	C8-C10-C11-C12
21	24	404	CL7	C8-C10-C11-C12
21	3B	602	CL7	C5-C6-C7-C8
21	3C	503	CL7	C10-C11-C12-C13
21	32	516	CL7	C15-C16-C17-C18
21	32	517	CL7	C8-C10-C11-C12
21	4B	603	CL7	C5-C6-C7-C8
21	4C	503	CL7	C10-C11-C12-C13
21	42	516	CL7	C15-C16-C17-C18
21	42	517	CL7	C8-C10-C11-C12
32	13	525	ZEX	C25-C26-C27-C28
32	14	403	ZEX	C25-C26-C27-C28
32	14	418	ZEX	C25-C26-C27-C28
32	14	420	ZEX	C25-C26-C27-C28
32	23	401	ZEX	C25-C26-C27-C28
32	24	403	ZEX	C25-C26-C27-C28
32	24	418	ZEX	C25-C26-C27-C28
32	24	420	ZEX	C25-C26-C27-C28
32	33	525	ZEX	C25-C26-C27-C28
32	34	403	ZEX	C25-C26-C27-C28
32	34	418	ZEX	C25-C26-C27-C28
32	34	420	ZEX	C25-C26-C27-C28
32	43	401	ZEX	C25-C26-C27-C28
32	44	403	ZEX	C25-C26-C27-C28
32	44	418	ZEX	C25-C26-C27-C28
32	44	420	ZEX	C25-C26-C27-C28
26	2A	408	LHG	C1-C2-C3-O3
26	3A	408	LHG	C1-C2-C3-O3
21	13	501	CL7	C4-C3-C5-C6
21	13	505	CL7	C4-C3-C5-C6
21	23	402	CL7	C4-C3-C5-C6
21	23	406	CL7	C4-C3-C5-C6
21	32	503	CL7	C4-C3-C5-C6
21	33	501	CL7	C4-C3-C5-C6
21	33	505	CL7	C4-C3-C5-C6
21	42	503	CL7	C4-C3-C5-C6
21	43	402	CL7	C4-C3-C5-C6
21	43	406	CL7	C4-C3-C5-C6
21	13	512	CL7	C2-C3-C5-C6
21	23	413	CL7	C2-C3-C5-C6
21	33	512	CL7	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	413	CL7	C2-C3-C5-C6
21	1C	510	CL7	C15-C16-C17-C18
21	13	507	CL7	C13-C15-C16-C17
21	14	411	CL7	C13-C15-C16-C17
21	2C	510	CL7	C15-C16-C17-C18
21	23	408	CL7	C13-C15-C16-C17
21	24	411	CL7	C13-C15-C16-C17
21	3C	510	CL7	C15-C16-C17-C18
21	33	507	CL7	C13-C15-C16-C17
21	34	411	CL7	C13-C15-C16-C17
21	4C	510	CL7	C15-C16-C17-C18
21	43	408	CL7	C13-C15-C16-C17
21	44	411	CL7	C13-C15-C16-C17
21	1D	402	CL7	C2A-CAA-CBA-CGA
21	2D	402	CL7	C2A-CAA-CBA-CGA
21	3D	402	CL7	C2A-CAA-CBA-CGA
21	4D	402	CL7	C2A-CAA-CBA-CGA
21	12	518	CL7	C16-C17-C18-C19
21	22	518	CL7	C16-C17-C18-C19
21	32	518	CL7	C16-C17-C18-C19
21	42	518	CL7	C16-C17-C18-C19
21	1B	607	CL7	C3-C5-C6-C7
21	1B	612	CL7	C3-C5-C6-C7
21	12	517	CL7	C3-C5-C6-C7
21	2B	608	CL7	C3-C5-C6-C7
21	2B	613	CL7	C3-C5-C6-C7
21	22	517	CL7	C3-C5-C6-C7
21	3B	607	CL7	C3-C5-C6-C7
21	3B	612	CL7	C3-C5-C6-C7
21	32	517	CL7	C3-C5-C6-C7
21	4B	608	CL7	C3-C5-C6-C7
21	4B	613	CL7	C3-C5-C6-C7
21	42	517	CL7	C3-C5-C6-C7
23	14	402	8CT	C12-C13-C14-C15
23	24	402	8CT	C12-C13-C14-C15
23	34	402	8CT	C12-C13-C14-C15
23	44	402	8CT	C12-C13-C14-C15
32	12	522	ZEX	C29-C30-C31-C32
32	14	403	ZEX	C29-C30-C31-C32
32	22	522	ZEX	C29-C30-C31-C32
32	24	403	ZEX	C29-C30-C31-C32
32	32	522	ZEX	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	34	403	ZEX	C29-C30-C31-C32
32	42	522	ZEX	C29-C30-C31-C32
32	44	403	ZEX	C29-C30-C31-C32
21	11	420	CL7	C4C-C3C-CAC-CBC
21	21	420	CL7	C4C-C3C-CAC-CBC
21	31	420	CL7	C4C-C3C-CAC-CBC
21	41	420	CL7	C4C-C3C-CAC-CBC
24	1A	405	LMG	C11-C10-O7-C8
24	2A	405	LMG	C11-C10-O7-C8
24	3A	405	LMG	C11-C10-O7-C8
24	4A	405	LMG	C11-C10-O7-C8
21	12	517	CL7	C10-C11-C12-C13
21	22	517	CL7	C10-C11-C12-C13
21	32	517	CL7	C10-C11-C12-C13
21	42	517	CL7	C10-C11-C12-C13
21	12	506	CL7	O1D-CGD-O2D-CED
21	22	506	CL7	O1D-CGD-O2D-CED
21	32	506	CL7	O1D-CGD-O2D-CED
21	42	506	CL7	O1D-CGD-O2D-CED
21	12	517	CL7	C15-C16-C17-C18
21	22	517	CL7	C15-C16-C17-C18
21	32	517	CL7	C15-C16-C17-C18
21	42	517	CL7	C15-C16-C17-C18
27	1C	516	DGD	C3B-C4B-C5B-C6B
27	4C	516	DGD	C3B-C4B-C5B-C6B
21	13	511	CL7	C3-C5-C6-C7
21	23	412	CL7	C3-C5-C6-C7
21	33	511	CL7	C3-C5-C6-C7
21	43	412	CL7	C3-C5-C6-C7
27	2C	516	DGD	C3B-C4B-C5B-C6B
27	3C	516	DGD	C3B-C4B-C5B-C6B
21	12	501	CL7	C5-C6-C7-C8
21	22	501	CL7	C5-C6-C7-C8
21	32	501	CL7	C5-C6-C7-C8
21	42	501	CL7	C5-C6-C7-C8
21	13	514	CL7	O1D-CGD-O2D-CED
21	23	415	CL7	O1D-CGD-O2D-CED
21	33	514	CL7	O1D-CGD-O2D-CED
21	43	415	CL7	O1D-CGD-O2D-CED
21	1B	611	CL7	C4-C3-C5-C6
21	2B	612	CL7	C4-C3-C5-C6
21	3B	611	CL7	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4B	612	CL7	C4-C3-C5-C6
21	1B	604	CL7	C11-C12-C13-C14
21	1B	608	CL7	C6-C7-C8-C9
21	1B	611	CL7	C6-C7-C8-C9
21	12	501	CL7	C11-C12-C13-C14
21	12	509	CL7	C6-C7-C8-C9
21	13	508	CL7	C11-C10-C8-C9
21	2B	609	CL7	C6-C7-C8-C9
21	2B	612	CL7	C6-C7-C8-C9
21	22	501	CL7	C11-C12-C13-C14
21	22	509	CL7	C6-C7-C8-C9
21	23	409	CL7	C11-C10-C8-C9
21	3B	604	CL7	C11-C12-C13-C14
21	3B	608	CL7	C6-C7-C8-C9
21	3B	611	CL7	C6-C7-C8-C9
21	32	501	CL7	C11-C12-C13-C14
21	32	509	CL7	C6-C7-C8-C9
21	33	508	CL7	C11-C10-C8-C9
21	4B	605	CL7	C11-C12-C13-C14
21	4B	609	CL7	C6-C7-C8-C9
21	4B	612	CL7	C6-C7-C8-C9
21	42	501	CL7	C11-C12-C13-C14
21	42	509	CL7	C6-C7-C8-C9
21	43	409	CL7	C11-C10-C8-C9
21	12	509	CL7	C8-C10-C11-C12
21	22	509	CL7	C8-C10-C11-C12
21	32	509	CL7	C8-C10-C11-C12
21	42	509	CL7	C8-C10-C11-C12
21	1B	615	CL7	C2A-CAA-CBA-CGA
21	2B	616	CL7	C2A-CAA-CBA-CGA
21	3B	615	CL7	C2A-CAA-CBA-CGA
21	4B	616	CL7	C2A-CAA-CBA-CGA
23	1B	618	8CT	C14-C15-C16-C39
23	1B	626	8CT	C10-C11-C12-C40
23	1D	406	8CT	C22-C21-C23-C24
23	2B	601	8CT	C10-C11-C12-C40
23	2B	619	8CT	C14-C15-C16-C39
23	2D	406	8CT	C22-C21-C23-C24
23	3B	618	8CT	C14-C15-C16-C39
23	3B	626	8CT	C10-C11-C12-C40
23	3D	406	8CT	C22-C21-C23-C24
23	4B	601	8CT	C10-C11-C12-C40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4B	619	8CT	C14-C15-C16-C39
23	4D	406	8CT	C22-C21-C23-C24
32	12	520	ZEX	C7-C8-C9-C19
32	11	422	ZEX	C7-C8-C9-C19
32	14	419	ZEX	C7-C8-C9-C19
32	14	420	ZEX	C31-C32-C33-C40
32	22	520	ZEX	C7-C8-C9-C19
32	21	422	ZEX	C7-C8-C9-C19
32	24	419	ZEX	C7-C8-C9-C19
32	24	420	ZEX	C31-C32-C33-C40
32	32	520	ZEX	C7-C8-C9-C19
32	31	422	ZEX	C7-C8-C9-C19
32	34	419	ZEX	C7-C8-C9-C19
32	34	420	ZEX	C31-C32-C33-C40
32	42	520	ZEX	C7-C8-C9-C19
32	41	422	ZEX	C7-C8-C9-C19
32	44	419	ZEX	C7-C8-C9-C19
32	44	420	ZEX	C31-C32-C33-C40
23	1B	618	8CT	C14-C15-C16-C17
23	1B	626	8CT	C10-C11-C12-C13
23	1C	514	8CT	C25-C26-C28-C29
23	1D	406	8CT	C20-C21-C23-C24
23	2B	601	8CT	C10-C11-C12-C13
23	2B	619	8CT	C14-C15-C16-C17
23	2C	514	8CT	C25-C26-C28-C29
23	2D	406	8CT	C20-C21-C23-C24
23	3B	618	8CT	C14-C15-C16-C17
23	3B	626	8CT	C10-C11-C12-C13
23	3C	514	8CT	C25-C26-C28-C29
23	3D	406	8CT	C20-C21-C23-C24
23	4B	601	8CT	C10-C11-C12-C13
23	4B	619	8CT	C14-C15-C16-C17
23	4C	514	8CT	C25-C26-C28-C29
23	4D	406	8CT	C20-C21-C23-C24
32	13	520	ZEX	C7-C8-C9-C10
32	14	420	ZEX	C31-C32-C33-C34
32	23	421	ZEX	C7-C8-C9-C10
32	24	420	ZEX	C31-C32-C33-C34
32	33	520	ZEX	C7-C8-C9-C10
32	34	420	ZEX	C31-C32-C33-C34
32	43	421	ZEX	C7-C8-C9-C10
32	44	420	ZEX	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	518	CL7	C16-C17-C18-C20
21	22	518	CL7	C16-C17-C18-C20
21	32	518	CL7	C16-C17-C18-C20
21	42	518	CL7	C16-C17-C18-C20
21	1D	402	CL7	O1D-CGD-O2D-CED
21	2D	402	CL7	O1D-CGD-O2D-CED
21	3D	402	CL7	O1D-CGD-O2D-CED
21	4D	402	CL7	O1D-CGD-O2D-CED
21	14	406	CL7	CBD-CGD-O2D-CED
21	24	406	CL7	CBD-CGD-O2D-CED
21	34	406	CL7	CBD-CGD-O2D-CED
21	44	406	CL7	CBD-CGD-O2D-CED
21	12	503	CL7	O1D-CGD-O2D-CED
21	2A	407	CL7	O1D-CGD-O2D-CED
21	3A	407	CL7	O1D-CGD-O2D-CED
21	32	503	CL7	O1D-CGD-O2D-CED
21	4A	407	CL7	O1D-CGD-O2D-CED
21	1B	605	CL7	C10-C11-C12-C13
21	1B	612	CL7	C13-C15-C16-C17
21	2B	606	CL7	C10-C11-C12-C13
21	2B	613	CL7	C13-C15-C16-C17
21	21	402	CL7	C8-C10-C11-C12
21	3B	605	CL7	C10-C11-C12-C13
21	3B	612	CL7	C13-C15-C16-C17
21	31	402	CL7	C8-C10-C11-C12
21	4B	606	CL7	C10-C11-C12-C13
21	4B	613	CL7	C13-C15-C16-C17
21	1C	505	CL7	O1D-CGD-O2D-CED
21	2C	505	CL7	O1D-CGD-O2D-CED
21	22	503	CL7	O1D-CGD-O2D-CED
21	3C	505	CL7	O1D-CGD-O2D-CED
21	4C	505	CL7	O1D-CGD-O2D-CED
21	42	503	CL7	O1D-CGD-O2D-CED
21	1A	407	CL7	O1D-CGD-O2D-CED
21	1B	614	CL7	C3A-C2A-CAA-CBA
21	1C	503	CL7	C3A-C2A-CAA-CBA
21	1C	504	CL7	C3A-C2A-CAA-CBA
21	12	507	CL7	C3A-C2A-CAA-CBA
21	12	510	CL7	C3A-C2A-CAA-CBA
21	12	512	CL7	C3A-C2A-CAA-CBA
21	12	513	CL7	C3A-C2A-CAA-CBA
21	13	504	CL7	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	13	512	CL7	C3A-C2A-CAA-CBA
21	14	412	CL7	C3A-C2A-CAA-CBA
21	14	414	CL7	C3A-C2A-CAA-CBA
21	2B	615	CL7	C3A-C2A-CAA-CBA
21	2C	503	CL7	C3A-C2A-CAA-CBA
21	2C	504	CL7	C3A-C2A-CAA-CBA
21	22	507	CL7	C3A-C2A-CAA-CBA
21	22	510	CL7	C3A-C2A-CAA-CBA
21	22	512	CL7	C3A-C2A-CAA-CBA
21	22	513	CL7	C3A-C2A-CAA-CBA
21	23	405	CL7	C3A-C2A-CAA-CBA
21	23	413	CL7	C3A-C2A-CAA-CBA
21	24	412	CL7	C3A-C2A-CAA-CBA
21	24	414	CL7	C3A-C2A-CAA-CBA
21	3B	614	CL7	C3A-C2A-CAA-CBA
21	3C	503	CL7	C3A-C2A-CAA-CBA
21	3C	504	CL7	C3A-C2A-CAA-CBA
21	32	507	CL7	C3A-C2A-CAA-CBA
21	32	510	CL7	C3A-C2A-CAA-CBA
21	32	512	CL7	C3A-C2A-CAA-CBA
21	32	513	CL7	C3A-C2A-CAA-CBA
21	33	504	CL7	C3A-C2A-CAA-CBA
21	33	512	CL7	C3A-C2A-CAA-CBA
21	34	412	CL7	C3A-C2A-CAA-CBA
21	34	414	CL7	C3A-C2A-CAA-CBA
21	4B	615	CL7	C3A-C2A-CAA-CBA
21	4C	503	CL7	C3A-C2A-CAA-CBA
21	4C	504	CL7	C3A-C2A-CAA-CBA
21	42	507	CL7	C3A-C2A-CAA-CBA
21	42	510	CL7	C3A-C2A-CAA-CBA
21	42	512	CL7	C3A-C2A-CAA-CBA
21	42	513	CL7	C3A-C2A-CAA-CBA
21	43	405	CL7	C3A-C2A-CAA-CBA
21	43	413	CL7	C3A-C2A-CAA-CBA
21	44	412	CL7	C3A-C2A-CAA-CBA
21	44	414	CL7	C3A-C2A-CAA-CBA
21	11	402	CL7	C8-C10-C11-C12
21	41	402	CL7	C8-C10-C11-C12
23	1C	515	8CT	C12-C13-C14-C15
23	2C	515	8CT	C12-C13-C14-C15
23	3C	515	8CT	C12-C13-C14-C15
23	4C	515	8CT	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1C	501	CL7	C16-C17-C18-C19
21	2C	501	CL7	C16-C17-C18-C19
21	3C	501	CL7	C16-C17-C18-C19
21	4C	501	CL7	C16-C17-C18-C19
27	1C	516	DGD	CCB-CDB-CEB-CFB
27	2C	516	DGD	CCB-CDB-CEB-CFB
27	3C	516	DGD	CCB-CDB-CEB-CFB
27	4C	516	DGD	CCB-CDB-CEB-CFB
21	1C	506	CL7	O2A-C1-C2-C3
21	1C	507	CL7	O2A-C1-C2-C3
21	2C	506	CL7	O2A-C1-C2-C3
21	2C	507	CL7	O2A-C1-C2-C3
21	3C	506	CL7	O2A-C1-C2-C3
21	3C	507	CL7	O2A-C1-C2-C3
21	4C	506	CL7	O2A-C1-C2-C3
21	4C	507	CL7	O2A-C1-C2-C3
21	1A	407	CL7	C3-C5-C6-C7
21	2A	407	CL7	C3-C5-C6-C7
21	3A	407	CL7	C3-C5-C6-C7
21	4A	407	CL7	C3-C5-C6-C7
21	1C	505	CL7	C10-C11-C12-C13
21	2C	505	CL7	C10-C11-C12-C13
21	4C	505	CL7	C10-C11-C12-C13
21	12	503	CL7	C4-C3-C5-C6
21	22	503	CL7	C4-C3-C5-C6
21	2B	612	CL7	C2-C3-C5-C6
21	3C	505	CL7	C10-C11-C12-C13
27	2C	516	DGD	C8A-C9A-CAA-CBA
27	4C	516	DGD	C8A-C9A-CAA-CBA
27	1C	516	DGD	C8A-C9A-CAA-CBA
27	3C	516	DGD	C8A-C9A-CAA-CBA
21	14	405	CL7	C10-C11-C12-C13
21	24	405	CL7	C10-C11-C12-C13
21	34	405	CL7	C10-C11-C12-C13
21	44	405	CL7	C10-C11-C12-C13
21	32	503	CL7	C3-C5-C6-C7
21	42	503	CL7	C3-C5-C6-C7
21	1A	401	CL7	C4C-C3C-CAC-CBC
21	2A	401	CL7	C4C-C3C-CAC-CBC
21	3A	401	CL7	C4C-C3C-CAC-CBC
21	4A	401	CL7	C4C-C3C-CAC-CBC
27	1C	516	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	2C	516	DGD	O6E-C5E-C6E-O5E
27	3C	516	DGD	O6E-C5E-C6E-O5E
27	4C	516	DGD	O6E-C5E-C6E-O5E
24	1A	405	LMG	O9-C10-O7-C8
24	2A	405	LMG	O9-C10-O7-C8
24	3A	405	LMG	O9-C10-O7-C8
24	4A	405	LMG	O9-C10-O7-C8
21	12	518	CL7	C10-C11-C12-C13
21	22	518	CL7	C10-C11-C12-C13
21	32	518	CL7	C10-C11-C12-C13
21	42	518	CL7	C10-C11-C12-C13
21	12	503	CL7	C3-C5-C6-C7
21	22	503	CL7	C3-C5-C6-C7
23	1B	626	8CT	C02-C03-C10-C11
23	1C	514	8CT	C04-C03-C10-C11
23	1C	518	8CT	C04-C03-C10-C11
23	1D	406	8CT	C02-C03-C10-C11
23	1K	101	8CT	C04-C03-C10-C11
23	2B	601	8CT	C02-C03-C10-C11
23	2C	514	8CT	C04-C03-C10-C11
23	2C	518	8CT	C04-C03-C10-C11
23	2D	406	8CT	C02-C03-C10-C11
23	2K	101	8CT	C04-C03-C10-C11
23	3B	626	8CT	C02-C03-C10-C11
23	3C	514	8CT	C04-C03-C10-C11
23	3C	518	8CT	C04-C03-C10-C11
23	3D	406	8CT	C02-C03-C10-C11
23	3K	101	8CT	C04-C03-C10-C11
23	4B	601	8CT	C02-C03-C10-C11
23	4C	514	8CT	C04-C03-C10-C11
23	4C	518	8CT	C04-C03-C10-C11
23	4D	406	8CT	C02-C03-C10-C11
23	4K	101	8CT	C04-C03-C10-C11
32	12	519	ZEX	C5-C6-C7-C8
32	12	520	ZEX	C5-C6-C7-C8
32	12	524	ZEX	C1-C6-C7-C8
32	12	524	ZEX	C5-C6-C7-C8
32	11	421	ZEX	C1-C6-C7-C8
32	11	421	ZEX	C5-C6-C7-C8
32	11	422	ZEX	C1-C6-C7-C8
32	11	422	ZEX	C5-C6-C7-C8
32	13	519	ZEX	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	13	519	ZEX	C5-C6-C7-C8
32	13	522	ZEX	C5-C6-C7-C8
32	14	403	ZEX	C1-C6-C7-C8
32	22	519	ZEX	C5-C6-C7-C8
32	22	520	ZEX	C5-C6-C7-C8
32	22	524	ZEX	C1-C6-C7-C8
32	22	524	ZEX	C5-C6-C7-C8
32	21	421	ZEX	C1-C6-C7-C8
32	21	421	ZEX	C5-C6-C7-C8
32	21	422	ZEX	C1-C6-C7-C8
32	21	422	ZEX	C5-C6-C7-C8
32	23	420	ZEX	C1-C6-C7-C8
32	23	420	ZEX	C5-C6-C7-C8
32	23	423	ZEX	C5-C6-C7-C8
32	24	403	ZEX	C1-C6-C7-C8
32	32	519	ZEX	C5-C6-C7-C8
32	32	520	ZEX	C5-C6-C7-C8
32	32	524	ZEX	C1-C6-C7-C8
32	32	524	ZEX	C5-C6-C7-C8
32	31	421	ZEX	C1-C6-C7-C8
32	31	421	ZEX	C5-C6-C7-C8
32	31	422	ZEX	C1-C6-C7-C8
32	31	422	ZEX	C5-C6-C7-C8
32	33	519	ZEX	C1-C6-C7-C8
32	33	519	ZEX	C5-C6-C7-C8
32	33	522	ZEX	C5-C6-C7-C8
32	34	403	ZEX	C1-C6-C7-C8
32	42	519	ZEX	C5-C6-C7-C8
32	42	520	ZEX	C5-C6-C7-C8
32	42	524	ZEX	C1-C6-C7-C8
32	42	524	ZEX	C5-C6-C7-C8
32	41	421	ZEX	C1-C6-C7-C8
32	41	421	ZEX	C5-C6-C7-C8
32	41	422	ZEX	C1-C6-C7-C8
32	41	422	ZEX	C5-C6-C7-C8
32	43	420	ZEX	C1-C6-C7-C8
32	43	420	ZEX	C5-C6-C7-C8
32	43	423	ZEX	C5-C6-C7-C8
32	44	403	ZEX	C1-C6-C7-C8
21	14	406	CL7	C10-C11-C12-C13
21	24	406	CL7	C10-C11-C12-C13
21	33	508	CL7	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	34	406	CL7	C10-C11-C12-C13
21	44	406	CL7	C10-C11-C12-C13
21	1A	407	CL7	C10-C11-C12-C13
21	13	508	CL7	C5-C6-C7-C8
21	2A	407	CL7	C10-C11-C12-C13
21	23	409	CL7	C5-C6-C7-C8
21	3A	407	CL7	C10-C11-C12-C13
21	4A	407	CL7	C10-C11-C12-C13
21	43	409	CL7	C5-C6-C7-C8
21	1C	510	CL7	O1D-CGD-O2D-CED
21	3C	510	CL7	O1D-CGD-O2D-CED
21	1B	608	CL7	C6-C7-C8-C10
21	1B	611	CL7	C2-C3-C5-C6
21	1B	611	CL7	C6-C7-C8-C10
21	1B	612	CL7	C12-C13-C15-C16
21	1C	508	CL7	C11-C10-C8-C7
21	1C	510	CL7	C6-C7-C8-C10
21	1C	510	CL7	C11-C10-C8-C7
21	12	505	CL7	C11-C12-C13-C15
21	12	505	CL7	C12-C13-C15-C16
21	12	511	CL7	C6-C7-C8-C10
21	12	517	CL7	C12-C13-C15-C16
21	11	418	CL7	C11-C10-C8-C7
21	13	504	CL7	C11-C10-C8-C7
21	13	508	CL7	C11-C10-C8-C7
21	2B	609	CL7	C6-C7-C8-C10
21	2B	612	CL7	C6-C7-C8-C10
21	2B	613	CL7	C12-C13-C15-C16
21	2C	508	CL7	C11-C10-C8-C7
21	2C	510	CL7	C6-C7-C8-C10
21	2C	510	CL7	C11-C10-C8-C7
21	22	505	CL7	C11-C12-C13-C15
21	22	505	CL7	C12-C13-C15-C16
21	22	511	CL7	C6-C7-C8-C10
21	22	517	CL7	C12-C13-C15-C16
21	21	418	CL7	C11-C10-C8-C7
21	23	405	CL7	C11-C10-C8-C7
21	23	409	CL7	C11-C10-C8-C7
21	3B	608	CL7	C6-C7-C8-C10
21	3B	611	CL7	C2-C3-C5-C6
21	3B	611	CL7	C6-C7-C8-C10
21	3B	612	CL7	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3C	508	CL7	C11-C10-C8-C7
21	3C	510	CL7	C6-C7-C8-C10
21	3C	510	CL7	C11-C10-C8-C7
21	32	505	CL7	C11-C12-C13-C15
21	32	505	CL7	C12-C13-C15-C16
21	32	511	CL7	C6-C7-C8-C10
21	32	517	CL7	C12-C13-C15-C16
21	31	418	CL7	C11-C10-C8-C7
21	33	504	CL7	C11-C10-C8-C7
21	33	508	CL7	C11-C10-C8-C7
21	4B	609	CL7	C6-C7-C8-C10
21	4B	612	CL7	C2-C3-C5-C6
21	4B	612	CL7	C6-C7-C8-C10
21	4B	613	CL7	C12-C13-C15-C16
21	4C	508	CL7	C11-C10-C8-C7
21	4C	510	CL7	C6-C7-C8-C10
21	4C	510	CL7	C11-C10-C8-C7
21	42	505	CL7	C11-C12-C13-C15
21	42	505	CL7	C12-C13-C15-C16
21	42	511	CL7	C6-C7-C8-C10
21	42	517	CL7	C12-C13-C15-C16
21	41	418	CL7	C11-C10-C8-C7
21	43	405	CL7	C11-C10-C8-C7
21	43	409	CL7	C11-C10-C8-C7
21	12	506	CL7	C8-C10-C11-C12
21	22	506	CL7	C8-C10-C11-C12
21	22	507	CL7	C8-C10-C11-C12
21	32	506	CL7	C8-C10-C11-C12
21	32	507	CL7	C8-C10-C11-C12
21	42	506	CL7	C8-C10-C11-C12
21	42	507	CL7	C8-C10-C11-C12
32	12	524	ZEX	C29-C30-C31-C32
32	14	420	ZEX	C33-C34-C35-C15
32	22	524	ZEX	C29-C30-C31-C32
32	24	420	ZEX	C33-C34-C35-C15
32	32	524	ZEX	C29-C30-C31-C32
32	34	420	ZEX	C33-C34-C35-C15
32	42	524	ZEX	C29-C30-C31-C32
32	44	420	ZEX	C33-C34-C35-C15
21	2C	510	CL7	O1D-CGD-O2D-CED
21	4C	510	CL7	O1D-CGD-O2D-CED
21	12	513	CL7	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	14	410	CL7	C2A-CAA-CBA-CGA
21	14	415	CL7	C2A-CAA-CBA-CGA
21	22	513	CL7	C2A-CAA-CBA-CGA
21	24	410	CL7	C2A-CAA-CBA-CGA
21	24	415	CL7	C2A-CAA-CBA-CGA
21	32	513	CL7	C2A-CAA-CBA-CGA
21	34	410	CL7	C2A-CAA-CBA-CGA
21	34	415	CL7	C2A-CAA-CBA-CGA
21	42	513	CL7	C2A-CAA-CBA-CGA
21	44	410	CL7	C2A-CAA-CBA-CGA
21	44	415	CL7	C2A-CAA-CBA-CGA
21	1B	603	CL7	C10-C11-C12-C13
21	1C	501	CL7	C13-C15-C16-C17
21	12	507	CL7	C8-C10-C11-C12
21	2B	604	CL7	C10-C11-C12-C13
21	2C	501	CL7	C13-C15-C16-C17
21	3B	603	CL7	C10-C11-C12-C13
21	3C	501	CL7	C13-C15-C16-C17
21	4B	604	CL7	C10-C11-C12-C13
21	4C	501	CL7	C13-C15-C16-C17
21	41	403	CL7	C10-C11-C12-C13
21	24	412	CL7	O1D-CGD-O2D-CED
21	34	412	CL7	O1D-CGD-O2D-CED
21	1C	506	CL7	C10-C11-C12-C13
21	11	403	CL7	C10-C11-C12-C13
21	2C	506	CL7	C10-C11-C12-C13
21	21	403	CL7	C10-C11-C12-C13
21	3C	506	CL7	C10-C11-C12-C13
21	31	403	CL7	C10-C11-C12-C13
21	4C	506	CL7	C10-C11-C12-C13
21	22	507	CL7	O1D-CGD-O2D-CED
21	32	507	CL7	O1D-CGD-O2D-CED
21	44	412	CL7	O1D-CGD-O2D-CED
21	11	418	CL7	C15-C16-C17-C18
21	21	418	CL7	C15-C16-C17-C18
21	41	418	CL7	C15-C16-C17-C18
21	12	507	CL7	O1D-CGD-O2D-CED
21	14	412	CL7	O1D-CGD-O2D-CED
21	42	507	CL7	O1D-CGD-O2D-CED
31	1F	101	HEM	C4B-C3B-CAB-CBB
31	1F	101	HEM	C4C-C3C-CAC-CBC
31	2F	101	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	2F	101	HEM	C4C-C3C-CAC-CBC
31	3F	101	HEM	C4B-C3B-CAB-CBB
31	3F	101	HEM	C4C-C3C-CAC-CBC
31	4F	101	HEM	C4B-C3B-CAB-CBB
31	4F	101	HEM	C4C-C3C-CAC-CBC
21	14	412	CL7	C13-C15-C16-C17
21	24	412	CL7	C13-C15-C16-C17
21	31	418	CL7	C15-C16-C17-C18
21	34	412	CL7	C13-C15-C16-C17
21	44	412	CL7	C13-C15-C16-C17
21	14	416	CL7	CBD-CGD-O2D-CED
21	24	416	CL7	CBD-CGD-O2D-CED
21	34	416	CL7	CBD-CGD-O2D-CED
21	44	416	CL7	CBD-CGD-O2D-CED
21	34	414	CL7	O1D-CGD-O2D-CED
21	14	414	CL7	O1D-CGD-O2D-CED
21	12	505	CL7	C10-C11-C12-C13
21	12	516	CL7	C5-C6-C7-C8
21	13	510	CL7	C8-C10-C11-C12
21	22	505	CL7	C10-C11-C12-C13
21	22	516	CL7	C5-C6-C7-C8
21	23	411	CL7	C8-C10-C11-C12
21	32	505	CL7	C10-C11-C12-C13
21	32	516	CL7	C5-C6-C7-C8
21	33	510	CL7	C8-C10-C11-C12
21	42	505	CL7	C10-C11-C12-C13
21	42	516	CL7	C5-C6-C7-C8
21	43	411	CL7	C8-C10-C11-C12
21	13	501	CL7	C2-C3-C5-C6
21	13	505	CL7	C2-C3-C5-C6
21	23	402	CL7	C2-C3-C5-C6
21	23	406	CL7	C2-C3-C5-C6
21	33	501	CL7	C2-C3-C5-C6
21	33	505	CL7	C2-C3-C5-C6
21	43	402	CL7	C2-C3-C5-C6
21	43	406	CL7	C2-C3-C5-C6
21	1A	407	CL7	C11-C10-C8-C9
21	1B	605	CL7	C14-C13-C15-C16
21	1B	612	CL7	C6-C7-C8-C9
21	1C	503	CL7	C11-C10-C8-C9
21	12	505	CL7	C11-C12-C13-C14
21	12	509	CL7	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	510	CL7	C14-C13-C15-C16
21	11	408	CL7	C14-C13-C15-C16
21	13	507	CL7	C14-C13-C15-C16
21	2A	407	CL7	C11-C10-C8-C9
21	2B	605	CL7	C11-C12-C13-C14
21	2B	606	CL7	C14-C13-C15-C16
21	2B	613	CL7	C6-C7-C8-C9
21	2C	503	CL7	C11-C10-C8-C9
21	22	505	CL7	C11-C12-C13-C14
21	22	509	CL7	C11-C12-C13-C14
21	22	510	CL7	C14-C13-C15-C16
21	21	408	CL7	C14-C13-C15-C16
21	23	408	CL7	C14-C13-C15-C16
21	3A	407	CL7	C11-C10-C8-C9
21	3B	605	CL7	C14-C13-C15-C16
21	3B	612	CL7	C6-C7-C8-C9
21	3C	503	CL7	C11-C10-C8-C9
21	32	505	CL7	C11-C12-C13-C14
21	32	509	CL7	C11-C12-C13-C14
21	32	510	CL7	C14-C13-C15-C16
21	31	408	CL7	C14-C13-C15-C16
21	33	507	CL7	C14-C13-C15-C16
21	4A	407	CL7	C11-C10-C8-C9
21	4B	606	CL7	C14-C13-C15-C16
21	4B	613	CL7	C6-C7-C8-C9
21	4C	503	CL7	C11-C10-C8-C9
21	42	505	CL7	C11-C12-C13-C14
21	42	509	CL7	C11-C12-C13-C14
21	42	510	CL7	C14-C13-C15-C16
21	41	408	CL7	C14-C13-C15-C16
21	43	408	CL7	C14-C13-C15-C16
21	24	414	CL7	O1D-CGD-O2D-CED
21	44	414	CL7	O1D-CGD-O2D-CED
21	3B	608	CL7	C2C-C3C-CAC-CBC
21	13	512	CL7	C3-C5-C6-C7
21	23	413	CL7	C3-C5-C6-C7
21	33	512	CL7	C3-C5-C6-C7
21	43	413	CL7	C3-C5-C6-C7
21	13	501	CL7	C2A-CAA-CBA-CGA
21	23	402	CL7	C2A-CAA-CBA-CGA
21	33	501	CL7	C2A-CAA-CBA-CGA
21	43	402	CL7	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2B	609	CL7	C2C-C3C-CAC-CBC
32	13	520	ZEX	C7-C8-C9-C19
32	23	421	ZEX	C7-C8-C9-C19
32	33	520	ZEX	C7-C8-C9-C19
32	43	421	ZEX	C7-C8-C9-C19
21	11	410	CL7	C5-C6-C7-C8
21	21	410	CL7	C5-C6-C7-C8
21	31	410	CL7	C5-C6-C7-C8
21	41	410	CL7	C5-C6-C7-C8
21	1B	608	CL7	C2C-C3C-CAC-CBC
21	4B	609	CL7	C2C-C3C-CAC-CBC
23	1C	515	8CT	C25-C26-C28-C29
23	2C	515	8CT	C25-C26-C28-C29
23	3C	515	8CT	C25-C26-C28-C29
23	4C	515	8CT	C25-C26-C28-C29
21	1B	609	CL7	C1A-C2A-CAA-CBA
21	1B	612	CL7	C1A-C2A-CAA-CBA
21	1B	614	CL7	C1A-C2A-CAA-CBA
21	1C	508	CL7	C1A-C2A-CAA-CBA
21	1C	510	CL7	C1A-C2A-CAA-CBA
21	1C	513	CL7	C1A-C2A-CAA-CBA
21	1D	402	CL7	C1A-C2A-CAA-CBA
21	12	501	CL7	C1A-C2A-CAA-CBA
21	12	507	CL7	C1A-C2A-CAA-CBA
21	12	510	CL7	C1A-C2A-CAA-CBA
21	12	511	CL7	C1A-C2A-CAA-CBA
21	12	512	CL7	C1A-C2A-CAA-CBA
21	12	516	CL7	C1A-C2A-CAA-CBA
21	11	417	CL7	C1A-C2A-CAA-CBA
21	11	418	CL7	C1A-C2A-CAA-CBA
21	13	503	CL7	C1A-C2A-CAA-CBA
21	13	514	CL7	C1A-C2A-CAA-CBA
21	13	516	CL7	C1A-C2A-CAA-CBA
21	14	404	CL7	C1A-C2A-CAA-CBA
21	14	414	CL7	C1A-C2A-CAA-CBA
21	2B	610	CL7	C1A-C2A-CAA-CBA
21	2B	613	CL7	C1A-C2A-CAA-CBA
21	2B	615	CL7	C1A-C2A-CAA-CBA
21	2C	508	CL7	C1A-C2A-CAA-CBA
21	2C	510	CL7	C1A-C2A-CAA-CBA
21	2C	513	CL7	C1A-C2A-CAA-CBA
21	2D	402	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	22	501	CL7	C1A-C2A-CAA-CBA
21	22	507	CL7	C1A-C2A-CAA-CBA
21	22	510	CL7	C1A-C2A-CAA-CBA
21	22	511	CL7	C1A-C2A-CAA-CBA
21	22	512	CL7	C1A-C2A-CAA-CBA
21	22	516	CL7	C1A-C2A-CAA-CBA
21	21	417	CL7	C1A-C2A-CAA-CBA
21	21	418	CL7	C1A-C2A-CAA-CBA
21	23	404	CL7	C1A-C2A-CAA-CBA
21	23	415	CL7	C1A-C2A-CAA-CBA
21	23	417	CL7	C1A-C2A-CAA-CBA
21	24	404	CL7	C1A-C2A-CAA-CBA
21	24	414	CL7	C1A-C2A-CAA-CBA
21	3B	609	CL7	C1A-C2A-CAA-CBA
21	3B	612	CL7	C1A-C2A-CAA-CBA
21	3B	614	CL7	C1A-C2A-CAA-CBA
21	3C	508	CL7	C1A-C2A-CAA-CBA
21	3C	510	CL7	C1A-C2A-CAA-CBA
21	3C	513	CL7	C1A-C2A-CAA-CBA
21	3D	402	CL7	C1A-C2A-CAA-CBA
21	32	501	CL7	C1A-C2A-CAA-CBA
21	32	507	CL7	C1A-C2A-CAA-CBA
21	32	510	CL7	C1A-C2A-CAA-CBA
21	32	511	CL7	C1A-C2A-CAA-CBA
21	32	512	CL7	C1A-C2A-CAA-CBA
21	32	516	CL7	C1A-C2A-CAA-CBA
21	31	417	CL7	C1A-C2A-CAA-CBA
21	31	418	CL7	C1A-C2A-CAA-CBA
21	33	503	CL7	C1A-C2A-CAA-CBA
21	33	514	CL7	C1A-C2A-CAA-CBA
21	33	516	CL7	C1A-C2A-CAA-CBA
21	34	404	CL7	C1A-C2A-CAA-CBA
21	34	414	CL7	C1A-C2A-CAA-CBA
21	4B	610	CL7	C1A-C2A-CAA-CBA
21	4B	613	CL7	C1A-C2A-CAA-CBA
21	4B	615	CL7	C1A-C2A-CAA-CBA
21	4C	508	CL7	C1A-C2A-CAA-CBA
21	4C	510	CL7	C1A-C2A-CAA-CBA
21	4C	513	CL7	C1A-C2A-CAA-CBA
21	4D	402	CL7	C1A-C2A-CAA-CBA
21	42	501	CL7	C1A-C2A-CAA-CBA
21	42	507	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	510	CL7	C1A-C2A-CAA-CBA
21	42	511	CL7	C1A-C2A-CAA-CBA
21	42	512	CL7	C1A-C2A-CAA-CBA
21	42	516	CL7	C1A-C2A-CAA-CBA
21	41	417	CL7	C1A-C2A-CAA-CBA
21	41	418	CL7	C1A-C2A-CAA-CBA
21	43	404	CL7	C1A-C2A-CAA-CBA
21	43	415	CL7	C1A-C2A-CAA-CBA
21	43	417	CL7	C1A-C2A-CAA-CBA
21	44	404	CL7	C1A-C2A-CAA-CBA
21	44	414	CL7	C1A-C2A-CAA-CBA
21	1C	503	CL7	C16-C17-C18-C20
21	2C	503	CL7	C16-C17-C18-C20
21	3C	503	CL7	C16-C17-C18-C20
21	4C	503	CL7	C16-C17-C18-C20
26	1B	625	LHG	C15-C16-C17-C18
26	2B	626	LHG	C15-C16-C17-C18
26	3B	625	LHG	C15-C16-C17-C18
26	4B	626	LHG	C15-C16-C17-C18
23	1K	101	8CT	C18-C19-C20-C21
23	2K	101	8CT	C18-C19-C20-C21
23	3K	101	8CT	C18-C19-C20-C21
23	4K	101	8CT	C18-C19-C20-C21
21	31	408	CL7	C4C-C3C-CAC-CBC
21	1C	510	CL7	C3-C5-C6-C7
21	2C	510	CL7	C3-C5-C6-C7
21	3C	510	CL7	C3-C5-C6-C7
21	4C	510	CL7	C3-C5-C6-C7
21	11	408	CL7	C4C-C3C-CAC-CBC
21	21	408	CL7	C4C-C3C-CAC-CBC
21	41	408	CL7	C4C-C3C-CAC-CBC
21	13	507	CL7	C5-C6-C7-C8
21	23	408	CL7	C5-C6-C7-C8
21	33	507	CL7	C5-C6-C7-C8
21	43	408	CL7	C5-C6-C7-C8
27	1B	624	DGD	C2A-C1A-O1G-C1G
27	2B	625	DGD	C2A-C1A-O1G-C1G
24	1D	410	LMG	O6-C5-C6-O5
24	2D	410	LMG	O6-C5-C6-O5
24	3D	410	LMG	O6-C5-C6-O5
24	4D	410	LMG	O6-C5-C6-O5
32	14	419	ZEX	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	24	419	ZEX	C25-C26-C27-C28
32	34	419	ZEX	C25-C26-C27-C28
32	44	419	ZEX	C25-C26-C27-C28
24	1B	621	LMG	C38-C39-C40-C41
24	2B	622	LMG	C38-C39-C40-C41
24	3B	621	LMG	C38-C39-C40-C41
24	4B	622	LMG	C38-C39-C40-C41
27	3B	624	DGD	C2A-C1A-O1G-C1G
27	4B	625	DGD	C2A-C1A-O1G-C1G
21	11	402	CL7	C4-C3-C5-C6
21	21	402	CL7	C4-C3-C5-C6
21	31	402	CL7	C4-C3-C5-C6
21	41	402	CL7	C4-C3-C5-C6
21	12	503	CL7	C2-C3-C5-C6
21	14	417	CL7	C3A-C2A-CAA-CBA
21	22	503	CL7	C2-C3-C5-C6
21	24	417	CL7	C3A-C2A-CAA-CBA
21	32	503	CL7	C2-C3-C5-C6
21	34	417	CL7	C3A-C2A-CAA-CBA
21	44	417	CL7	C3A-C2A-CAA-CBA
21	12	517	CL7	C2A-CAA-CBA-CGA
21	22	517	CL7	C2A-CAA-CBA-CGA
21	32	517	CL7	C2A-CAA-CBA-CGA
21	42	517	CL7	C2A-CAA-CBA-CGA
21	13	507	CL7	C3-C5-C6-C7
21	23	408	CL7	C3-C5-C6-C7
21	33	507	CL7	C3-C5-C6-C7
21	43	408	CL7	C3-C5-C6-C7
24	1A	405	LMG	O1-C7-C8-C9
24	1B	621	LMG	C7-C8-C9-O8
24	2A	405	LMG	O1-C7-C8-C9
24	2B	622	LMG	C7-C8-C9-O8
24	3A	405	LMG	O1-C7-C8-C9
24	3B	621	LMG	C7-C8-C9-O8
24	4A	405	LMG	O1-C7-C8-C9
24	4B	622	LMG	C7-C8-C9-O8
25	13	523	SQD	C45-C44-O6-C1
25	23	424	SQD	C45-C44-O6-C1
25	33	523	SQD	C45-C44-O6-C1
25	43	424	SQD	C45-C44-O6-C1
21	11	415	CL7	C4C-C3C-CAC-CBC
21	21	415	CL7	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	31	415	CL7	C4C-C3C-CAC-CBC
21	41	415	CL7	C4C-C3C-CAC-CBC
21	14	414	CL7	C5-C6-C7-C8
21	34	414	CL7	C5-C6-C7-C8
21	1D	404	CL7	O1D-CGD-O2D-CED
21	4D	404	CL7	O1D-CGD-O2D-CED
24	11	401	LMG	O6-C5-C6-O5
24	21	401	LMG	O6-C5-C6-O5
24	31	401	LMG	O6-C5-C6-O5
24	41	401	LMG	O6-C5-C6-O5
21	24	414	CL7	C5-C6-C7-C8
21	44	414	CL7	C5-C6-C7-C8
21	12	503	CL7	C10-C11-C12-C13
21	22	503	CL7	C10-C11-C12-C13
21	32	503	CL7	C10-C11-C12-C13
21	42	503	CL7	C10-C11-C12-C13
21	1C	501	CL7	C2B-C3B-CAB-OBB
21	1C	503	CL7	C2B-C3B-CAB-OBB
21	1C	512	CL7	C2B-C3B-CAB-OBB
21	1D	404	CL7	C2B-C3B-CAB-OBB
21	12	508	CL7	C2B-C3B-CAB-OBB
21	12	516	CL7	C2B-C3B-CAB-OBB
21	11	402	CL7	C2B-C3B-CAB-OBB
21	14	405	CL7	C2B-C3B-CAB-OBB
21	2C	501	CL7	C2B-C3B-CAB-OBB
21	2C	503	CL7	C2B-C3B-CAB-OBB
21	2C	512	CL7	C2B-C3B-CAB-OBB
21	2D	404	CL7	C2B-C3B-CAB-OBB
21	22	508	CL7	C2B-C3B-CAB-OBB
21	22	516	CL7	C2B-C3B-CAB-OBB
21	21	402	CL7	C2B-C3B-CAB-OBB
21	24	405	CL7	C2B-C3B-CAB-OBB
21	3C	501	CL7	C2B-C3B-CAB-OBB
21	3C	503	CL7	C2B-C3B-CAB-OBB
21	3C	512	CL7	C2B-C3B-CAB-OBB
21	3D	404	CL7	C2B-C3B-CAB-OBB
21	32	508	CL7	C2B-C3B-CAB-OBB
21	32	516	CL7	C2B-C3B-CAB-OBB
21	31	402	CL7	C2B-C3B-CAB-OBB
21	34	405	CL7	C2B-C3B-CAB-OBB
21	4C	501	CL7	C2B-C3B-CAB-OBB
21	4C	503	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4C	512	CL7	C2B-C3B-CAB-OBB
21	4D	404	CL7	C2B-C3B-CAB-OBB
21	42	508	CL7	C2B-C3B-CAB-OBB
21	42	516	CL7	C2B-C3B-CAB-OBB
21	41	402	CL7	C2B-C3B-CAB-OBB
21	44	405	CL7	C2B-C3B-CAB-OBB
21	2D	404	CL7	O1D-CGD-O2D-CED
21	3D	404	CL7	O1D-CGD-O2D-CED
21	12	512	CL7	C10-C11-C12-C13
21	22	512	CL7	C10-C11-C12-C13
21	42	503	CL7	C2-C3-C5-C6
21	14	415	CL7	CBD-CGD-O2D-CED
21	24	415	CL7	CBD-CGD-O2D-CED
21	34	415	CL7	CBD-CGD-O2D-CED
21	44	415	CL7	CBD-CGD-O2D-CED
21	1B	609	CL7	C13-C15-C16-C17
21	2B	610	CL7	C13-C15-C16-C17
21	3B	609	CL7	C13-C15-C16-C17
21	4B	610	CL7	C13-C15-C16-C17
21	1B	606	CL7	C4B-C3B-CAB-OBB
21	1B	613	CL7	C4B-C3B-CAB-OBB
21	11	405	CL7	C4B-C3B-CAB-OBB
21	14	415	CL7	C4B-C3B-CAB-OBB
21	2B	607	CL7	C4B-C3B-CAB-OBB
21	2B	614	CL7	C4B-C3B-CAB-OBB
21	21	405	CL7	C4B-C3B-CAB-OBB
21	24	415	CL7	C4B-C3B-CAB-OBB
21	3B	606	CL7	C4B-C3B-CAB-OBB
21	3B	613	CL7	C4B-C3B-CAB-OBB
21	31	405	CL7	C4B-C3B-CAB-OBB
21	34	415	CL7	C4B-C3B-CAB-OBB
21	4B	607	CL7	C4B-C3B-CAB-OBB
21	4B	614	CL7	C4B-C3B-CAB-OBB
21	41	405	CL7	C4B-C3B-CAB-OBB
21	44	415	CL7	C4B-C3B-CAB-OBB
21	11	410	CL7	C15-C16-C17-C18
21	21	410	CL7	C15-C16-C17-C18
21	32	512	CL7	C10-C11-C12-C13
21	31	410	CL7	C15-C16-C17-C18
21	42	512	CL7	C10-C11-C12-C13
21	41	410	CL7	C15-C16-C17-C18
21	14	409	CL7	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	24	409	CL7	C5-C6-C7-C8
21	34	409	CL7	C5-C6-C7-C8
21	44	409	CL7	C5-C6-C7-C8
26	1D	409	LHG	O6-C4-C5-O7
26	2D	409	LHG	O6-C4-C5-O7
26	3D	409	LHG	O6-C4-C5-O7
26	4D	409	LHG	O6-C4-C5-O7
21	1B	609	CL7	C16-C17-C18-C19
21	1B	609	CL7	C16-C17-C18-C20
21	1C	503	CL7	C16-C17-C18-C19
21	2B	610	CL7	C16-C17-C18-C20
21	2C	503	CL7	C16-C17-C18-C19
21	3B	609	CL7	C16-C17-C18-C19
21	3B	609	CL7	C16-C17-C18-C20
21	3C	503	CL7	C16-C17-C18-C19
21	4B	610	CL7	C16-C17-C18-C19
21	4B	610	CL7	C16-C17-C18-C20
21	4C	503	CL7	C16-C17-C18-C19
21	2B	608	CL7	C8-C10-C11-C12
21	3B	607	CL7	C8-C10-C11-C12
21	11	415	CL7	O1D-CGD-O2D-CED
21	21	415	CL7	O1D-CGD-O2D-CED
21	41	415	CL7	O1D-CGD-O2D-CED
27	1B	624	DGD	O1A-C1A-O1G-C1G
27	2B	625	DGD	O1A-C1A-O1G-C1G
27	3B	624	DGD	O1A-C1A-O1G-C1G
27	4B	625	DGD	O1A-C1A-O1G-C1G
25	1B	620	SQD	C32-C33-C34-C35
25	3B	620	SQD	C32-C33-C34-C35
25	4B	621	SQD	C32-C33-C34-C35
21	13	512	CL7	CBD-CGD-O2D-CED
21	23	413	CL7	CBD-CGD-O2D-CED
21	1B	607	CL7	C8-C10-C11-C12
21	11	410	CL7	C10-C11-C12-C13
21	21	410	CL7	C10-C11-C12-C13
21	31	410	CL7	C10-C11-C12-C13
21	4B	608	CL7	C8-C10-C11-C12
24	1A	405	LMG	C2-C1-O1-C7
24	11	401	LMG	C2-C1-O1-C7
24	2A	405	LMG	C2-C1-O1-C7
24	21	401	LMG	C2-C1-O1-C7
24	3A	405	LMG	C2-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	31	401	LMG	C2-C1-O1-C7
24	4A	405	LMG	C2-C1-O1-C7
24	41	401	LMG	C2-C1-O1-C7
25	2B	621	SQD	C32-C33-C34-C35
24	1A	405	LMG	O1-C7-C8-O7
24	2A	405	LMG	O1-C7-C8-O7
24	3A	405	LMG	O1-C7-C8-O7
24	4A	405	LMG	O1-C7-C8-O7
21	1A	401	CL7	C10-C11-C12-C13
21	1B	604	CL7	C8-C10-C11-C12
21	2A	401	CL7	C10-C11-C12-C13
21	2B	605	CL7	C8-C10-C11-C12
21	3A	401	CL7	C10-C11-C12-C13
21	3B	604	CL7	C8-C10-C11-C12
21	4A	401	CL7	C10-C11-C12-C13
21	4B	605	CL7	C8-C10-C11-C12
21	41	410	CL7	C10-C11-C12-C13
22	1A	402	PHO	CHA-CBD-CGD-O1D
22	1A	402	PHO	CHA-CBD-CGD-O2D
22	1D	408	PHO	CHA-CBD-CGD-O1D
22	1D	408	PHO	CHA-CBD-CGD-O2D
22	2A	402	PHO	CHA-CBD-CGD-O1D
22	2A	402	PHO	CHA-CBD-CGD-O2D
22	2D	408	PHO	CHA-CBD-CGD-O1D
22	2D	408	PHO	CHA-CBD-CGD-O2D
22	3A	402	PHO	CHA-CBD-CGD-O1D
22	3A	402	PHO	CHA-CBD-CGD-O2D
22	3D	408	PHO	CHA-CBD-CGD-O1D
22	3D	408	PHO	CHA-CBD-CGD-O2D
22	4A	402	PHO	CHA-CBD-CGD-O1D
22	4A	402	PHO	CHA-CBD-CGD-O2D
22	4D	408	PHO	CHA-CBD-CGD-O1D
22	4D	408	PHO	CHA-CBD-CGD-O2D
21	12	507	CL7	C4-C3-C5-C6
21	13	502	CL7	C4-C3-C5-C6
21	22	507	CL7	C4-C3-C5-C6
21	32	507	CL7	C4-C3-C5-C6
21	33	502	CL7	C4-C3-C5-C6
21	42	507	CL7	C4-C3-C5-C6
21	43	403	CL7	C4-C3-C5-C6
21	1B	603	CL7	C11-C10-C8-C7
21	1B	604	CL7	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	605	CL7	C12-C13-C15-C16
21	1B	609	CL7	C6-C7-C8-C10
21	1B	612	CL7	C11-C10-C8-C7
21	1C	503	CL7	C11-C10-C8-C7
21	1C	505	CL7	C12-C13-C15-C16
21	1C	506	CL7	C11-C10-C8-C7
21	1C	510	CL7	C12-C13-C15-C16
21	12	503	CL7	C12-C13-C15-C16
21	12	507	CL7	C11-C10-C8-C7
21	12	510	CL7	C6-C7-C8-C10
21	12	510	CL7	C11-C10-C8-C7
21	11	408	CL7	C11-C10-C8-C7
21	13	501	CL7	C12-C13-C15-C16
21	13	507	CL7	C6-C7-C8-C10
21	14	411	CL7	C11-C12-C13-C15
21	2B	604	CL7	C11-C10-C8-C7
21	2B	605	CL7	C12-C13-C15-C16
21	2B	606	CL7	C12-C13-C15-C16
21	2B	610	CL7	C6-C7-C8-C10
21	2B	613	CL7	C11-C10-C8-C7
21	2C	503	CL7	C11-C10-C8-C7
21	2C	505	CL7	C12-C13-C15-C16
21	2C	506	CL7	C11-C10-C8-C7
21	2C	510	CL7	C12-C13-C15-C16
21	22	503	CL7	C12-C13-C15-C16
21	22	507	CL7	C11-C10-C8-C7
21	22	510	CL7	C6-C7-C8-C10
21	22	510	CL7	C11-C10-C8-C7
21	21	408	CL7	C11-C10-C8-C7
21	23	402	CL7	C12-C13-C15-C16
21	23	408	CL7	C6-C7-C8-C10
21	24	411	CL7	C11-C12-C13-C15
21	3B	603	CL7	C11-C10-C8-C7
21	3B	604	CL7	C12-C13-C15-C16
21	3B	605	CL7	C12-C13-C15-C16
21	3B	609	CL7	C6-C7-C8-C10
21	3B	612	CL7	C11-C10-C8-C7
21	3C	503	CL7	C11-C10-C8-C7
21	3C	505	CL7	C12-C13-C15-C16
21	3C	506	CL7	C11-C10-C8-C7
21	3C	510	CL7	C12-C13-C15-C16
21	32	503	CL7	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	32	507	CL7	C11-C10-C8-C7
21	32	510	CL7	C6-C7-C8-C10
21	32	510	CL7	C11-C10-C8-C7
21	31	408	CL7	C11-C10-C8-C7
21	33	501	CL7	C12-C13-C15-C16
21	33	507	CL7	C6-C7-C8-C10
21	34	411	CL7	C11-C12-C13-C15
21	4B	604	CL7	C11-C10-C8-C7
21	4B	605	CL7	C12-C13-C15-C16
21	4B	606	CL7	C12-C13-C15-C16
21	4B	610	CL7	C6-C7-C8-C10
21	4B	613	CL7	C11-C10-C8-C7
21	4C	503	CL7	C11-C10-C8-C7
21	4C	505	CL7	C12-C13-C15-C16
21	4C	506	CL7	C11-C10-C8-C7
21	4C	510	CL7	C12-C13-C15-C16
21	42	503	CL7	C12-C13-C15-C16
21	42	507	CL7	C11-C10-C8-C7
21	42	510	CL7	C6-C7-C8-C10
21	42	510	CL7	C11-C10-C8-C7
21	41	408	CL7	C11-C10-C8-C7
21	43	402	CL7	C12-C13-C15-C16
21	43	408	CL7	C6-C7-C8-C10
21	44	411	CL7	C11-C12-C13-C15
21	33	516	CL7	C4C-C3C-CAC-CBC
21	43	417	CL7	C4C-C3C-CAC-CBC
21	1B	612	CL7	C11-C10-C8-C9
21	1C	510	CL7	C14-C13-C15-C16
21	12	501	CL7	C6-C7-C8-C9
21	12	503	CL7	C14-C13-C15-C16
21	12	505	CL7	C11-C10-C8-C9
21	12	512	CL7	C11-C10-C8-C9
21	11	402	CL7	C6-C7-C8-C9
21	11	406	CL7	C14-C13-C15-C16
21	11	418	CL7	C14-C13-C15-C16
21	13	501	CL7	C14-C13-C15-C16
21	13	503	CL7	C6-C7-C8-C9
21	13	503	CL7	C11-C10-C8-C9
21	13	504	CL7	C11-C12-C13-C14
21	13	509	CL7	C11-C10-C8-C9
21	13	511	CL7	C14-C13-C15-C16
21	2B	613	CL7	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2C	510	CL7	C14-C13-C15-C16
21	22	501	CL7	C6-C7-C8-C9
21	22	503	CL7	C14-C13-C15-C16
21	22	505	CL7	C11-C10-C8-C9
21	22	512	CL7	C11-C10-C8-C9
21	21	402	CL7	C6-C7-C8-C9
21	21	406	CL7	C14-C13-C15-C16
21	21	418	CL7	C14-C13-C15-C16
21	23	402	CL7	C14-C13-C15-C16
21	23	404	CL7	C6-C7-C8-C9
21	23	404	CL7	C11-C10-C8-C9
21	23	405	CL7	C11-C12-C13-C14
21	23	410	CL7	C11-C10-C8-C9
21	23	412	CL7	C14-C13-C15-C16
21	3B	612	CL7	C11-C10-C8-C9
21	3C	510	CL7	C14-C13-C15-C16
21	32	501	CL7	C6-C7-C8-C9
21	32	503	CL7	C14-C13-C15-C16
21	32	505	CL7	C11-C10-C8-C9
21	32	512	CL7	C11-C10-C8-C9
21	31	402	CL7	C6-C7-C8-C9
21	31	406	CL7	C14-C13-C15-C16
21	31	418	CL7	C14-C13-C15-C16
21	33	501	CL7	C14-C13-C15-C16
21	33	503	CL7	C6-C7-C8-C9
21	33	503	CL7	C11-C10-C8-C9
21	33	504	CL7	C11-C12-C13-C14
21	33	509	CL7	C11-C10-C8-C9
21	33	511	CL7	C14-C13-C15-C16
21	4B	613	CL7	C11-C10-C8-C9
21	4C	510	CL7	C14-C13-C15-C16
21	42	501	CL7	C6-C7-C8-C9
21	42	503	CL7	C14-C13-C15-C16
21	42	505	CL7	C11-C10-C8-C9
21	42	512	CL7	C11-C10-C8-C9
21	41	402	CL7	C6-C7-C8-C9
21	41	406	CL7	C14-C13-C15-C16
21	41	418	CL7	C14-C13-C15-C16
21	43	402	CL7	C14-C13-C15-C16
21	43	404	CL7	C6-C7-C8-C9
21	43	404	CL7	C11-C10-C8-C9
21	43	405	CL7	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	410	CL7	C11-C10-C8-C9
21	43	412	CL7	C14-C13-C15-C16
21	31	415	CL7	O1D-CGD-O2D-CED
21	33	512	CL7	CBD-CGD-O2D-CED
21	43	413	CL7	CBD-CGD-O2D-CED
21	13	516	CL7	C4C-C3C-CAC-CBC
21	23	417	CL7	C4C-C3C-CAC-CBC
21	11	402	CL7	C5-C6-C7-C8
21	14	413	CL7	C10-C11-C12-C13
21	21	402	CL7	C5-C6-C7-C8
21	24	413	CL7	C10-C11-C12-C13
21	31	402	CL7	C5-C6-C7-C8
21	34	413	CL7	C10-C11-C12-C13
21	44	413	CL7	C10-C11-C12-C13
21	23	418	CL7	O1D-CGD-O2D-CED
21	33	517	CL7	O1D-CGD-O2D-CED
23	1K	101	8CT	C10-C11-C12-C40
23	2K	101	8CT	C10-C11-C12-C40
23	3K	101	8CT	C10-C11-C12-C40
23	4K	101	8CT	C10-C11-C12-C40
32	13	520	ZEX	C31-C32-C33-C40
32	14	420	ZEX	C11-C12-C13-C20
32	23	421	ZEX	C31-C32-C33-C40
32	24	420	ZEX	C11-C12-C13-C20
32	33	520	ZEX	C31-C32-C33-C40
32	34	420	ZEX	C11-C12-C13-C20
32	43	421	ZEX	C31-C32-C33-C40
32	44	420	ZEX	C11-C12-C13-C20
21	2B	610	CL7	C16-C17-C18-C19
21	13	517	CL7	O1D-CGD-O2D-CED
21	43	418	CL7	O1D-CGD-O2D-CED
23	1B	619	8CT	C25-C26-C28-C29
23	1K	101	8CT	C10-C11-C12-C13
23	2B	620	8CT	C25-C26-C28-C29
23	2K	101	8CT	C10-C11-C12-C13
23	3B	619	8CT	C25-C26-C28-C29
23	3K	101	8CT	C10-C11-C12-C13
23	4B	620	8CT	C25-C26-C28-C29
23	4K	101	8CT	C10-C11-C12-C13
32	12	524	ZEX	C7-C8-C9-C10
32	22	524	ZEX	C7-C8-C9-C10
32	32	524	ZEX	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	42	524	ZEX	C7-C8-C9-C10
21	41	402	CL7	C5-C6-C7-C8
21	13	504	CL7	C4C-C3C-CAC-CBC
21	23	405	CL7	C4C-C3C-CAC-CBC
21	33	504	CL7	C4C-C3C-CAC-CBC
21	43	405	CL7	C4C-C3C-CAC-CBC
21	4C	501	CL7	CBD-CGD-O2D-CED
21	23	403	CL7	C4-C3-C5-C6
21	12	518	CL7	C15-C16-C17-C18
21	22	518	CL7	C15-C16-C17-C18
21	32	518	CL7	C15-C16-C17-C18
21	42	518	CL7	C15-C16-C17-C18
21	1B	616	CL7	O1D-CGD-O2D-CED
21	2B	617	CL7	O1D-CGD-O2D-CED
21	3B	616	CL7	O1D-CGD-O2D-CED
21	4B	617	CL7	O1D-CGD-O2D-CED
21	1C	505	CL7	C3A-C2A-CAA-CBA
21	1C	509	CL7	C3A-C2A-CAA-CBA
21	12	503	CL7	C3A-C2A-CAA-CBA
21	12	515	CL7	C3A-C2A-CAA-CBA
21	11	405	CL7	C3A-C2A-CAA-CBA
21	11	418	CL7	C3A-C2A-CAA-CBA
21	13	501	CL7	C3A-C2A-CAA-CBA
21	13	503	CL7	C3A-C2A-CAA-CBA
21	13	513	CL7	C3A-C2A-CAA-CBA
21	14	411	CL7	C3A-C2A-CAA-CBA
21	2C	505	CL7	C3A-C2A-CAA-CBA
21	2C	509	CL7	C3A-C2A-CAA-CBA
21	22	503	CL7	C3A-C2A-CAA-CBA
21	22	515	CL7	C3A-C2A-CAA-CBA
21	21	405	CL7	C3A-C2A-CAA-CBA
21	21	418	CL7	C3A-C2A-CAA-CBA
21	23	402	CL7	C3A-C2A-CAA-CBA
21	23	404	CL7	C3A-C2A-CAA-CBA
21	24	411	CL7	C3A-C2A-CAA-CBA
21	3C	505	CL7	C3A-C2A-CAA-CBA
21	3C	509	CL7	C3A-C2A-CAA-CBA
21	32	503	CL7	C3A-C2A-CAA-CBA
21	32	515	CL7	C3A-C2A-CAA-CBA
21	31	405	CL7	C3A-C2A-CAA-CBA
21	31	418	CL7	C3A-C2A-CAA-CBA
21	33	501	CL7	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	33	503	CL7	C3A-C2A-CAA-CBA
21	33	513	CL7	C3A-C2A-CAA-CBA
21	34	411	CL7	C3A-C2A-CAA-CBA
21	4C	505	CL7	C3A-C2A-CAA-CBA
21	4C	509	CL7	C3A-C2A-CAA-CBA
21	42	503	CL7	C3A-C2A-CAA-CBA
21	42	515	CL7	C3A-C2A-CAA-CBA
21	41	405	CL7	C3A-C2A-CAA-CBA
21	41	418	CL7	C3A-C2A-CAA-CBA
21	43	402	CL7	C3A-C2A-CAA-CBA
21	43	404	CL7	C3A-C2A-CAA-CBA
21	44	411	CL7	C3A-C2A-CAA-CBA
23	1A	404	8CT	C23-C24-C25-C26
23	2A	404	8CT	C23-C24-C25-C26
23	3A	404	8CT	C23-C24-C25-C26
23	4A	404	8CT	C23-C24-C25-C26
27	4B	625	DGD	C6B-C7B-C8B-C9B
21	1C	501	CL7	CBD-CGD-O2D-CED
21	13	503	CL7	C8-C10-C11-C12
21	13	503	CL7	C10-C11-C12-C13
21	33	503	CL7	C10-C11-C12-C13
21	33	505	CL7	C2C-C3C-CAC-CBC
27	3B	624	DGD	C6B-C7B-C8B-C9B
21	1C	504	CL7	C6-C7-C8-C10
21	2C	504	CL7	C6-C7-C8-C10
21	3C	504	CL7	C6-C7-C8-C10
21	4C	504	CL7	C6-C7-C8-C10
21	23	406	CL7	C2C-C3C-CAC-CBC
27	1B	624	DGD	C6B-C7B-C8B-C9B
27	2B	625	DGD	C6B-C7B-C8B-C9B
21	1B	612	CL7	C10-C11-C12-C13
21	2B	613	CL7	C10-C11-C12-C13
21	3B	612	CL7	C10-C11-C12-C13
21	4B	613	CL7	C10-C11-C12-C13
21	3C	501	CL7	CBD-CGD-O2D-CED
21	13	505	CL7	C2C-C3C-CAC-CBC
22	1A	402	PHO	O2A-C1-C2-C3
22	2A	402	PHO	O2A-C1-C2-C3
22	3A	402	PHO	O2A-C1-C2-C3
22	4A	402	PHO	O2A-C1-C2-C3
21	23	404	CL7	C10-C11-C12-C13
21	33	503	CL7	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	404	CL7	C10-C11-C12-C13
21	12	511	CL7	C3-C5-C6-C7
21	22	511	CL7	C3-C5-C6-C7
21	32	511	CL7	C3-C5-C6-C7
21	42	511	CL7	C3-C5-C6-C7
21	43	406	CL7	C2C-C3C-CAC-CBC
21	23	404	CL7	C8-C10-C11-C12
21	43	404	CL7	C8-C10-C11-C12
21	1B	613	CL7	C4-C3-C5-C6
21	2B	614	CL7	C4-C3-C5-C6
21	3B	613	CL7	C4-C3-C5-C6
21	4B	614	CL7	C4-C3-C5-C6
21	2C	501	CL7	CBD-CGD-O2D-CED
21	4C	502	CL7	C10-C11-C12-C13
26	1A	408	LHG	C3-O3-P-O6
26	2A	408	LHG	C3-O3-P-O6
26	3A	408	LHG	C3-O3-P-O6
26	4A	408	LHG	C3-O3-P-O6
21	1C	502	CL7	C10-C11-C12-C13
21	2C	502	CL7	C10-C11-C12-C13
21	3C	502	CL7	C10-C11-C12-C13
21	2C	505	CL7	C4C-C3C-CAC-CBC
21	1C	505	CL7	C4C-C3C-CAC-CBC
21	3C	505	CL7	C4C-C3C-CAC-CBC
21	4C	505	CL7	C4C-C3C-CAC-CBC
26	1B	625	LHG	C1-C2-C3-O3
26	2B	626	LHG	C1-C2-C3-O3
26	3B	625	LHG	C1-C2-C3-O3
26	4B	626	LHG	C1-C2-C3-O3
21	12	501	CL7	C2-C1-O2A-CGA
21	12	509	CL7	C2-C1-O2A-CGA
21	11	402	CL7	C2-C1-O2A-CGA
21	11	417	CL7	C2-C1-O2A-CGA
21	22	501	CL7	C2-C1-O2A-CGA
21	22	509	CL7	C2-C1-O2A-CGA
21	21	402	CL7	C2-C1-O2A-CGA
21	21	417	CL7	C2-C1-O2A-CGA
21	32	501	CL7	C2-C1-O2A-CGA
21	32	509	CL7	C2-C1-O2A-CGA
21	31	402	CL7	C2-C1-O2A-CGA
21	31	417	CL7	C2-C1-O2A-CGA
21	42	501	CL7	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	509	CL7	C2-C1-O2A-CGA
21	41	402	CL7	C2-C1-O2A-CGA
21	41	417	CL7	C2-C1-O2A-CGA
21	2B	605	CL7	C13-C15-C16-C17
21	3B	604	CL7	C13-C15-C16-C17
21	4B	605	CL7	C13-C15-C16-C17
21	1B	607	CL7	C11-C10-C8-C9
21	1C	507	CL7	C6-C7-C8-C9
21	1C	507	CL7	C14-C13-C15-C16
21	12	503	CL7	C11-C10-C8-C9
21	12	509	CL7	C14-C13-C15-C16
21	12	511	CL7	C11-C10-C8-C9
21	12	518	CL7	C14-C13-C15-C16
21	13	503	CL7	C14-C13-C15-C16
21	13	508	CL7	C6-C7-C8-C9
21	13	508	CL7	C14-C13-C15-C16
21	2B	608	CL7	C11-C10-C8-C9
21	2C	507	CL7	C6-C7-C8-C9
21	2C	507	CL7	C14-C13-C15-C16
21	22	503	CL7	C11-C10-C8-C9
21	22	509	CL7	C14-C13-C15-C16
21	22	511	CL7	C11-C10-C8-C9
21	22	518	CL7	C14-C13-C15-C16
21	23	404	CL7	C14-C13-C15-C16
21	23	409	CL7	C6-C7-C8-C9
21	23	409	CL7	C14-C13-C15-C16
21	3B	607	CL7	C11-C10-C8-C9
21	3C	507	CL7	C6-C7-C8-C9
21	3C	507	CL7	C14-C13-C15-C16
21	32	503	CL7	C11-C10-C8-C9
21	32	509	CL7	C14-C13-C15-C16
21	32	511	CL7	C11-C10-C8-C9
21	32	518	CL7	C14-C13-C15-C16
21	33	503	CL7	C14-C13-C15-C16
21	33	508	CL7	C6-C7-C8-C9
21	33	508	CL7	C14-C13-C15-C16
21	4B	608	CL7	C11-C10-C8-C9
21	4C	507	CL7	C6-C7-C8-C9
21	4C	507	CL7	C14-C13-C15-C16
21	42	503	CL7	C11-C10-C8-C9
21	42	509	CL7	C14-C13-C15-C16
21	42	511	CL7	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	518	CL7	C14-C13-C15-C16
21	43	404	CL7	C14-C13-C15-C16
21	43	409	CL7	C6-C7-C8-C9
21	43	409	CL7	C14-C13-C15-C16
27	1B	624	DGD	CBB-CCB-CDB-CEB
27	2B	625	DGD	CBB-CCB-CDB-CEB
27	3B	624	DGD	CBB-CCB-CDB-CEB
27	4B	625	DGD	CBB-CCB-CDB-CEB
21	24	406	CL7	O1D-CGD-O2D-CED
21	1B	604	CL7	C13-C15-C16-C17
21	11	408	CL7	C13-C15-C16-C17
21	21	408	CL7	C13-C15-C16-C17
21	31	408	CL7	C13-C15-C16-C17
21	41	408	CL7	C13-C15-C16-C17
32	14	403	ZEX	C21-C26-C27-C28
32	24	403	ZEX	C21-C26-C27-C28
32	34	403	ZEX	C21-C26-C27-C28
32	44	403	ZEX	C21-C26-C27-C28
21	1C	501	CL7	C16-C17-C18-C20
21	2C	501	CL7	C16-C17-C18-C20
21	3C	501	CL7	C16-C17-C18-C20
21	4C	501	CL7	C16-C17-C18-C20
23	1B	618	8CT	C02-C03-C10-C11
23	1B	626	8CT	C04-C03-C10-C11
23	14	402	8CT	C02-C03-C10-C11
23	2B	601	8CT	C04-C03-C10-C11
23	2B	619	8CT	C02-C03-C10-C11
23	24	402	8CT	C02-C03-C10-C11
23	3B	618	8CT	C02-C03-C10-C11
23	3B	626	8CT	C04-C03-C10-C11
23	34	402	8CT	C02-C03-C10-C11
23	4B	619	8CT	C02-C03-C10-C11
23	44	402	8CT	C02-C03-C10-C11
32	12	520	ZEX	C1-C6-C7-C8
32	13	520	ZEX	C1-C6-C7-C8
32	13	520	ZEX	C5-C6-C7-C8
32	14	418	ZEX	C1-C6-C7-C8
32	14	418	ZEX	C5-C6-C7-C8
32	14	420	ZEX	C1-C6-C7-C8
32	14	420	ZEX	C5-C6-C7-C8
32	22	520	ZEX	C1-C6-C7-C8
32	23	421	ZEX	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	23	421	ZEX	C5-C6-C7-C8
32	24	418	ZEX	C1-C6-C7-C8
32	24	418	ZEX	C5-C6-C7-C8
32	24	420	ZEX	C1-C6-C7-C8
32	24	420	ZEX	C5-C6-C7-C8
32	32	520	ZEX	C1-C6-C7-C8
32	33	520	ZEX	C1-C6-C7-C8
32	33	520	ZEX	C5-C6-C7-C8
32	34	418	ZEX	C1-C6-C7-C8
32	34	418	ZEX	C5-C6-C7-C8
32	34	420	ZEX	C1-C6-C7-C8
32	34	420	ZEX	C5-C6-C7-C8
32	42	520	ZEX	C1-C6-C7-C8
32	43	421	ZEX	C1-C6-C7-C8
32	43	421	ZEX	C5-C6-C7-C8
32	44	418	ZEX	C1-C6-C7-C8
32	44	418	ZEX	C5-C6-C7-C8
32	44	420	ZEX	C1-C6-C7-C8
32	44	420	ZEX	C5-C6-C7-C8
23	1B	619	8CT	C27-C26-C28-C29
23	2B	620	8CT	C27-C26-C28-C29
23	3B	619	8CT	C27-C26-C28-C29
23	4B	620	8CT	C27-C26-C28-C29
21	14	406	CL7	O1D-CGD-O2D-CED
21	24	416	CL7	O1D-CGD-O2D-CED
21	34	406	CL7	O1D-CGD-O2D-CED
23	1C	514	8CT	C20-C21-C23-C24
23	2C	514	8CT	C20-C21-C23-C24
23	3C	514	8CT	C20-C21-C23-C24
23	4C	514	8CT	C20-C21-C23-C24
21	13	511	CL7	C5-C6-C7-C8
21	23	412	CL7	C5-C6-C7-C8
21	33	511	CL7	C5-C6-C7-C8
21	43	412	CL7	C5-C6-C7-C8
21	14	416	CL7	O1D-CGD-O2D-CED
21	34	416	CL7	O1D-CGD-O2D-CED
21	44	406	CL7	O1D-CGD-O2D-CED
21	14	405	CL7	C16-C17-C18-C19
21	24	405	CL7	C16-C17-C18-C19
21	34	405	CL7	C16-C17-C18-C19
21	44	405	CL7	C16-C17-C18-C19
21	44	416	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	14	401	LHG	O6-C4-C5-C6
26	24	401	LHG	O6-C4-C5-C6
26	34	401	LHG	O6-C4-C5-C6
26	44	401	LHG	O6-C4-C5-C6
21	1B	608	CL7	C11-C10-C8-C7
21	1C	501	CL7	C12-C13-C15-C16
21	1C	509	CL7	C12-C13-C15-C16
21	1D	404	CL7	C11-C10-C8-C7
21	12	512	CL7	C11-C10-C8-C7
21	11	402	CL7	C6-C7-C8-C10
21	11	404	CL7	C11-C12-C13-C15
21	13	503	CL7	C6-C7-C8-C10
21	13	508	CL7	C12-C13-C15-C16
21	13	509	CL7	C11-C10-C8-C7
21	13	511	CL7	C11-C10-C8-C7
21	14	404	CL7	C11-C10-C8-C7
21	2B	609	CL7	C11-C10-C8-C7
21	2C	501	CL7	C12-C13-C15-C16
21	2C	509	CL7	C12-C13-C15-C16
21	2D	404	CL7	C11-C10-C8-C7
21	22	512	CL7	C11-C10-C8-C7
21	21	402	CL7	C6-C7-C8-C10
21	21	404	CL7	C11-C12-C13-C15
21	23	404	CL7	C6-C7-C8-C10
21	23	409	CL7	C12-C13-C15-C16
21	23	410	CL7	C11-C10-C8-C7
21	23	412	CL7	C11-C10-C8-C7
21	24	404	CL7	C11-C10-C8-C7
21	3B	608	CL7	C11-C10-C8-C7
21	3C	501	CL7	C12-C13-C15-C16
21	3C	509	CL7	C12-C13-C15-C16
21	3D	404	CL7	C11-C10-C8-C7
21	32	512	CL7	C11-C10-C8-C7
21	31	402	CL7	C6-C7-C8-C10
21	31	404	CL7	C11-C12-C13-C15
21	33	503	CL7	C6-C7-C8-C10
21	33	508	CL7	C12-C13-C15-C16
21	33	509	CL7	C11-C10-C8-C7
21	33	511	CL7	C11-C10-C8-C7
21	34	404	CL7	C11-C10-C8-C7
21	4B	609	CL7	C11-C10-C8-C7
21	4C	501	CL7	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4C	509	CL7	C12-C13-C15-C16
21	4D	404	CL7	C11-C10-C8-C7
21	42	512	CL7	C11-C10-C8-C7
21	41	402	CL7	C6-C7-C8-C10
21	41	404	CL7	C11-C12-C13-C15
21	43	404	CL7	C6-C7-C8-C10
21	43	409	CL7	C12-C13-C15-C16
21	43	410	CL7	C11-C10-C8-C7
21	43	412	CL7	C11-C10-C8-C7
21	44	404	CL7	C11-C10-C8-C7
21	14	406	CL7	C5-C6-C7-C8
21	24	406	CL7	C5-C6-C7-C8
21	34	406	CL7	C5-C6-C7-C8
21	44	406	CL7	C5-C6-C7-C8
23	1C	515	8CT	C16-C17-C18-C19
23	2C	515	8CT	C16-C17-C18-C19
23	3C	515	8CT	C16-C17-C18-C19
23	4C	515	8CT	C16-C17-C18-C19
21	12	517	CL7	C16-C17-C18-C19
21	22	517	CL7	C16-C17-C18-C19
21	32	517	CL7	C16-C17-C18-C19
21	42	517	CL7	C16-C17-C18-C19
21	13	516	CL7	C5-C6-C7-C8
21	23	417	CL7	C5-C6-C7-C8
21	33	516	CL7	C5-C6-C7-C8
21	43	417	CL7	C5-C6-C7-C8
21	11	403	CL7	C2A-CAA-CBA-CGA
21	13	514	CL7	C2A-CAA-CBA-CGA
21	21	403	CL7	C2A-CAA-CBA-CGA
21	31	403	CL7	C2A-CAA-CBA-CGA
21	41	403	CL7	C2A-CAA-CBA-CGA
21	43	415	CL7	C2A-CAA-CBA-CGA
21	12	507	CL7	C16-C17-C18-C19
27	1C	516	DGD	C2A-C1A-O1G-C1G
27	2C	516	DGD	C2A-C1A-O1G-C1G
27	3C	516	DGD	C2A-C1A-O1G-C1G
27	4C	516	DGD	C2A-C1A-O1G-C1G
21	1B	603	CL7	CAD-CBD-CGD-O2D
21	1B	604	CL7	CAD-CBD-CGD-O2D
21	1B	612	CL7	CAD-CBD-CGD-O2D
21	1B	613	CL7	CAD-CBD-CGD-O2D
21	1B	622	CL7	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1C	501	CL7	CAD-CBD-CGD-O2D
21	1C	502	CL7	CAD-CBD-CGD-O2D
21	1C	505	CL7	CAD-CBD-CGD-O2D
21	12	505	CL7	CAD-CBD-CGD-O2D
21	12	509	CL7	CAD-CBD-CGD-O2D
21	12	515	CL7	CAD-CBD-CGD-O2D
21	11	404	CL7	CAD-CBD-CGD-O2D
21	11	410	CL7	CAD-CBD-CGD-O2D
21	11	411	CL7	CAD-CBD-CGD-O2D
21	11	412	CL7	CAD-CBD-CGD-O2D
21	13	504	CL7	CAD-CBD-CGD-O2D
21	13	509	CL7	CAD-CBD-CGD-O2D
21	13	510	CL7	CAD-CBD-CGD-O2D
21	14	411	CL7	CAD-CBD-CGD-O2D
21	2A	401	CL7	CAD-CBD-CGD-O2D
21	2B	604	CL7	CAD-CBD-CGD-O2D
21	2B	605	CL7	CAD-CBD-CGD-O2D
21	2B	613	CL7	CAD-CBD-CGD-O2D
21	2B	614	CL7	CAD-CBD-CGD-O2D
21	2B	623	CL7	CAD-CBD-CGD-O2D
21	2C	501	CL7	CAD-CBD-CGD-O2D
21	2C	502	CL7	CAD-CBD-CGD-O2D
21	2C	505	CL7	CAD-CBD-CGD-O2D
21	22	505	CL7	CAD-CBD-CGD-O2D
21	22	509	CL7	CAD-CBD-CGD-O2D
21	22	515	CL7	CAD-CBD-CGD-O2D
21	21	404	CL7	CAD-CBD-CGD-O2D
21	21	410	CL7	CAD-CBD-CGD-O2D
21	21	411	CL7	CAD-CBD-CGD-O2D
21	21	412	CL7	CAD-CBD-CGD-O2D
21	23	405	CL7	CAD-CBD-CGD-O2D
21	23	410	CL7	CAD-CBD-CGD-O2D
21	23	411	CL7	CAD-CBD-CGD-O2D
21	24	411	CL7	CAD-CBD-CGD-O2D
21	3A	401	CL7	CAD-CBD-CGD-O2D
21	3B	603	CL7	CAD-CBD-CGD-O2D
21	3B	604	CL7	CAD-CBD-CGD-O2D
21	3B	612	CL7	CAD-CBD-CGD-O2D
21	3B	613	CL7	CAD-CBD-CGD-O2D
21	3B	622	CL7	CAD-CBD-CGD-O2D
21	3C	501	CL7	CAD-CBD-CGD-O2D
21	3C	502	CL7	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3C	505	CL7	CAD-CBD-CGD-O2D
21	32	505	CL7	CAD-CBD-CGD-O2D
21	32	509	CL7	CAD-CBD-CGD-O2D
21	32	515	CL7	CAD-CBD-CGD-O2D
21	31	404	CL7	CAD-CBD-CGD-O2D
21	31	410	CL7	CAD-CBD-CGD-O2D
21	31	411	CL7	CAD-CBD-CGD-O2D
21	31	412	CL7	CAD-CBD-CGD-O2D
21	33	504	CL7	CAD-CBD-CGD-O2D
21	33	509	CL7	CAD-CBD-CGD-O2D
21	33	510	CL7	CAD-CBD-CGD-O2D
21	34	411	CL7	CAD-CBD-CGD-O2D
21	4A	401	CL7	CAD-CBD-CGD-O2D
21	4B	604	CL7	CAD-CBD-CGD-O2D
21	4B	605	CL7	CAD-CBD-CGD-O2D
21	4B	613	CL7	CAD-CBD-CGD-O2D
21	4B	614	CL7	CAD-CBD-CGD-O2D
21	4B	623	CL7	CAD-CBD-CGD-O2D
21	4C	501	CL7	CAD-CBD-CGD-O2D
21	4C	502	CL7	CAD-CBD-CGD-O2D
21	4C	505	CL7	CAD-CBD-CGD-O2D
21	42	505	CL7	CAD-CBD-CGD-O2D
21	42	509	CL7	CAD-CBD-CGD-O2D
21	42	515	CL7	CAD-CBD-CGD-O2D
21	41	404	CL7	CAD-CBD-CGD-O2D
21	41	410	CL7	CAD-CBD-CGD-O2D
21	41	411	CL7	CAD-CBD-CGD-O2D
21	41	412	CL7	CAD-CBD-CGD-O2D
21	43	405	CL7	CAD-CBD-CGD-O2D
21	43	410	CL7	CAD-CBD-CGD-O2D
21	43	411	CL7	CAD-CBD-CGD-O2D
21	44	411	CL7	CAD-CBD-CGD-O2D
30	1D	407	PL9	C17-C18-C19-C20
30	2D	407	PL9	C17-C18-C19-C20
30	3D	407	PL9	C17-C18-C19-C20
30	4D	407	PL9	C17-C18-C19-C20
21	1B	606	CL7	C5-C6-C7-C8
21	13	507	CL7	C15-C16-C17-C18
21	14	406	CL7	C8-C10-C11-C12
21	2B	607	CL7	C5-C6-C7-C8
21	23	408	CL7	C15-C16-C17-C18
21	24	406	CL7	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3B	606	CL7	C5-C6-C7-C8
21	33	507	CL7	C15-C16-C17-C18
21	34	406	CL7	C8-C10-C11-C12
21	4B	607	CL7	C5-C6-C7-C8
21	43	408	CL7	C15-C16-C17-C18
21	44	406	CL7	C8-C10-C11-C12
21	1C	504	CL7	C6-C7-C8-C9
21	2C	504	CL7	C6-C7-C8-C9
21	22	507	CL7	C16-C17-C18-C19
21	3C	504	CL7	C6-C7-C8-C9
21	32	507	CL7	C16-C17-C18-C19
21	4C	504	CL7	C6-C7-C8-C9
21	42	507	CL7	C16-C17-C18-C19
24	1D	410	LMG	O6-C1-O1-C7
24	2D	410	LMG	O6-C1-O1-C7
24	3D	410	LMG	O6-C1-O1-C7
24	4D	410	LMG	O6-C1-O1-C7
21	13	507	CL7	C10-C11-C12-C13
21	23	408	CL7	C10-C11-C12-C13
21	33	507	CL7	C10-C11-C12-C13
21	43	408	CL7	C10-C11-C12-C13
26	13	524	LHG	C2-C3-O3-P
26	23	425	LHG	C2-C3-O3-P
26	33	524	LHG	C2-C3-O3-P
26	43	425	LHG	C2-C3-O3-P
26	14	401	LHG	O6-C4-C5-O7
26	24	401	LHG	O6-C4-C5-O7
26	34	401	LHG	O6-C4-C5-O7
26	44	401	LHG	O6-C4-C5-O7
21	11	418	CL7	C8-C10-C11-C12
21	21	418	CL7	C8-C10-C11-C12
21	31	418	CL7	C8-C10-C11-C12
21	41	418	CL7	C8-C10-C11-C12
21	23	415	CL7	C2A-CAA-CBA-CGA
21	33	514	CL7	C2A-CAA-CBA-CGA
21	4B	617	CL7	C2A-CAA-CBA-CGA
21	14	404	CL7	C16-C17-C18-C20
21	24	404	CL7	C16-C17-C18-C20
21	34	404	CL7	C16-C17-C18-C20
21	44	404	CL7	C16-C17-C18-C20
21	1B	605	CL7	CHA-CBD-CGD-O1D
21	1B	608	CL7	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	610	CL7	CHA-CBD-CGD-O1D
21	1B	615	CL7	CHA-CBD-CGD-O2D
21	1B	615	CL7	CHA-CBD-CGD-O1D
21	1C	504	CL7	CHA-CBD-CGD-O1D
21	1C	509	CL7	CHA-CBD-CGD-O2D
21	1C	509	CL7	CHA-CBD-CGD-O1D
21	12	502	CL7	CHA-CBD-CGD-O2D
21	12	502	CL7	CHA-CBD-CGD-O1D
21	12	506	CL7	CHA-CBD-CGD-O2D
21	12	506	CL7	CHA-CBD-CGD-O1D
21	12	513	CL7	CHA-CBD-CGD-O2D
21	11	408	CL7	CHA-CBD-CGD-O2D
21	11	408	CL7	CHA-CBD-CGD-O1D
21	13	502	CL7	CHA-CBD-CGD-O1D
21	13	506	CL7	CHA-CBD-CGD-O2D
21	14	409	CL7	CHA-CBD-CGD-O2D
21	14	409	CL7	CHA-CBD-CGD-O1D
21	2B	606	CL7	CHA-CBD-CGD-O1D
21	2B	609	CL7	CHA-CBD-CGD-O1D
21	2B	611	CL7	CHA-CBD-CGD-O1D
21	2B	616	CL7	CHA-CBD-CGD-O2D
21	2B	616	CL7	CHA-CBD-CGD-O1D
21	2C	504	CL7	CHA-CBD-CGD-O1D
21	2C	509	CL7	CHA-CBD-CGD-O2D
21	2C	509	CL7	CHA-CBD-CGD-O1D
21	22	502	CL7	CHA-CBD-CGD-O1D
21	22	506	CL7	CHA-CBD-CGD-O2D
21	22	506	CL7	CHA-CBD-CGD-O1D
21	22	513	CL7	CHA-CBD-CGD-O2D
21	21	408	CL7	CHA-CBD-CGD-O2D
21	21	408	CL7	CHA-CBD-CGD-O1D
21	23	403	CL7	CHA-CBD-CGD-O1D
21	23	407	CL7	CHA-CBD-CGD-O2D
21	24	409	CL7	CHA-CBD-CGD-O2D
21	24	409	CL7	CHA-CBD-CGD-O1D
21	3B	605	CL7	CHA-CBD-CGD-O1D
21	3B	608	CL7	CHA-CBD-CGD-O1D
21	3B	610	CL7	CHA-CBD-CGD-O1D
21	3B	615	CL7	CHA-CBD-CGD-O2D
21	3B	615	CL7	CHA-CBD-CGD-O1D
21	3C	504	CL7	CHA-CBD-CGD-O1D
21	3C	509	CL7	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	3C	509	CL7	CHA-CBD-CGD-O1D
21	32	502	CL7	CHA-CBD-CGD-O2D
21	32	502	CL7	CHA-CBD-CGD-O1D
21	32	506	CL7	CHA-CBD-CGD-O2D
21	32	506	CL7	CHA-CBD-CGD-O1D
21	32	513	CL7	CHA-CBD-CGD-O2D
21	31	408	CL7	CHA-CBD-CGD-O2D
21	31	408	CL7	CHA-CBD-CGD-O1D
21	33	502	CL7	CHA-CBD-CGD-O1D
21	33	506	CL7	CHA-CBD-CGD-O2D
21	34	409	CL7	CHA-CBD-CGD-O2D
21	34	409	CL7	CHA-CBD-CGD-O1D
21	4B	606	CL7	CHA-CBD-CGD-O1D
21	4B	609	CL7	CHA-CBD-CGD-O1D
21	4B	611	CL7	CHA-CBD-CGD-O1D
21	4B	616	CL7	CHA-CBD-CGD-O2D
21	4B	616	CL7	CHA-CBD-CGD-O1D
21	4C	504	CL7	CHA-CBD-CGD-O1D
21	4C	509	CL7	CHA-CBD-CGD-O2D
21	4C	509	CL7	CHA-CBD-CGD-O1D
21	42	502	CL7	CHA-CBD-CGD-O2D
21	42	502	CL7	CHA-CBD-CGD-O1D
21	42	506	CL7	CHA-CBD-CGD-O2D
21	42	506	CL7	CHA-CBD-CGD-O1D
21	42	513	CL7	CHA-CBD-CGD-O2D
21	41	408	CL7	CHA-CBD-CGD-O2D
21	41	408	CL7	CHA-CBD-CGD-O1D
21	43	403	CL7	CHA-CBD-CGD-O1D
21	43	407	CL7	CHA-CBD-CGD-O2D
21	44	409	CL7	CHA-CBD-CGD-O2D
21	44	409	CL7	CHA-CBD-CGD-O1D
21	14	415	CL7	O1D-CGD-O2D-CED
21	24	415	CL7	O1D-CGD-O2D-CED
21	44	415	CL7	O1D-CGD-O2D-CED
21	2A	401	CL7	O1A-CGA-O2A-C1
21	4A	401	CL7	O1A-CGA-O2A-C1
21	34	415	CL7	O1D-CGD-O2D-CED
21	1B	601	CL7	C4C-C3C-CAC-CBC
21	3B	601	CL7	C4C-C3C-CAC-CBC
21	33	512	CL7	O1D-CGD-O2D-CED
21	43	413	CL7	O1D-CGD-O2D-CED
21	1C	507	CL7	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1C	510	CL7	C6-C7-C8-C9
21	2C	507	CL7	C11-C10-C8-C9
21	2C	510	CL7	C6-C7-C8-C9
21	3C	507	CL7	C11-C10-C8-C9
21	3C	510	CL7	C6-C7-C8-C9
21	34	406	CL7	C6-C7-C8-C9
21	4C	507	CL7	C11-C10-C8-C9
21	4C	510	CL7	C6-C7-C8-C9
21	13	512	CL7	O1D-CGD-O2D-CED
21	23	413	CL7	O1D-CGD-O2D-CED
21	2B	602	CL7	C4C-C3C-CAC-CBC
21	4B	602	CL7	C4C-C3C-CAC-CBC
21	1A	401	CL7	O1A-CGA-O2A-C1
21	3A	401	CL7	O1A-CGA-O2A-C1
21	12	505	CL7	C8-C10-C11-C12
21	22	505	CL7	C8-C10-C11-C12
21	32	505	CL7	C8-C10-C11-C12
21	42	505	CL7	C8-C10-C11-C12
21	1B	616	CL7	C2A-CAA-CBA-CGA
21	1C	505	CL7	C2A-CAA-CBA-CGA
21	2B	617	CL7	C2A-CAA-CBA-CGA
21	2C	505	CL7	C2A-CAA-CBA-CGA
21	3B	616	CL7	C2A-CAA-CBA-CGA
21	3C	505	CL7	C2A-CAA-CBA-CGA
21	4C	505	CL7	C2A-CAA-CBA-CGA
23	1A	404	8CT	C22-C21-C23-C24
23	1B	617	8CT	C10-C11-C12-C40
23	2A	404	8CT	C22-C21-C23-C24
23	2B	618	8CT	C10-C11-C12-C40
23	3A	404	8CT	C22-C21-C23-C24
23	3B	617	8CT	C10-C11-C12-C40
23	4A	404	8CT	C22-C21-C23-C24
23	4B	618	8CT	C10-C11-C12-C40
32	12	524	ZEX	C7-C8-C9-C19
32	22	524	ZEX	C7-C8-C9-C19
32	32	524	ZEX	C7-C8-C9-C19
32	42	524	ZEX	C7-C8-C9-C19
23	1B	617	8CT	C10-C11-C12-C13
23	2B	618	8CT	C10-C11-C12-C13
23	3B	617	8CT	C10-C11-C12-C13
23	4B	618	8CT	C10-C11-C12-C13
21	11	404	CL7	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	21	404	CL7	C1A-C2A-CAA-CBA
21	31	404	CL7	C1A-C2A-CAA-CBA
21	41	404	CL7	C1A-C2A-CAA-CBA
21	12	512	CL7	C16-C17-C18-C20
21	22	512	CL7	C16-C17-C18-C20
21	32	512	CL7	C16-C17-C18-C20
21	42	512	CL7	C16-C17-C18-C20
21	1B	611	CL7	C10-C11-C12-C13
21	3B	611	CL7	C10-C11-C12-C13
21	4B	612	CL7	C10-C11-C12-C13
21	1B	614	CL7	C2-C1-O2A-CGA
21	14	409	CL7	C2-C1-O2A-CGA
21	2B	615	CL7	C2-C1-O2A-CGA
21	24	409	CL7	C2-C1-O2A-CGA
21	3B	614	CL7	C2-C1-O2A-CGA
21	34	409	CL7	C2-C1-O2A-CGA
21	4B	615	CL7	C2-C1-O2A-CGA
21	44	409	CL7	C2-C1-O2A-CGA
21	2B	612	CL7	C10-C11-C12-C13
21	12	512	CL7	C4-C3-C5-C6
21	22	512	CL7	C4-C3-C5-C6
21	32	512	CL7	C4-C3-C5-C6
21	42	512	CL7	C4-C3-C5-C6
21	11	402	CL7	C2-C3-C5-C6
21	21	402	CL7	C2-C3-C5-C6
21	31	402	CL7	C2-C3-C5-C6
21	41	402	CL7	C2-C3-C5-C6
26	1D	409	LHG	C3-O3-P-O4
26	1D	409	LHG	C4-O6-P-O4
26	13	524	LHG	C3-O3-P-O5
26	14	401	LHG	C4-O6-P-O4
26	2D	409	LHG	C3-O3-P-O4
26	2D	409	LHG	C4-O6-P-O4
26	23	425	LHG	C3-O3-P-O5
26	24	401	LHG	C4-O6-P-O4
26	3D	409	LHG	C3-O3-P-O4
26	3D	409	LHG	C4-O6-P-O4
26	33	524	LHG	C3-O3-P-O5
26	34	401	LHG	C4-O6-P-O4
26	4D	409	LHG	C3-O3-P-O4
26	4D	409	LHG	C4-O6-P-O4
26	43	425	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	44	401	LHG	C4-O6-P-O4
21	4B	605	CL7	CBD-CGD-O2D-CED
26	1B	623	LHG	C10-C11-C12-C13
26	3B	623	LHG	C10-C11-C12-C13
21	1C	505	CL7	C8-C10-C11-C12
21	2C	505	CL7	C8-C10-C11-C12
21	4C	505	CL7	C8-C10-C11-C12
21	12	508	CL7	C2A-CAA-CBA-CGA
21	22	508	CL7	C2A-CAA-CBA-CGA
21	32	508	CL7	C2A-CAA-CBA-CGA
21	42	508	CL7	C2A-CAA-CBA-CGA
26	2B	624	LHG	C10-C11-C12-C13
21	12	505	CL7	C4C-C3C-CAC-CBC
21	22	505	CL7	C4C-C3C-CAC-CBC
26	4B	624	LHG	C10-C11-C12-C13
21	12	503	CL7	C16-C17-C18-C19
21	22	503	CL7	C16-C17-C18-C19
21	32	503	CL7	C16-C17-C18-C19
21	42	503	CL7	C16-C17-C18-C19
21	32	505	CL7	C4C-C3C-CAC-CBC
21	1B	601	CL7	CAD-CBD-CGD-O1D
21	12	502	CL7	CAD-CBD-CGD-O1D
21	12	506	CL7	CAD-CBD-CGD-O1D
21	12	511	CL7	CAD-CBD-CGD-O1D
21	12	513	CL7	CAD-CBD-CGD-O1D
21	11	409	CL7	CAD-CBD-CGD-O1D
21	2B	602	CL7	CAD-CBD-CGD-O1D
21	22	502	CL7	CAD-CBD-CGD-O1D
21	22	506	CL7	CAD-CBD-CGD-O1D
21	22	511	CL7	CAD-CBD-CGD-O1D
21	22	513	CL7	CAD-CBD-CGD-O1D
21	21	409	CL7	CAD-CBD-CGD-O1D
21	3B	601	CL7	CAD-CBD-CGD-O1D
21	32	502	CL7	CAD-CBD-CGD-O1D
21	32	506	CL7	CAD-CBD-CGD-O1D
21	32	511	CL7	CAD-CBD-CGD-O1D
21	32	513	CL7	CAD-CBD-CGD-O1D
21	31	409	CL7	CAD-CBD-CGD-O1D
21	4B	602	CL7	CAD-CBD-CGD-O1D
21	42	502	CL7	CAD-CBD-CGD-O1D
21	42	506	CL7	CAD-CBD-CGD-O1D
21	42	511	CL7	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	513	CL7	CAD-CBD-CGD-O1D
21	41	409	CL7	CAD-CBD-CGD-O1D
25	1B	620	SQD	O5-C5-C6-S
25	2B	621	SQD	O5-C5-C6-S
25	3B	620	SQD	O5-C5-C6-S
25	4B	621	SQD	O5-C5-C6-S
21	3C	505	CL7	C8-C10-C11-C12
21	42	505	CL7	C4C-C3C-CAC-CBC
21	24	411	CL7	C5-C6-C7-C8
21	1C	509	CL7	C16-C17-C18-C19
21	2C	509	CL7	C16-C17-C18-C19
21	3C	509	CL7	C16-C17-C18-C19
21	4C	509	CL7	C16-C17-C18-C19
21	13	516	CL7	C4-C3-C5-C6
21	23	417	CL7	C4-C3-C5-C6
21	33	516	CL7	C4-C3-C5-C6
21	43	417	CL7	C4-C3-C5-C6
21	1B	605	CL7	C6-C7-C8-C10
21	1B	611	CL7	C11-C10-C8-C7
21	1B	611	CL7	C11-C12-C13-C15
21	1C	501	CL7	C11-C10-C8-C7
21	1C	510	CL7	C11-C12-C13-C15
21	12	506	CL7	C11-C12-C13-C15
21	12	508	CL7	C3A-C2A-CAA-CBA
21	11	412	CL7	C3A-C2A-CAA-CBA
21	13	501	CL7	C6-C7-C8-C10
21	13	501	CL7	C11-C12-C13-C15
21	13	509	CL7	C12-C13-C15-C16
21	13	510	CL7	C3A-C2A-CAA-CBA
21	14	404	CL7	C6-C7-C8-C10
21	14	409	CL7	C11-C10-C8-C7
21	2B	606	CL7	C6-C7-C8-C10
21	2B	612	CL7	C11-C10-C8-C7
21	2B	612	CL7	C11-C12-C13-C15
21	2C	501	CL7	C11-C10-C8-C7
21	2C	510	CL7	C11-C12-C13-C15
21	22	506	CL7	C11-C12-C13-C15
21	22	508	CL7	C3A-C2A-CAA-CBA
21	21	412	CL7	C3A-C2A-CAA-CBA
21	23	402	CL7	C6-C7-C8-C10
21	23	402	CL7	C11-C12-C13-C15
21	23	410	CL7	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	23	411	CL7	C3A-C2A-CAA-CBA
21	23	414	CL7	C3A-C2A-CAA-CBA
21	24	404	CL7	C6-C7-C8-C10
21	24	409	CL7	C11-C10-C8-C7
21	3B	605	CL7	C6-C7-C8-C10
21	3B	611	CL7	C11-C10-C8-C7
21	3B	611	CL7	C11-C12-C13-C15
21	3C	501	CL7	C11-C10-C8-C7
21	3C	510	CL7	C11-C12-C13-C15
21	32	506	CL7	C11-C12-C13-C15
21	32	508	CL7	C3A-C2A-CAA-CBA
21	31	412	CL7	C3A-C2A-CAA-CBA
21	33	501	CL7	C6-C7-C8-C10
21	33	501	CL7	C11-C12-C13-C15
21	33	509	CL7	C12-C13-C15-C16
21	33	510	CL7	C3A-C2A-CAA-CBA
21	34	404	CL7	C6-C7-C8-C10
21	34	409	CL7	C11-C10-C8-C7
21	4B	606	CL7	C6-C7-C8-C10
21	4B	612	CL7	C11-C10-C8-C7
21	4B	612	CL7	C11-C12-C13-C15
21	4C	501	CL7	C11-C10-C8-C7
21	4C	510	CL7	C11-C12-C13-C15
21	42	506	CL7	C11-C12-C13-C15
21	42	508	CL7	C3A-C2A-CAA-CBA
21	41	412	CL7	C3A-C2A-CAA-CBA
21	43	402	CL7	C6-C7-C8-C10
21	43	402	CL7	C11-C12-C13-C15
21	43	410	CL7	C12-C13-C15-C16
21	43	411	CL7	C3A-C2A-CAA-CBA
21	43	414	CL7	C3A-C2A-CAA-CBA
21	44	404	CL7	C6-C7-C8-C10
21	44	409	CL7	C11-C10-C8-C7
23	1B	626	8CT	C28-C29-C30-C31
23	1C	514	8CT	C28-C29-C30-C31
23	1K	101	8CT	C28-C29-C30-C31
23	14	402	8CT	C28-C29-C30-C31
23	2B	601	8CT	C28-C29-C30-C31
23	2C	514	8CT	C28-C29-C30-C31
23	24	402	8CT	C28-C29-C30-C31
23	3B	626	8CT	C28-C29-C30-C31
23	3C	514	8CT	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	34	402	8CT	C28-C29-C30-C31
23	4B	601	8CT	C28-C29-C30-C31
23	4C	514	8CT	C28-C29-C30-C31
23	44	402	8CT	C28-C29-C30-C31
23	1B	617	8CT	C16-C17-C18-C19
23	2B	618	8CT	C16-C17-C18-C19
23	3B	617	8CT	C16-C17-C18-C19
23	4B	618	8CT	C16-C17-C18-C19
32	14	419	ZEX	C33-C34-C35-C15
32	24	419	ZEX	C33-C34-C35-C15
32	34	419	ZEX	C33-C34-C35-C15
32	44	419	ZEX	C33-C34-C35-C15
21	1B	604	CL7	CBD-CGD-O2D-CED
21	2B	605	CL7	CBD-CGD-O2D-CED
21	14	411	CL7	C5-C6-C7-C8
21	24	412	CL7	C5-C6-C7-C8
21	34	411	CL7	C5-C6-C7-C8
21	34	412	CL7	C5-C6-C7-C8
25	13	523	SQD	C9-C10-C11-C12
25	23	424	SQD	C9-C10-C11-C12
25	33	523	SQD	C9-C10-C11-C12
25	43	424	SQD	C9-C10-C11-C12
27	1C	516	DGD	O1A-C1A-O1G-C1G
27	2C	516	DGD	O1A-C1A-O1G-C1G
27	3C	516	DGD	O1A-C1A-O1G-C1G
21	14	412	CL7	C5-C6-C7-C8
21	44	411	CL7	C5-C6-C7-C8
21	44	412	CL7	C5-C6-C7-C8
21	3B	604	CL7	CBD-CGD-O2D-CED
21	1A	407	CL7	C16-C17-C18-C19
21	12	517	CL7	C16-C17-C18-C20
21	2A	407	CL7	C16-C17-C18-C19
21	22	517	CL7	C16-C17-C18-C20
21	3A	407	CL7	C16-C17-C18-C19
21	32	517	CL7	C16-C17-C18-C20
21	4A	407	CL7	C16-C17-C18-C19
21	42	517	CL7	C16-C17-C18-C20
27	4C	516	DGD	O1A-C1A-O1G-C1G
24	1B	621	LMG	O7-C8-C9-O8
24	2B	622	LMG	O7-C8-C9-O8
24	3B	621	LMG	O7-C8-C9-O8
24	4B	622	LMG	O7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	12	521	SQD	O47-C45-C46-O48
25	22	521	SQD	O47-C45-C46-O48
25	32	521	SQD	O47-C45-C46-O48
25	42	521	SQD	O47-C45-C46-O48
25	4A	406	SQD	C9-C10-C11-C12
25	12	521	SQD	C45-C44-O6-C1
25	13	521	SQD	C45-C44-O6-C1
25	22	521	SQD	C45-C44-O6-C1
25	23	422	SQD	C45-C44-O6-C1
25	32	521	SQD	C45-C44-O6-C1
25	33	521	SQD	C45-C44-O6-C1
25	42	521	SQD	C45-C44-O6-C1
25	43	422	SQD	C45-C44-O6-C1
21	3C	501	CL7	O1D-CGD-O2D-CED
21	1B	614	CL7	C11-C12-C13-C15
21	2B	615	CL7	C11-C12-C13-C15
21	3B	614	CL7	C11-C12-C13-C15
21	4B	615	CL7	C11-C12-C13-C15
21	22	503	CL7	C13-C15-C16-C17
21	32	503	CL7	C13-C15-C16-C17
25	2A	406	SQD	C9-C10-C11-C12
21	2C	501	CL7	O1D-CGD-O2D-CED
25	1A	406	SQD	C9-C10-C11-C12
21	1C	501	CL7	O1D-CGD-O2D-CED
21	4C	501	CL7	O1D-CGD-O2D-CED
21	12	503	CL7	C13-C15-C16-C17
21	42	503	CL7	C13-C15-C16-C17
30	1D	407	PL9	C35-C34-C36-C37
30	1D	407	PL9	C45-C44-C46-C47
30	2D	407	PL9	C35-C34-C36-C37
30	2D	407	PL9	C45-C44-C46-C47
30	3D	407	PL9	C35-C34-C36-C37
30	3D	407	PL9	C45-C44-C46-C47
30	4D	407	PL9	C35-C34-C36-C37
30	4D	407	PL9	C45-C44-C46-C47
21	1A	401	CL7	CBA-CGA-O2A-C1
21	2A	401	CL7	CBA-CGA-O2A-C1
21	3A	401	CL7	CBA-CGA-O2A-C1
21	4A	401	CL7	CBA-CGA-O2A-C1
25	2B	621	SQD	C17-C18-C19-C20
25	3B	620	SQD	C17-C18-C19-C20
25	1B	620	SQD	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	4B	621	SQD	C17-C18-C19-C20
21	1B	609	CL7	C6-C7-C8-C9
21	1C	501	CL7	C11-C10-C8-C9
21	1C	501	CL7	C14-C13-C15-C16
21	1C	502	CL7	C6-C7-C8-C9
21	12	501	CL7	C11-C10-C8-C9
21	12	502	CL7	C11-C10-C8-C9
21	12	507	CL7	C11-C10-C8-C9
21	12	507	CL7	C11-C12-C13-C14
21	12	511	CL7	C6-C7-C8-C9
21	11	404	CL7	C11-C12-C13-C14
21	13	509	CL7	C11-C12-C13-C14
21	13	510	CL7	C6-C7-C8-C9
21	13	511	CL7	C6-C7-C8-C9
21	14	405	CL7	C11-C12-C13-C14
21	14	406	CL7	C6-C7-C8-C9
21	14	409	CL7	C11-C10-C8-C9
21	14	411	CL7	C11-C12-C13-C14
21	2B	610	CL7	C6-C7-C8-C9
21	2C	501	CL7	C11-C10-C8-C9
21	2C	501	CL7	C14-C13-C15-C16
21	2C	502	CL7	C6-C7-C8-C9
21	22	501	CL7	C11-C10-C8-C9
21	22	502	CL7	C11-C10-C8-C9
21	22	507	CL7	C11-C10-C8-C9
21	22	507	CL7	C11-C12-C13-C14
21	22	511	CL7	C6-C7-C8-C9
21	21	404	CL7	C11-C12-C13-C14
21	23	410	CL7	C11-C12-C13-C14
21	23	411	CL7	C6-C7-C8-C9
21	23	412	CL7	C6-C7-C8-C9
21	24	405	CL7	C11-C12-C13-C14
21	24	406	CL7	C6-C7-C8-C9
21	24	409	CL7	C11-C10-C8-C9
21	24	411	CL7	C11-C12-C13-C14
21	3B	609	CL7	C6-C7-C8-C9
21	3C	501	CL7	C11-C10-C8-C9
21	3C	501	CL7	C14-C13-C15-C16
21	3C	502	CL7	C6-C7-C8-C9
21	32	501	CL7	C11-C10-C8-C9
21	32	502	CL7	C11-C10-C8-C9
21	32	507	CL7	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	32	507	CL7	C11-C12-C13-C14
21	32	511	CL7	C6-C7-C8-C9
21	31	404	CL7	C11-C12-C13-C14
21	33	509	CL7	C11-C12-C13-C14
21	33	510	CL7	C6-C7-C8-C9
21	33	511	CL7	C6-C7-C8-C9
21	34	405	CL7	C11-C12-C13-C14
21	34	409	CL7	C11-C10-C8-C9
21	34	411	CL7	C11-C12-C13-C14
21	4B	610	CL7	C6-C7-C8-C9
21	4C	501	CL7	C11-C10-C8-C9
21	4C	501	CL7	C14-C13-C15-C16
21	4C	502	CL7	C6-C7-C8-C9
21	42	501	CL7	C11-C10-C8-C9
21	42	502	CL7	C11-C10-C8-C9
21	42	507	CL7	C11-C10-C8-C9
21	42	507	CL7	C11-C12-C13-C14
21	42	511	CL7	C6-C7-C8-C9
21	41	404	CL7	C11-C12-C13-C14
21	43	410	CL7	C11-C12-C13-C14
21	43	411	CL7	C6-C7-C8-C9
21	43	412	CL7	C6-C7-C8-C9
21	44	405	CL7	C11-C12-C13-C14
21	44	406	CL7	C6-C7-C8-C9
21	44	409	CL7	C11-C10-C8-C9
21	44	411	CL7	C11-C12-C13-C14
22	1D	408	PHO	C6-C7-C8-C9
22	2D	408	PHO	C6-C7-C8-C9
22	3D	408	PHO	C6-C7-C8-C9
22	4D	408	PHO	C6-C7-C8-C9
25	3A	406	SQD	C9-C10-C11-C12
21	13	505	CL7	C16-C17-C18-C19
21	23	406	CL7	C16-C17-C18-C19
21	33	505	CL7	C16-C17-C18-C19
21	43	406	CL7	C16-C17-C18-C19
21	13	510	CL7	CAA-CBA-CGA-O2A
21	23	411	CL7	CAA-CBA-CGA-O2A
21	33	510	CL7	CAA-CBA-CGA-O2A
21	43	411	CL7	CAA-CBA-CGA-O2A
21	1B	614	CL7	C2B-C3B-CAB-OBB
21	1C	510	CL7	C2B-C3B-CAB-OBB
21	12	505	CL7	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	511	CL7	C2B-C3B-CAB-OBB
21	12	512	CL7	C2B-C3B-CAB-OBB
21	12	518	CL7	C2B-C3B-CAB-OBB
21	11	411	CL7	C2B-C3B-CAB-OBB
21	13	506	CL7	C2B-C3B-CAB-OBB
21	13	517	CL7	C2B-C3B-CAB-OBB
21	14	406	CL7	C2B-C3B-CAB-OBB
21	14	408	CL7	C2B-C3B-CAB-OBB
21	2B	615	CL7	C2B-C3B-CAB-OBB
21	2C	510	CL7	C2B-C3B-CAB-OBB
21	22	505	CL7	C2B-C3B-CAB-OBB
21	22	511	CL7	C2B-C3B-CAB-OBB
21	22	512	CL7	C2B-C3B-CAB-OBB
21	22	518	CL7	C2B-C3B-CAB-OBB
21	21	411	CL7	C2B-C3B-CAB-OBB
21	23	407	CL7	C2B-C3B-CAB-OBB
21	23	418	CL7	C2B-C3B-CAB-OBB
21	24	406	CL7	C2B-C3B-CAB-OBB
21	24	408	CL7	C2B-C3B-CAB-OBB
21	3B	614	CL7	C2B-C3B-CAB-OBB
21	3C	510	CL7	C2B-C3B-CAB-OBB
21	32	505	CL7	C2B-C3B-CAB-OBB
21	32	511	CL7	C2B-C3B-CAB-OBB
21	32	512	CL7	C2B-C3B-CAB-OBB
21	32	518	CL7	C2B-C3B-CAB-OBB
21	31	411	CL7	C2B-C3B-CAB-OBB
21	33	506	CL7	C2B-C3B-CAB-OBB
21	33	517	CL7	C2B-C3B-CAB-OBB
21	34	406	CL7	C2B-C3B-CAB-OBB
21	34	408	CL7	C2B-C3B-CAB-OBB
21	4B	615	CL7	C2B-C3B-CAB-OBB
21	4C	510	CL7	C2B-C3B-CAB-OBB
21	42	505	CL7	C2B-C3B-CAB-OBB
21	42	511	CL7	C2B-C3B-CAB-OBB
21	42	512	CL7	C2B-C3B-CAB-OBB
21	42	518	CL7	C2B-C3B-CAB-OBB
21	41	411	CL7	C2B-C3B-CAB-OBB
21	43	407	CL7	C2B-C3B-CAB-OBB
21	43	418	CL7	C2B-C3B-CAB-OBB
21	44	406	CL7	C2B-C3B-CAB-OBB
21	44	408	CL7	C2B-C3B-CAB-OBB
32	33	520	ZEX	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	43	421	ZEX	C31-C32-C33-C34
21	1B	608	CL7	C8-C10-C11-C12
21	2B	609	CL7	C8-C10-C11-C12
21	3B	608	CL7	C8-C10-C11-C12
21	4B	609	CL7	C8-C10-C11-C12
21	4B	612	CL7	C13-C15-C16-C17
21	24	405	CL7	C16-C17-C18-C20
21	34	405	CL7	C16-C17-C18-C20
27	2C	516	DGD	CDB-CEB-CFB-CGB
27	1C	516	DGD	CDB-CEB-CFB-CGB
21	1B	611	CL7	C13-C15-C16-C17
21	2B	612	CL7	C13-C15-C16-C17
21	3B	611	CL7	C13-C15-C16-C17
21	1B	605	CL7	C4B-C3B-CAB-OBB
21	1C	503	CL7	C4B-C3B-CAB-OBB
21	1C	512	CL7	C4B-C3B-CAB-OBB
21	11	402	CL7	C4B-C3B-CAB-OBB
21	2B	606	CL7	C4B-C3B-CAB-OBB
21	2C	503	CL7	C4B-C3B-CAB-OBB
21	2C	512	CL7	C4B-C3B-CAB-OBB
21	21	402	CL7	C4B-C3B-CAB-OBB
21	3B	605	CL7	C4B-C3B-CAB-OBB
21	3C	503	CL7	C4B-C3B-CAB-OBB
21	3C	512	CL7	C4B-C3B-CAB-OBB
21	31	402	CL7	C4B-C3B-CAB-OBB
21	4B	606	CL7	C4B-C3B-CAB-OBB
21	4C	503	CL7	C4B-C3B-CAB-OBB
21	4C	512	CL7	C4B-C3B-CAB-OBB
21	41	402	CL7	C4B-C3B-CAB-OBB
27	3C	516	DGD	CDB-CEB-CFB-CGB
27	4C	516	DGD	CDB-CEB-CFB-CGB
24	21	401	LMG	C37-C38-C39-C40
21	12	516	CL7	C2A-CAA-CBA-CGA
21	12	518	CL7	C2A-CAA-CBA-CGA
21	22	516	CL7	C2A-CAA-CBA-CGA
21	22	518	CL7	C2A-CAA-CBA-CGA
21	32	516	CL7	C2A-CAA-CBA-CGA
21	42	516	CL7	C2A-CAA-CBA-CGA
21	42	518	CL7	C2A-CAA-CBA-CGA
24	41	401	LMG	C37-C38-C39-C40
21	1B	602	CL7	C2-C1-O2A-CGA
21	12	516	CL7	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	11	410	CL7	C2-C1-O2A-CGA
21	13	517	CL7	C2-C1-O2A-CGA
21	14	405	CL7	C2-C1-O2A-CGA
21	2B	603	CL7	C2-C1-O2A-CGA
21	22	516	CL7	C2-C1-O2A-CGA
21	21	410	CL7	C2-C1-O2A-CGA
21	23	418	CL7	C2-C1-O2A-CGA
21	24	405	CL7	C2-C1-O2A-CGA
21	3B	602	CL7	C2-C1-O2A-CGA
21	32	516	CL7	C2-C1-O2A-CGA
21	31	410	CL7	C2-C1-O2A-CGA
21	33	517	CL7	C2-C1-O2A-CGA
21	34	405	CL7	C2-C1-O2A-CGA
21	4B	603	CL7	C2-C1-O2A-CGA
21	42	516	CL7	C2-C1-O2A-CGA
21	41	410	CL7	C2-C1-O2A-CGA
21	43	418	CL7	C2-C1-O2A-CGA
21	44	405	CL7	C2-C1-O2A-CGA
26	1B	623	LHG	C28-C29-C30-C31
21	14	405	CL7	C16-C17-C18-C20
21	44	405	CL7	C16-C17-C18-C20
26	4B	624	LHG	C28-C29-C30-C31
24	11	401	LMG	C37-C38-C39-C40
26	2B	624	LHG	C28-C29-C30-C31
32	13	525	ZEX	C21-C26-C27-C28
32	23	401	ZEX	C21-C26-C27-C28
32	33	525	ZEX	C21-C26-C27-C28
32	43	401	ZEX	C21-C26-C27-C28
26	3B	623	LHG	C28-C29-C30-C31
24	31	401	LMG	C37-C38-C39-C40
21	11	418	CL7	C4-C3-C5-C6
21	21	418	CL7	C4-C3-C5-C6
21	31	418	CL7	C4-C3-C5-C6
21	41	418	CL7	C4-C3-C5-C6
26	2B	626	LHG	C11-C12-C13-C14
26	3B	625	LHG	C11-C12-C13-C14
23	4B	601	8CT	C04-C03-C10-C11
21	12	507	CL7	C2-C3-C5-C6
21	22	507	CL7	C2-C3-C5-C6
21	32	507	CL7	C2-C3-C5-C6
21	42	507	CL7	C2-C3-C5-C6
25	1B	620	SQD	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	3B	620	SQD	C14-C15-C16-C17
26	4B	626	LHG	C11-C12-C13-C14
25	2B	621	SQD	C14-C15-C16-C17
25	4B	621	SQD	C14-C15-C16-C17
26	1B	625	LHG	C11-C12-C13-C14
21	32	518	CL7	C2A-CAA-CBA-CGA
25	13	523	SQD	O47-C45-C46-O48
25	23	424	SQD	O47-C45-C46-O48
25	33	523	SQD	O47-C45-C46-O48
25	43	424	SQD	O47-C45-C46-O48
24	1A	405	LMG	C29-C28-O8-C9
24	2A	405	LMG	C29-C28-O8-C9
24	3A	405	LMG	C29-C28-O8-C9
24	4A	405	LMG	C29-C28-O8-C9
21	1C	507	CL7	C12-C13-C15-C16
21	12	501	CL7	C11-C10-C8-C7
21	12	502	CL7	C6-C7-C8-C10
21	12	502	CL7	C11-C10-C8-C7
21	12	516	CL7	C12-C13-C15-C16
21	13	502	CL7	C2-C3-C5-C6
21	13	507	CL7	C11-C10-C8-C7
21	13	507	CL7	C12-C13-C15-C16
21	2C	507	CL7	C12-C13-C15-C16
21	22	501	CL7	C11-C10-C8-C7
21	22	502	CL7	C6-C7-C8-C10
21	22	502	CL7	C11-C10-C8-C7
21	22	516	CL7	C12-C13-C15-C16
21	23	403	CL7	C2-C3-C5-C6
21	23	408	CL7	C11-C10-C8-C7
21	23	408	CL7	C12-C13-C15-C16
21	3C	507	CL7	C12-C13-C15-C16
21	32	501	CL7	C11-C10-C8-C7
21	32	502	CL7	C6-C7-C8-C10
21	32	502	CL7	C11-C10-C8-C7
21	32	516	CL7	C12-C13-C15-C16
21	33	502	CL7	C2-C3-C5-C6
21	33	507	CL7	C11-C10-C8-C7
21	33	507	CL7	C12-C13-C15-C16
21	4C	507	CL7	C12-C13-C15-C16
21	42	501	CL7	C11-C10-C8-C7
21	42	502	CL7	C6-C7-C8-C10
21	42	502	CL7	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	516	CL7	C12-C13-C15-C16
21	43	403	CL7	C2-C3-C5-C6
21	43	408	CL7	C11-C10-C8-C7
21	43	408	CL7	C12-C13-C15-C16
21	1B	605	CL7	C6-C7-C8-C9
21	12	502	CL7	C6-C7-C8-C9
21	12	506	CL7	C11-C12-C13-C14
21	12	512	CL7	C11-C12-C13-C14
21	13	501	CL7	C6-C7-C8-C9
21	14	404	CL7	C6-C7-C8-C9
21	2B	606	CL7	C6-C7-C8-C9
21	22	502	CL7	C6-C7-C8-C9
21	22	506	CL7	C11-C12-C13-C14
21	22	512	CL7	C11-C12-C13-C14
21	23	402	CL7	C6-C7-C8-C9
21	24	404	CL7	C6-C7-C8-C9
21	3B	605	CL7	C6-C7-C8-C9
21	32	502	CL7	C6-C7-C8-C9
21	32	506	CL7	C11-C12-C13-C14
21	32	512	CL7	C11-C12-C13-C14
21	33	501	CL7	C6-C7-C8-C9
21	34	404	CL7	C6-C7-C8-C9
21	4B	606	CL7	C6-C7-C8-C9
21	42	502	CL7	C6-C7-C8-C9
21	42	506	CL7	C11-C12-C13-C14
21	42	512	CL7	C11-C12-C13-C14
21	43	402	CL7	C6-C7-C8-C9
21	44	404	CL7	C6-C7-C8-C9
21	44	413	CL7	C11-C10-C8-C9
21	2B	612	CL7	C15-C16-C17-C18
32	11	421	ZEX	C9-C10-C11-C12
32	21	421	ZEX	C9-C10-C11-C12
32	31	421	ZEX	C9-C10-C11-C12
32	41	421	ZEX	C9-C10-C11-C12
21	1B	603	CL7	C16-C17-C18-C20
21	2B	604	CL7	C16-C17-C18-C20
21	3B	603	CL7	C16-C17-C18-C20
21	4B	604	CL7	C16-C17-C18-C20
21	4B	612	CL7	C15-C16-C17-C18
21	13	505	CL7	C2A-CAA-CBA-CGA
21	23	406	CL7	C2A-CAA-CBA-CGA
21	33	505	CL7	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	406	CL7	C2A-CAA-CBA-CGA
21	1B	611	CL7	C15-C16-C17-C18
21	3B	611	CL7	C15-C16-C17-C18
27	2B	625	DGD	CCA-CDA-CEA-CFA
24	1B	621	LMG	C36-C37-C38-C39
24	3B	621	LMG	C36-C37-C38-C39
27	1B	624	DGD	CCA-CDA-CEA-CFA
27	3B	624	DGD	CCA-CDA-CEA-CFA
27	4B	625	DGD	CCA-CDA-CEA-CFA
24	4B	622	LMG	C36-C37-C38-C39
24	2B	622	LMG	C36-C37-C38-C39
21	13	503	CL7	C13-C15-C16-C17
21	23	404	CL7	C13-C15-C16-C17
21	43	404	CL7	C13-C15-C16-C17
32	13	520	ZEX	C31-C32-C33-C34
32	23	421	ZEX	C31-C32-C33-C34
21	33	503	CL7	C13-C15-C16-C17
21	41	418	CL7	CAA-CBA-CGA-O2A
21	14	404	CL7	C16-C17-C18-C19
21	34	404	CL7	C16-C17-C18-C19
21	44	404	CL7	C16-C17-C18-C19
21	11	402	CL7	CBD-CGD-O2D-CED
27	3B	624	DGD	C8B-C9B-CAB-CBB
27	2B	625	DGD	C8B-C9B-CAB-CBB
27	4B	625	DGD	C8B-C9B-CAB-CBB
21	1C	503	CL7	CAA-CBA-CGA-O2A
21	11	418	CL7	CAA-CBA-CGA-O2A
21	2C	503	CL7	CAA-CBA-CGA-O2A
21	21	418	CL7	CAA-CBA-CGA-O2A
21	3C	503	CL7	CAA-CBA-CGA-O2A
21	31	418	CL7	CAA-CBA-CGA-O2A
21	4C	503	CL7	CAA-CBA-CGA-O2A
27	1B	624	DGD	C8B-C9B-CAB-CBB
21	13	509	CL7	C15-C16-C17-C18
21	23	410	CL7	C15-C16-C17-C18
21	33	509	CL7	C15-C16-C17-C18
21	43	410	CL7	C15-C16-C17-C18
21	21	402	CL7	CBD-CGD-O2D-CED
21	31	402	CL7	CBD-CGD-O2D-CED
21	41	402	CL7	CBD-CGD-O2D-CED
21	24	404	CL7	C16-C17-C18-C19
21	34	411	CL7	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	11	421	ZEX	C33-C34-C35-C15
32	14	419	ZEX	C9-C10-C11-C12
32	14	420	ZEX	C9-C10-C11-C12
32	21	421	ZEX	C33-C34-C35-C15
32	24	419	ZEX	C9-C10-C11-C12
32	24	420	ZEX	C9-C10-C11-C12
32	31	421	ZEX	C33-C34-C35-C15
32	34	419	ZEX	C9-C10-C11-C12
32	34	420	ZEX	C9-C10-C11-C12
32	41	421	ZEX	C33-C34-C35-C15
32	44	419	ZEX	C9-C10-C11-C12
32	44	420	ZEX	C9-C10-C11-C12
30	1D	407	PL9	C16-C17-C18-C19
30	2D	407	PL9	C16-C17-C18-C19
30	3D	407	PL9	C16-C17-C18-C19
30	4D	407	PL9	C16-C17-C18-C19
21	14	411	CL7	C16-C17-C18-C20
21	24	411	CL7	C16-C17-C18-C20
21	44	411	CL7	C16-C17-C18-C20
21	1D	405	CL7	C4C-C3C-CAC-CBC
21	2D	405	CL7	C4C-C3C-CAC-CBC
21	14	408	CL7	CAA-CBA-CGA-O2A
21	24	408	CL7	CAA-CBA-CGA-O2A
21	11	403	CL7	C2-C1-O2A-CGA
21	14	412	CL7	C2-C1-O2A-CGA
21	2C	502	CL7	C2-C1-O2A-CGA
21	21	403	CL7	C2-C1-O2A-CGA
21	24	412	CL7	C2-C1-O2A-CGA
21	3C	502	CL7	C2-C1-O2A-CGA
21	31	403	CL7	C2-C1-O2A-CGA
21	34	412	CL7	C2-C1-O2A-CGA
21	4C	502	CL7	C2-C1-O2A-CGA
21	41	403	CL7	C2-C1-O2A-CGA
21	44	412	CL7	C2-C1-O2A-CGA
21	3D	405	CL7	C4C-C3C-CAC-CBC
21	4D	405	CL7	C4C-C3C-CAC-CBC
21	1B	614	CL7	C11-C12-C13-C14
21	12	507	CL7	C16-C17-C18-C20
21	2B	615	CL7	C11-C12-C13-C14
21	22	507	CL7	C16-C17-C18-C20
21	3B	614	CL7	C11-C12-C13-C14
21	32	507	CL7	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4B	615	CL7	C11-C12-C13-C14
21	42	507	CL7	C16-C17-C18-C20
21	34	408	CL7	CAA-CBA-CGA-O2A
21	44	408	CL7	CAA-CBA-CGA-O2A
21	13	513	CL7	C2A-CAA-CBA-CGA
21	23	414	CL7	C2A-CAA-CBA-CGA
21	33	513	CL7	C2A-CAA-CBA-CGA
21	43	414	CL7	C2A-CAA-CBA-CGA
21	13	505	CL7	C3A-C2A-CAA-CBA
21	23	406	CL7	C3A-C2A-CAA-CBA
21	33	505	CL7	C3A-C2A-CAA-CBA
21	43	406	CL7	C3A-C2A-CAA-CBA
21	11	418	CL7	C16-C17-C18-C19
21	11	418	CL7	C16-C17-C18-C20
21	21	418	CL7	C16-C17-C18-C19
21	31	418	CL7	C16-C17-C18-C19
32	14	403	ZEX	C33-C34-C35-C15
32	24	403	ZEX	C33-C34-C35-C15
32	34	403	ZEX	C33-C34-C35-C15
32	44	403	ZEX	C33-C34-C35-C15
21	13	506	CL7	C2C-C3C-CAC-CBC
21	23	407	CL7	C2C-C3C-CAC-CBC
21	2B	605	CL7	O1D-CGD-O2D-CED
21	33	506	CL7	C2C-C3C-CAC-CBC
21	43	407	CL7	C2C-C3C-CAC-CBC
21	1A	401	CL7	C11-C10-C8-C9
21	1B	611	CL7	C14-C13-C15-C16
21	12	506	CL7	C11-C10-C8-C9
21	11	406	CL7	C11-C12-C13-C14
21	13	502	CL7	C11-C10-C8-C9
21	14	406	CL7	C14-C13-C15-C16
21	14	413	CL7	C11-C10-C8-C9
21	2A	401	CL7	C11-C10-C8-C9
21	2B	612	CL7	C14-C13-C15-C16
21	22	506	CL7	C11-C10-C8-C9
21	21	406	CL7	C11-C12-C13-C14
21	21	418	CL7	C11-C10-C8-C9
21	23	403	CL7	C11-C10-C8-C9
21	24	406	CL7	C14-C13-C15-C16
21	24	413	CL7	C11-C10-C8-C9
21	3A	401	CL7	C11-C10-C8-C9
21	3B	611	CL7	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	32	506	CL7	C11-C10-C8-C9
21	31	406	CL7	C11-C12-C13-C14
21	33	502	CL7	C11-C10-C8-C9
21	34	406	CL7	C14-C13-C15-C16
21	34	413	CL7	C11-C10-C8-C9
21	4A	401	CL7	C11-C10-C8-C9
21	4B	612	CL7	C14-C13-C15-C16
21	42	506	CL7	C11-C10-C8-C9
21	41	406	CL7	C11-C12-C13-C14
21	43	403	CL7	C11-C10-C8-C9
21	44	406	CL7	C14-C13-C15-C16
21	1B	606	CL7	C6-C7-C8-C9
21	11	417	CL7	C6-C7-C8-C9
21	2B	607	CL7	C6-C7-C8-C9
21	21	417	CL7	C6-C7-C8-C9
21	21	418	CL7	C16-C17-C18-C20
21	3B	606	CL7	C6-C7-C8-C9
21	31	417	CL7	C6-C7-C8-C9
21	31	418	CL7	C16-C17-C18-C20
21	4B	607	CL7	C6-C7-C8-C9
21	41	417	CL7	C6-C7-C8-C9
21	41	418	CL7	C16-C17-C18-C19
21	41	418	CL7	C16-C17-C18-C20
21	13	506	CL7	CAA-CBA-CGA-O1A
21	23	407	CL7	CAA-CBA-CGA-O1A
21	33	506	CL7	CAA-CBA-CGA-O1A
21	43	407	CL7	CAA-CBA-CGA-O1A
21	12	505	CL7	C13-C15-C16-C17
21	22	505	CL7	C13-C15-C16-C17
21	32	505	CL7	C13-C15-C16-C17
21	42	505	CL7	C13-C15-C16-C17
23	1B	626	8CT	C39-C16-C17-C18
23	2B	601	8CT	C39-C16-C17-C18
23	3B	626	8CT	C39-C16-C17-C18
23	4B	601	8CT	C39-C16-C17-C18
21	3B	615	CL7	C2C-C3C-CAC-CBC
31	1F	101	HEM	CAA-CBA-CGA-O1A
31	2F	101	HEM	CAA-CBA-CGA-O1A
31	3F	101	HEM	CAA-CBA-CGA-O1A
31	4F	101	HEM	CAA-CBA-CGA-O1A
21	3B	604	CL7	O1D-CGD-O2D-CED
21	4B	605	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1C	508	CL7	C16-C17-C18-C20
21	2C	508	CL7	C16-C17-C18-C20
21	3C	508	CL7	C16-C17-C18-C20
21	4C	508	CL7	C16-C17-C18-C20
21	1A	407	CL7	O2A-C1-C2-C3
21	1C	510	CL7	O2A-C1-C2-C3
21	12	509	CL7	O2A-C1-C2-C3
21	2A	407	CL7	O2A-C1-C2-C3
21	2C	510	CL7	O2A-C1-C2-C3
21	22	509	CL7	O2A-C1-C2-C3
21	3A	407	CL7	O2A-C1-C2-C3
21	3C	510	CL7	O2A-C1-C2-C3
21	32	509	CL7	O2A-C1-C2-C3
21	4A	407	CL7	O2A-C1-C2-C3
21	4C	510	CL7	O2A-C1-C2-C3
21	42	509	CL7	O2A-C1-C2-C3
21	1B	604	CL7	O1D-CGD-O2D-CED
21	1B	615	CL7	C2C-C3C-CAC-CBC
31	2F	101	HEM	CAD-CBD-CGD-O1D
31	3F	101	HEM	CAD-CBD-CGD-O1D
31	4F	101	HEM	CAD-CBD-CGD-O1D
25	1B	620	SQD	C46-C45-O47-C7
25	2B	621	SQD	C46-C45-O47-C7
25	3B	620	SQD	C46-C45-O47-C7
25	4B	621	SQD	C46-C45-O47-C7
21	12	506	CL7	C1A-C2A-CAA-CBA
21	12	515	CL7	C1A-C2A-CAA-CBA
21	14	405	CL7	C1A-C2A-CAA-CBA
21	22	506	CL7	C1A-C2A-CAA-CBA
21	22	515	CL7	C1A-C2A-CAA-CBA
21	24	405	CL7	C1A-C2A-CAA-CBA
21	32	506	CL7	C1A-C2A-CAA-CBA
21	32	515	CL7	C1A-C2A-CAA-CBA
21	34	405	CL7	C1A-C2A-CAA-CBA
21	42	506	CL7	C1A-C2A-CAA-CBA
21	42	515	CL7	C1A-C2A-CAA-CBA
21	44	405	CL7	C1A-C2A-CAA-CBA
21	2B	616	CL7	C2C-C3C-CAC-CBC
21	1C	508	CL7	C16-C17-C18-C19
21	2C	508	CL7	C16-C17-C18-C19
21	4C	508	CL7	C16-C17-C18-C19
21	1A	407	CL7	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	612	CL7	C11-C12-C13-C15
21	12	501	CL7	C11-C12-C13-C15
21	13	503	CL7	C11-C12-C13-C15
21	13	511	CL7	C11-C12-C13-C15
21	14	404	CL7	C12-C13-C15-C16
21	14	412	CL7	C12-C13-C15-C16
21	2A	407	CL7	C11-C10-C8-C7
21	2B	613	CL7	C11-C12-C13-C15
21	22	501	CL7	C11-C12-C13-C15
21	23	404	CL7	C11-C12-C13-C15
21	23	412	CL7	C11-C12-C13-C15
21	24	404	CL7	C12-C13-C15-C16
21	24	412	CL7	C12-C13-C15-C16
21	3A	407	CL7	C11-C10-C8-C7
21	3B	612	CL7	C11-C12-C13-C15
21	32	501	CL7	C11-C12-C13-C15
21	33	503	CL7	C11-C12-C13-C15
21	33	511	CL7	C11-C12-C13-C15
21	34	404	CL7	C12-C13-C15-C16
21	34	412	CL7	C12-C13-C15-C16
21	4A	407	CL7	C11-C10-C8-C7
21	4B	613	CL7	C11-C12-C13-C15
21	42	501	CL7	C11-C12-C13-C15
21	43	404	CL7	C11-C12-C13-C15
21	43	412	CL7	C11-C12-C13-C15
21	44	404	CL7	C12-C13-C15-C16
21	44	412	CL7	C12-C13-C15-C16
21	4B	616	CL7	C2C-C3C-CAC-CBC
21	12	514	CL7	CAA-CBA-CGA-O2A
21	22	514	CL7	CAA-CBA-CGA-O2A
21	32	514	CL7	CAA-CBA-CGA-O2A
21	42	514	CL7	CAA-CBA-CGA-O2A
31	1F	101	HEM	CAD-CBD-CGD-O1D
21	12	514	CL7	CAA-CBA-CGA-O1A
21	22	514	CL7	CAA-CBA-CGA-O1A
21	32	514	CL7	CAA-CBA-CGA-O1A
21	3C	508	CL7	C16-C17-C18-C19
21	1A	401	CL7	C2A-CAA-CBA-CGA
21	12	501	CL7	C2A-CAA-CBA-CGA
21	11	402	CL7	C2A-CAA-CBA-CGA
21	14	405	CL7	C2A-CAA-CBA-CGA
21	2A	401	CL7	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	22	501	CL7	C2A-CAA-CBA-CGA
21	21	402	CL7	C2A-CAA-CBA-CGA
21	24	405	CL7	C2A-CAA-CBA-CGA
21	3A	401	CL7	C2A-CAA-CBA-CGA
21	32	501	CL7	C2A-CAA-CBA-CGA
21	31	402	CL7	C2A-CAA-CBA-CGA
21	34	405	CL7	C2A-CAA-CBA-CGA
21	4A	401	CL7	C2A-CAA-CBA-CGA
21	42	501	CL7	C2A-CAA-CBA-CGA
21	41	402	CL7	C2A-CAA-CBA-CGA
21	44	405	CL7	C2A-CAA-CBA-CGA
21	1B	612	CL7	C5-C6-C7-C8
21	2B	613	CL7	C5-C6-C7-C8
21	3B	612	CL7	C5-C6-C7-C8
21	4B	613	CL7	C5-C6-C7-C8
21	42	514	CL7	CAA-CBA-CGA-O1A
21	13	506	CL7	CAA-CBA-CGA-O2A
21	23	407	CL7	CAA-CBA-CGA-O2A
21	33	506	CL7	CAA-CBA-CGA-O2A
21	34	410	CL7	CAA-CBA-CGA-O1A
21	43	407	CL7	CAA-CBA-CGA-O2A
21	1C	507	CL7	C8-C10-C11-C12
21	2C	507	CL7	C8-C10-C11-C12
21	3C	507	CL7	C8-C10-C11-C12
21	4C	507	CL7	C8-C10-C11-C12
21	31	402	CL7	O1D-CGD-O2D-CED
21	32	518	CL7	C3-C5-C6-C7
23	1B	626	8CT	C15-C16-C17-C18
23	2B	601	8CT	C15-C16-C17-C18
23	3B	626	8CT	C15-C16-C17-C18
23	4B	601	8CT	C15-C16-C17-C18
21	14	410	CL7	CAA-CBA-CGA-O1A
24	11	401	LMG	O7-C8-C9-O8
24	21	401	LMG	O7-C8-C9-O8
24	31	401	LMG	O7-C8-C9-O8
24	41	401	LMG	O7-C8-C9-O8
26	14	401	LHG	O7-C5-C6-O8
26	24	401	LHG	O7-C5-C6-O8
26	34	401	LHG	O7-C5-C6-O8
26	44	401	LHG	O7-C5-C6-O8
21	11	402	CL7	O1D-CGD-O2D-CED
21	21	402	CL7	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	24	410	CL7	CAA-CBA-CGA-O1A
21	44	410	CL7	CAA-CBA-CGA-O1A
31	2F	101	HEM	CAA-CBA-CGA-O2A
31	3F	101	HEM	CAA-CBA-CGA-O2A
31	4F	101	HEM	CAA-CBA-CGA-O2A
21	1C	507	CL7	C13-C15-C16-C17
21	3C	507	CL7	C13-C15-C16-C17
21	41	402	CL7	O1D-CGD-O2D-CED
21	13	504	CL7	C16-C17-C18-C19
21	2C	507	CL7	C13-C15-C16-C17
21	4C	507	CL7	C13-C15-C16-C17
31	1F	101	HEM	CAA-CBA-CGA-O2A
21	14	411	CL7	C4-C3-C5-C6
21	24	411	CL7	C4-C3-C5-C6
21	34	411	CL7	C4-C3-C5-C6
21	44	411	CL7	C4-C3-C5-C6
21	1C	508	CL7	C2-C1-O2A-CGA
21	13	508	CL7	C2-C1-O2A-CGA
21	13	511	CL7	C2-C1-O2A-CGA
21	2C	508	CL7	C2-C1-O2A-CGA
21	23	409	CL7	C2-C1-O2A-CGA
21	23	412	CL7	C2-C1-O2A-CGA
21	3C	508	CL7	C2-C1-O2A-CGA
21	33	508	CL7	C2-C1-O2A-CGA
21	33	511	CL7	C2-C1-O2A-CGA
21	4C	508	CL7	C2-C1-O2A-CGA
21	43	409	CL7	C2-C1-O2A-CGA
21	43	412	CL7	C2-C1-O2A-CGA
21	2C	507	CL7	C15-C16-C17-C18
21	32	517	CL7	C13-C15-C16-C17
21	4C	507	CL7	C15-C16-C17-C18
21	43	405	CL7	C16-C17-C18-C19
21	1C	501	CL7	C11-C12-C13-C14
21	11	418	CL7	C11-C10-C8-C9
21	2C	501	CL7	C11-C12-C13-C14
21	3C	501	CL7	C11-C12-C13-C14
21	31	418	CL7	C11-C10-C8-C9
21	4C	501	CL7	C11-C12-C13-C14
21	41	418	CL7	C11-C10-C8-C9
21	42	517	CL7	C13-C15-C16-C17
21	42	518	CL7	C3-C5-C6-C7
21	24	410	CL7	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	34	410	CL7	CAA-CBA-CGA-O2A
21	44	410	CL7	CAA-CBA-CGA-O2A
21	12	517	CL7	C13-C15-C16-C17
21	22	517	CL7	C13-C15-C16-C17
21	3C	507	CL7	C15-C16-C17-C18
32	13	520	ZEX	C21-C26-C27-C28
32	23	421	ZEX	C21-C26-C27-C28
32	33	520	ZEX	C21-C26-C27-C28
32	43	421	ZEX	C21-C26-C27-C28
21	1C	507	CL7	C15-C16-C17-C18
21	33	504	CL7	C16-C17-C18-C19
21	4A	403	CL7	C6-C7-C8-C9
21	14	410	CL7	CAA-CBA-CGA-O2A
21	44	408	CL7	CAA-CBA-CGA-O1A
21	12	518	CL7	C3-C5-C6-C7
21	22	518	CL7	C3-C5-C6-C7
23	1D	406	8CT	C04-C03-C10-C11
23	3D	406	8CT	C04-C03-C10-C11
21	1C	509	CL7	CAA-CBA-CGA-O2A
21	2C	509	CL7	CAA-CBA-CGA-O2A
21	3C	509	CL7	CAA-CBA-CGA-O2A
21	4C	509	CL7	CAA-CBA-CGA-O2A
21	14	408	CL7	CAA-CBA-CGA-O1A
21	24	408	CL7	CAA-CBA-CGA-O1A
21	34	408	CL7	CAA-CBA-CGA-O1A
32	11	421	ZEX	C29-C30-C31-C32
32	14	418	ZEX	C29-C30-C31-C32
32	21	421	ZEX	C29-C30-C31-C32
32	24	418	ZEX	C29-C30-C31-C32
32	31	421	ZEX	C29-C30-C31-C32
32	34	418	ZEX	C29-C30-C31-C32
32	41	421	ZEX	C29-C30-C31-C32
32	44	418	ZEX	C29-C30-C31-C32
21	1B	604	CL7	C4-C3-C5-C6
21	2B	605	CL7	C4-C3-C5-C6
21	3B	604	CL7	C4-C3-C5-C6
21	4B	605	CL7	C4-C3-C5-C6
32	14	420	ZEX	C11-C12-C13-C14
32	24	420	ZEX	C11-C12-C13-C14
32	34	420	ZEX	C11-C12-C13-C14
32	44	420	ZEX	C11-C12-C13-C14
21	1A	403	CL7	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	23	405	CL7	C16-C17-C18-C19
21	3A	403	CL7	C6-C7-C8-C9
30	1D	407	PL9	C33-C34-C36-C37
30	1D	407	PL9	C43-C44-C46-C47
30	2D	407	PL9	C33-C34-C36-C37
30	2D	407	PL9	C43-C44-C46-C47
30	3D	407	PL9	C33-C34-C36-C37
30	3D	407	PL9	C43-C44-C46-C47
30	4D	407	PL9	C33-C34-C36-C37
30	4D	407	PL9	C43-C44-C46-C47
21	11	410	CL7	C3-C5-C6-C7
21	21	410	CL7	C3-C5-C6-C7
21	31	410	CL7	C3-C5-C6-C7
21	41	410	CL7	C3-C5-C6-C7
21	13	513	CL7	CAA-CBA-CGA-O2A
21	23	414	CL7	CAA-CBA-CGA-O2A
21	33	513	CL7	CAA-CBA-CGA-O2A
26	2A	408	LHG	C9-C10-C11-C12
26	4A	408	LHG	C9-C10-C11-C12
21	14	406	CL7	C16-C17-C18-C20
21	2A	403	CL7	C6-C7-C8-C9
21	24	406	CL7	C16-C17-C18-C20
21	34	406	CL7	C16-C17-C18-C20
21	44	406	CL7	C16-C17-C18-C20
26	1A	408	LHG	C9-C10-C11-C12
26	3A	408	LHG	C9-C10-C11-C12
21	43	414	CL7	CAA-CBA-CGA-O2A
21	33	518	CL7	CAA-CBA-CGA-O2A
21	34	405	CL7	C8-C10-C11-C12
21	44	405	CL7	C8-C10-C11-C12
26	1D	409	LHG	O6-C4-C5-C6
26	2D	409	LHG	O6-C4-C5-C6
26	3D	409	LHG	O6-C4-C5-C6
26	4D	409	LHG	O6-C4-C5-C6
27	1B	624	DGD	O2G-C1B-C2B-C3B
27	2B	625	DGD	O2G-C1B-C2B-C3B
27	3B	624	DGD	O2G-C1B-C2B-C3B
27	4B	625	DGD	O2G-C1B-C2B-C3B
21	12	506	CL7	C4-C3-C5-C6
21	14	414	CL7	C4-C3-C5-C6
21	22	506	CL7	C4-C3-C5-C6
21	24	414	CL7	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	32	506	CL7	C4-C3-C5-C6
21	34	414	CL7	C4-C3-C5-C6
21	42	506	CL7	C4-C3-C5-C6
21	44	414	CL7	C4-C3-C5-C6
21	1B	609	CL7	C12-C13-C15-C16
21	12	505	CL7	C6-C7-C8-C10
21	13	516	CL7	C2-C3-C5-C6
21	14	411	CL7	C2-C3-C5-C6
21	2B	610	CL7	C12-C13-C15-C16
21	22	505	CL7	C6-C7-C8-C10
21	23	417	CL7	C2-C3-C5-C6
21	24	411	CL7	C2-C3-C5-C6
21	3B	609	CL7	C12-C13-C15-C16
21	32	505	CL7	C6-C7-C8-C10
21	33	516	CL7	C2-C3-C5-C6
21	34	411	CL7	C2-C3-C5-C6
21	4B	610	CL7	C12-C13-C15-C16
21	42	505	CL7	C6-C7-C8-C10
21	43	417	CL7	C2-C3-C5-C6
21	44	411	CL7	C2-C3-C5-C6
21	13	518	CL7	CAA-CBA-CGA-O2A
21	23	419	CL7	CAA-CBA-CGA-O2A
21	43	419	CL7	CAA-CBA-CGA-O2A
21	14	405	CL7	C8-C10-C11-C12
21	24	405	CL7	C8-C10-C11-C12
23	1D	406	8CT	C18-C19-C20-C21
21	1A	401	CL7	CAA-CBA-CGA-O2A
21	3A	401	CL7	CAA-CBA-CGA-O2A
21	1B	605	CL7	C2B-C3B-CAB-OBB
21	2B	606	CL7	C2B-C3B-CAB-OBB
21	3B	605	CL7	C2B-C3B-CAB-OBB
21	4B	606	CL7	C2B-C3B-CAB-OBB
21	3B	622	CL7	CAA-CBA-CGA-O2A
21	2A	401	CL7	CAA-CBA-CGA-O2A
21	4A	401	CL7	CAA-CBA-CGA-O2A
21	1D	404	CL7	C2A-CAA-CBA-CGA
21	11	412	CL7	C2A-CAA-CBA-CGA
21	2D	404	CL7	C2A-CAA-CBA-CGA
21	21	412	CL7	C2A-CAA-CBA-CGA
21	3D	404	CL7	C2A-CAA-CBA-CGA
21	31	412	CL7	C2A-CAA-CBA-CGA
21	4D	404	CL7	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	41	412	CL7	C2A-CAA-CBA-CGA
21	23	414	CL7	C2C-C3C-CAC-CBC
21	33	513	CL7	C2C-C3C-CAC-CBC
21	1B	622	CL7	CAA-CBA-CGA-O2A
21	2B	623	CL7	CAA-CBA-CGA-O2A
21	34	415	CL7	CAA-CBA-CGA-O2A
21	4B	623	CL7	CAA-CBA-CGA-O2A
21	44	415	CL7	CAA-CBA-CGA-O2A
21	13	513	CL7	C2C-C3C-CAC-CBC
21	43	414	CL7	C2C-C3C-CAC-CBC
21	1B	605	CL7	C4-C3-C5-C6
21	1C	506	CL7	C4-C3-C5-C6
21	1C	510	CL7	C4-C3-C5-C6
21	12	502	CL7	C4-C3-C5-C6
21	2B	606	CL7	C4-C3-C5-C6
21	2C	506	CL7	C4-C3-C5-C6
21	2C	510	CL7	C4-C3-C5-C6
21	22	502	CL7	C4-C3-C5-C6
21	3B	605	CL7	C4-C3-C5-C6
21	3C	506	CL7	C4-C3-C5-C6
21	3C	510	CL7	C4-C3-C5-C6
21	32	502	CL7	C4-C3-C5-C6
21	4C	506	CL7	C4-C3-C5-C6
21	4C	510	CL7	C4-C3-C5-C6
21	42	502	CL7	C4-C3-C5-C6
30	1D	407	PL9	C20-C19-C21-C22
30	2D	407	PL9	C20-C19-C21-C22
30	3D	407	PL9	C20-C19-C21-C22
30	4D	407	PL9	C20-C19-C21-C22
21	14	415	CL7	CAA-CBA-CGA-O2A
21	21	412	CL7	CAA-CBA-CGA-O2A
21	24	415	CL7	CAA-CBA-CGA-O2A
21	1B	613	CL7	C2-C3-C5-C6
21	12	512	CL7	C2-C3-C5-C6
21	2B	614	CL7	C2-C3-C5-C6
21	22	512	CL7	C2-C3-C5-C6
21	3B	613	CL7	C2-C3-C5-C6
21	32	512	CL7	C2-C3-C5-C6
21	4B	614	CL7	C2-C3-C5-C6
21	42	512	CL7	C2-C3-C5-C6
21	1B	605	CL7	C11-C12-C13-C14
21	1B	612	CL7	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1C	503	CL7	C11-C12-C13-C14
21	12	507	CL7	C14-C13-C15-C16
21	14	412	CL7	C11-C10-C8-C9
21	14	412	CL7	C14-C13-C15-C16
21	2B	606	CL7	C11-C12-C13-C14
21	2C	503	CL7	C11-C12-C13-C14
21	22	507	CL7	C14-C13-C15-C16
21	24	412	CL7	C11-C10-C8-C9
21	24	412	CL7	C14-C13-C15-C16
21	3B	605	CL7	C11-C12-C13-C14
21	3C	503	CL7	C11-C12-C13-C14
21	34	412	CL7	C11-C10-C8-C9
21	34	412	CL7	C14-C13-C15-C16
21	4B	606	CL7	C11-C12-C13-C14
21	4C	503	CL7	C11-C12-C13-C14
21	44	412	CL7	C11-C10-C8-C9
21	44	412	CL7	C14-C13-C15-C16
21	11	412	CL7	CAA-CBA-CGA-O2A
21	31	412	CL7	CAA-CBA-CGA-O2A
21	41	412	CL7	CAA-CBA-CGA-O2A
21	12	504	CL7	C3A-C2A-CAA-CBA
21	11	419	CL7	C3A-C2A-CAA-CBA
21	22	504	CL7	C3A-C2A-CAA-CBA
21	21	419	CL7	C3A-C2A-CAA-CBA
21	32	504	CL7	C3A-C2A-CAA-CBA
21	31	419	CL7	C3A-C2A-CAA-CBA
21	42	504	CL7	C3A-C2A-CAA-CBA
21	41	419	CL7	C3A-C2A-CAA-CBA
21	11	411	CL7	CAA-CBA-CGA-O2A
21	11	419	CL7	CAA-CBA-CGA-O2A
21	21	411	CL7	CAA-CBA-CGA-O2A
21	21	419	CL7	CAA-CBA-CGA-O2A
21	31	411	CL7	CAA-CBA-CGA-O2A
21	31	419	CL7	CAA-CBA-CGA-O2A
21	41	411	CL7	CAA-CBA-CGA-O2A
21	41	419	CL7	CAA-CBA-CGA-O2A
21	1A	401	CL7	CAD-CBD-CGD-O2D
21	1B	609	CL7	CAD-CBD-CGD-O2D
21	1C	503	CL7	CAD-CBD-CGD-O2D
21	1C	508	CL7	CAD-CBD-CGD-O2D
21	1C	517	CL7	CAD-CBD-CGD-O2D
21	1D	404	CL7	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	12	508	CL7	CAD-CBD-CGD-O2D
21	11	420	CL7	CAD-CBD-CGD-O2D
21	13	501	CL7	CAD-CBD-CGD-O2D
21	13	503	CL7	CAD-CBD-CGD-O2D
21	13	507	CL7	CAD-CBD-CGD-O2D
21	13	508	CL7	CAD-CBD-CGD-O2D
21	13	511	CL7	CAD-CBD-CGD-O2D
21	13	512	CL7	CAD-CBD-CGD-O2D
21	13	513	CL7	CAD-CBD-CGD-O2D
21	2B	610	CL7	CAD-CBD-CGD-O2D
21	2C	503	CL7	CAD-CBD-CGD-O2D
21	2C	508	CL7	CAD-CBD-CGD-O2D
21	2C	517	CL7	CAD-CBD-CGD-O2D
21	2D	404	CL7	CAD-CBD-CGD-O2D
21	22	508	CL7	CAD-CBD-CGD-O2D
21	21	420	CL7	CAD-CBD-CGD-O2D
21	23	402	CL7	CAD-CBD-CGD-O2D
21	23	404	CL7	CAD-CBD-CGD-O2D
21	23	408	CL7	CAD-CBD-CGD-O2D
21	23	409	CL7	CAD-CBD-CGD-O2D
21	23	412	CL7	CAD-CBD-CGD-O2D
21	23	413	CL7	CAD-CBD-CGD-O2D
21	23	414	CL7	CAD-CBD-CGD-O2D
21	3B	609	CL7	CAD-CBD-CGD-O2D
21	3C	503	CL7	CAD-CBD-CGD-O2D
21	3C	508	CL7	CAD-CBD-CGD-O2D
21	3C	517	CL7	CAD-CBD-CGD-O2D
21	3D	404	CL7	CAD-CBD-CGD-O2D
21	32	508	CL7	CAD-CBD-CGD-O2D
21	31	420	CL7	CAD-CBD-CGD-O2D
21	33	501	CL7	CAD-CBD-CGD-O2D
21	33	503	CL7	CAD-CBD-CGD-O2D
21	33	507	CL7	CAD-CBD-CGD-O2D
21	33	508	CL7	CAD-CBD-CGD-O2D
21	33	511	CL7	CAD-CBD-CGD-O2D
21	33	512	CL7	CAD-CBD-CGD-O2D
21	33	513	CL7	CAD-CBD-CGD-O2D
21	4B	610	CL7	CAD-CBD-CGD-O2D
21	4C	503	CL7	CAD-CBD-CGD-O2D
21	4C	508	CL7	CAD-CBD-CGD-O2D
21	4C	517	CL7	CAD-CBD-CGD-O2D
21	4D	404	CL7	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	508	CL7	CAD-CBD-CGD-O2D
21	41	420	CL7	CAD-CBD-CGD-O2D
21	43	402	CL7	CAD-CBD-CGD-O2D
21	43	404	CL7	CAD-CBD-CGD-O2D
21	43	408	CL7	CAD-CBD-CGD-O2D
21	43	409	CL7	CAD-CBD-CGD-O2D
21	43	412	CL7	CAD-CBD-CGD-O2D
21	43	413	CL7	CAD-CBD-CGD-O2D
21	43	414	CL7	CAD-CBD-CGD-O2D
21	2C	503	CL7	C8-C10-C11-C12
23	2D	406	8CT	C18-C19-C20-C21
23	3D	406	8CT	C18-C19-C20-C21
23	4D	406	8CT	C18-C19-C20-C21
21	1C	502	CL7	C2-C1-O2A-CGA
31	1F	101	HEM	CAD-CBD-CGD-O2D
31	2F	101	HEM	CAD-CBD-CGD-O2D
31	3F	101	HEM	CAD-CBD-CGD-O2D
31	4F	101	HEM	CAD-CBD-CGD-O2D
21	14	406	CL7	CAA-CBA-CGA-O2A
21	24	406	CL7	CAA-CBA-CGA-O2A
21	34	406	CL7	CAA-CBA-CGA-O2A
21	44	406	CL7	CAA-CBA-CGA-O2A
21	1C	503	CL7	C8-C10-C11-C12
21	3C	503	CL7	C8-C10-C11-C12
21	4C	503	CL7	C8-C10-C11-C12
21	4B	606	CL7	C4-C3-C5-C6
21	12	516	CL7	C16-C17-C18-C19
21	42	516	CL7	C16-C17-C18-C19
21	11	405	CL7	CAA-CBA-CGA-O1A
21	11	405	CL7	CAA-CBA-CGA-O2A
21	13	513	CL7	CAA-CBA-CGA-O1A
21	21	405	CL7	CAA-CBA-CGA-O2A
21	23	414	CL7	CAA-CBA-CGA-O1A
21	31	405	CL7	CAA-CBA-CGA-O2A
21	41	405	CL7	CAA-CBA-CGA-O2A
21	43	414	CL7	CAA-CBA-CGA-O1A
21	12	501	CL7	CAA-CBA-CGA-O2A
21	22	501	CL7	CAA-CBA-CGA-O2A
21	32	501	CL7	CAA-CBA-CGA-O2A
21	42	501	CL7	CAA-CBA-CGA-O2A
23	1A	404	8CT	C20-C21-C23-C24
23	2A	404	8CT	C20-C21-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	3A	404	8CT	C20-C21-C23-C24
23	4A	404	8CT	C20-C21-C23-C24
25	12	521	SQD	C44-C45-C46-O48
25	22	521	SQD	C44-C45-C46-O48
25	32	521	SQD	C44-C45-C46-O48
25	42	521	SQD	C44-C45-C46-O48
21	33	513	CL7	CAA-CBA-CGA-O1A
21	11	406	CL7	O1D-CGD-O2D-CED
21	41	406	CL7	O1D-CGD-O2D-CED
21	2B	610	CL7	CAA-CBA-CGA-O2A
21	4B	610	CL7	CAA-CBA-CGA-O2A
21	32	516	CL7	C16-C17-C18-C19
21	21	405	CL7	CAA-CBA-CGA-O1A
21	21	411	CL7	CAA-CBA-CGA-O1A
21	23	419	CL7	CAA-CBA-CGA-O1A
21	31	405	CL7	CAA-CBA-CGA-O1A
21	41	405	CL7	CAA-CBA-CGA-O1A
21	41	412	CL7	CAA-CBA-CGA-O1A
21	43	419	CL7	CAA-CBA-CGA-O1A
26	2B	624	LHG	C25-C26-C27-C28
26	3B	623	LHG	C25-C26-C27-C28
26	4B	624	LHG	C25-C26-C27-C28
21	33	501	CL7	C5-C6-C7-C8
21	1B	610	CL7	O2A-C1-C2-C3
21	1C	505	CL7	O2A-C1-C2-C3
21	14	413	CL7	O2A-C1-C2-C3
21	2B	611	CL7	O2A-C1-C2-C3
21	2C	505	CL7	O2A-C1-C2-C3
21	24	413	CL7	O2A-C1-C2-C3
21	3B	610	CL7	O2A-C1-C2-C3
21	3C	505	CL7	O2A-C1-C2-C3
21	34	413	CL7	O2A-C1-C2-C3
21	4B	611	CL7	O2A-C1-C2-C3
21	4C	505	CL7	O2A-C1-C2-C3
21	44	413	CL7	O2A-C1-C2-C3
26	1B	623	LHG	C25-C26-C27-C28
26	2D	409	LHG	C31-C32-C33-C34
26	4D	409	LHG	C31-C32-C33-C34
26	1D	409	LHG	C31-C32-C33-C34
26	3D	409	LHG	C31-C32-C33-C34
21	1B	609	CL7	CAA-CBA-CGA-O2A
21	3B	609	CL7	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	11	412	CL7	CAA-CBA-CGA-O1A
21	13	518	CL7	CAA-CBA-CGA-O1A
21	21	412	CL7	CAA-CBA-CGA-O1A
21	31	411	CL7	CAA-CBA-CGA-O1A
21	31	412	CL7	CAA-CBA-CGA-O1A
21	33	518	CL7	CAA-CBA-CGA-O1A
21	41	411	CL7	CAA-CBA-CGA-O1A
21	32	503	CL7	C5-C6-C7-C8
21	42	503	CL7	C5-C6-C7-C8
21	22	516	CL7	C16-C17-C18-C19
21	1A	407	CL7	CHA-CBD-CGD-O2D
21	1B	605	CL7	CHA-CBD-CGD-O2D
21	1B	608	CL7	CHA-CBD-CGD-O2D
21	1B	610	CL7	CHA-CBD-CGD-O2D
21	1B	616	CL7	CHA-CBD-CGD-O2D
21	1C	504	CL7	CHA-CBD-CGD-O2D
21	1C	510	CL7	CHA-CBD-CGD-O1D
21	12	507	CL7	CHA-CBD-CGD-O2D
21	12	517	CL7	CHA-CBD-CGD-O2D
21	12	517	CL7	CHA-CBD-CGD-O1D
21	11	405	CL7	CHA-CBD-CGD-O2D
21	11	405	CL7	CHA-CBD-CGD-O1D
21	13	502	CL7	CHA-CBD-CGD-O2D
21	13	505	CL7	CHA-CBD-CGD-O2D
21	13	505	CL7	CHA-CBD-CGD-O1D
21	13	512	CL7	CHA-CBD-CGD-O1D
21	13	516	CL7	CHA-CBD-CGD-O2D
21	13	516	CL7	CHA-CBD-CGD-O1D
21	2A	407	CL7	CHA-CBD-CGD-O2D
21	2B	606	CL7	CHA-CBD-CGD-O2D
21	2B	609	CL7	CHA-CBD-CGD-O2D
21	2B	611	CL7	CHA-CBD-CGD-O2D
21	2B	617	CL7	CHA-CBD-CGD-O2D
21	2C	504	CL7	CHA-CBD-CGD-O2D
21	2C	510	CL7	CHA-CBD-CGD-O1D
21	22	502	CL7	CHA-CBD-CGD-O2D
21	22	507	CL7	CHA-CBD-CGD-O2D
21	22	517	CL7	CHA-CBD-CGD-O2D
21	22	517	CL7	CHA-CBD-CGD-O1D
21	21	405	CL7	CHA-CBD-CGD-O2D
21	21	405	CL7	CHA-CBD-CGD-O1D
21	23	403	CL7	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	23	406	CL7	CHA-CBD-CGD-O2D
21	23	406	CL7	CHA-CBD-CGD-O1D
21	23	413	CL7	CHA-CBD-CGD-O1D
21	23	417	CL7	CHA-CBD-CGD-O2D
21	23	417	CL7	CHA-CBD-CGD-O1D
21	3A	407	CL7	CHA-CBD-CGD-O2D
21	3B	605	CL7	CHA-CBD-CGD-O2D
21	3B	608	CL7	CHA-CBD-CGD-O2D
21	3B	610	CL7	CHA-CBD-CGD-O2D
21	3B	616	CL7	CHA-CBD-CGD-O2D
21	3C	504	CL7	CHA-CBD-CGD-O2D
21	3C	510	CL7	CHA-CBD-CGD-O1D
21	32	507	CL7	CHA-CBD-CGD-O2D
21	32	517	CL7	CHA-CBD-CGD-O2D
21	32	517	CL7	CHA-CBD-CGD-O1D
21	31	405	CL7	CHA-CBD-CGD-O2D
21	31	405	CL7	CHA-CBD-CGD-O1D
21	33	502	CL7	CHA-CBD-CGD-O2D
21	33	505	CL7	CHA-CBD-CGD-O2D
21	33	505	CL7	CHA-CBD-CGD-O1D
21	33	512	CL7	CHA-CBD-CGD-O1D
21	33	516	CL7	CHA-CBD-CGD-O2D
21	33	516	CL7	CHA-CBD-CGD-O1D
21	4A	407	CL7	CHA-CBD-CGD-O2D
21	4B	606	CL7	CHA-CBD-CGD-O2D
21	4B	609	CL7	CHA-CBD-CGD-O2D
21	4B	611	CL7	CHA-CBD-CGD-O2D
21	4B	617	CL7	CHA-CBD-CGD-O2D
21	4C	504	CL7	CHA-CBD-CGD-O2D
21	4C	510	CL7	CHA-CBD-CGD-O1D
21	42	507	CL7	CHA-CBD-CGD-O2D
21	42	517	CL7	CHA-CBD-CGD-O2D
21	42	517	CL7	CHA-CBD-CGD-O1D
21	41	405	CL7	CHA-CBD-CGD-O2D
21	41	405	CL7	CHA-CBD-CGD-O1D
21	43	403	CL7	CHA-CBD-CGD-O2D
21	43	406	CL7	CHA-CBD-CGD-O2D
21	43	406	CL7	CHA-CBD-CGD-O1D
21	43	413	CL7	CHA-CBD-CGD-O1D
21	43	417	CL7	CHA-CBD-CGD-O2D
21	43	417	CL7	CHA-CBD-CGD-O1D
21	43	402	CL7	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	11	411	CL7	CAA-CBA-CGA-O1A
21	11	419	CL7	CAA-CBA-CGA-O1A
21	21	419	CL7	CAA-CBA-CGA-O1A
21	31	419	CL7	CAA-CBA-CGA-O1A
21	41	419	CL7	CAA-CBA-CGA-O1A
30	1D	407	PL9	C17-C18-C19-C21
30	2D	407	PL9	C17-C18-C19-C21
30	3D	407	PL9	C17-C18-C19-C21
30	4D	407	PL9	C17-C18-C19-C21
21	31	406	CL7	O1D-CGD-O2D-CED
21	12	503	CL7	C5-C6-C7-C8
21	13	501	CL7	C5-C6-C7-C8
21	23	402	CL7	C5-C6-C7-C8
21	32	511	CL7	C11-C12-C13-C14
22	2D	408	PHO	C16-C17-C18-C20
21	22	503	CL7	C5-C6-C7-C8
21	12	510	CL7	CAA-CBA-CGA-O2A
21	12	512	CL7	CAA-CBA-CGA-O2A
21	22	510	CL7	CAA-CBA-CGA-O2A
21	24	412	CL7	CAA-CBA-CGA-O2A
21	32	510	CL7	CAA-CBA-CGA-O2A
21	42	512	CL7	CAA-CBA-CGA-O2A
21	21	406	CL7	O1D-CGD-O2D-CED
21	1C	508	CL7	C8-C10-C11-C12
21	14	413	CL7	C8-C10-C11-C12
21	2C	508	CL7	C8-C10-C11-C12
21	24	413	CL7	C8-C10-C11-C12
21	3C	508	CL7	C8-C10-C11-C12
21	4C	508	CL7	C8-C10-C11-C12
21	44	413	CL7	C8-C10-C11-C12
21	34	413	CL7	C8-C10-C11-C12
21	13	501	CL7	CAA-CBA-CGA-O2A
21	22	512	CL7	CAA-CBA-CGA-O2A
21	23	402	CL7	CAA-CBA-CGA-O2A
21	32	512	CL7	CAA-CBA-CGA-O2A
21	33	501	CL7	CAA-CBA-CGA-O2A
21	34	412	CL7	CAA-CBA-CGA-O2A
21	42	510	CL7	CAA-CBA-CGA-O2A
21	43	402	CL7	CAA-CBA-CGA-O2A
21	44	412	CL7	CAA-CBA-CGA-O2A
21	12	511	CL7	C11-C12-C13-C14
21	22	511	CL7	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	42	511	CL7	C11-C12-C13-C14
22	1D	408	PHO	C16-C17-C18-C20
22	3D	408	PHO	C16-C17-C18-C20
22	4D	408	PHO	C16-C17-C18-C20
21	1D	404	CL7	C3-C5-C6-C7
21	2D	404	CL7	C3-C5-C6-C7
21	3D	404	CL7	C3-C5-C6-C7
21	4D	404	CL7	C3-C5-C6-C7
24	1D	410	LMG	C11-C10-O7-C8
24	2D	410	LMG	C11-C10-O7-C8
24	3D	410	LMG	C11-C10-O7-C8
24	4D	410	LMG	C11-C10-O7-C8
21	14	409	CL7	CAA-CBA-CGA-O2A
21	14	412	CL7	CAA-CBA-CGA-O2A
21	24	409	CL7	CAA-CBA-CGA-O2A
21	34	409	CL7	CAA-CBA-CGA-O2A
21	44	409	CL7	CAA-CBA-CGA-O2A
21	11	418	CL7	C6-C7-C8-C10
21	21	418	CL7	C6-C7-C8-C10
21	31	418	CL7	C6-C7-C8-C10
21	41	418	CL7	C6-C7-C8-C10
24	1D	410	LMG	O7-C10-C11-C12
24	2D	410	LMG	O7-C10-C11-C12
24	3D	410	LMG	O7-C10-C11-C12
24	4D	410	LMG	O7-C10-C11-C12
21	2B	623	CL7	CAA-CBA-CGA-O1A
21	1B	604	CL7	C14-C13-C15-C16
21	12	517	CL7	C14-C13-C15-C16
21	11	408	CL7	C11-C12-C13-C14
21	13	503	CL7	C11-C12-C13-C14
21	13	511	CL7	C11-C12-C13-C14
21	2B	605	CL7	C14-C13-C15-C16
21	2B	613	CL7	C14-C13-C15-C16
21	22	517	CL7	C14-C13-C15-C16
21	21	408	CL7	C11-C12-C13-C14
21	23	404	CL7	C11-C12-C13-C14
21	23	412	CL7	C11-C12-C13-C14
21	3B	604	CL7	C14-C13-C15-C16
21	3B	612	CL7	C14-C13-C15-C16
21	32	507	CL7	C14-C13-C15-C16
21	32	517	CL7	C14-C13-C15-C16
21	31	408	CL7	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	33	503	CL7	C11-C12-C13-C14
21	33	511	CL7	C11-C12-C13-C14
21	4B	605	CL7	C14-C13-C15-C16
21	4B	613	CL7	C14-C13-C15-C16
21	42	507	CL7	C14-C13-C15-C16
21	42	517	CL7	C14-C13-C15-C16
21	43	404	CL7	C11-C12-C13-C14
21	43	412	CL7	C11-C12-C13-C14
23	14	402	8CT	C23-C24-C25-C26
23	24	402	8CT	C23-C24-C25-C26
23	34	402	8CT	C23-C24-C25-C26
23	44	402	8CT	C23-C24-C25-C26
26	34	401	LHG	C15-C16-C17-C18
21	1B	622	CL7	CAA-CBA-CGA-O1A
21	3B	622	CL7	CAA-CBA-CGA-O1A
21	4B	623	CL7	CAA-CBA-CGA-O1A
26	14	401	LHG	C15-C16-C17-C18
26	24	401	LHG	C15-C16-C17-C18
26	44	401	LHG	C15-C16-C17-C18
21	23	418	CL7	CAA-CBA-CGA-O2A
25	1A	406	SQD	C4-C5-C6-S
25	11	423	SQD	C4-C5-C6-S
25	2A	406	SQD	C4-C5-C6-S
25	21	423	SQD	C4-C5-C6-S
25	3A	406	SQD	C4-C5-C6-S
25	31	423	SQD	C4-C5-C6-S
25	4A	406	SQD	C4-C5-C6-S
25	41	423	SQD	C4-C5-C6-S
21	21	406	CL7	CBD-CGD-O2D-CED
21	23	406	CL7	C16-C17-C18-C20
21	33	505	CL7	C16-C17-C18-C20
21	14	415	CL7	CAA-CBA-CGA-O1A
21	24	415	CL7	CAA-CBA-CGA-O1A
21	34	415	CL7	CAA-CBA-CGA-O1A
21	44	415	CL7	CAA-CBA-CGA-O1A
21	11	406	CL7	CBD-CGD-O2D-CED
21	41	406	CL7	CBD-CGD-O2D-CED
21	1A	401	CL7	CAA-CBA-CGA-O1A
21	32	501	CL7	CAA-CBA-CGA-O1A
21	4A	401	CL7	CAA-CBA-CGA-O1A
21	42	501	CL7	CAA-CBA-CGA-O1A
21	13	517	CL7	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	33	517	CL7	CAA-CBA-CGA-O2A
21	43	418	CL7	CAA-CBA-CGA-O2A
21	1B	609	CL7	CAA-CBA-CGA-O1A
21	2A	401	CL7	CAA-CBA-CGA-O1A
21	3A	401	CL7	CAA-CBA-CGA-O1A
21	3B	609	CL7	CAA-CBA-CGA-O1A
21	4B	610	CL7	CAA-CBA-CGA-O1A
21	11	408	CL7	C10-C11-C12-C13
21	41	408	CL7	C10-C11-C12-C13
21	12	512	CL7	C16-C17-C18-C19
21	13	505	CL7	C16-C17-C18-C20
21	22	512	CL7	C16-C17-C18-C19
21	32	512	CL7	C16-C17-C18-C19
21	42	512	CL7	C16-C17-C18-C19
21	43	406	CL7	C16-C17-C18-C20
21	21	408	CL7	C10-C11-C12-C13
21	31	408	CL7	C10-C11-C12-C13
26	3B	625	LHG	C14-C15-C16-C17
21	12	501	CL7	CAA-CBA-CGA-O1A
21	22	501	CL7	CAA-CBA-CGA-O1A
21	14	413	CL7	C5-C6-C7-C8
21	24	413	CL7	C5-C6-C7-C8
21	44	413	CL7	C5-C6-C7-C8
26	1B	625	LHG	C14-C15-C16-C17
26	2B	626	LHG	C14-C15-C16-C17
26	4B	626	LHG	C14-C15-C16-C17
21	11	405	CL7	C1A-C2A-CAA-CBA
21	13	505	CL7	C1A-C2A-CAA-CBA
21	13	512	CL7	C1A-C2A-CAA-CBA
21	21	405	CL7	C1A-C2A-CAA-CBA
21	23	406	CL7	C1A-C2A-CAA-CBA
21	23	413	CL7	C1A-C2A-CAA-CBA
21	31	405	CL7	C1A-C2A-CAA-CBA
21	33	505	CL7	C1A-C2A-CAA-CBA
21	33	512	CL7	C1A-C2A-CAA-CBA
21	41	405	CL7	C1A-C2A-CAA-CBA
21	43	406	CL7	C1A-C2A-CAA-CBA
21	43	413	CL7	C1A-C2A-CAA-CBA
21	2C	507	CL7	C16-C17-C18-C20
21	3C	507	CL7	C16-C17-C18-C20
21	4C	507	CL7	C16-C17-C18-C20
21	2B	610	CL7	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	34	413	CL7	C5-C6-C7-C8
21	23	412	CL7	C15-C16-C17-C18
21	33	511	CL7	C15-C16-C17-C18
21	43	412	CL7	C15-C16-C17-C18
21	12	503	CL7	C2A-CAA-CBA-CGA
21	22	503	CL7	C2A-CAA-CBA-CGA
21	32	503	CL7	C2A-CAA-CBA-CGA
21	42	503	CL7	C2A-CAA-CBA-CGA
21	31	406	CL7	CBD-CGD-O2D-CED
24	1A	405	LMG	C39-C40-C41-C42
24	3A	405	LMG	C39-C40-C41-C42
26	2B	626	LHG	C17-C18-C19-C20
26	3B	625	LHG	C17-C18-C19-C20
21	1B	607	CL7	C11-C12-C13-C14
21	1C	507	CL7	C16-C17-C18-C20
21	12	501	CL7	C16-C17-C18-C19
21	2B	608	CL7	C11-C12-C13-C14
21	22	501	CL7	C16-C17-C18-C19
21	3B	604	CL7	C16-C17-C18-C20
21	3B	607	CL7	C11-C12-C13-C14
21	32	501	CL7	C16-C17-C18-C19
21	4B	605	CL7	C16-C17-C18-C20
21	4B	608	CL7	C11-C12-C13-C14
21	42	501	CL7	C16-C17-C18-C19
21	13	511	CL7	C15-C16-C17-C18
21	22	502	CL7	C10-C11-C12-C13
24	4A	405	LMG	C39-C40-C41-C42
26	1B	625	LHG	C17-C18-C19-C20
24	2A	405	LMG	C39-C40-C41-C42
26	4B	626	LHG	C17-C18-C19-C20
21	12	507	CL7	CAA-CBA-CGA-O2A
21	22	507	CL7	CAA-CBA-CGA-O2A
21	32	507	CL7	CAA-CBA-CGA-O2A
21	42	507	CL7	CAA-CBA-CGA-O2A
21	12	502	CL7	C10-C11-C12-C13
21	32	502	CL7	C10-C11-C12-C13
21	42	502	CL7	C10-C11-C12-C13
32	14	419	ZEX	C21-C26-C27-C28
32	24	419	ZEX	C21-C26-C27-C28
32	34	419	ZEX	C21-C26-C27-C28
32	44	419	ZEX	C21-C26-C27-C28
21	11	418	CL7	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	21	418	CL7	C2-C3-C5-C6
21	31	418	CL7	C2-C3-C5-C6
21	41	418	CL7	C2-C3-C5-C6
26	14	401	LHG	C3-O3-P-O5
26	24	401	LHG	C3-O3-P-O5
26	34	401	LHG	C3-O3-P-O5
26	44	401	LHG	C3-O3-P-O5
21	1B	604	CL7	C16-C17-C18-C20
21	13	509	CL7	C16-C17-C18-C20
21	2B	605	CL7	C16-C17-C18-C20
21	22	503	CL7	C16-C17-C18-C20
21	23	410	CL7	C16-C17-C18-C20
21	33	509	CL7	C16-C17-C18-C20
21	42	503	CL7	C16-C17-C18-C20
21	43	410	CL7	C16-C17-C18-C20
21	23	418	CL7	CAA-CBA-CGA-O1A
21	2C	510	CL7	CAA-CBA-CGA-O2A
21	3C	510	CL7	CAA-CBA-CGA-O2A
21	4C	510	CL7	CAA-CBA-CGA-O2A
21	1D	404	CL7	C10-C11-C12-C13
21	4D	404	CL7	C10-C11-C12-C13
23	2D	406	8CT	C04-C03-C10-C11
23	4D	406	8CT	C04-C03-C10-C11
21	2D	404	CL7	C10-C11-C12-C13
21	3D	404	CL7	C10-C11-C12-C13
21	12	516	CL7	C13-C15-C16-C17
21	22	516	CL7	C13-C15-C16-C17
21	32	516	CL7	C13-C15-C16-C17
21	42	507	CL7	C13-C15-C16-C17
21	42	516	CL7	C13-C15-C16-C17
21	12	512	CL7	CAA-CBA-CGA-O1A
21	13	517	CL7	CAA-CBA-CGA-O1A
21	22	512	CL7	CAA-CBA-CGA-O1A
21	24	406	CL7	CAA-CBA-CGA-O1A
21	32	512	CL7	CAA-CBA-CGA-O1A
21	33	517	CL7	CAA-CBA-CGA-O1A
21	34	406	CL7	CAA-CBA-CGA-O1A
21	42	512	CL7	CAA-CBA-CGA-O1A
21	1C	510	CL7	CAA-CBA-CGA-O2A
21	12	507	CL7	C13-C15-C16-C17
21	22	507	CL7	C13-C15-C16-C17
24	2D	410	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1B	610	CL7	C16-C17-C18-C20
21	12	503	CL7	C16-C17-C18-C20
21	3B	610	CL7	C16-C17-C18-C20
21	32	503	CL7	C16-C17-C18-C20
21	43	417	CL7	C6-C7-C8-C9
21	1A	407	CL7	C2A-CAA-CBA-CGA
21	2A	407	CL7	C2A-CAA-CBA-CGA
21	4A	407	CL7	C2A-CAA-CBA-CGA
21	24	409	CL7	CAA-CBA-CGA-O1A
21	43	418	CL7	CAA-CBA-CGA-O1A
24	2D	410	LMG	O9-C10-C11-C12
21	32	507	CL7	C13-C15-C16-C17
21	14	406	CL7	CAA-CBA-CGA-O1A
21	14	409	CL7	CAA-CBA-CGA-O1A
21	34	409	CL7	CAA-CBA-CGA-O1A
21	44	406	CL7	CAA-CBA-CGA-O1A
21	44	409	CL7	CAA-CBA-CGA-O1A
24	4D	410	LMG	O9-C10-C11-C12
24	2B	622	LMG	C35-C36-C37-C38
21	41	418	CL7	C10-C11-C12-C13
21	13	516	CL7	C6-C7-C8-C9
21	2B	611	CL7	C16-C17-C18-C20
21	23	417	CL7	C6-C7-C8-C9
21	33	516	CL7	C6-C7-C8-C9
21	4B	611	CL7	C16-C17-C18-C20
24	3B	621	LMG	C35-C36-C37-C38
24	4B	622	LMG	C35-C36-C37-C38
21	1A	403	CL7	CAD-CBD-CGD-O1D
21	1C	504	CL7	CAD-CBD-CGD-O1D
21	1C	506	CL7	CAD-CBD-CGD-O1D
21	12	510	CL7	CAD-CBD-CGD-O1D
21	12	518	CL7	CAD-CBD-CGD-O1D
21	13	502	CL7	CAD-CBD-CGD-O1D
21	14	404	CL7	CAD-CBD-CGD-O1D
21	14	407	CL7	CAD-CBD-CGD-O1D
21	14	410	CL7	CAD-CBD-CGD-O1D
21	14	413	CL7	CAD-CBD-CGD-O1D
21	14	415	CL7	CAD-CBD-CGD-O1D
21	2A	403	CL7	CAD-CBD-CGD-O1D
21	2C	504	CL7	CAD-CBD-CGD-O1D
21	2C	506	CL7	CAD-CBD-CGD-O1D
21	22	510	CL7	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	22	518	CL7	CAD-CBD-CGD-O1D
21	23	403	CL7	CAD-CBD-CGD-O1D
21	24	404	CL7	CAD-CBD-CGD-O1D
21	24	407	CL7	CAD-CBD-CGD-O1D
21	24	410	CL7	CAD-CBD-CGD-O1D
21	24	413	CL7	CAD-CBD-CGD-O1D
21	24	415	CL7	CAD-CBD-CGD-O1D
21	3A	403	CL7	CAD-CBD-CGD-O1D
21	3C	504	CL7	CAD-CBD-CGD-O1D
21	3C	506	CL7	CAD-CBD-CGD-O1D
21	32	510	CL7	CAD-CBD-CGD-O1D
21	32	518	CL7	CAD-CBD-CGD-O1D
21	33	502	CL7	CAD-CBD-CGD-O1D
21	34	407	CL7	CAD-CBD-CGD-O1D
21	34	410	CL7	CAD-CBD-CGD-O1D
21	34	413	CL7	CAD-CBD-CGD-O1D
21	34	415	CL7	CAD-CBD-CGD-O1D
21	4A	403	CL7	CAD-CBD-CGD-O1D
21	4C	504	CL7	CAD-CBD-CGD-O1D
21	4C	506	CL7	CAD-CBD-CGD-O1D
21	42	510	CL7	CAD-CBD-CGD-O1D
21	42	518	CL7	CAD-CBD-CGD-O1D
21	43	403	CL7	CAD-CBD-CGD-O1D
21	44	407	CL7	CAD-CBD-CGD-O1D
21	44	410	CL7	CAD-CBD-CGD-O1D
21	44	413	CL7	CAD-CBD-CGD-O1D
21	44	415	CL7	CAD-CBD-CGD-O1D
25	1A	406	SQD	O5-C5-C6-S
25	11	423	SQD	O5-C5-C6-S
25	13	523	SQD	C46-C45-O47-C7
25	2A	406	SQD	O5-C5-C6-S
25	21	423	SQD	O5-C5-C6-S
25	23	424	SQD	C46-C45-O47-C7
25	3A	406	SQD	O5-C5-C6-S
25	31	423	SQD	O5-C5-C6-S
25	33	523	SQD	C46-C45-O47-C7
25	4A	406	SQD	O5-C5-C6-S
25	41	423	SQD	O5-C5-C6-S
25	43	424	SQD	C46-C45-O47-C7
24	1D	410	LMG	O9-C10-C11-C12
24	1B	621	LMG	C35-C36-C37-C38
21	1D	404	CL7	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2D	404	CL7	CAA-CBA-CGA-O2A
21	3D	404	CL7	CAA-CBA-CGA-O2A
21	11	418	CL7	C10-C11-C12-C13
21	1B	610	CL7	C14-C13-C15-C16
21	1C	505	CL7	C11-C12-C13-C14
21	14	405	CL7	C6-C7-C8-C9
21	2B	611	CL7	C14-C13-C15-C16
21	2C	505	CL7	C11-C12-C13-C14
21	24	405	CL7	C6-C7-C8-C9
21	3B	610	CL7	C14-C13-C15-C16
21	3C	505	CL7	C11-C12-C13-C14
21	34	405	CL7	C6-C7-C8-C9
21	4B	611	CL7	C14-C13-C15-C16
21	4C	505	CL7	C11-C12-C13-C14
21	41	408	CL7	C11-C12-C13-C14
21	44	405	CL7	C6-C7-C8-C9
21	31	418	CL7	C10-C11-C12-C13
27	1C	516	DGD	C1A-C2A-C3A-C4A
27	2C	516	DGD	C1A-C2A-C3A-C4A
27	3C	516	DGD	C1A-C2A-C3A-C4A
27	4C	516	DGD	C1A-C2A-C3A-C4A
24	3D	410	LMG	O9-C10-C11-C12
21	1C	509	CL7	C16-C17-C18-C20
21	3C	509	CL7	C16-C17-C18-C20
21	2C	501	CL7	CAA-CBA-CGA-O2A
21	4D	404	CL7	CAA-CBA-CGA-O2A
24	21	401	LMG	O7-C10-C11-C12
24	31	401	LMG	O7-C10-C11-C12
24	41	401	LMG	O7-C10-C11-C12
21	21	418	CL7	C10-C11-C12-C13
21	1D	405	CL7	C2A-CAA-CBA-CGA
21	2D	405	CL7	C2A-CAA-CBA-CGA
21	3D	405	CL7	C2A-CAA-CBA-CGA
21	4D	405	CL7	C2A-CAA-CBA-CGA
21	1C	501	CL7	CAA-CBA-CGA-O2A
21	13	512	CL7	CAA-CBA-CGA-O2A
21	21	406	CL7	CAA-CBA-CGA-O2A
21	3C	501	CL7	CAA-CBA-CGA-O2A
21	31	406	CL7	CAA-CBA-CGA-O2A
21	33	512	CL7	CAA-CBA-CGA-O2A
21	43	413	CL7	CAA-CBA-CGA-O2A
24	11	401	LMG	O7-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	1D	410	LMG	O9-C10-O7-C8
24	4D	410	LMG	O9-C10-O7-C8
21	2C	509	CL7	C16-C17-C18-C20
21	4C	509	CL7	C16-C17-C18-C20
21	12	509	CL7	C4-C3-C5-C6
21	22	509	CL7	C4-C3-C5-C6
21	32	509	CL7	C4-C3-C5-C6
21	42	509	CL7	C4-C3-C5-C6
25	13	523	SQD	C11-C12-C13-C14
25	23	424	SQD	C11-C12-C13-C14
25	33	523	SQD	C11-C12-C13-C14
21	1B	610	CL7	C11-C12-C13-C15
21	1C	507	CL7	C11-C12-C13-C15
21	12	501	CL7	C6-C7-C8-C10
21	12	505	CL7	C11-C10-C8-C7
21	12	510	CL7	C11-C12-C13-C15
21	12	511	CL7	C11-C10-C8-C7
21	11	404	CL7	C12-C13-C15-C16
21	13	502	CL7	C11-C10-C8-C7
21	2B	611	CL7	C11-C12-C13-C15
21	2C	507	CL7	C11-C12-C13-C15
21	22	501	CL7	C6-C7-C8-C10
21	22	505	CL7	C11-C10-C8-C7
21	22	510	CL7	C11-C12-C13-C15
21	22	511	CL7	C11-C10-C8-C7
21	21	404	CL7	C12-C13-C15-C16
21	23	403	CL7	C11-C10-C8-C7
21	3B	610	CL7	C11-C12-C13-C15
21	3C	507	CL7	C11-C12-C13-C15
21	32	501	CL7	C6-C7-C8-C10
21	32	505	CL7	C11-C10-C8-C7
21	32	510	CL7	C11-C12-C13-C15
21	32	511	CL7	C11-C10-C8-C7
21	31	404	CL7	C12-C13-C15-C16
21	33	502	CL7	C11-C10-C8-C7
21	4B	611	CL7	C11-C12-C13-C15
21	4C	507	CL7	C11-C12-C13-C15
21	42	501	CL7	C6-C7-C8-C10
21	42	505	CL7	C11-C10-C8-C7
21	42	510	CL7	C11-C12-C13-C15
21	42	511	CL7	C11-C10-C8-C7
21	41	404	CL7	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	43	403	CL7	C11-C10-C8-C7
23	1B	617	8CT	C28-C29-C30-C31
23	2B	618	8CT	C28-C29-C30-C31
23	2K	101	8CT	C28-C29-C30-C31
23	3B	617	8CT	C28-C29-C30-C31
23	3K	101	8CT	C28-C29-C30-C31
23	4B	618	8CT	C28-C29-C30-C31
23	4K	101	8CT	C28-C29-C30-C31
21	42	507	CL7	CAA-CBA-CGA-O1A
25	43	424	SQD	C13-C14-C15-C16
21	11	406	CL7	CAA-CBA-CGA-O2A
21	23	413	CL7	CAA-CBA-CGA-O2A
21	4C	501	CL7	CAA-CBA-CGA-O2A
21	41	406	CL7	CAA-CBA-CGA-O2A
22	1D	408	PHO	CAA-CBA-CGA-O2A
22	2D	408	PHO	CAA-CBA-CGA-O2A
22	3D	408	PHO	CAA-CBA-CGA-O2A
25	13	523	SQD	C13-C14-C15-C16
25	43	424	SQD	C11-C12-C13-C14
21	12	507	CL7	CAA-CBA-CGA-O1A
21	11	406	CL7	CAA-CBA-CGA-O1A
21	22	507	CL7	CAA-CBA-CGA-O1A
21	21	406	CL7	CAA-CBA-CGA-O1A
21	32	507	CL7	CAA-CBA-CGA-O1A
21	31	406	CL7	CAA-CBA-CGA-O1A
21	41	406	CL7	CAA-CBA-CGA-O1A
32	12	519	ZEX	C33-C34-C35-C15
32	22	519	ZEX	C33-C34-C35-C15
32	32	519	ZEX	C33-C34-C35-C15
32	42	519	ZEX	C33-C34-C35-C15
21	1B	603	CL7	C16-C17-C18-C19
21	2B	604	CL7	C16-C17-C18-C19
21	3B	603	CL7	C16-C17-C18-C19
21	4B	604	CL7	C16-C17-C18-C19
22	4D	408	PHO	CAA-CBA-CGA-O2A
25	23	424	SQD	C13-C14-C15-C16
25	33	523	SQD	C13-C14-C15-C16
21	1C	504	CL7	C4C-C3C-CAC-CBC
21	12	510	CL7	CAA-CBA-CGA-O1A
21	14	412	CL7	CAA-CBA-CGA-O1A
21	22	510	CL7	CAA-CBA-CGA-O1A
21	24	412	CL7	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	32	510	CL7	CAA-CBA-CGA-O1A
21	34	412	CL7	CAA-CBA-CGA-O1A
21	44	412	CL7	CAA-CBA-CGA-O1A
22	1D	408	PHO	CAA-CBA-CGA-O1A
22	2D	408	PHO	CAA-CBA-CGA-O1A
22	3D	408	PHO	CAA-CBA-CGA-O1A
22	4D	408	PHO	CAA-CBA-CGA-O1A
21	3C	504	CL7	C4C-C3C-CAC-CBC
25	11	423	SQD	O48-C23-C24-C25
25	21	423	SQD	O48-C23-C24-C25
25	31	423	SQD	O48-C23-C24-C25
25	41	423	SQD	O48-C23-C24-C25
21	42	510	CL7	CAA-CBA-CGA-O1A
21	3A	407	CL7	C2A-CAA-CBA-CGA
21	2C	504	CL7	C4C-C3C-CAC-CBC
21	4C	504	CL7	C4C-C3C-CAC-CBC
21	43	411	CL7	C13-C15-C16-C17
21	13	505	CL7	CAA-CBA-CGA-O2A
21	23	406	CL7	CAA-CBA-CGA-O2A
21	33	505	CL7	CAA-CBA-CGA-O2A
21	43	406	CL7	CAA-CBA-CGA-O2A

There are no ring outliers.

540 monomers are involved in 2632 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	33	502	CL7	7	0
21	2C	508	CL7	4	0
21	3C	511	CL7	1	0
25	32	521	SQD	1	0
21	22	507	CL7	5	0
21	23	404	CL7	11	0
21	23	415	CL7	2	0
21	3C	503	CL7	8	0
21	4B	609	CL7	4	0
21	1B	608	CL7	4	0
21	33	513	CL7	12	0
32	22	519	ZEX	3	0
21	44	409	CL7	2	0
25	42	521	SQD	2	0
21	21	402	CL7	10	0
21	31	404	CL7	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	23	409	CL7	14	0
21	11	409	CL7	3	0
21	2B	610	CL7	4	0
21	14	406	CL7	13	0
21	3C	505	CL7	5	0
21	31	418	CL7	7	0
21	4D	405	CL7	2	0
21	13	507	CL7	10	0
21	43	410	CL7	8	0
32	14	419	ZEX	8	0
26	2B	626	LHG	2	0
21	2B	604	CL7	9	0
21	31	414	CL7	8	0
21	34	414	CL7	4	0
21	21	408	CL7	7	0
23	2C	518	8CT	1	0
21	32	510	CL7	6	0
27	1C	516	DGD	5	0
30	4D	407	PL9	7	0
21	34	404	CL7	5	0
21	14	405	CL7	7	0
21	2B	608	CL7	7	0
21	32	517	CL7	10	0
24	1B	621	LMG	5	0
21	41	412	CL7	2	0
32	13	525	ZEX	24	0
21	43	409	CL7	14	0
32	12	520	ZEX	33	0
32	34	420	ZEX	10	0
32	44	403	ZEX	21	0
32	34	418	ZEX	9	0
24	1A	405	LMG	2	0
21	22	501	CL7	7	0
21	12	508	CL7	4	0
32	12	524	ZEX	16	0
26	14	401	LHG	2	0
21	24	411	CL7	7	0
21	2C	506	CL7	3	0
24	4B	622	LMG	6	0
26	4B	626	LHG	2	0
21	4C	502	CL7	3	0
21	43	407	CL7	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1C	504	CL7	3	0
24	3D	410	LMG	1	0
21	23	418	CL7	2	0
21	44	417	CL7	4	0
25	3B	620	SQD	2	0
22	4D	408	PHO	3	0
21	12	512	CL7	8	0
21	1B	615	CL7	4	0
21	14	404	CL7	6	0
21	34	408	CL7	4	0
21	41	410	CL7	6	0
32	12	522	ZEX	18	0
21	42	506	CL7	2	0
21	24	408	CL7	4	0
21	42	509	CL7	7	0
23	3C	518	8CT	1	0
26	23	425	LHG	1	0
21	2B	605	CL7	7	0
21	42	518	CL7	10	0
21	34	413	CL7	4	0
21	42	516	CL7	6	0
24	3A	405	LMG	2	0
21	3A	401	CL7	19	0
21	33	518	CL7	3	0
21	44	415	CL7	4	0
25	43	422	SQD	3	0
21	12	518	CL7	11	0
21	3C	507	CL7	4	0
21	13	512	CL7	6	0
32	22	520	ZEX	29	0
32	32	520	ZEX	30	0
32	21	421	ZEX	15	0
21	3C	508	CL7	3	0
21	31	413	CL7	6	0
21	31	405	CL7	5	0
21	44	408	CL7	4	0
32	23	423	ZEX	26	0
21	2C	511	CL7	1	0
21	2C	504	CL7	3	0
21	3B	604	CL7	10	0
21	43	417	CL7	6	0
21	32	516	CL7	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2B	615	CL7	2	0
21	13	501	CL7	8	0
21	32	512	CL7	7	0
26	44	401	LHG	2	0
32	43	401	ZEX	24	0
32	32	522	ZEX	17	0
25	41	423	SQD	1	0
21	4C	507	CL7	3	0
32	23	420	ZEX	17	0
21	2B	616	CL7	4	0
21	42	511	CL7	7	0
21	23	413	CL7	7	0
21	33	504	CL7	9	0
21	2C	513	CL7	3	0
22	3D	408	PHO	4	0
21	32	513	CL7	6	0
21	43	415	CL7	2	0
24	3B	621	LMG	6	0
21	1C	505	CL7	6	0
21	33	503	CL7	10	0
23	1C	515	8CT	1	0
32	41	422	ZEX	23	0
21	1C	510	CL7	4	0
21	43	406	CL7	18	0
21	3C	513	CL7	3	0
21	3B	606	CL7	5	0
32	32	524	ZEX	16	0
21	21	410	CL7	7	0
25	4A	406	SQD	2	0
21	23	416	CL7	2	0
21	3A	403	CL7	2	0
21	31	409	CL7	3	0
21	3C	509	CL7	4	0
32	12	519	ZEX	3	0
21	2C	507	CL7	5	0
23	4C	518	8CT	1	0
21	13	517	CL7	2	0
24	21	401	LMG	2	0
21	41	413	CL7	6	0
32	43	420	ZEX	17	0
21	43	413	CL7	8	0
26	3D	409	LHG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1B	611	CL7	4	0
21	11	416	CL7	1	0
21	1B	605	CL7	7	0
32	23	421	ZEX	10	0
21	32	515	CL7	2	0
21	23	402	CL7	10	0
21	14	409	CL7	2	0
21	2C	502	CL7	4	0
26	1B	623	LHG	6	0
21	32	502	CL7	8	0
21	42	507	CL7	5	0
21	2A	401	CL7	17	0
21	41	416	CL7	1	0
21	3B	602	CL7	4	0
21	41	414	CL7	2	0
32	42	519	ZEX	3	0
32	24	419	ZEX	7	0
21	13	506	CL7	5	0
21	33	516	CL7	5	0
21	4B	608	CL7	8	0
21	13	509	CL7	9	0
21	3C	502	CL7	3	0
21	44	412	CL7	2	0
21	1C	508	CL7	3	0
21	22	513	CL7	6	0
21	32	504	CL7	3	0
21	14	410	CL7	2	0
21	4A	403	CL7	2	0
22	2D	408	PHO	3	0
21	1C	503	CL7	7	0
21	23	411	CL7	4	0
30	1D	407	PL9	7	0
21	21	418	CL7	7	0
21	43	402	CL7	9	0
25	21	423	SQD	1	0
21	42	512	CL7	7	0
27	2C	516	DGD	4	0
32	33	525	ZEX	24	0
32	44	420	ZEX	12	0
21	33	509	CL7	8	0
21	11	414	CL7	2	0
23	1C	518	8CT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	34	415	CL7	4	0
21	31	420	CL7	6	0
21	21	403	CL7	5	0
21	21	417	CL7	5	0
21	3C	510	CL7	4	0
32	34	403	ZEX	21	0
21	4D	404	CL7	7	0
21	34	405	CL7	7	0
21	23	408	CL7	9	0
21	43	412	CL7	5	0
21	42	501	CL7	6	0
23	3C	515	8CT	1	0
21	24	404	CL7	6	0
21	2B	606	CL7	7	0
21	22	502	CL7	7	0
21	2B	607	CL7	6	0
21	44	406	CL7	12	0
21	33	508	CL7	14	0
21	3C	504	CL7	3	0
21	2B	612	CL7	4	0
21	4B	605	CL7	8	0
32	24	418	ZEX	10	0
21	3B	607	CL7	8	0
21	33	515	CL7	2	0
21	42	514	CL7	2	0
21	4C	506	CL7	4	0
21	32	507	CL7	5	0
22	1D	408	PHO	4	0
32	14	403	ZEX	22	0
21	4C	510	CL7	3	0
21	42	504	CL7	3	0
21	13	510	CL7	6	0
21	44	413	CL7	4	0
24	1D	410	LMG	1	0
21	4B	606	CL7	6	0
21	13	513	CL7	12	0
21	41	406	CL7	14	0
21	2A	403	CL7	2	0
21	24	414	CL7	3	0
21	14	415	CL7	4	0
32	34	419	ZEX	8	0
22	1A	402	PHO	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3B	612	CL7	3	0
21	12	517	CL7	8	0
21	22	505	CL7	17	0
21	33	514	CL7	2	0
21	22	510	CL7	6	0
21	1B	606	CL7	5	0
21	4C	511	CL7	1	0
21	42	517	CL7	10	0
21	12	514	CL7	2	0
21	32	506	CL7	2	0
25	33	521	SQD	4	0
32	33	519	ZEX	17	0
21	32	518	CL7	10	0
21	4B	616	CL7	4	0
21	13	505	CL7	17	0
21	4C	509	CL7	3	0
21	41	407	CL7	3	0
32	24	420	ZEX	12	0
26	34	401	LHG	2	0
32	13	522	ZEX	26	0
21	31	416	CL7	1	0
21	3D	405	CL7	2	0
21	3B	609	CL7	4	0
21	3B	613	CL7	2	0
32	43	421	ZEX	11	0
21	34	409	CL7	2	0
21	32	508	CL7	3	0
21	33	501	CL7	8	0
21	13	511	CL7	5	0
21	1C	513	CL7	3	0
32	44	418	ZEX	9	0
23	2C	515	8CT	1	0
21	4C	504	CL7	3	0
21	31	410	CL7	7	0
21	4A	401	CL7	18	0
24	11	401	LMG	2	0
21	41	404	CL7	8	0
21	14	414	CL7	4	0
21	2B	613	CL7	5	0
23	4C	515	8CT	1	0
21	13	516	CL7	5	0
21	1A	407	CL7	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	31	412	CL7	2	0
21	44	411	CL7	8	0
21	43	403	CL7	8	0
25	43	424	SQD	2	0
21	13	508	CL7	15	0
27	4C	516	DGD	4	0
27	3B	624	DGD	2	0
24	2D	410	LMG	1	0
21	11	417	CL7	3	0
21	3C	512	CL7	1	0
21	13	503	CL7	10	0
25	2B	621	SQD	2	0
21	22	516	CL7	6	0
21	33	506	CL7	5	0
21	24	410	CL7	2	0
21	1B	603	CL7	7	0
21	12	515	CL7	3	0
21	44	407	CL7	6	0
21	1C	502	CL7	4	0
21	41	420	CL7	6	0
21	43	408	CL7	10	0
21	22	515	CL7	3	0
32	33	522	ZEX	25	0
21	23	419	CL7	3	0
21	22	503	CL7	5	0
21	1B	610	CL7	3	0
21	43	414	CL7	13	0
21	32	503	CL7	9	0
21	4B	612	CL7	4	0
21	34	406	CL7	13	0
32	42	520	ZEX	31	0
21	42	513	CL7	6	0
21	43	411	CL7	6	0
21	11	407	CL7	3	0
21	24	405	CL7	6	0
21	2B	609	CL7	4	0
21	24	409	CL7	2	0
21	23	405	CL7	8	0
32	42	524	ZEX	17	0
21	31	406	CL7	13	0
21	34	410	CL7	2	0
21	3B	608	CL7	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1B	612	CL7	3	0
21	24	407	CL7	6	0
26	24	401	LHG	2	0
21	13	502	CL7	7	0
21	4C	505	CL7	6	0
32	11	421	ZEX	13	0
21	11	403	CL7	4	0
21	2B	614	CL7	2	0
26	13	524	LHG	1	0
21	21	420	CL7	6	0
21	4C	508	CL7	5	0
21	11	405	CL7	4	0
21	4B	607	CL7	4	0
22	3A	402	PHO	3	0
27	2B	625	DGD	2	0
21	21	413	CL7	6	0
32	31	421	ZEX	15	0
21	33	517	CL7	2	0
21	41	405	CL7	4	0
32	32	519	ZEX	4	0
21	3B	614	CL7	2	0
21	11	412	CL7	2	0
21	4C	512	CL7	1	0
21	3B	610	CL7	1	0
21	3D	404	CL7	6	0
32	23	401	ZEX	24	0
21	12	510	CL7	6	0
24	4D	410	LMG	1	0
21	21	416	CL7	1	0
21	12	513	CL7	6	0
21	13	515	CL7	2	0
32	31	422	ZEX	22	0
21	11	413	CL7	6	0
21	3B	615	CL7	4	0
21	1D	404	CL7	6	0
21	23	412	CL7	5	0
21	34	417	CL7	4	0
21	14	407	CL7	6	0
21	42	508	CL7	3	0
24	2A	405	LMG	2	0
31	1F	101	HEM	3	0
32	43	423	ZEX	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3B	605	CL7	6	0
25	33	523	SQD	1	0
21	32	514	CL7	2	0
32	21	422	ZEX	21	0
21	12	506	CL7	2	0
21	21	405	CL7	4	0
21	2B	611	CL7	3	0
21	14	417	CL7	4	0
21	33	505	CL7	18	0
21	22	509	CL7	4	0
21	31	403	CL7	5	0
32	42	522	ZEX	19	0
21	12	505	CL7	15	0
21	34	412	CL7	4	0
32	44	419	ZEX	9	0
32	14	418	ZEX	9	0
21	1C	511	CL7	1	0
21	1C	506	CL7	5	0
21	1B	609	CL7	4	0
21	24	415	CL7	4	0
21	31	408	CL7	7	0
21	43	418	CL7	2	0
21	12	501	CL7	5	0
21	21	406	CL7	13	0
21	44	414	CL7	4	0
32	33	520	ZEX	11	0
21	3B	611	CL7	5	0
21	21	414	CL7	8	0
25	23	422	SQD	4	0
21	21	404	CL7	8	0
21	31	411	CL7	2	0
27	3C	516	DGD	5	0
21	22	508	CL7	3	0
21	21	411	CL7	2	0
21	33	512	CL7	7	0
21	14	408	CL7	4	0
21	21	409	CL7	4	0
22	4A	402	PHO	3	0
26	1D	409	LHG	3	0
25	3A	406	SQD	1	0
21	23	407	CL7	5	0
21	1D	405	CL7	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	21	407	CL7	3	0
26	3B	623	LHG	6	0
21	12	516	CL7	5	0
21	4C	503	CL7	8	0
24	31	401	LMG	3	0
21	32	501	CL7	6	0
21	41	409	CL7	4	0
32	22	524	ZEX	16	0
31	2F	101	HEM	4	0
21	34	411	CL7	8	0
21	44	404	CL7	6	0
21	32	505	CL7	15	0
25	23	424	SQD	2	0
25	12	521	SQD	2	0
21	22	512	CL7	8	0
21	22	514	CL7	2	0
24	41	401	LMG	2	0
21	42	503	CL7	7	0
21	23	403	CL7	7	0
21	3B	603	CL7	6	0
21	4B	610	CL7	4	0
21	31	417	CL7	3	0
25	22	521	SQD	2	0
21	31	402	CL7	10	0
32	13	520	ZEX	11	0
21	4C	513	CL7	3	0
26	2B	624	LHG	6	0
21	13	504	CL7	8	0
21	1B	602	CL7	5	0
21	11	404	CL7	7	0
21	13	514	CL7	2	0
21	14	412	CL7	3	0
21	2C	503	CL7	7	0
27	4B	625	DGD	2	0
21	24	413	CL7	5	0
21	33	510	CL7	5	0
21	34	407	CL7	6	0
25	13	521	SQD	4	0
25	1B	620	SQD	3	0
25	1A	406	SQD	3	0
26	1B	625	LHG	1	0
21	23	406	CL7	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	24	417	CL7	4	0
32	24	403	ZEX	22	0
21	14	413	CL7	5	0
21	42	515	CL7	2	0
21	22	506	CL7	3	0
21	1C	509	CL7	3	0
21	14	411	CL7	7	0
21	41	403	CL7	5	0
32	41	421	ZEX	15	0
21	43	404	CL7	11	0
21	11	406	CL7	12	0
21	4B	603	CL7	3	0
21	3A	407	CL7	15	0
21	22	518	CL7	11	0
27	1B	624	DGD	2	0
21	44	410	CL7	2	0
31	3F	101	HEM	3	0
21	41	408	CL7	8	0
21	42	502	CL7	7	0
21	23	414	CL7	12	0
21	1A	401	CL7	18	0
21	1C	507	CL7	5	0
21	24	412	CL7	3	0
21	4B	614	CL7	2	0
32	22	522	ZEX	18	0
31	4F	101	HEM	4	0
21	4C	501	CL7	4	0
21	12	502	CL7	7	0
21	3C	501	CL7	4	0
21	2D	404	CL7	7	0
21	13	518	CL7	3	0
21	2D	405	CL7	2	0
21	11	410	CL7	8	0
25	2A	406	SQD	2	0
21	22	517	CL7	9	0
21	12	509	CL7	5	0
21	4B	604	CL7	8	0
30	3D	407	PL9	7	0
26	2D	409	LHG	4	0
21	12	511	CL7	8	0
21	1B	614	CL7	2	0
21	4B	611	CL7	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	41	418	CL7	6	0
24	2B	622	LMG	5	0
21	1B	607	CL7	8	0
21	4A	407	CL7	14	0
26	43	425	LHG	1	0
21	41	402	CL7	10	0
25	4B	621	SQD	3	0
21	12	504	CL7	3	0
21	23	417	CL7	5	0
21	2C	505	CL7	6	0
21	31	407	CL7	3	0
21	2C	510	CL7	4	0
21	22	511	CL7	8	0
21	1B	604	CL7	9	0
21	1C	512	CL7	1	0
21	3C	506	CL7	4	0
21	11	418	CL7	6	0
30	2D	407	PL9	7	0
21	12	503	CL7	9	0
21	11	402	CL7	10	0
25	11	423	SQD	1	0
21	33	511	CL7	6	0
21	44	405	CL7	8	0
21	11	411	CL7	2	0
21	2B	603	CL7	4	0
21	43	419	CL7	3	0
21	43	405	CL7	9	0
21	42	505	CL7	14	0
21	42	510	CL7	7	0
26	4D	409	LHG	3	0
21	24	406	CL7	13	0
21	2C	509	CL7	2	0
21	1C	501	CL7	3	0
21	32	509	CL7	5	0
21	4B	613	CL7	6	0
21	2C	512	CL7	1	0
25	31	423	SQD	1	0
32	11	422	ZEX	21	0
21	1A	403	CL7	2	0
21	41	411	CL7	2	0
21	33	507	CL7	10	0
26	4B	624	LHG	6	0

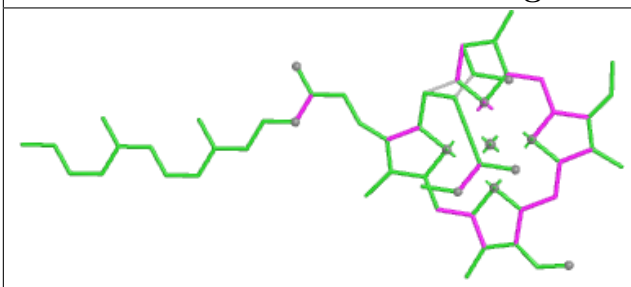
Continued on next page...

Continued from previous page...

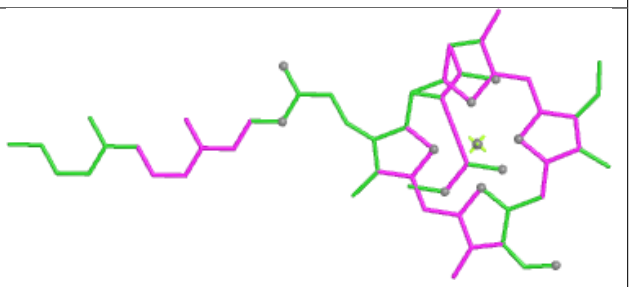
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4B	615	CL7	2	0
21	41	417	CL7	6	0
22	2A	402	PHO	3	0
24	4A	405	LMG	2	0
21	22	504	CL7	3	0
26	3B	625	LHG	1	0
21	11	408	CL7	7	0
25	13	523	SQD	2	0
21	32	511	CL7	9	0
21	43	416	CL7	2	0
21	11	420	CL7	6	0
26	33	524	LHG	1	0
32	13	519	ZEX	16	0
21	2A	407	CL7	14	0
21	23	410	CL7	10	0
32	14	420	ZEX	10	0
21	12	507	CL7	6	0
21	2C	501	CL7	5	0
21	1B	613	CL7	2	0
21	21	412	CL7	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

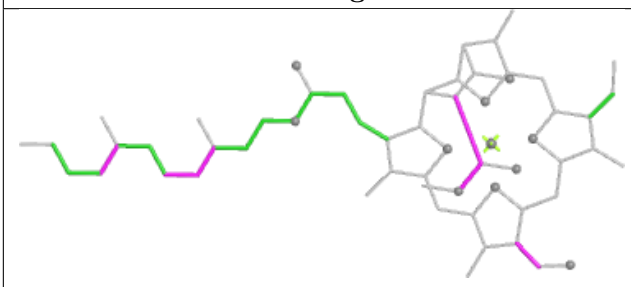
Ligand CL7 33 502



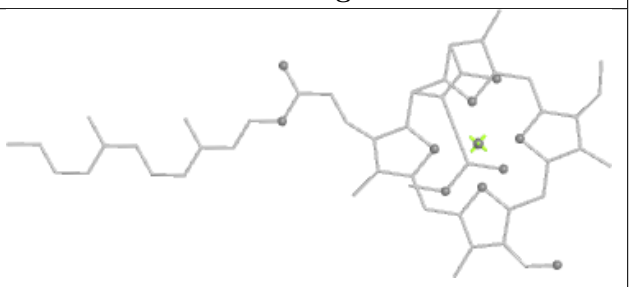
Bond lengths



Bond angles



Torsions

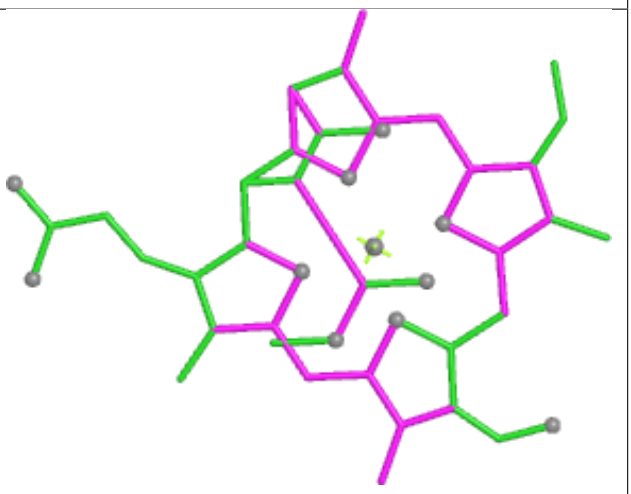


Rings

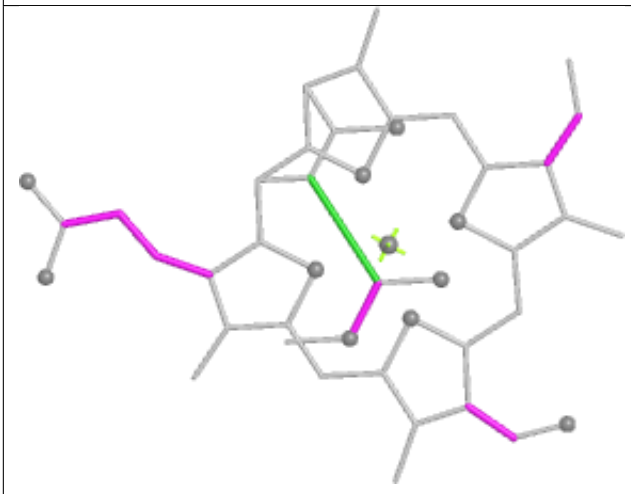
Ligand CL7 31 419



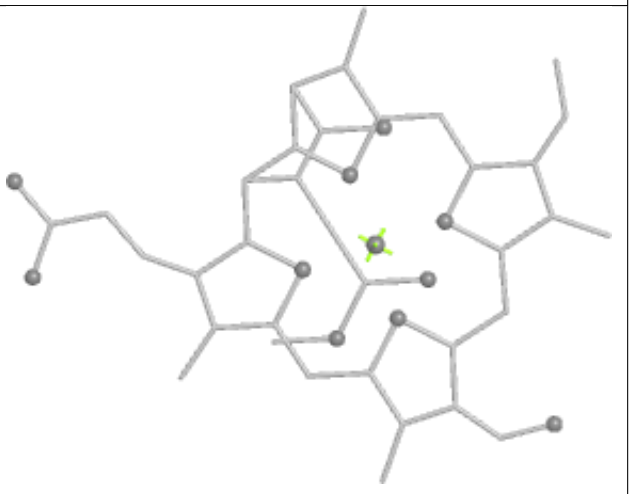
Bond lengths



Bond angles

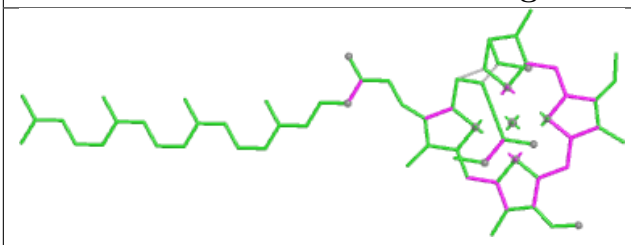


Torsions

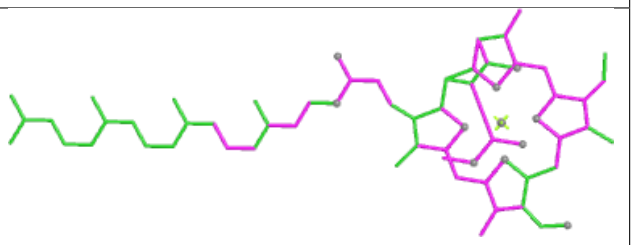


Rings

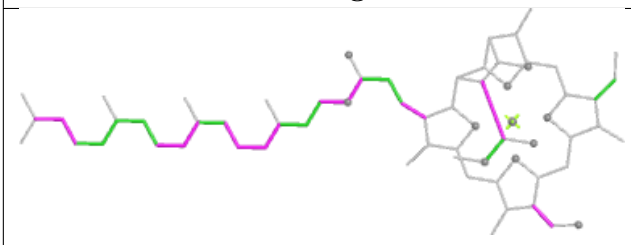
Ligand CL7 2C 508



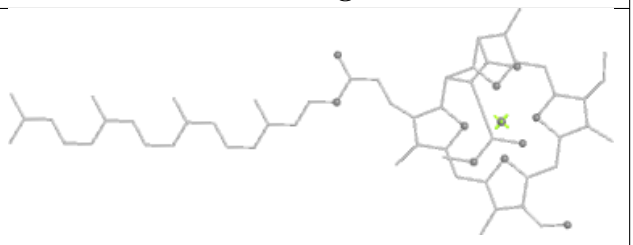
Bond lengths



Bond angles

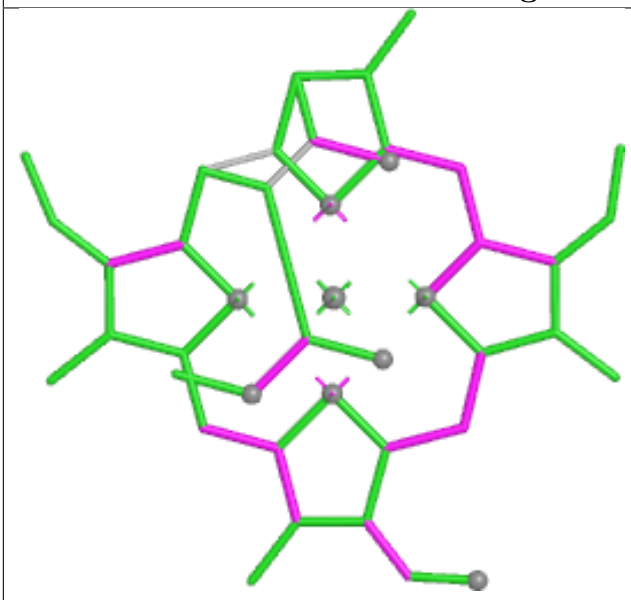


Torsions

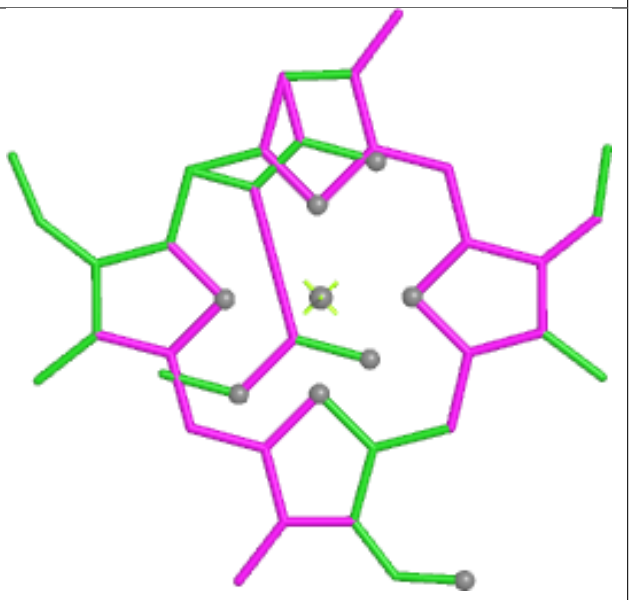


Rings

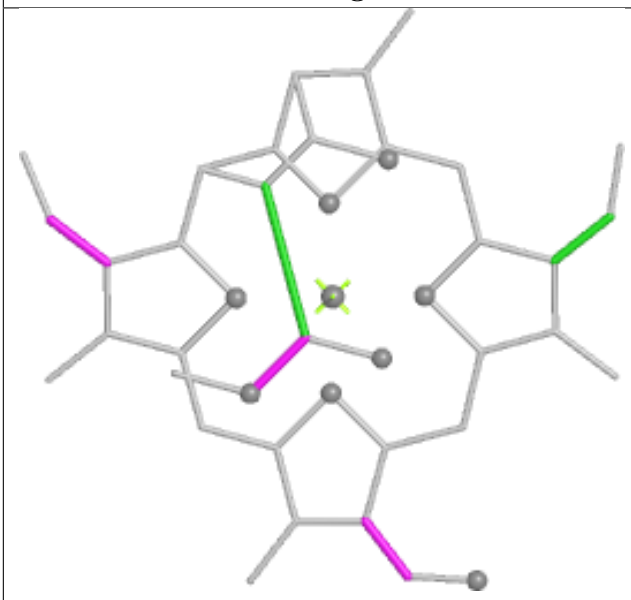
Ligand CL7 3C 511



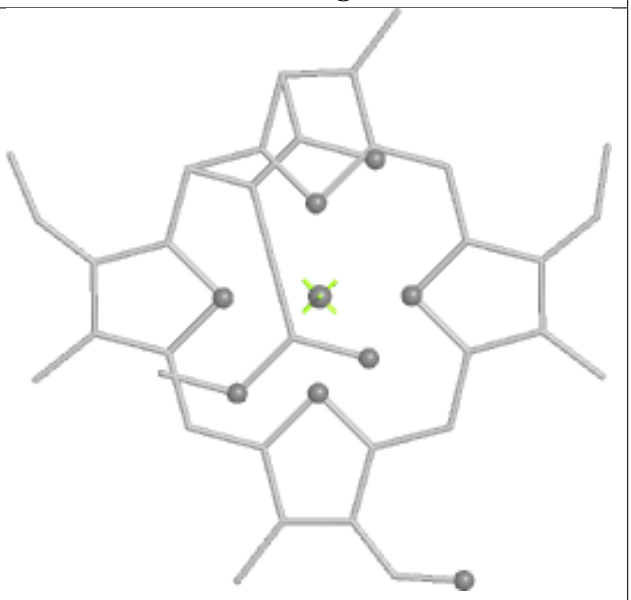
Bond lengths



Bond angles

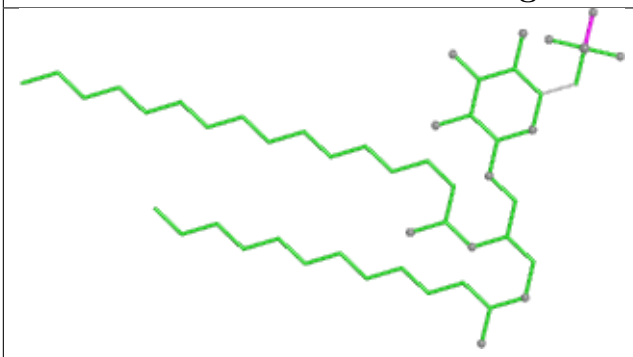


Torsions

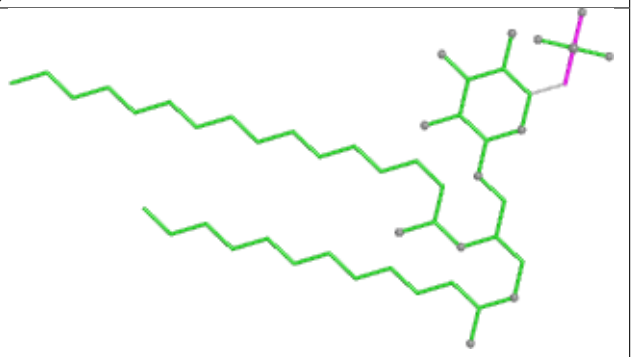


Rings

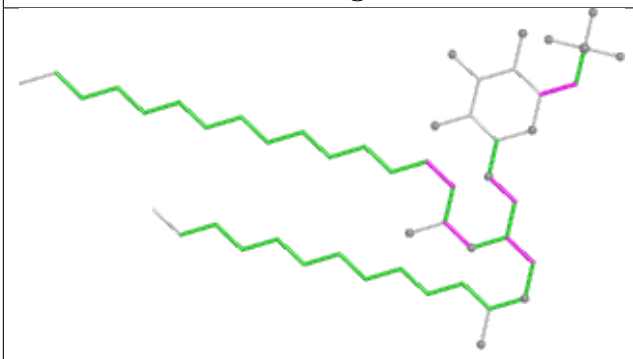
Ligand SQD 32 521



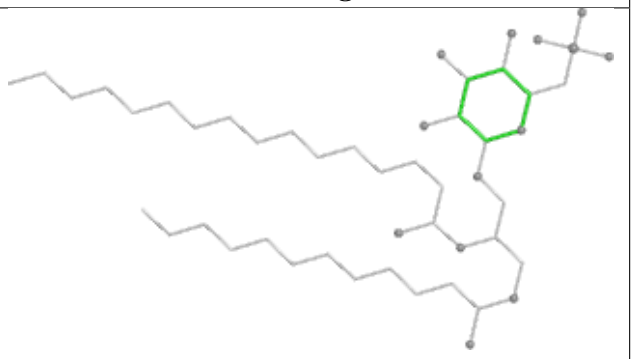
Bond lengths



Bond angles

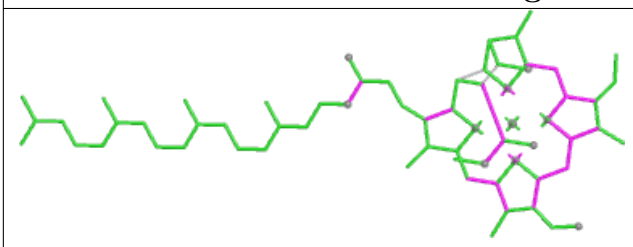


Torsions

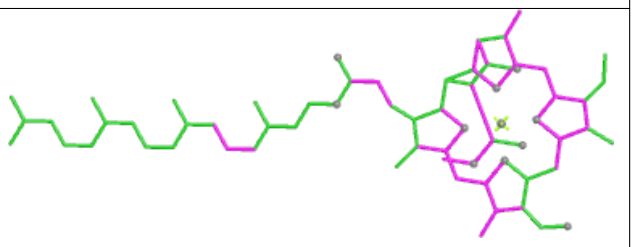


Rings

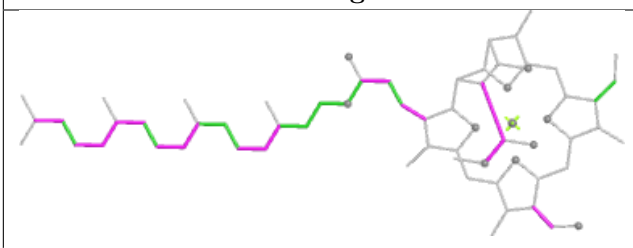
Ligand CL7 22 507



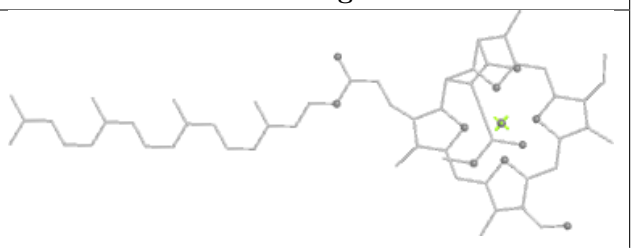
Bond lengths



Bond angles

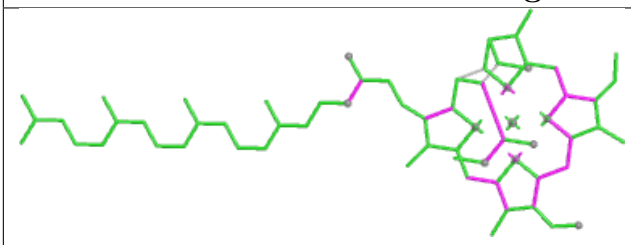


Torsions

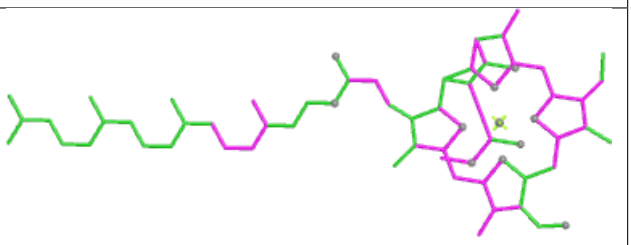


Rings

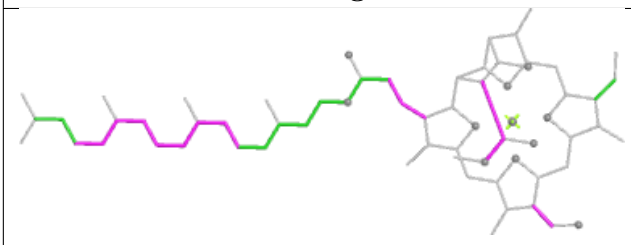
Ligand CL7 23 404



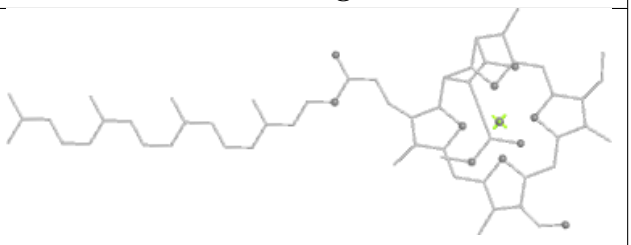
Bond lengths



Bond angles

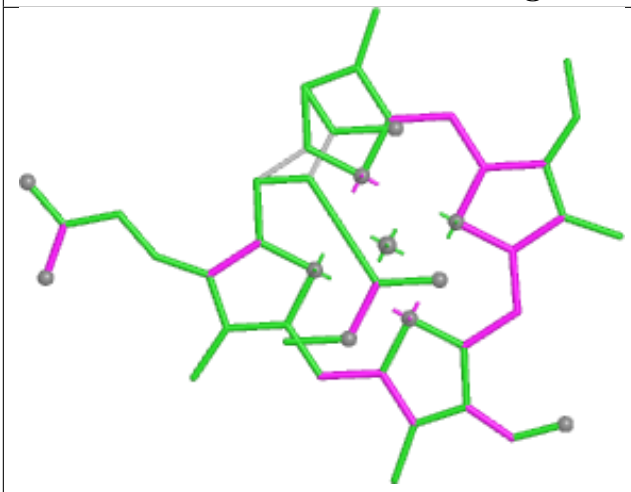


Torsions

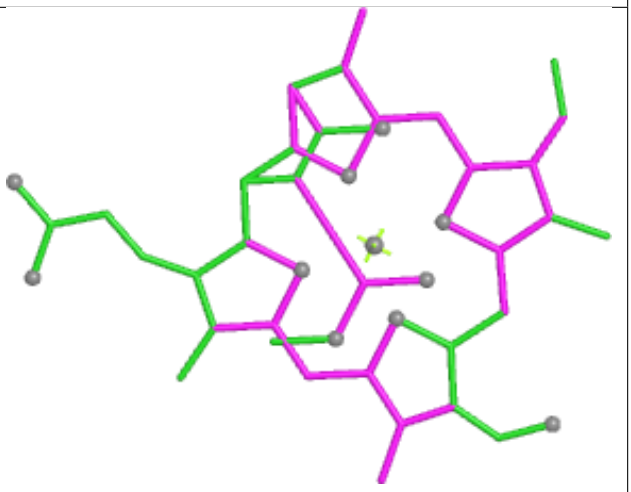


Rings

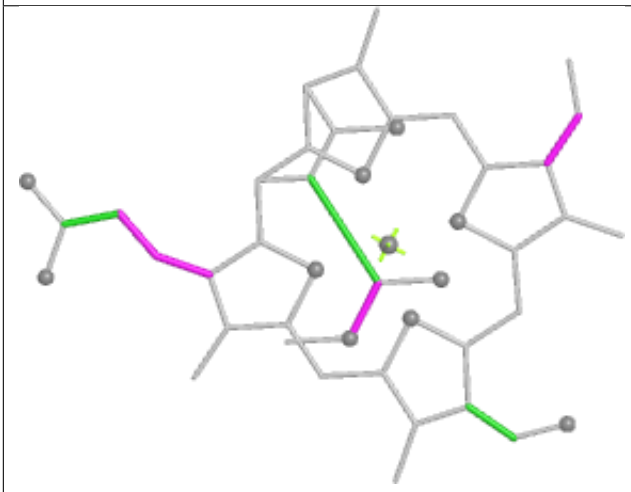
Ligand CL7 23 415



Bond lengths



Bond angles

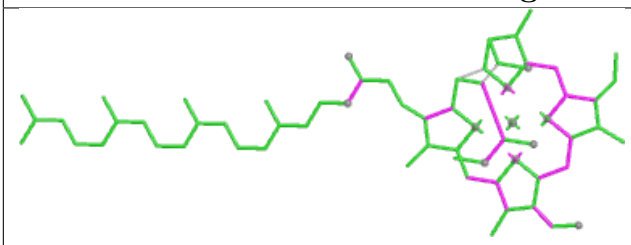


Torsions

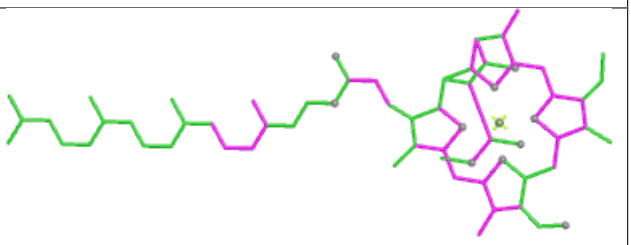


Rings

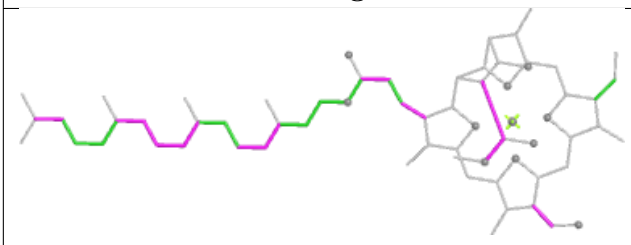
Ligand CL7 3C 503



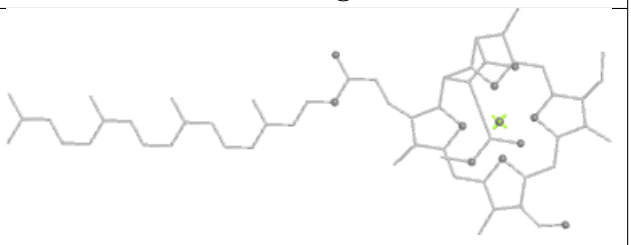
Bond lengths



Bond angles

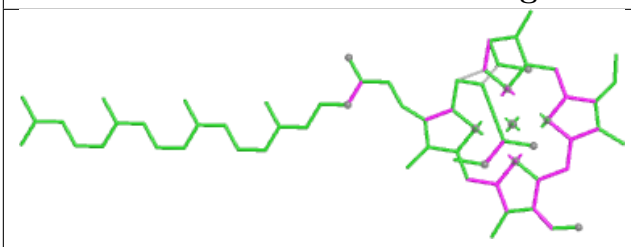


Torsions

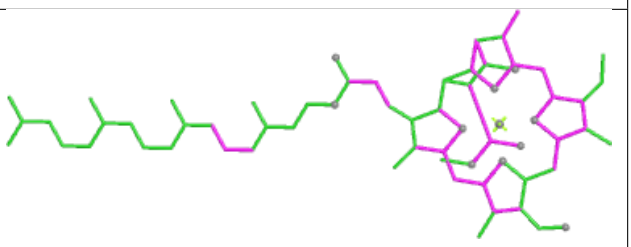


Rings

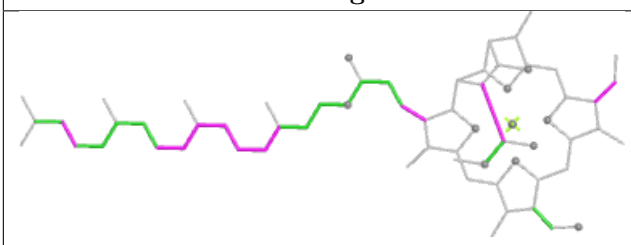
Ligand CL7 4B 609



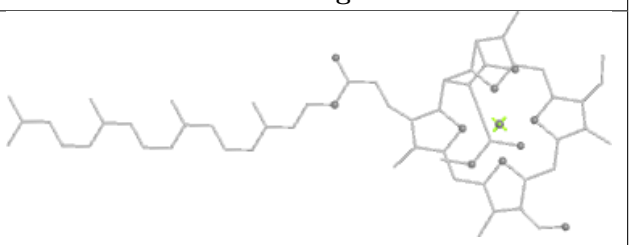
Bond lengths



Bond angles

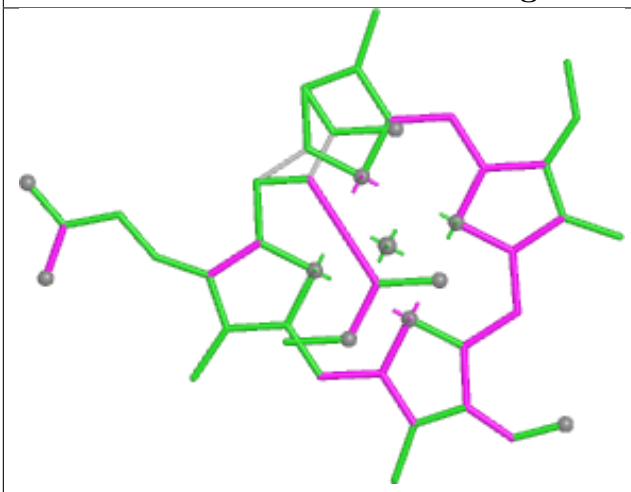


Torsions

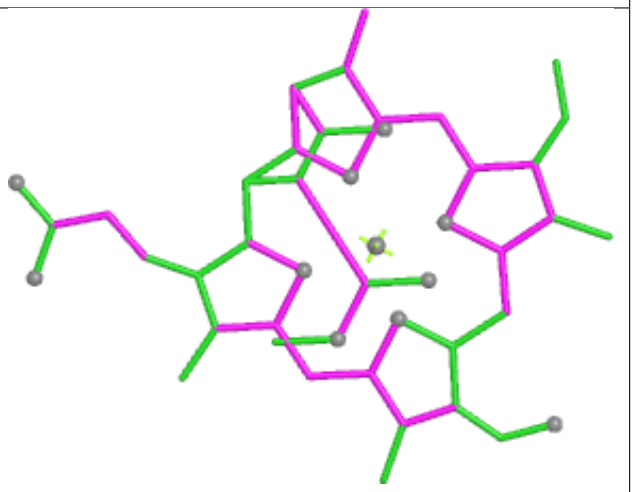


Rings

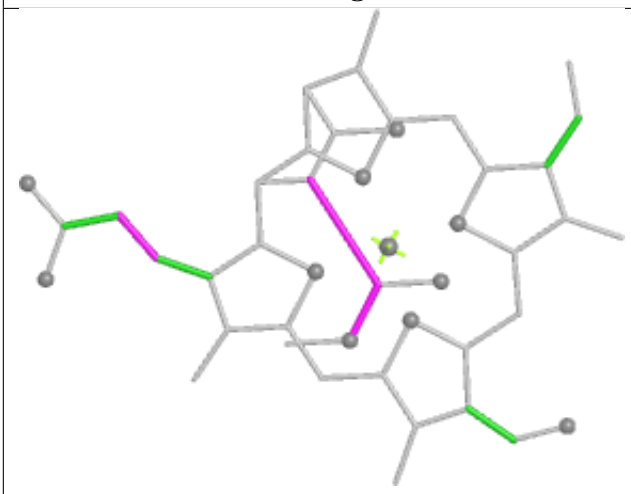
Ligand CL7 3B 616



Bond lengths



Bond angles

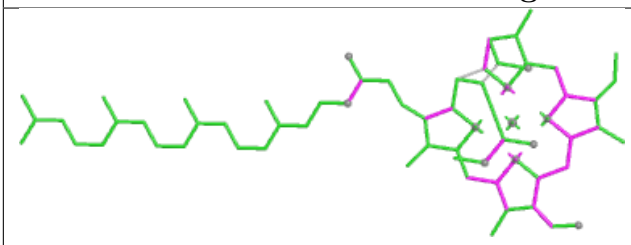


Torsions

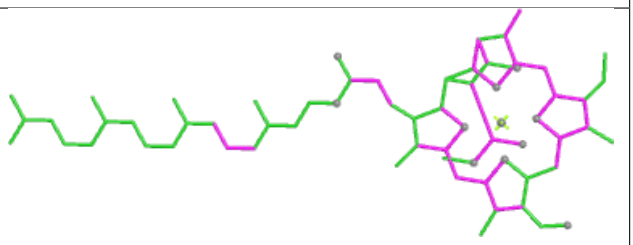


Rings

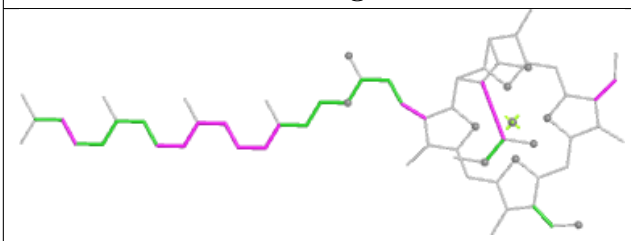
Ligand CL7 1B 608



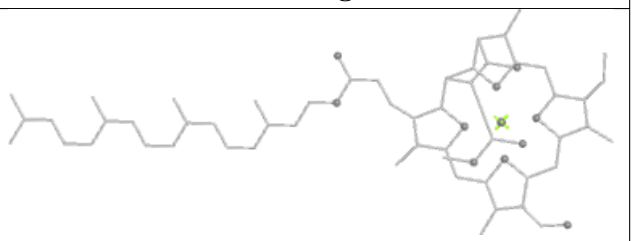
Bond lengths



Bond angles

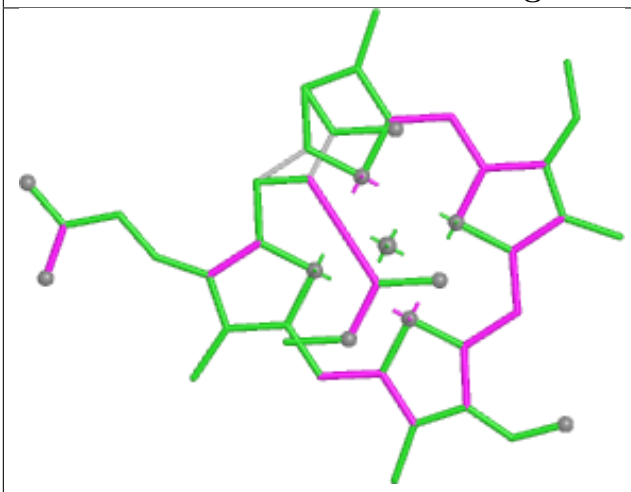


Torsions

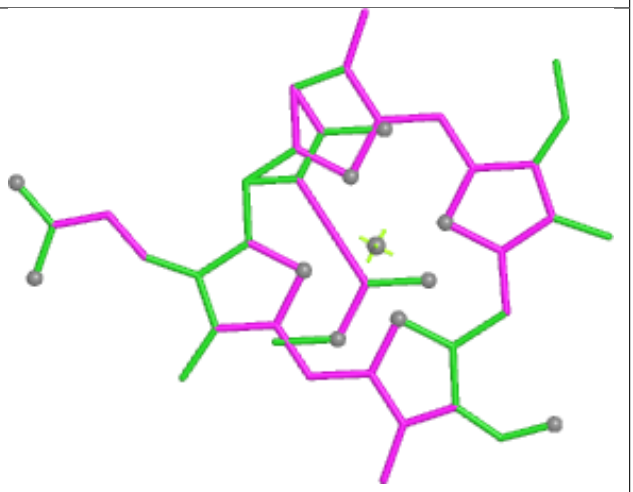


Rings

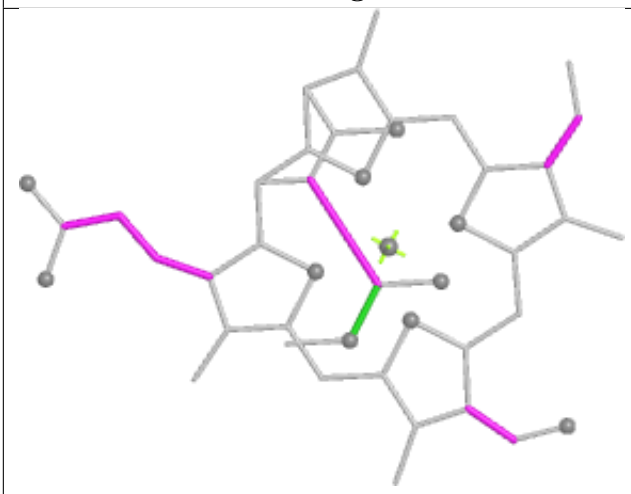
Ligand CL7 33 513



Bond lengths



Bond angles

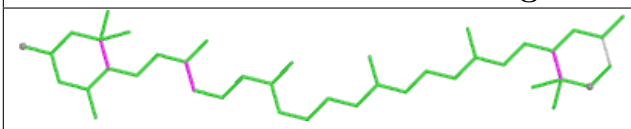


Torsions

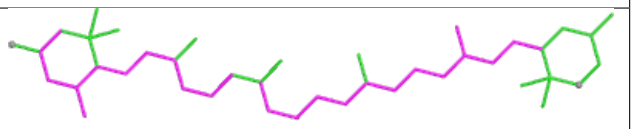


Rings

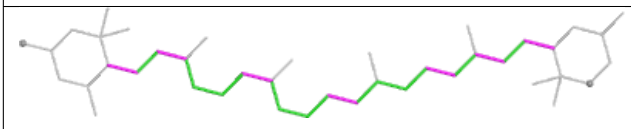
Ligand ZEX 22 519



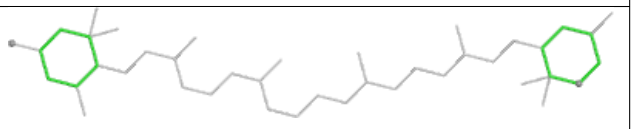
Bond lengths



Bond angles

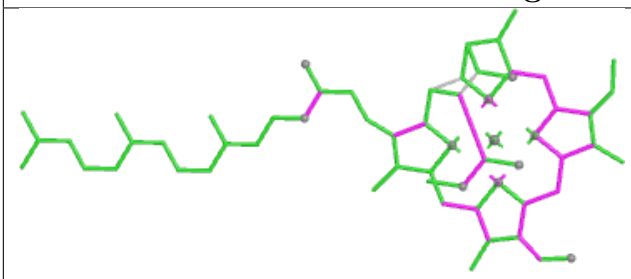


Torsions

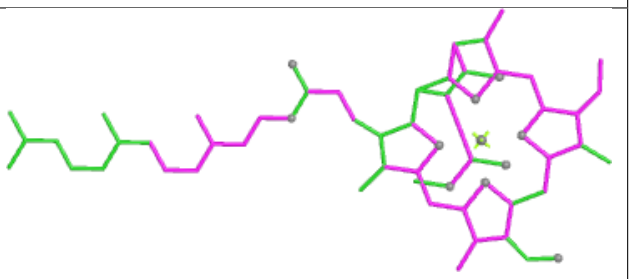


Rings

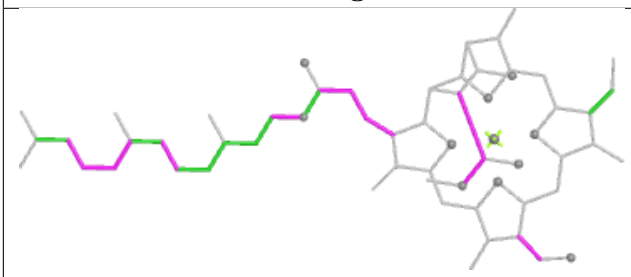
Ligand CL7 44 409



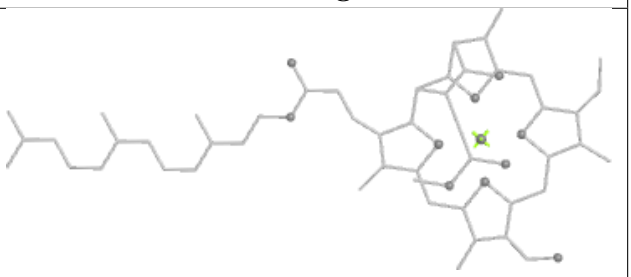
Bond lengths



Bond angles

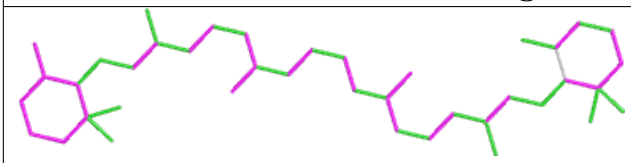


Torsions

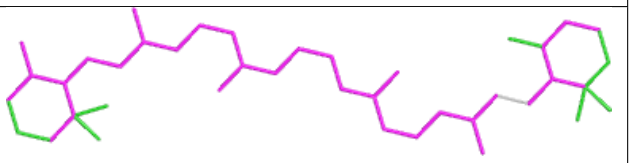


Rings

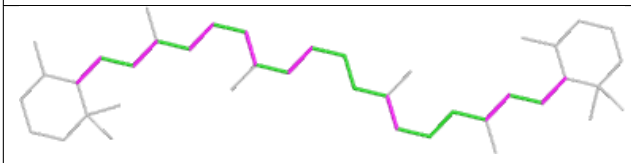
Ligand 8CT 3C 514



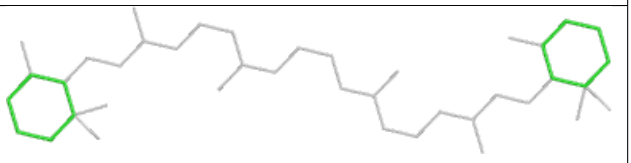
Bond lengths



Bond angles

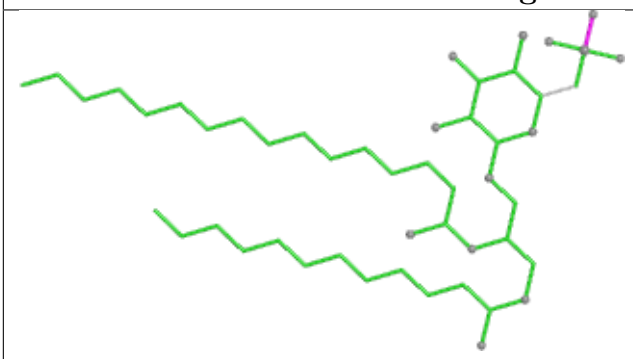


Torsions

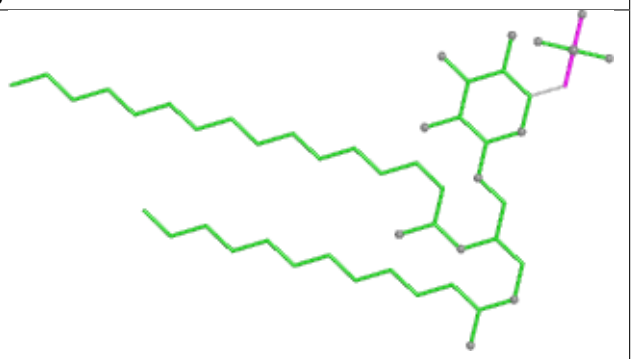


Rings

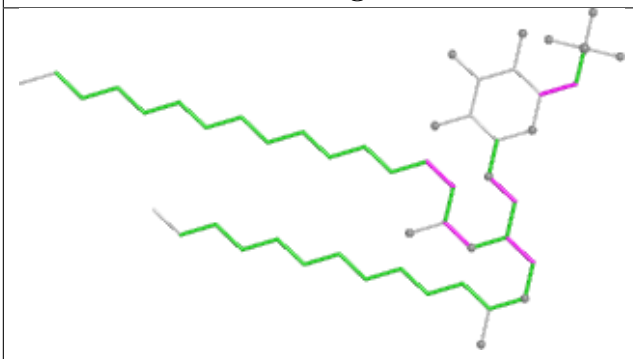
Ligand SQD 42 521



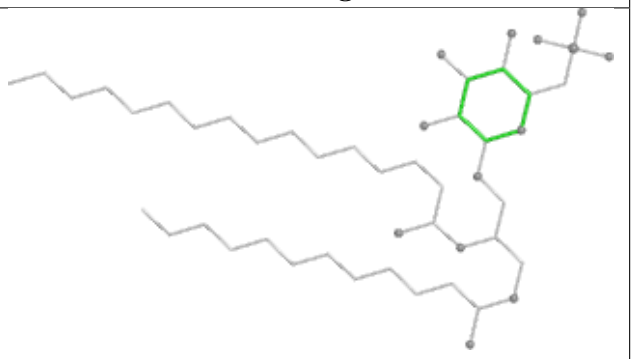
Bond lengths



Bond angles

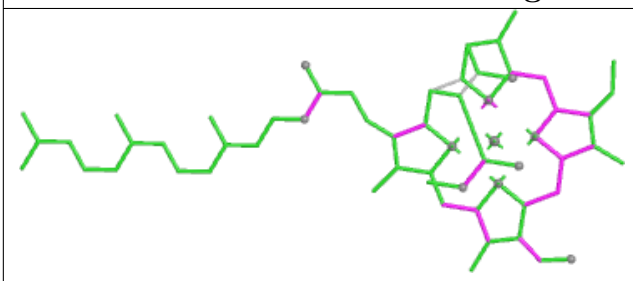


Torsions

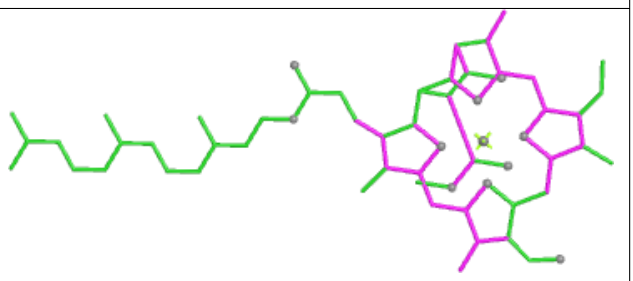


Rings

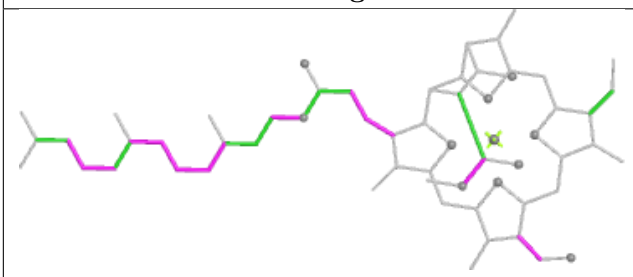
Ligand CL7 21 402



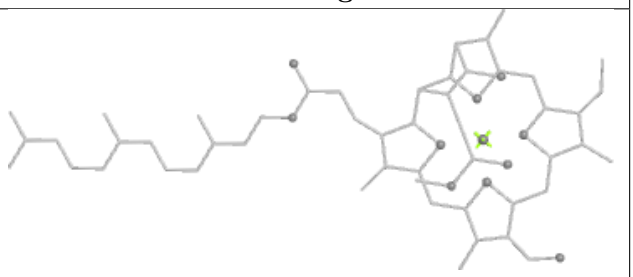
Bond lengths



Bond angles

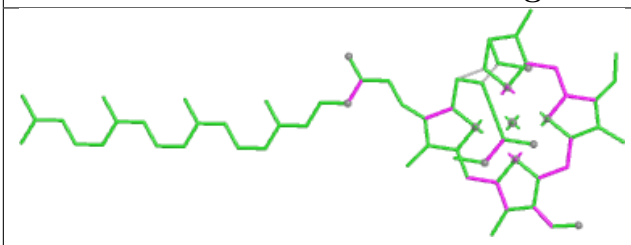


Torsions

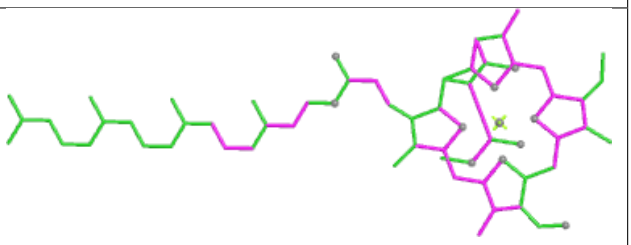


Rings

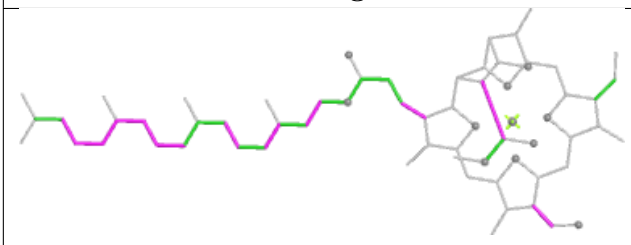
Ligand CL7 31 404



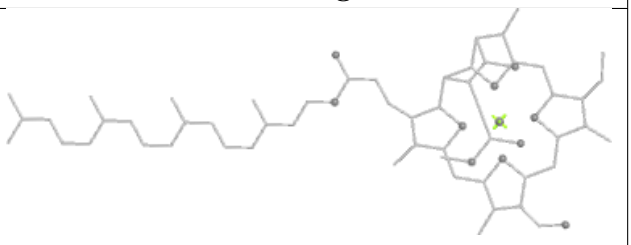
Bond lengths



Bond angles

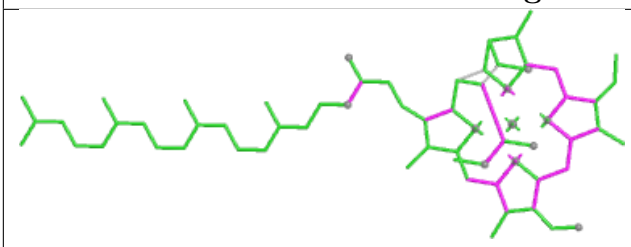


Torsions

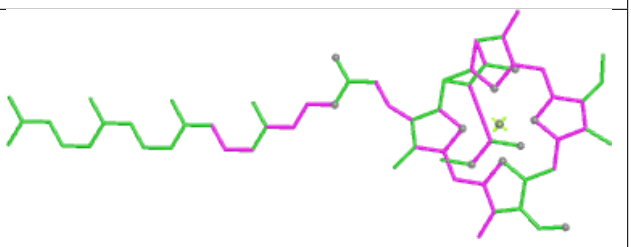


Rings

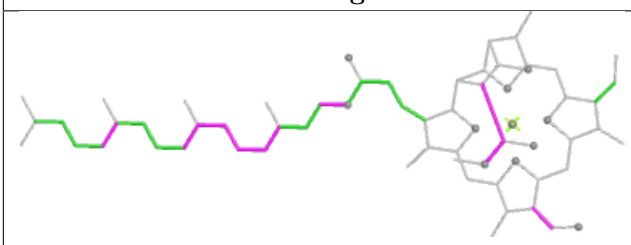
Ligand CL7 23 409



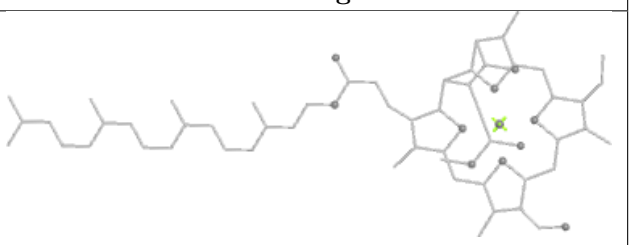
Bond lengths



Bond angles

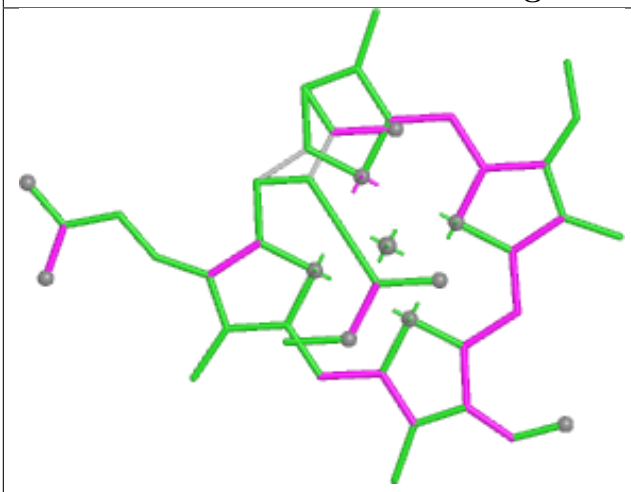


Torsions

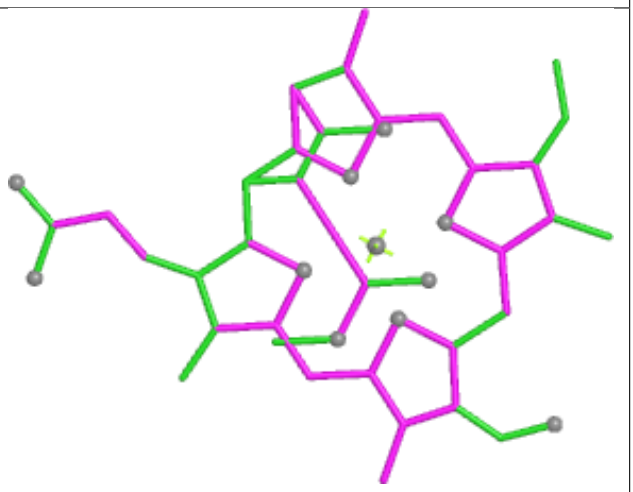


Rings

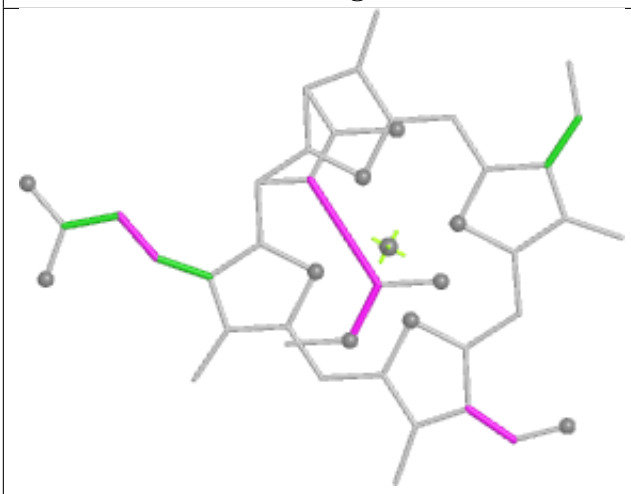
Ligand CL7 11 409



Bond lengths



Bond angles

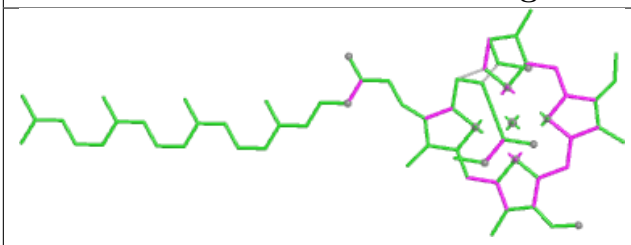


Torsions

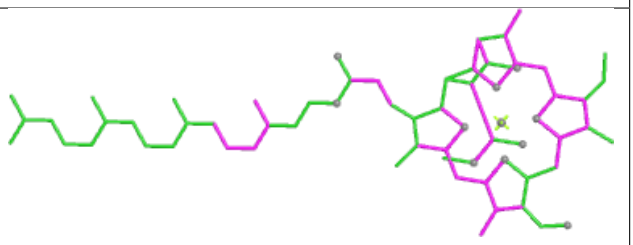


Rings

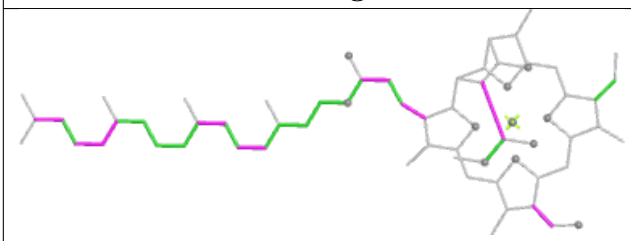
Ligand CL7 2B 610



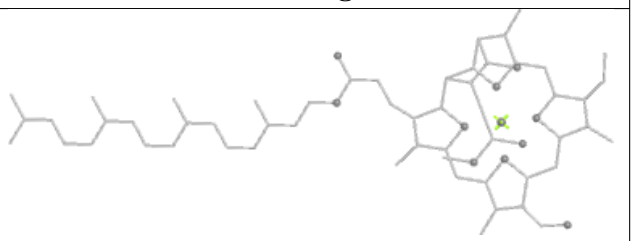
Bond lengths



Bond angles

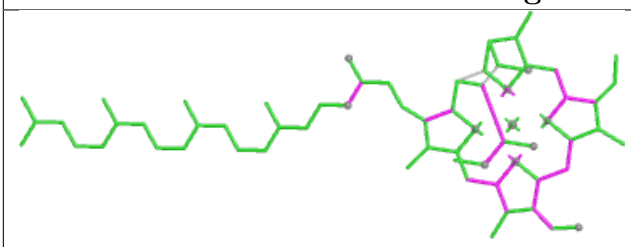


Torsions

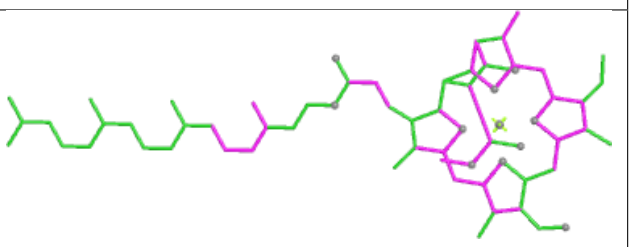


Rings

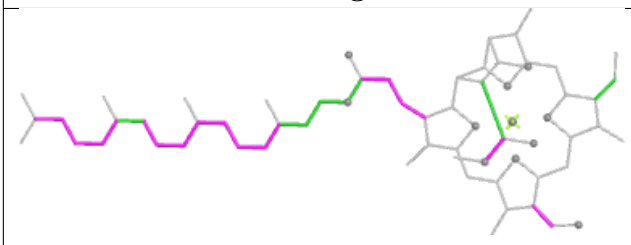
Ligand CL7 14 406



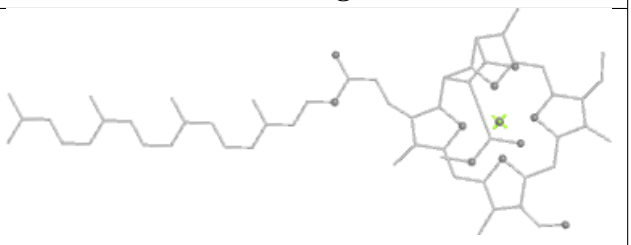
Bond lengths



Bond angles

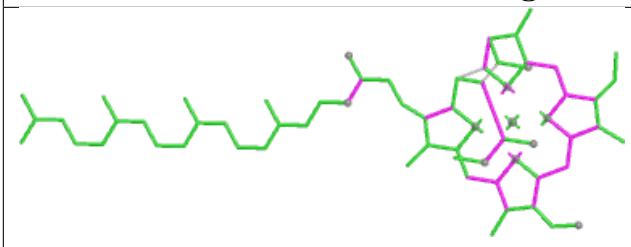


Torsions

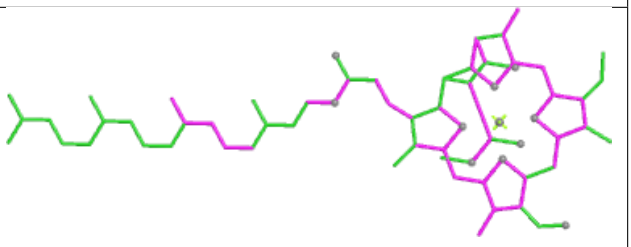


Rings

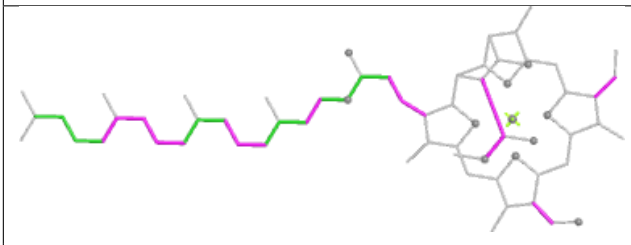
Ligand CL7 3C 505



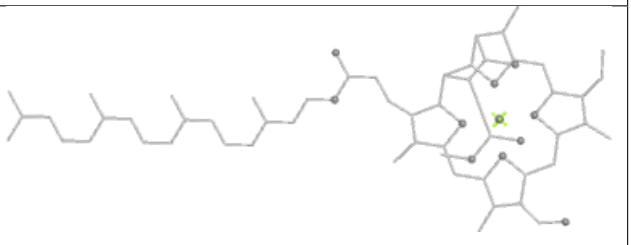
Bond lengths



Bond angles

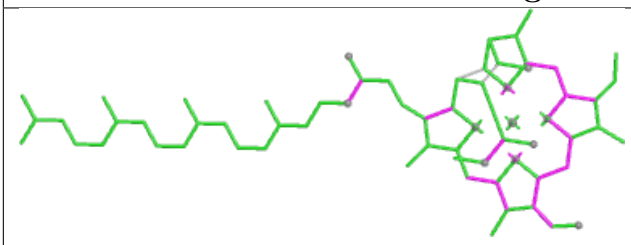


Torsions

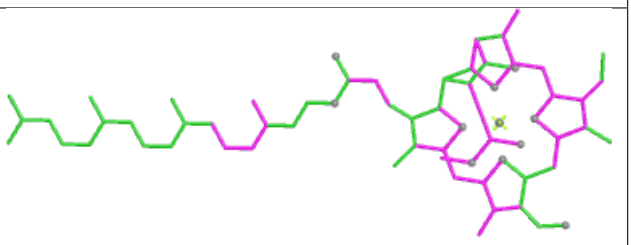


Rings

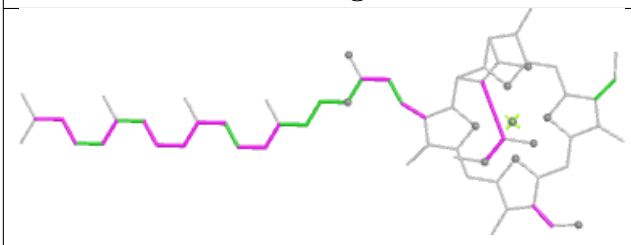
Ligand CL7 31 418



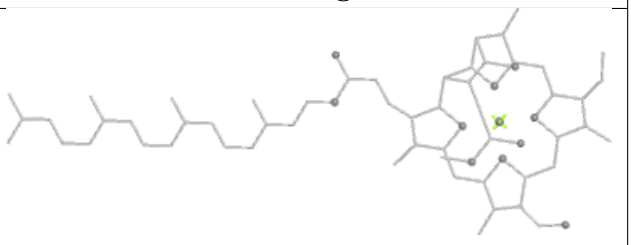
Bond lengths



Bond angles

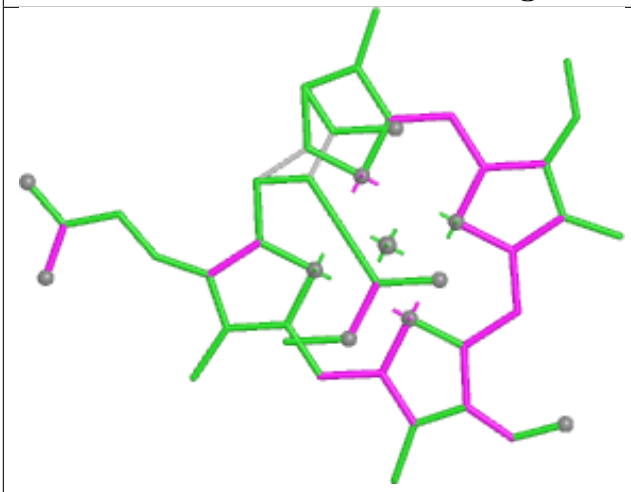


Torsions

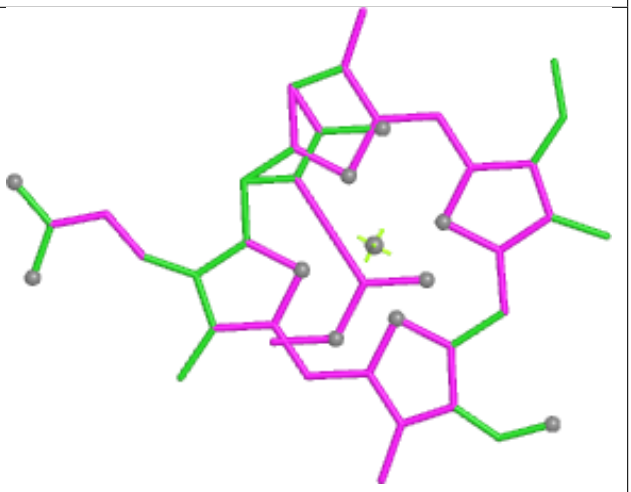


Rings

Ligand CL7 4D 405



Bond lengths



Bond angles

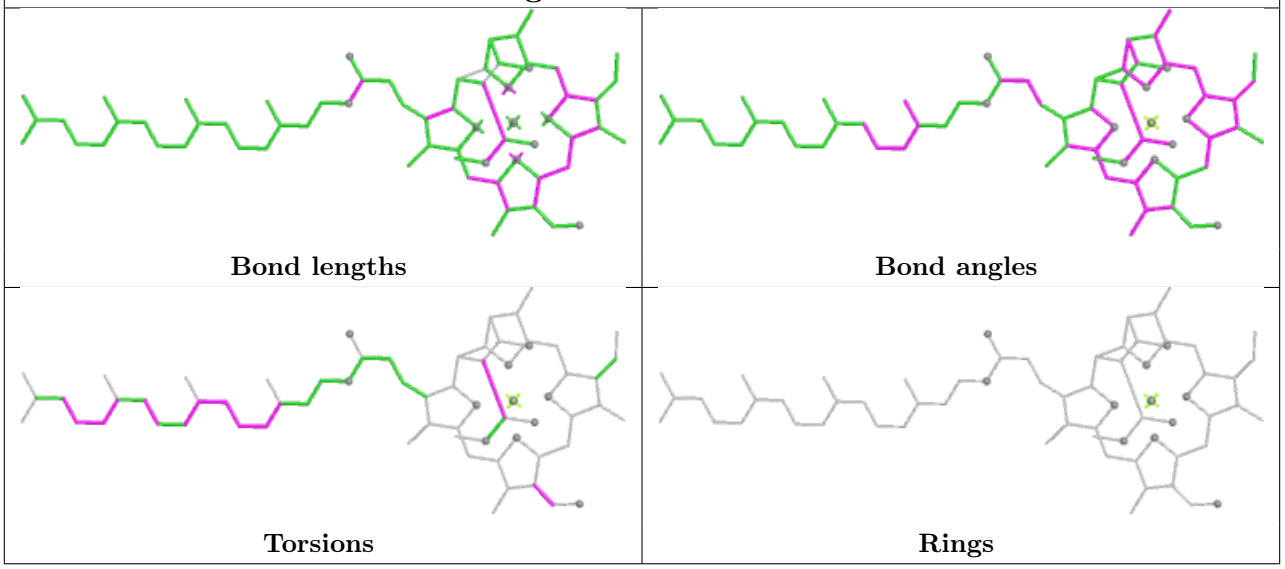


Torsions

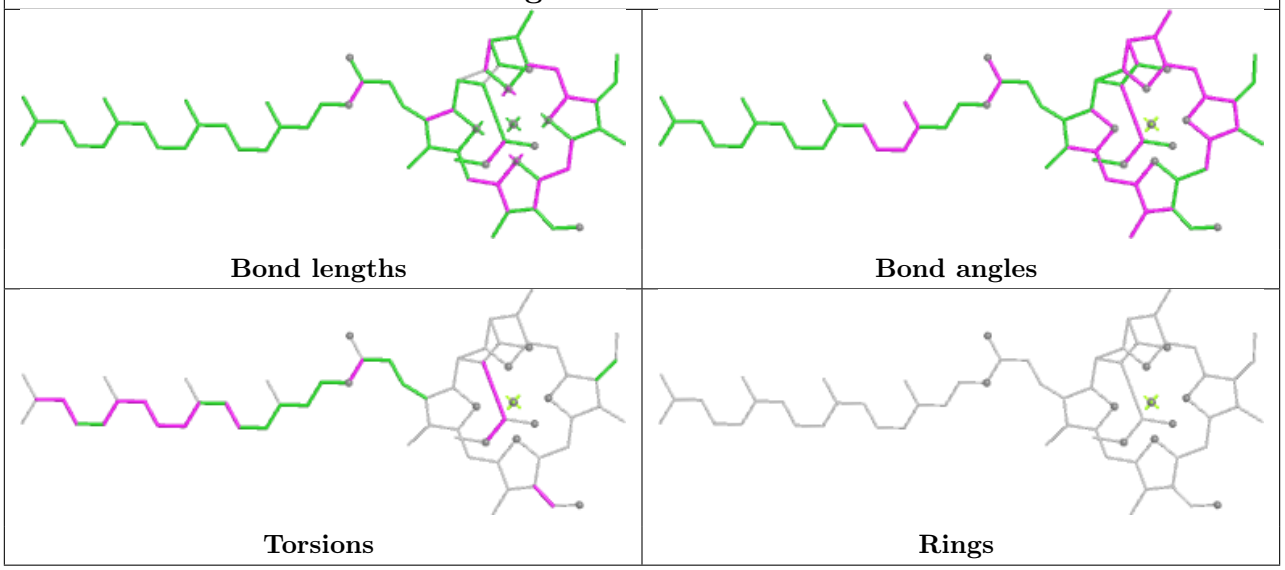


Rings

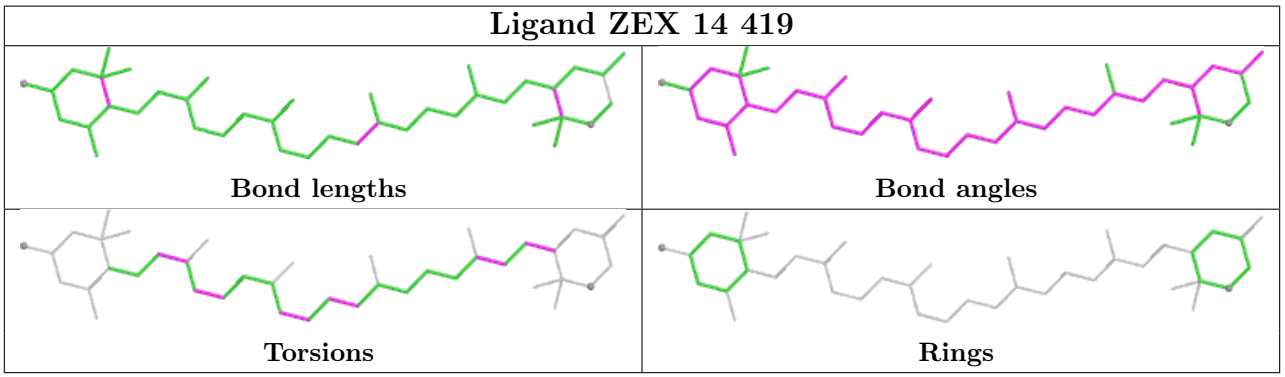
Ligand CL7 13 507



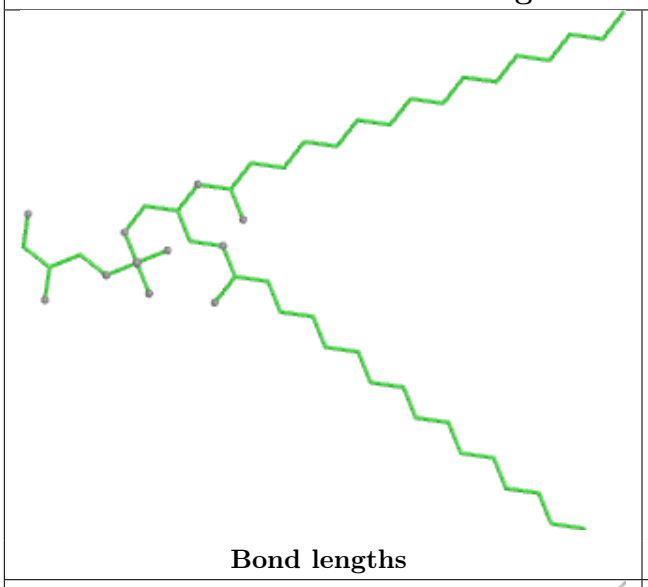
Ligand CL7 43 410



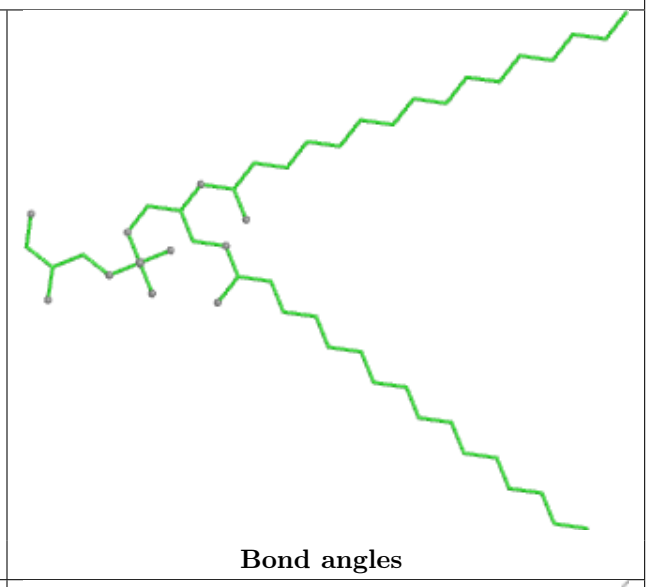
Ligand ZEX 14 419



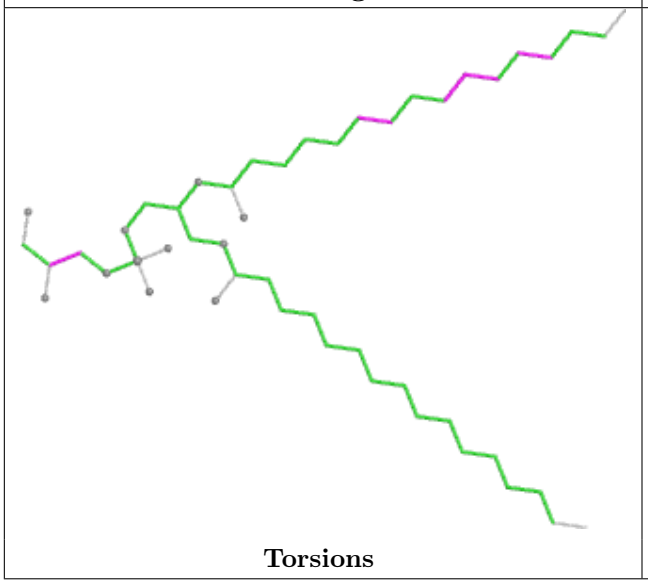
Ligand LHG 2B 626



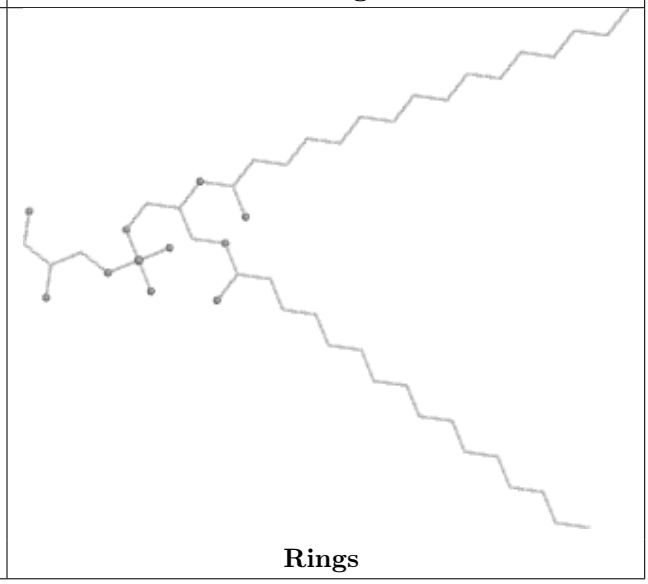
Bond lengths



Bond angles

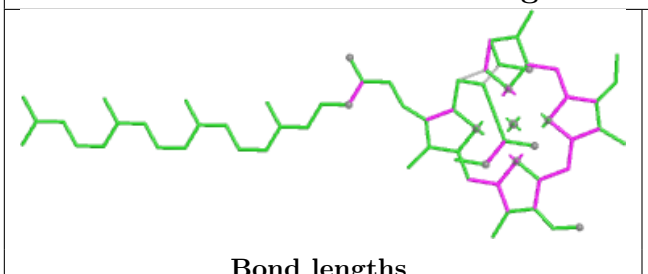


Torsions

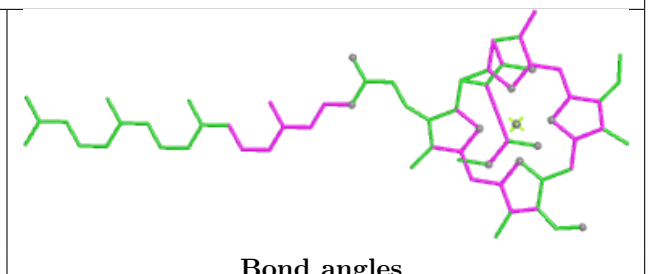


Rings

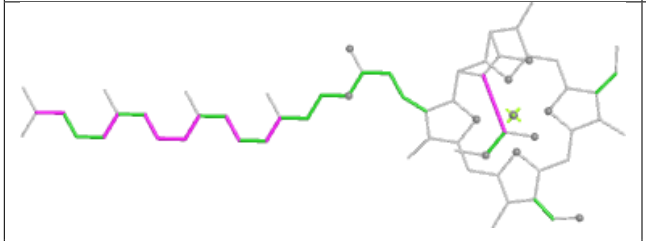
Ligand CL7 2B 604



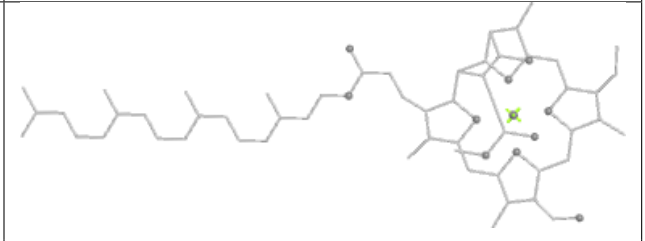
Bond lengths



Bond angles

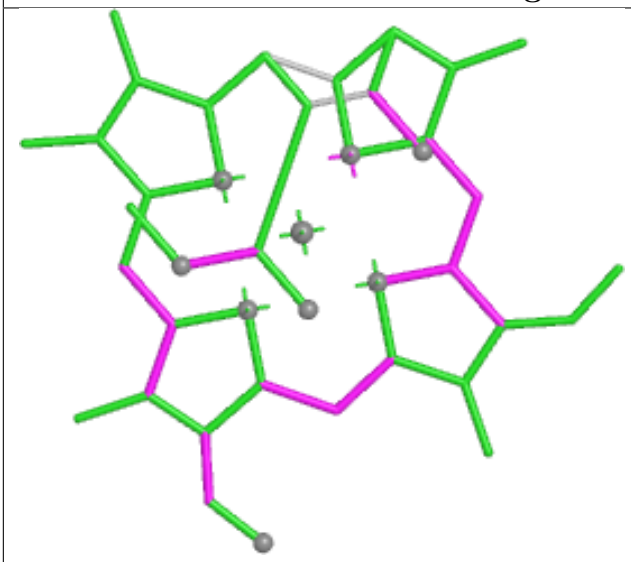


Torsions

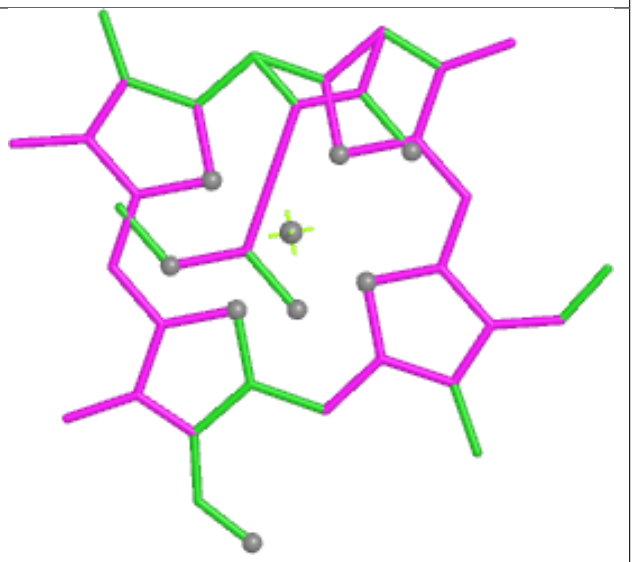


Rings

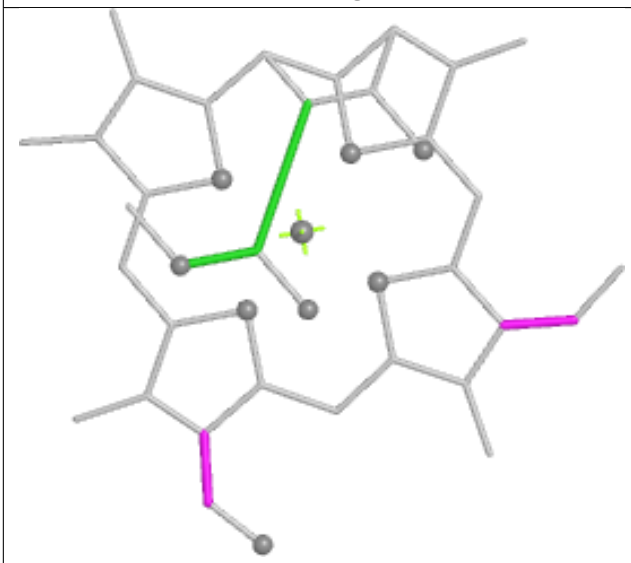
Ligand CL7 31 414



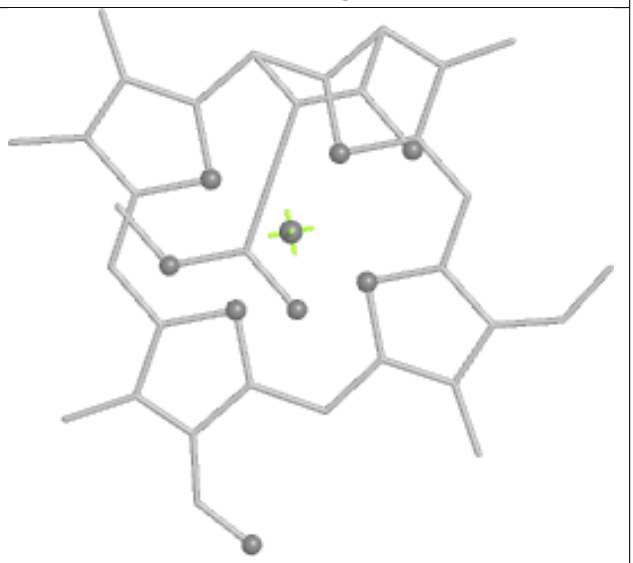
Bond lengths



Bond angles

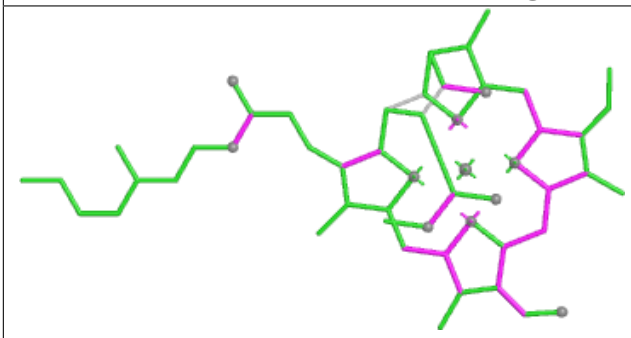


Torsions

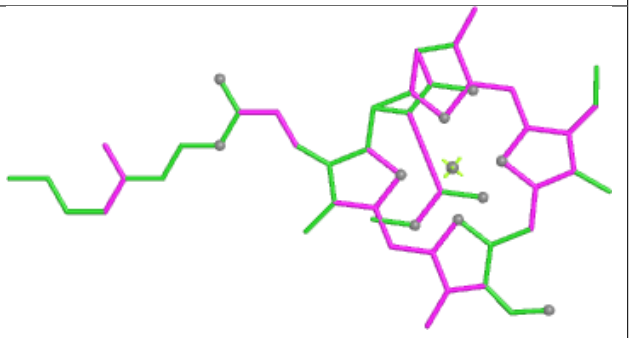


Rings

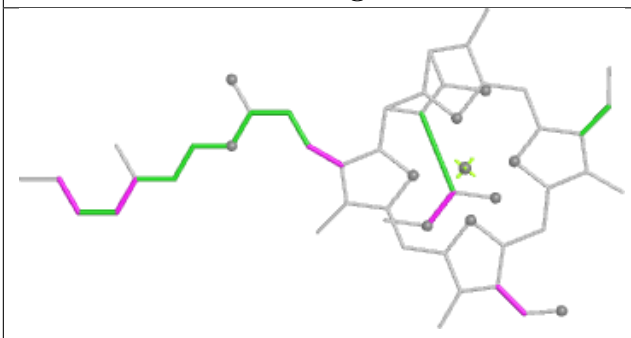
Ligand CL7 34 414



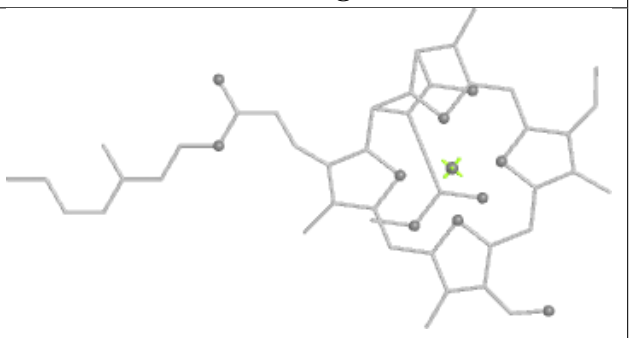
Bond lengths



Bond angles

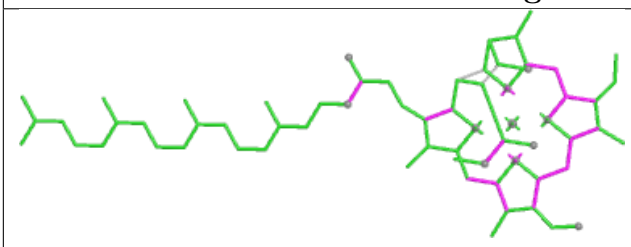


Torsions

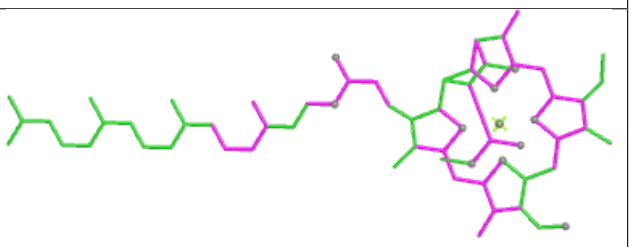


Rings

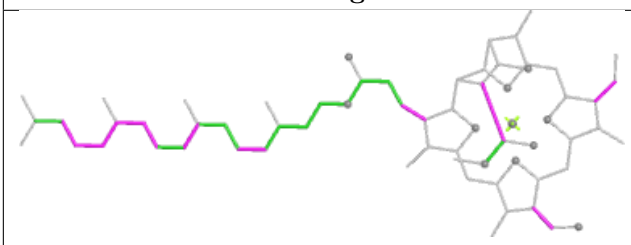
Ligand CL7 21 408



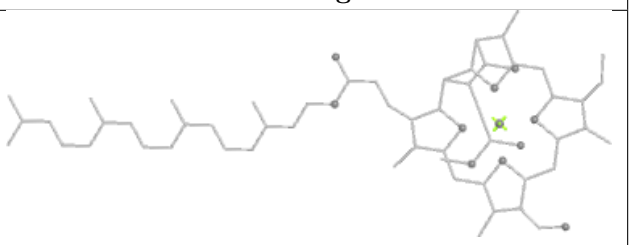
Bond lengths



Bond angles

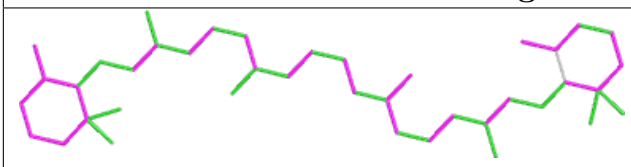


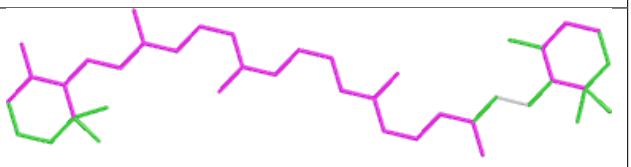
Torsions

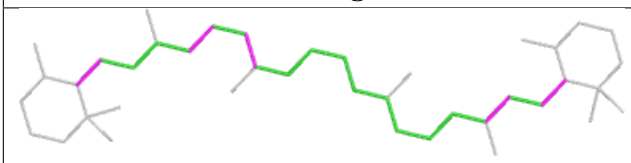


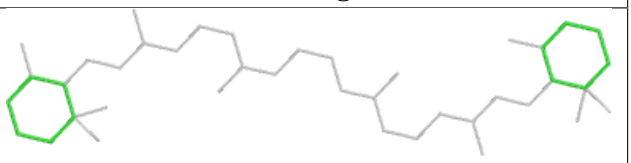
Rings

Ligand 8CT 2C 518

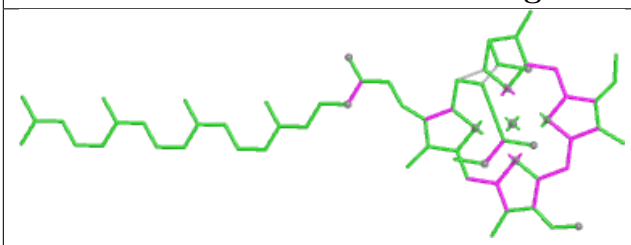

Bond lengths

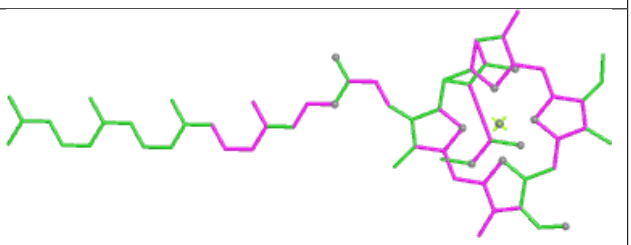

Bond angles

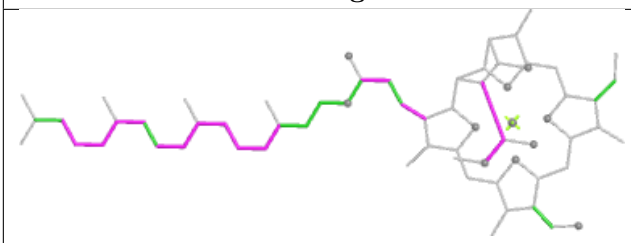

Torsions

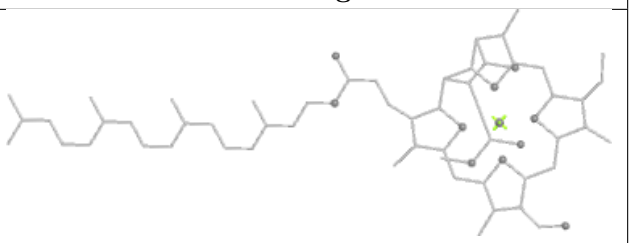

Rings

Ligand CL7 32 510

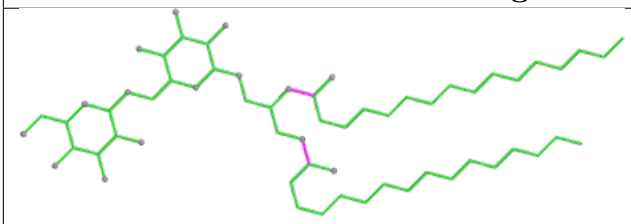

Bond lengths

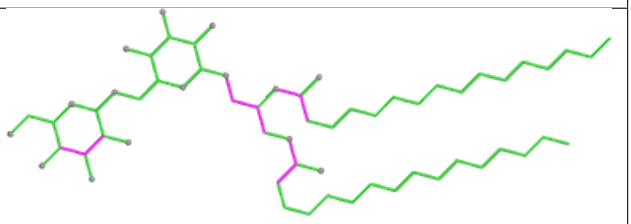

Bond angles

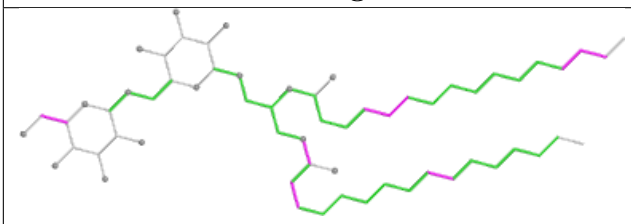

Torsions

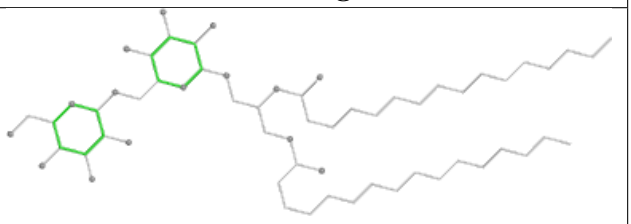

Rings

Ligand DGD 1C 516

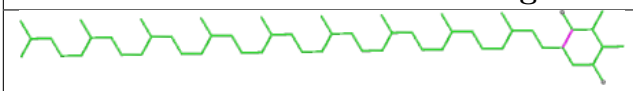

Bond lengths


Bond angles


Torsions


Rings

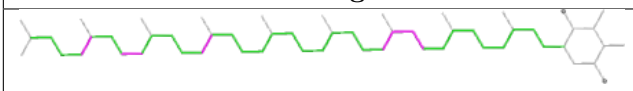
Ligand PL9 4D 407



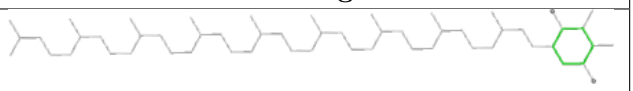
Bond lengths



Bond angles

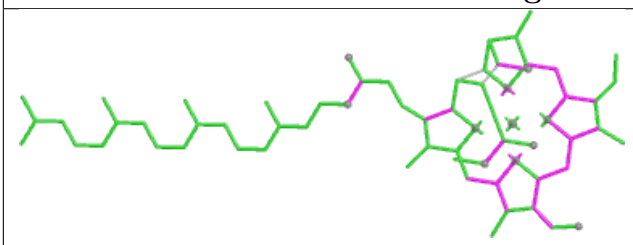


Torsions

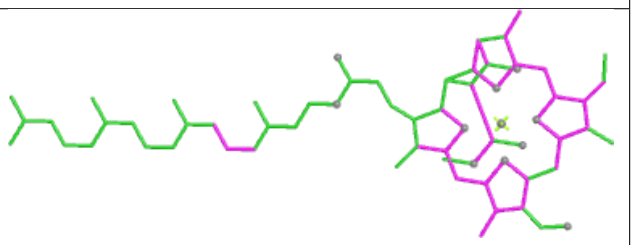


Rings

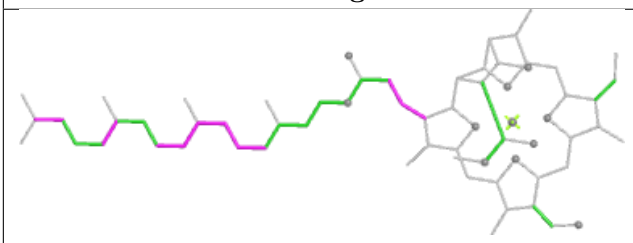
Ligand CL7 34 404



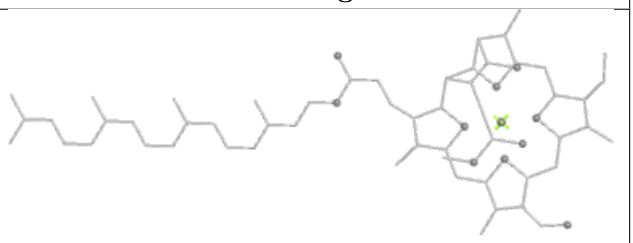
Bond lengths



Bond angles

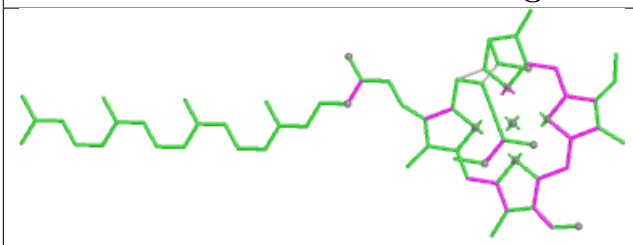


Torsions

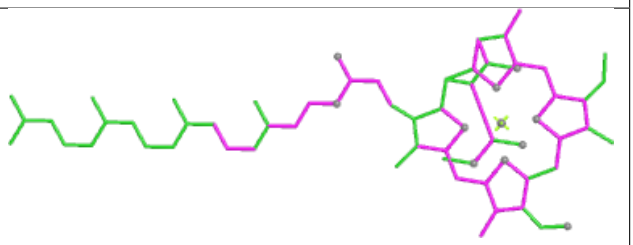


Rings

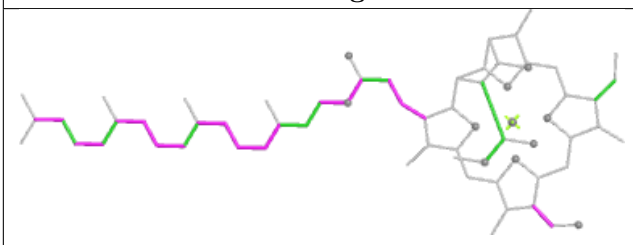
Ligand CL7 14 405



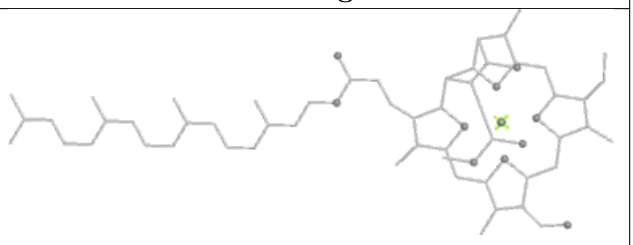
Bond lengths



Bond angles

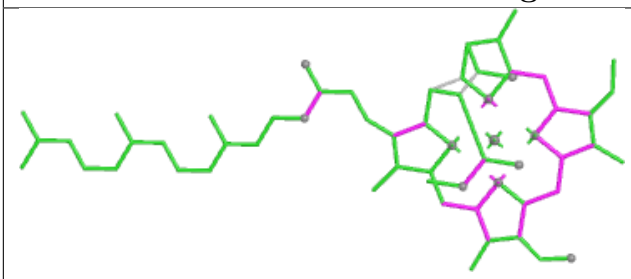


Torsions

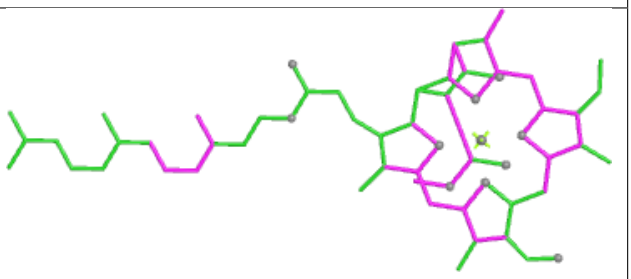


Rings

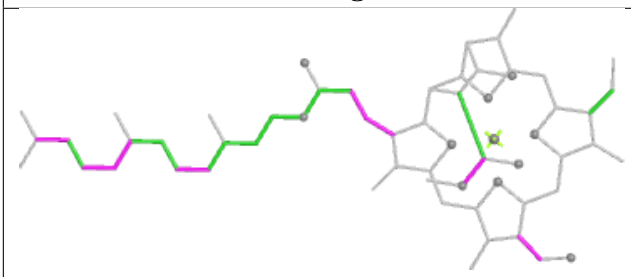
Ligand CL7 2B 608



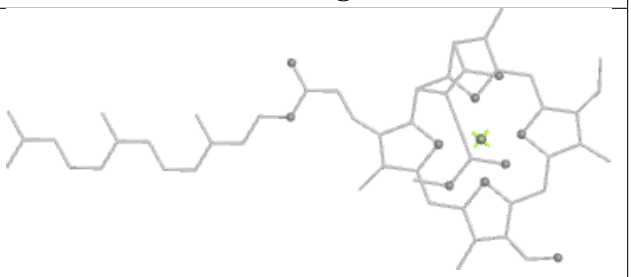
Bond lengths



Bond angles

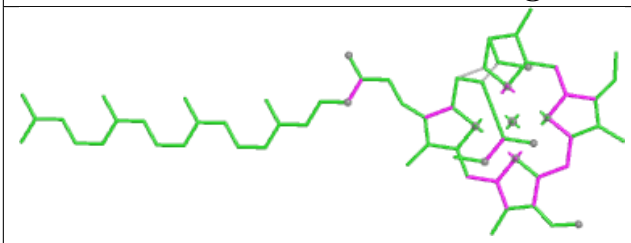


Torsions

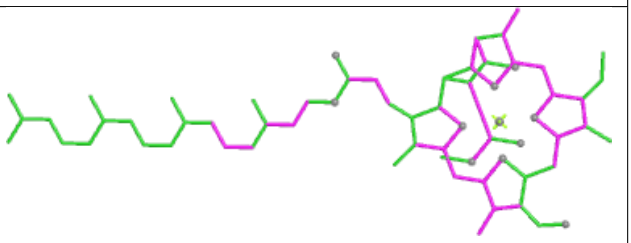


Rings

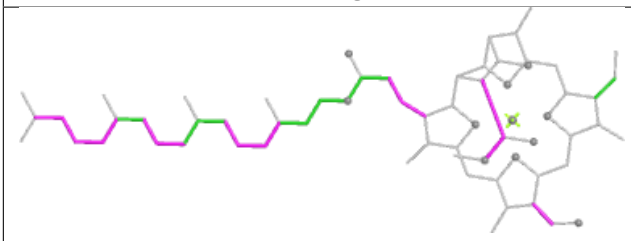
Ligand CL7 32 517



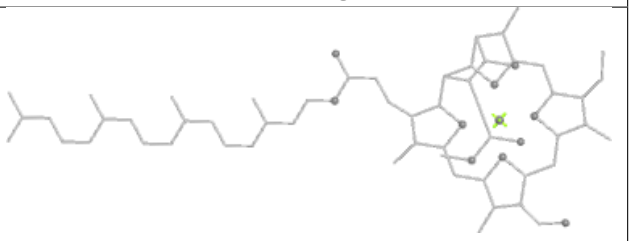
Bond lengths



Bond angles

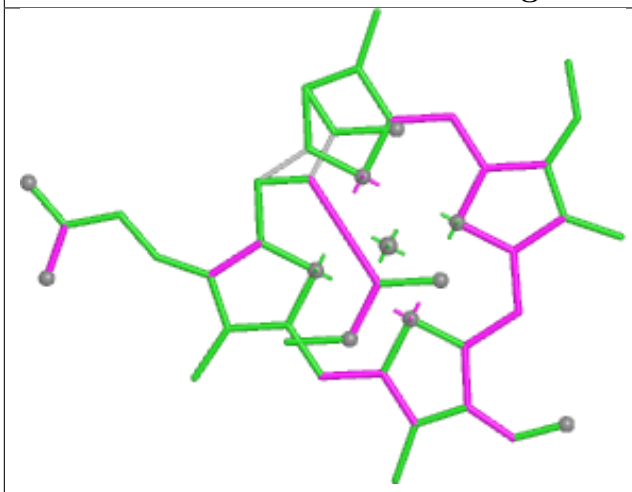


Torsions

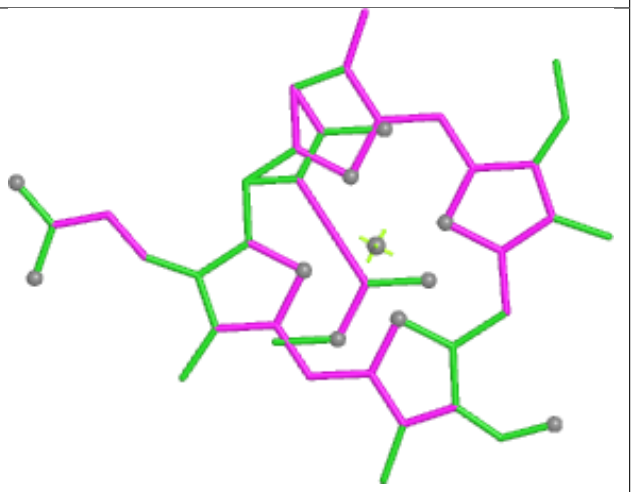


Rings

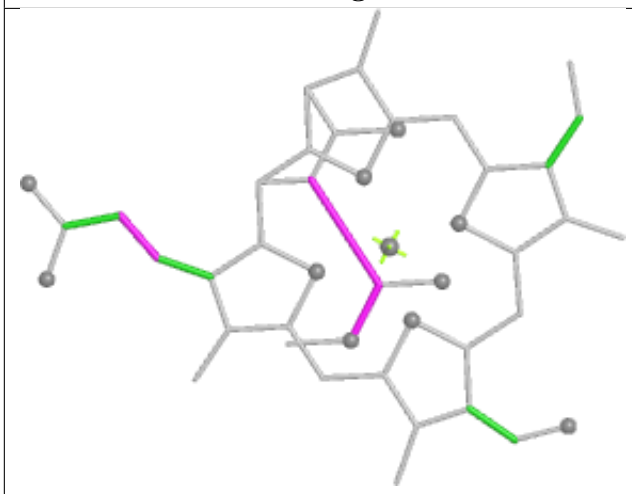
Ligand CL7 2B 617



Bond lengths



Bond angles

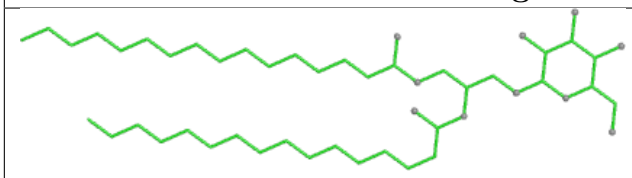


Torsions

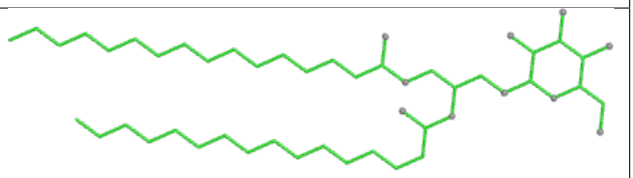


Rings

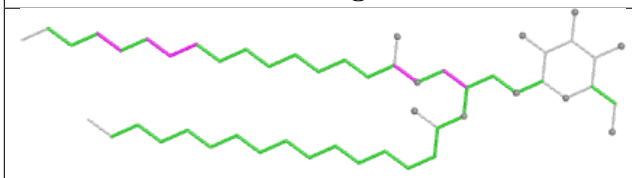
Ligand LMG 1B 621



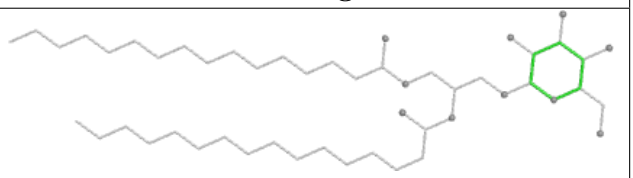
Bond lengths



Bond angles

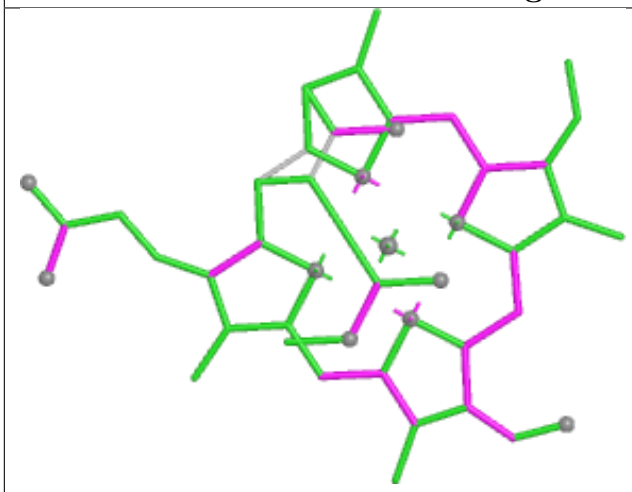


Torsions

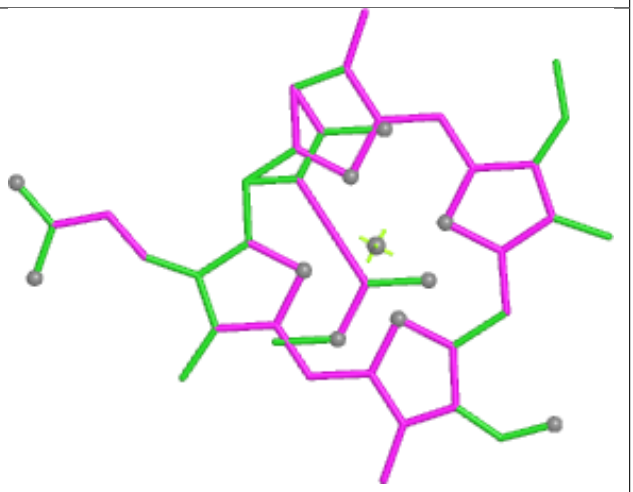


Rings

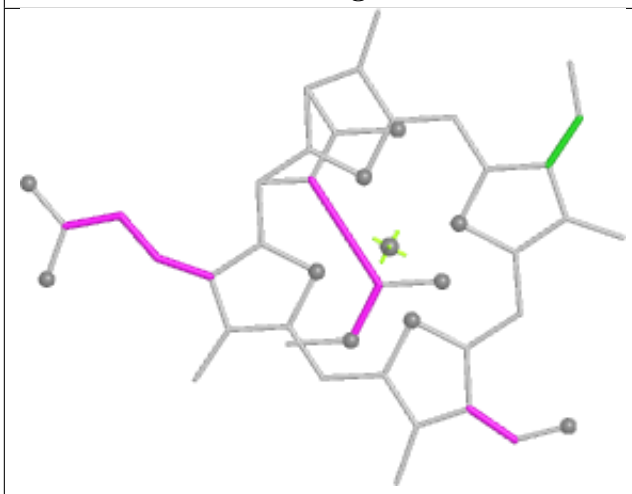
Ligand CL7 41 412



Bond lengths



Bond angles

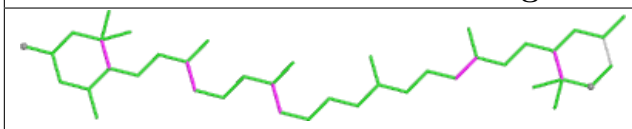


Torsions

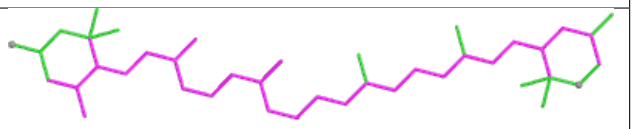


Rings

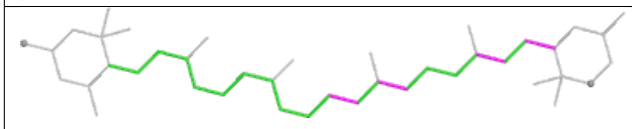
Ligand ZEX 13 525



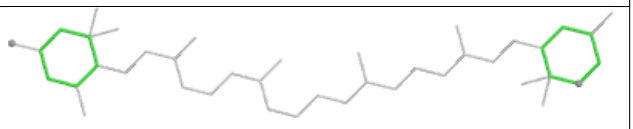
Bond lengths



Bond angles

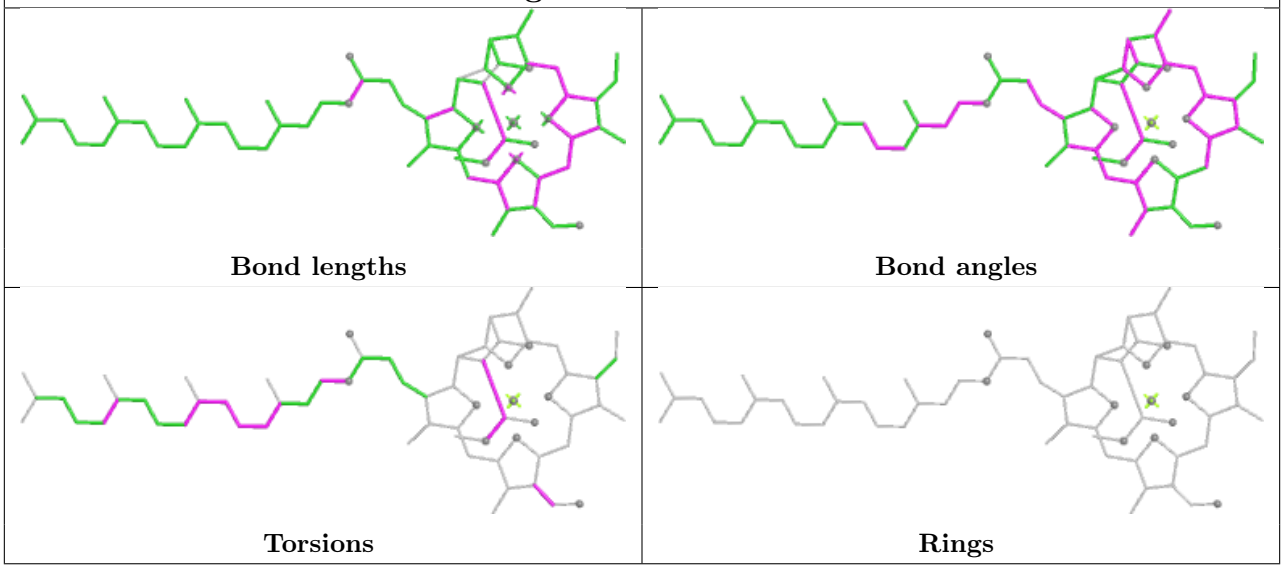


Torsions

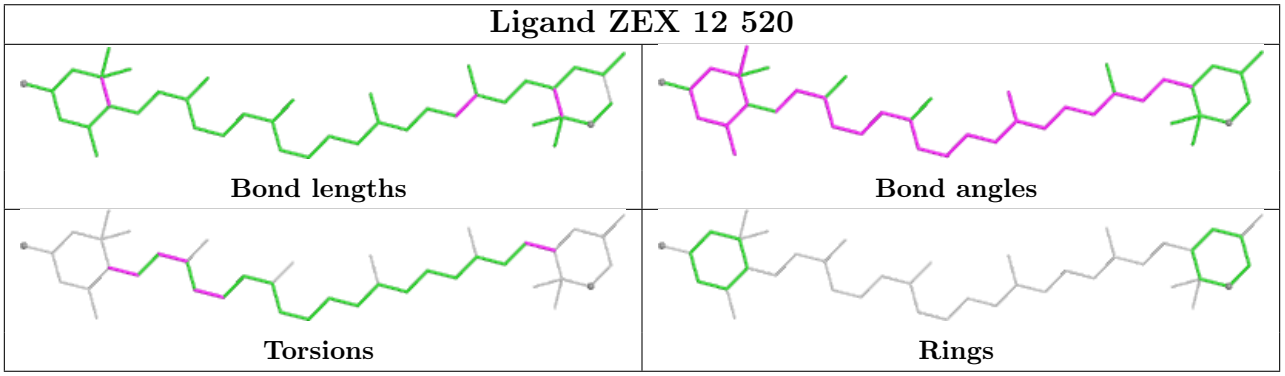


Rings

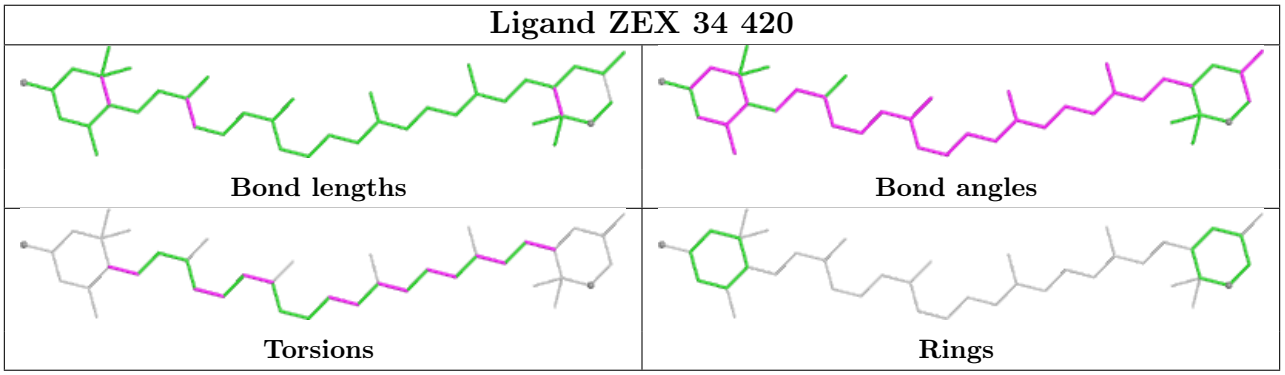
Ligand CL7 43 409



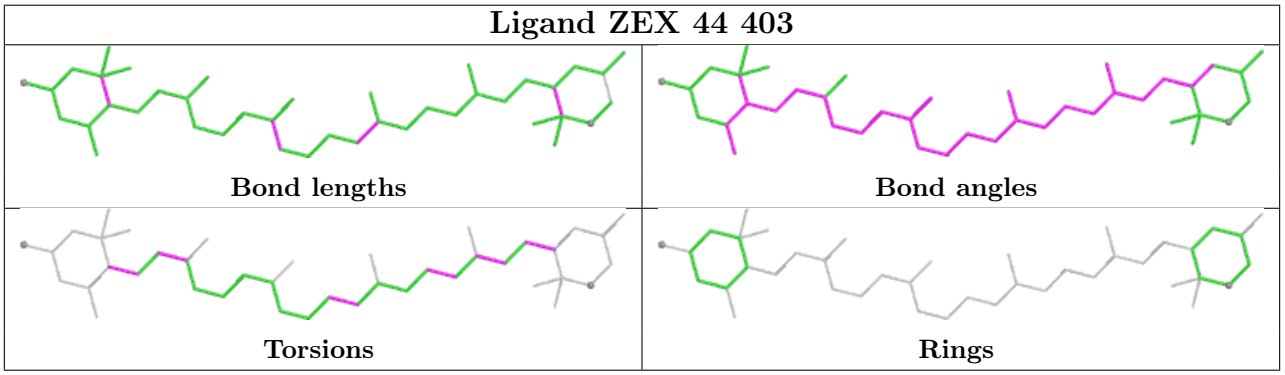
Ligand ZEX 12 520



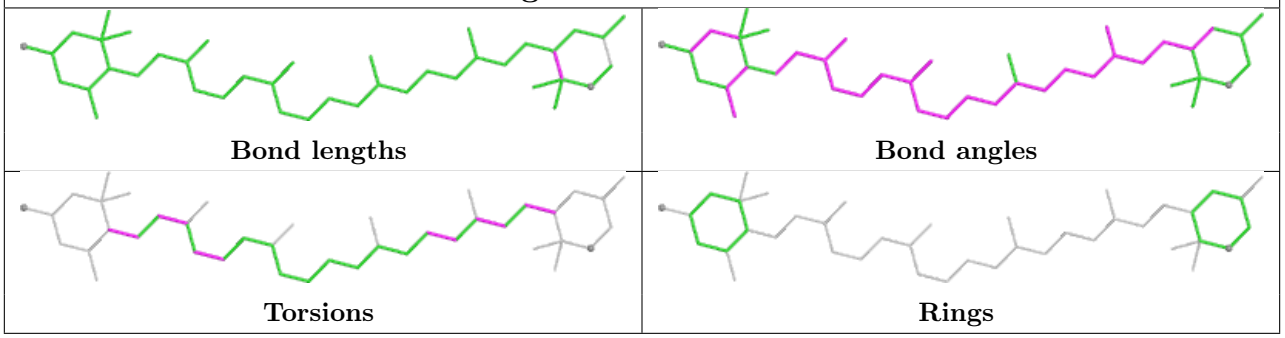
Ligand ZEX 34 420



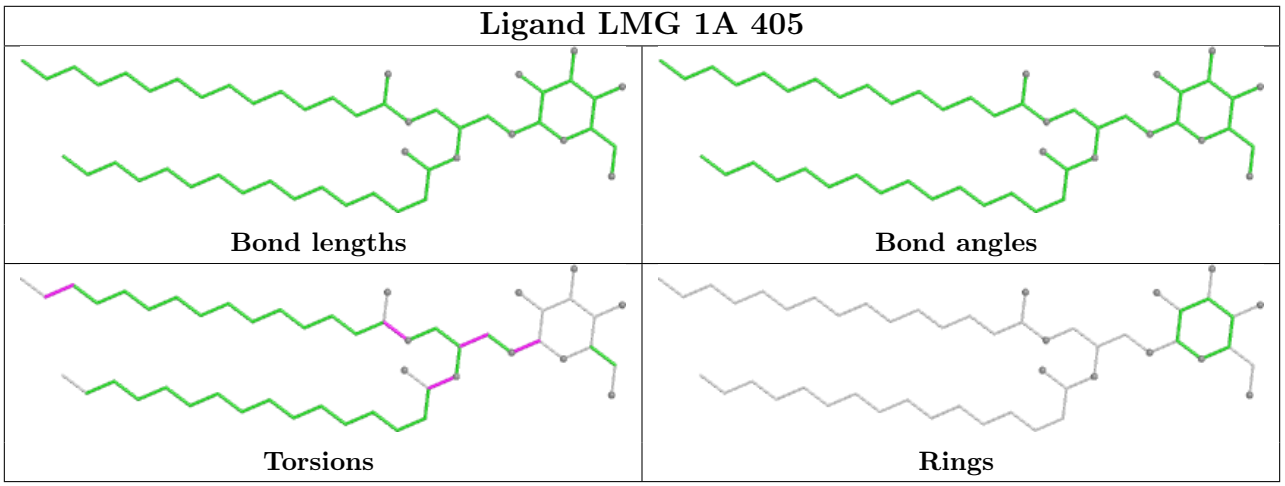
Ligand ZEX 44 403



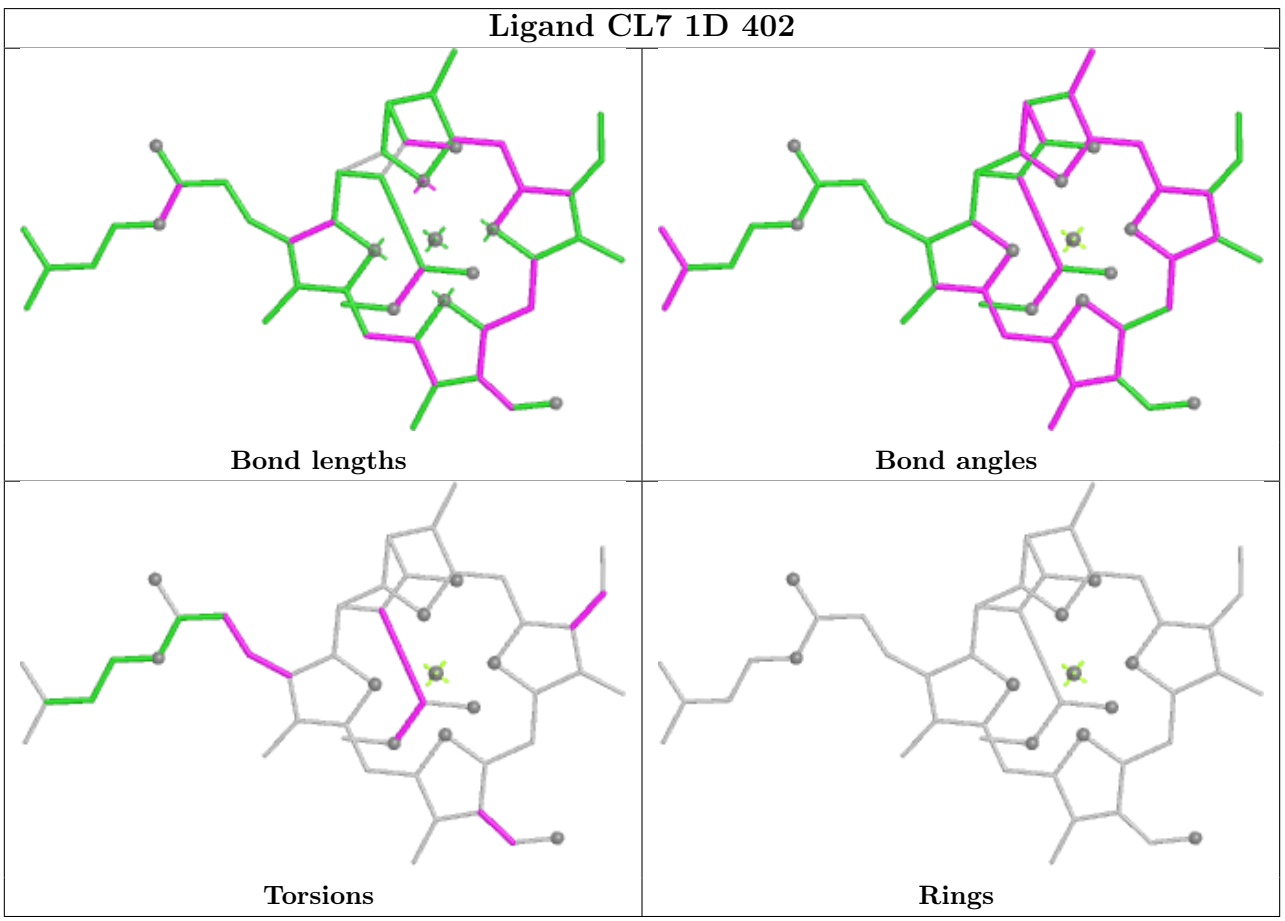
Ligand ZEX 34 418



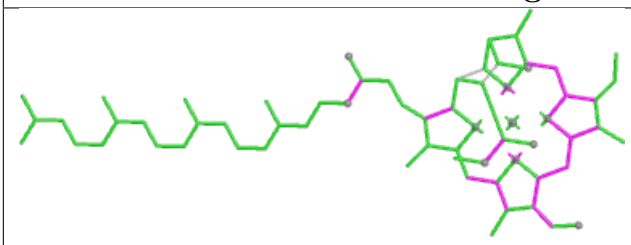
Ligand LMG 1A 405



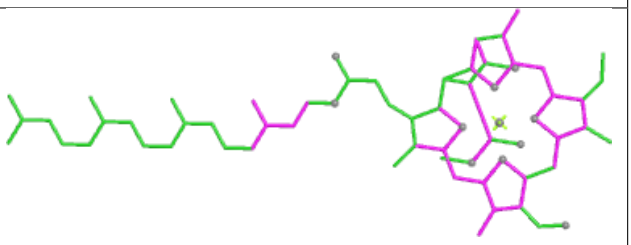
Ligand CL7 1D 402



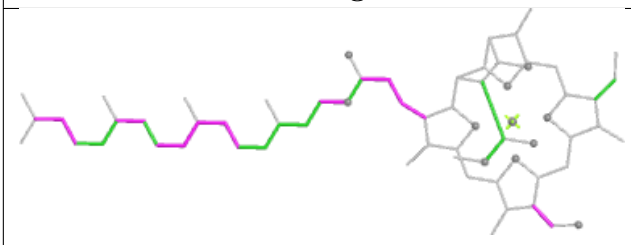
Ligand CL7 22 501



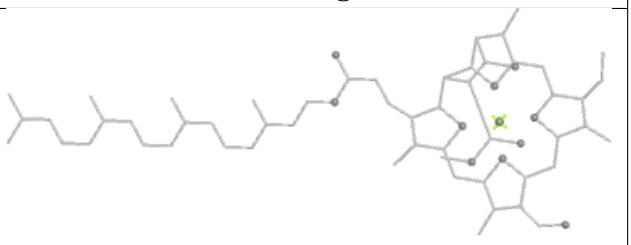
Bond lengths



Bond angles

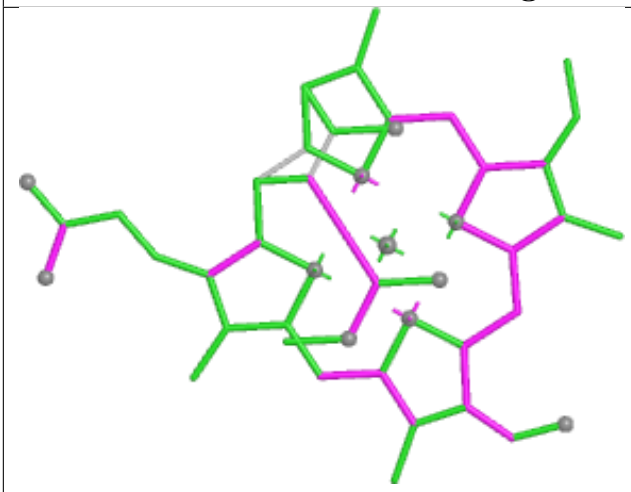


Torsions



Rings

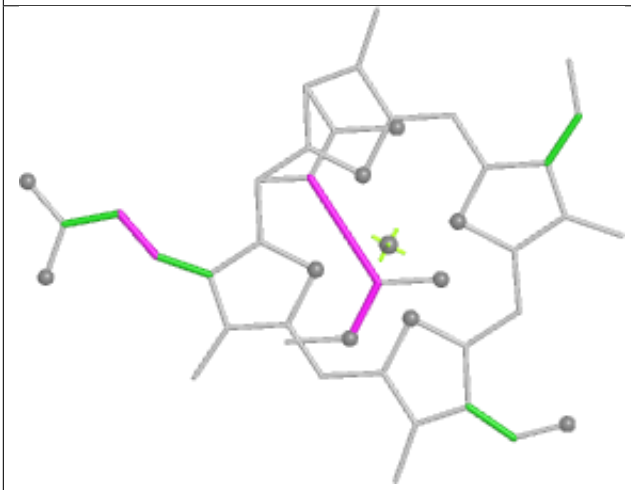
Ligand CL7 1B 616



Bond lengths



Bond angles

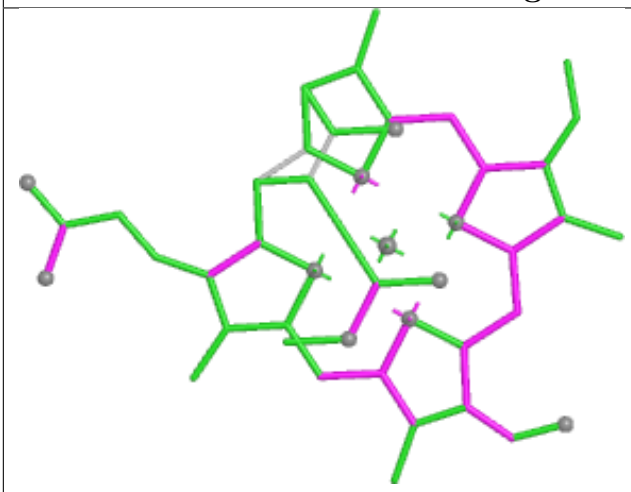


Torsions

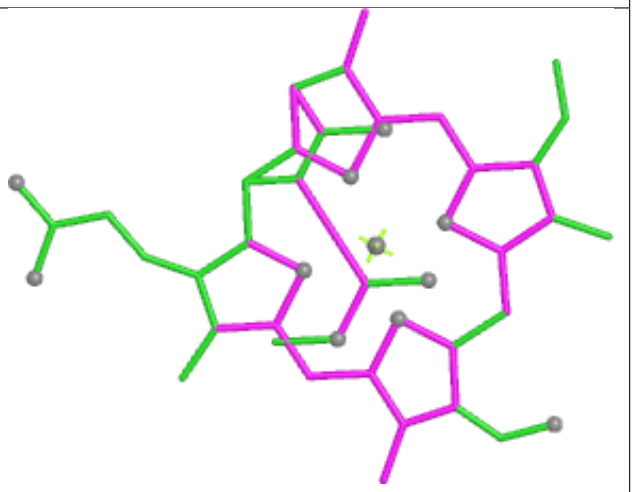


Rings

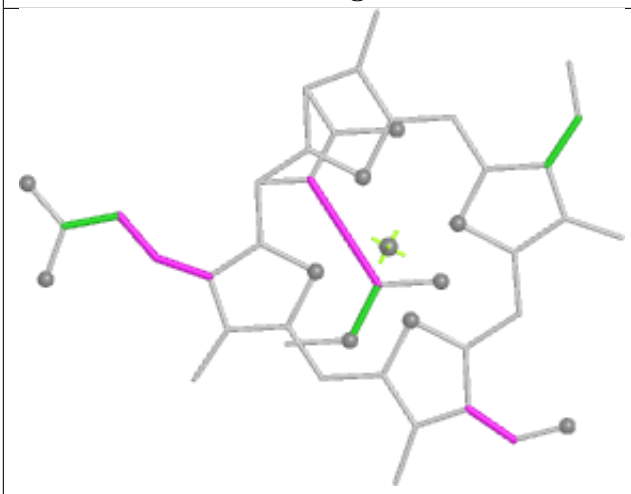
Ligand CL7 12 508



Bond lengths



Bond angles

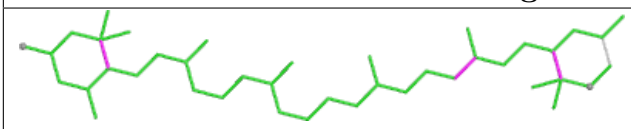


Torsions

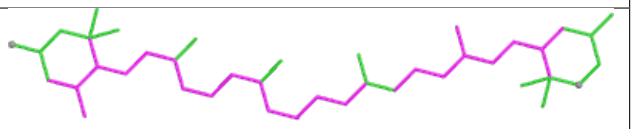


Rings

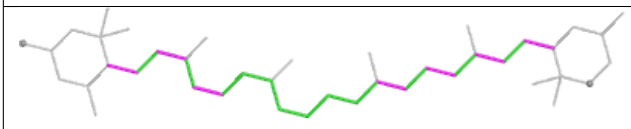
Ligand ZEX 12 524



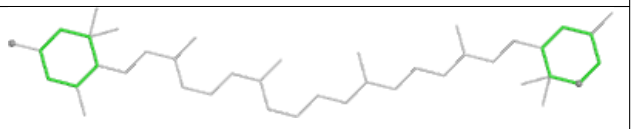
Bond lengths



Bond angles

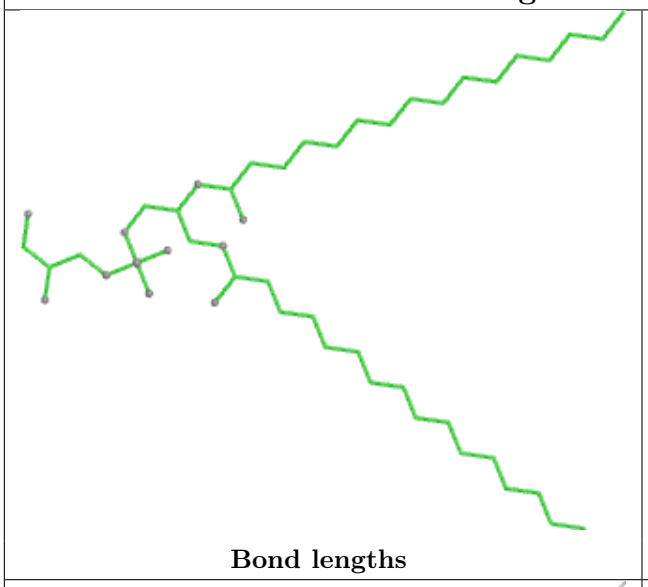


Torsions

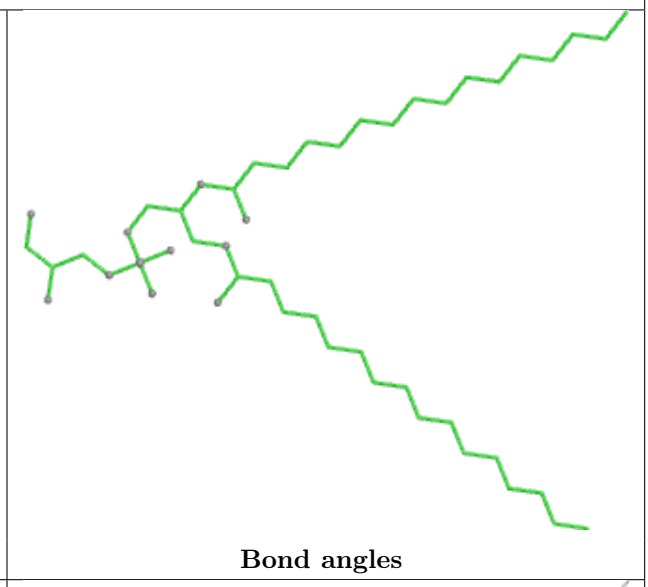


Rings

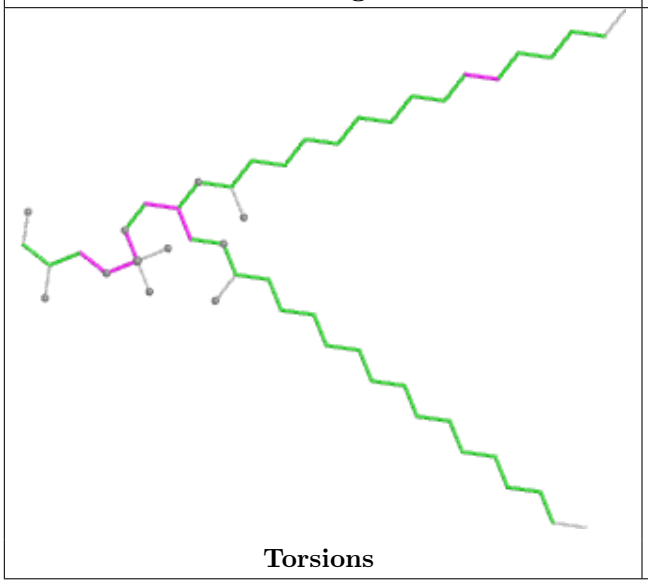
Ligand LHG 14 401



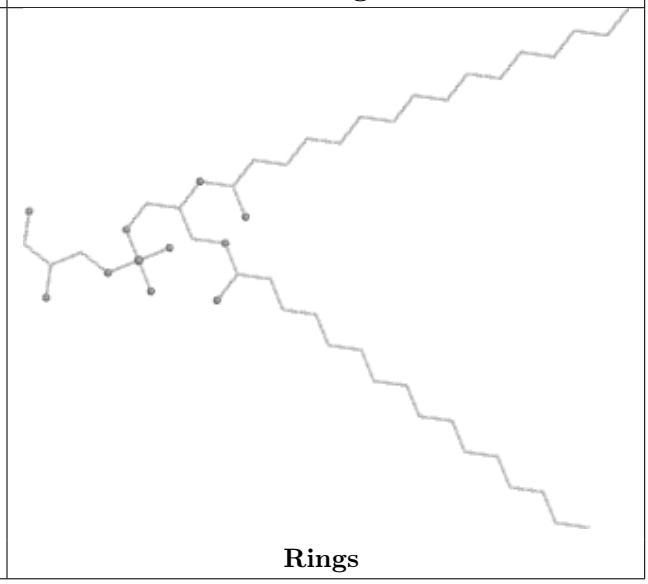
Bond lengths



Bond angles

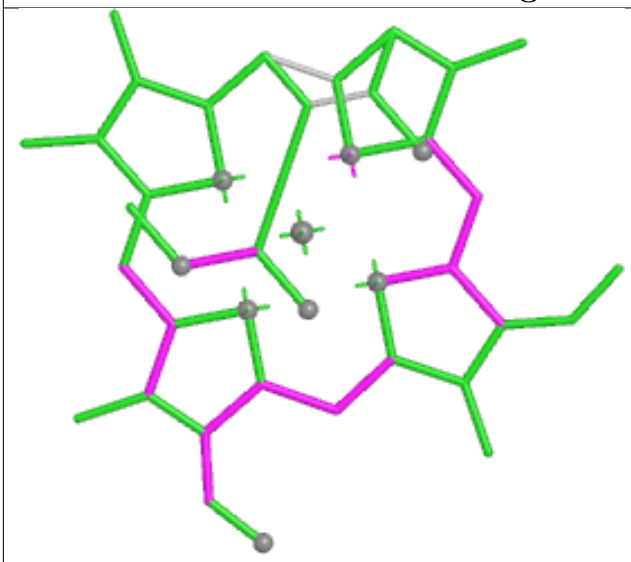


Torsions

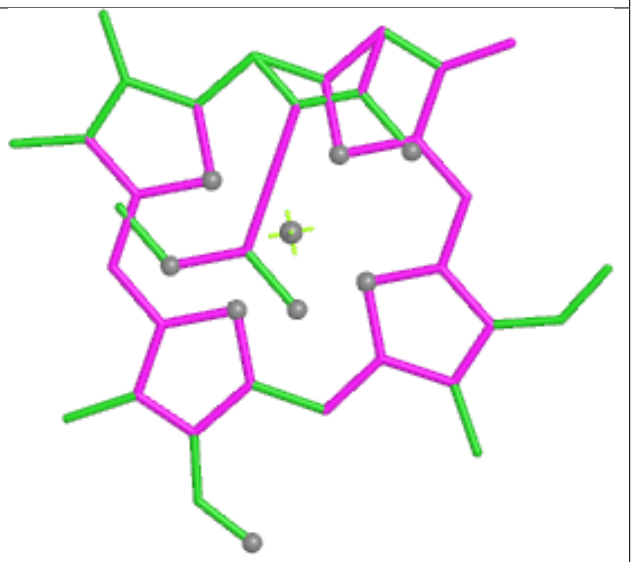


Rings

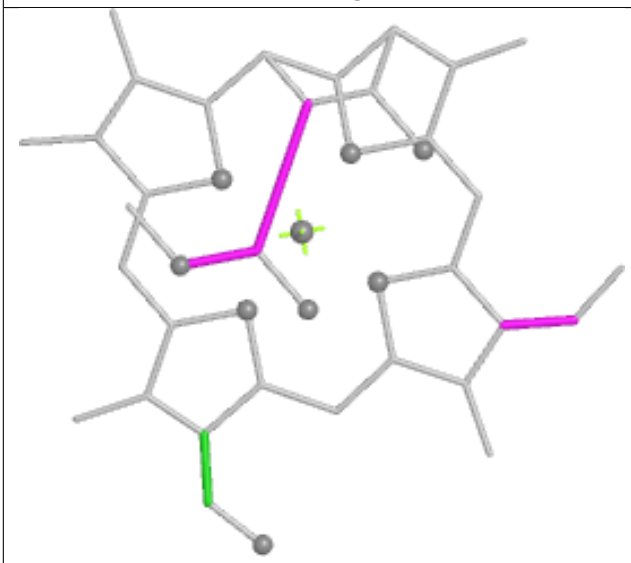
Ligand CL7 2B 602



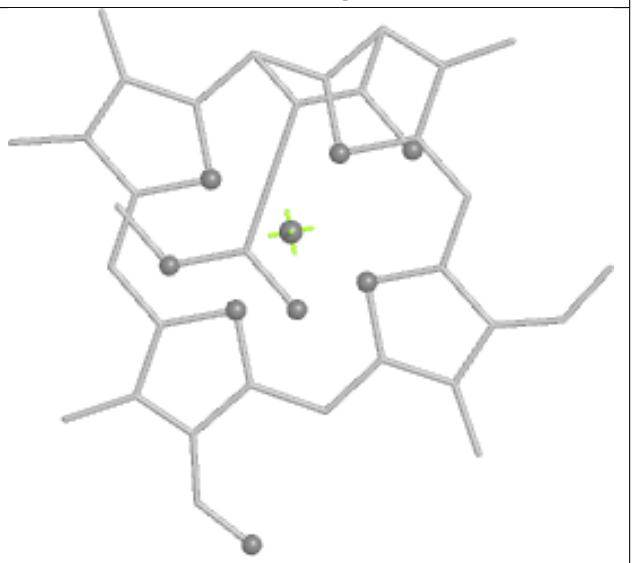
Bond lengths



Bond angles

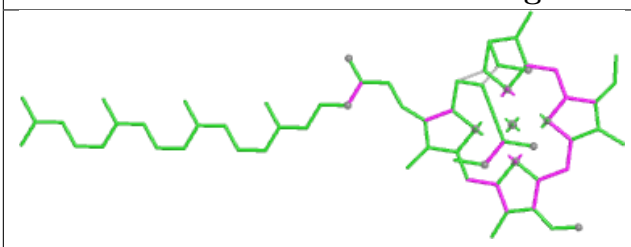


Torsions

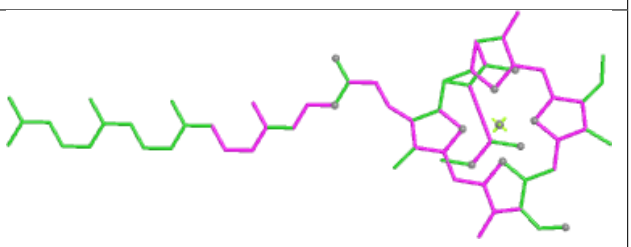


Rings

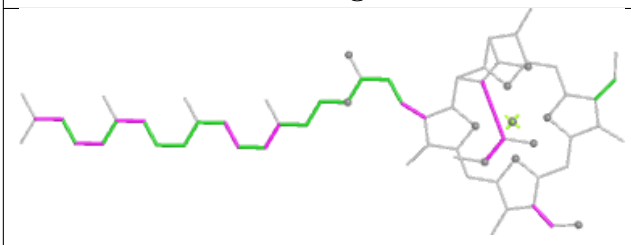
Ligand CL7 24 411



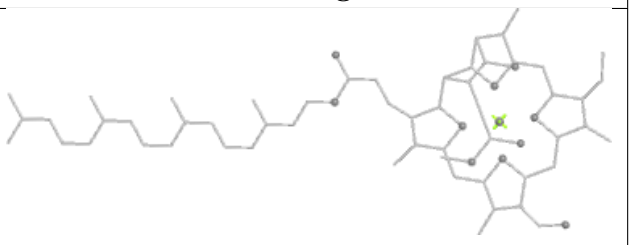
Bond lengths



Bond angles

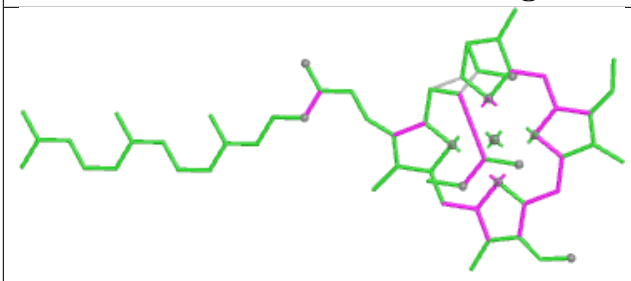


Torsions

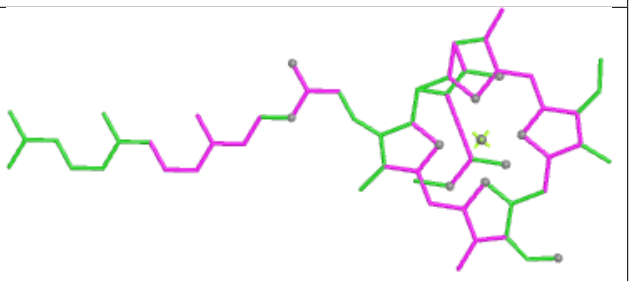


Rings

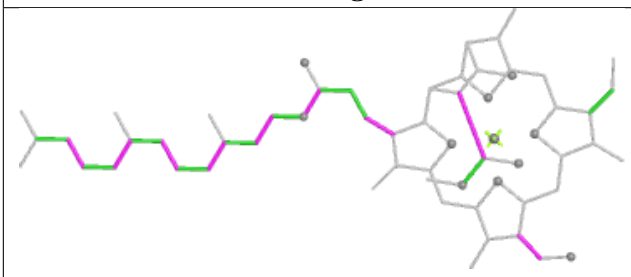
Ligand CL7 2C 506



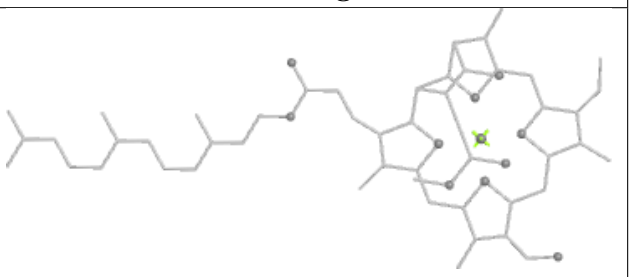
Bond lengths



Bond angles

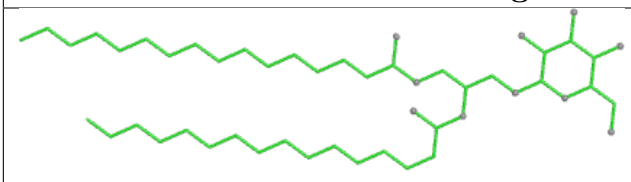


Torsions

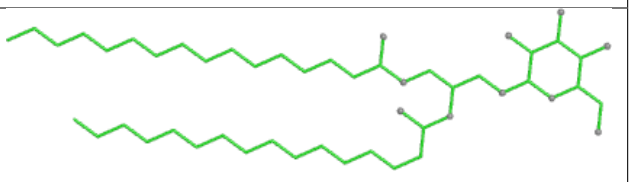


Rings

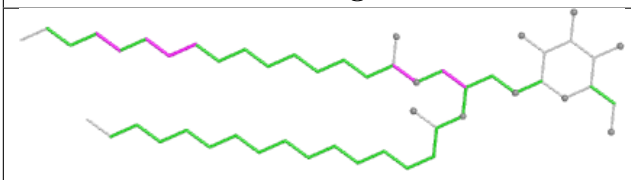
Ligand LMG 4B 622



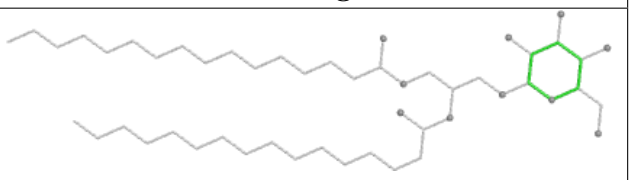
Bond lengths



Bond angles

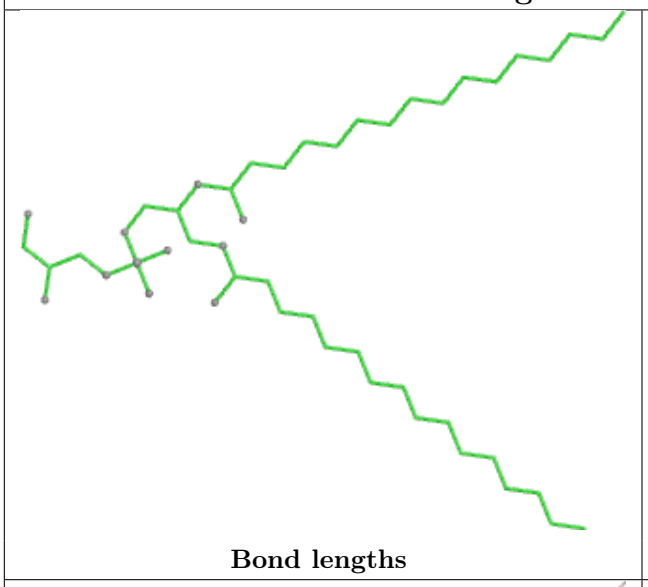


Torsions

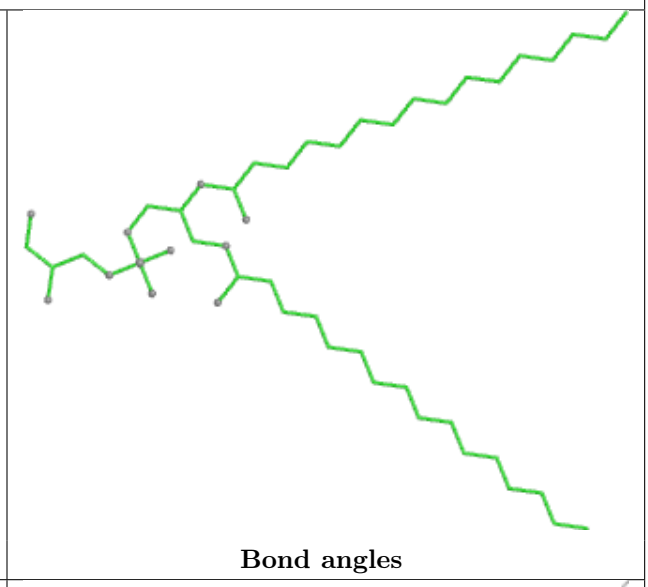


Rings

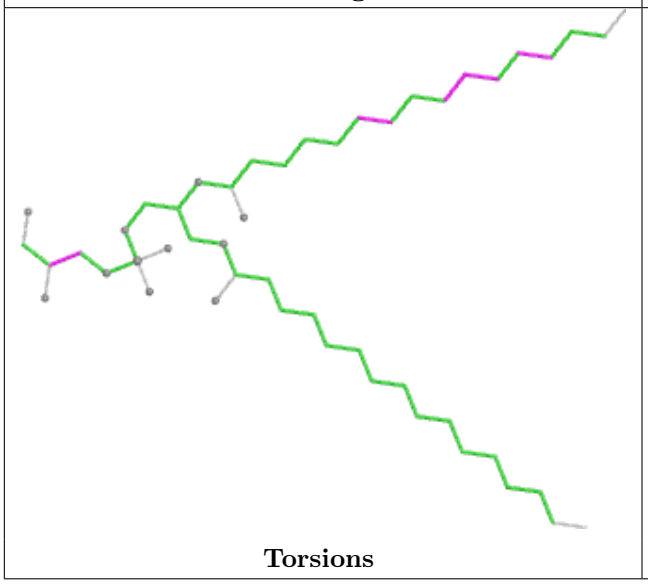
Ligand LHG 4B 626



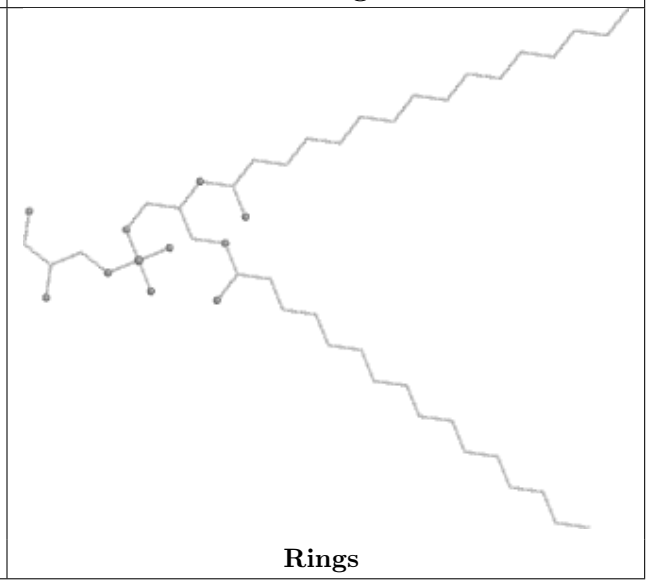
Bond lengths



Bond angles

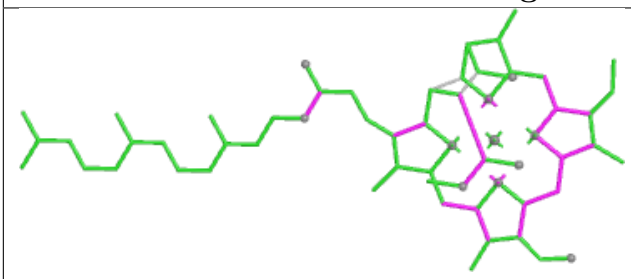


Torsions

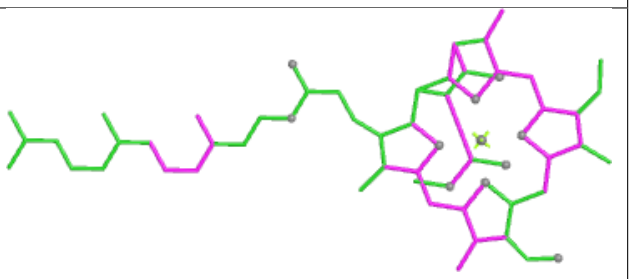


Rings

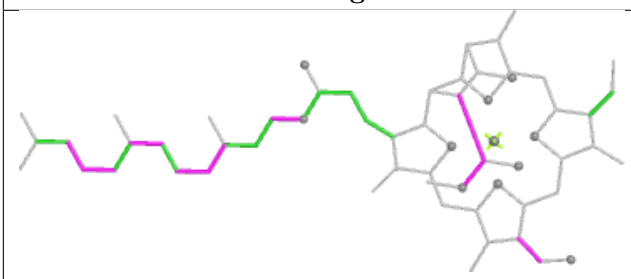
Ligand CL7 4C 502



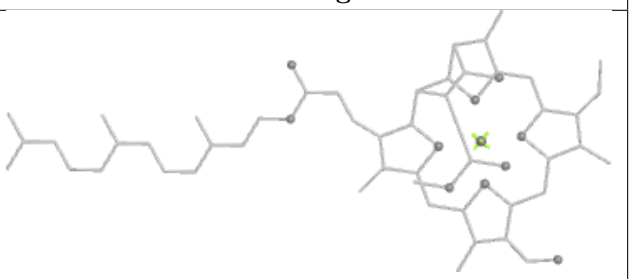
Bond lengths



Bond angles

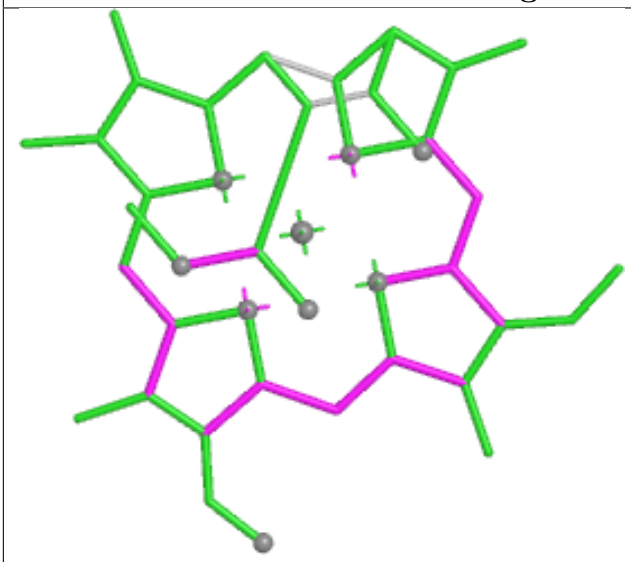


Torsions

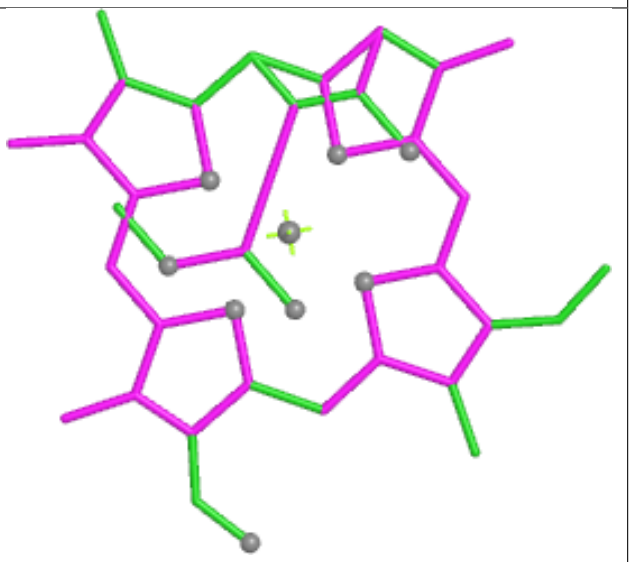


Rings

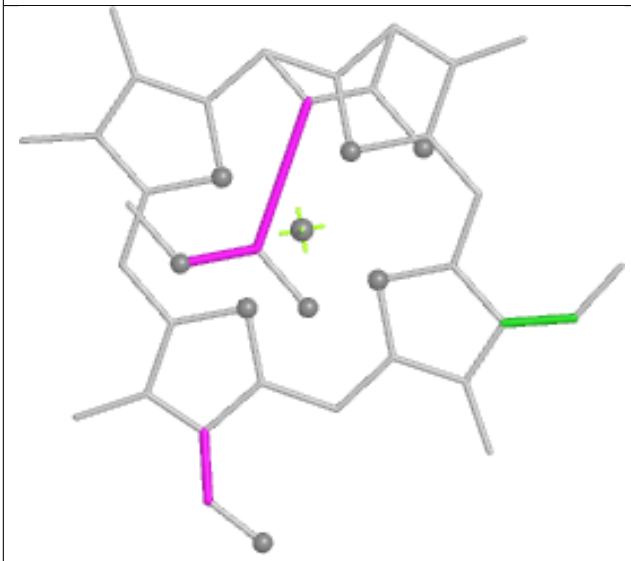
Ligand CL7 4C 517



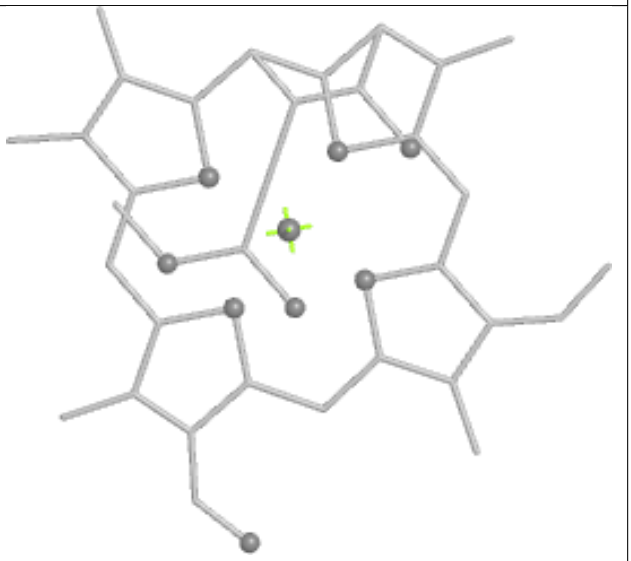
Bond lengths



Bond angles

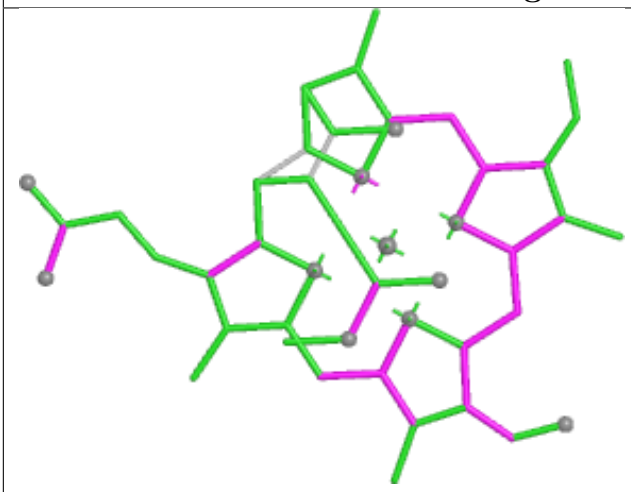


Torsions

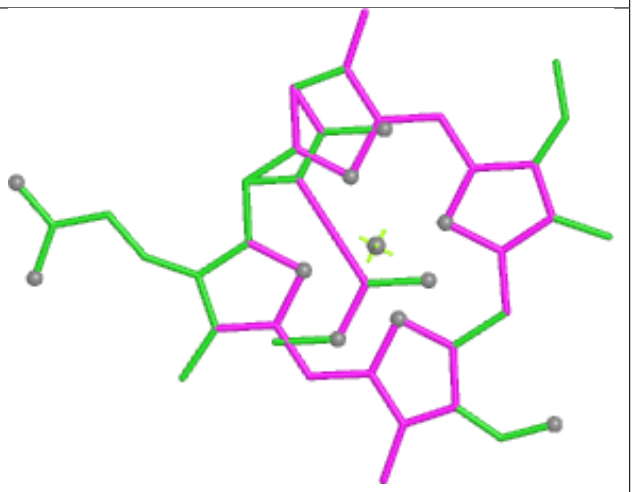


Rings

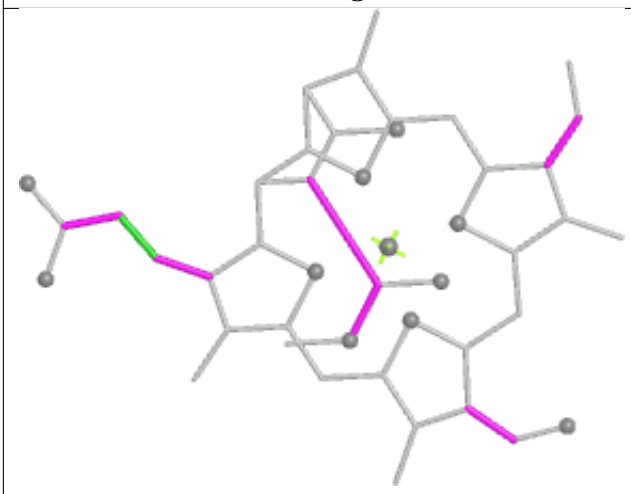
Ligand CL7 43 407



Bond lengths



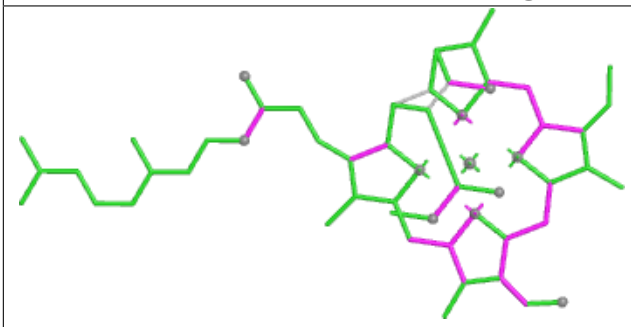
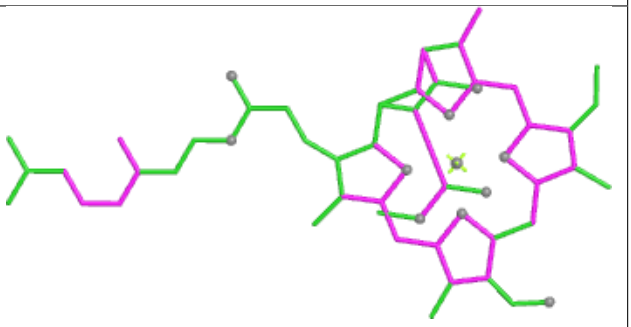
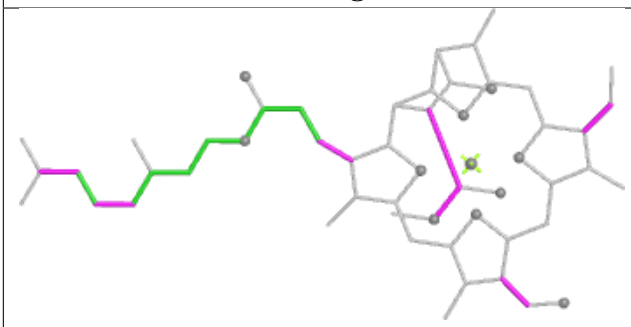
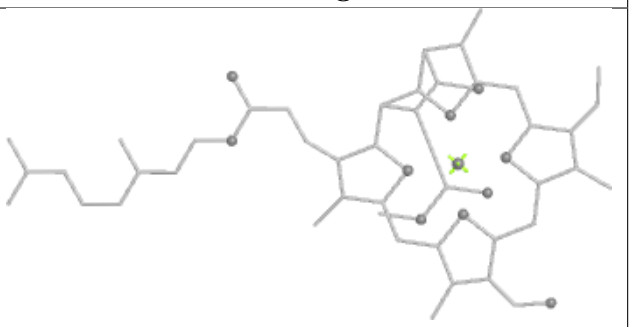
Bond angles

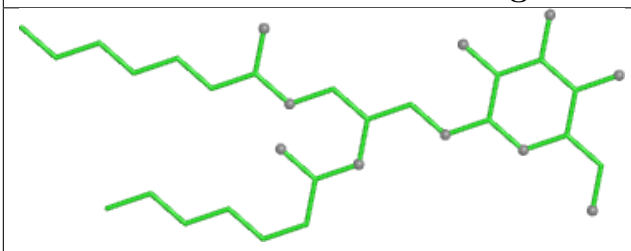
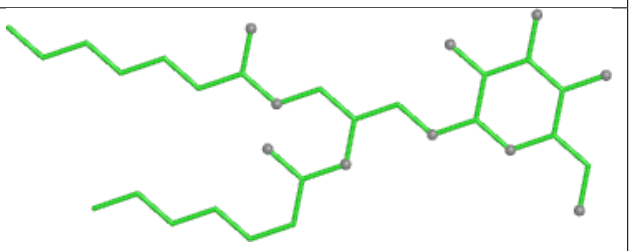
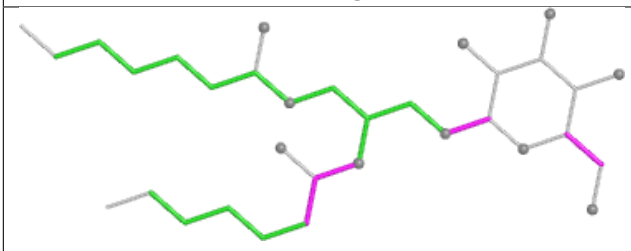
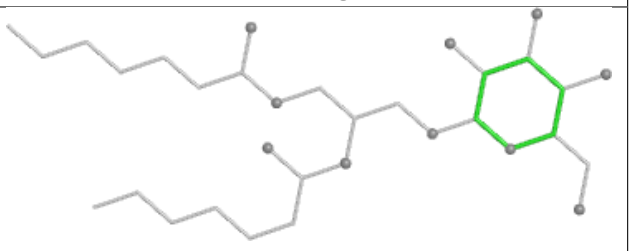


Torsions

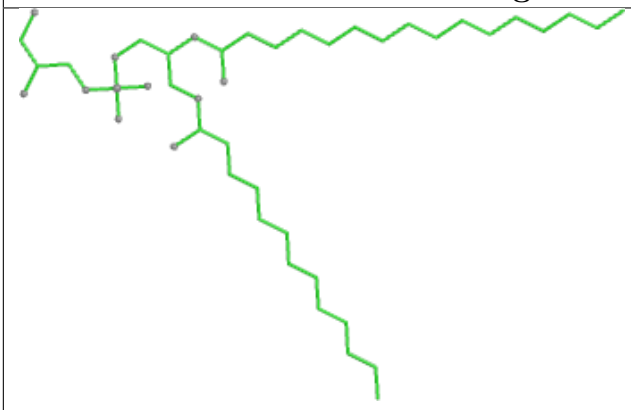


Rings

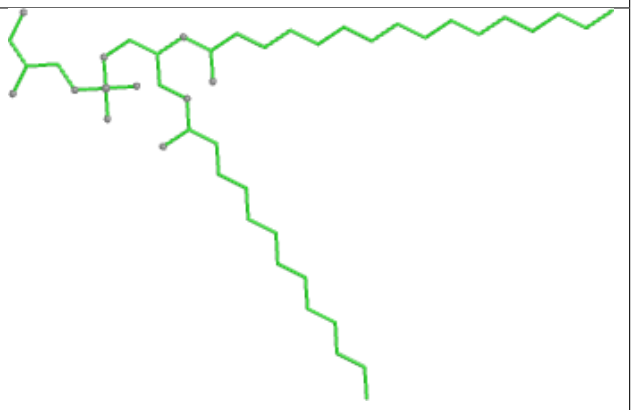
Ligand CL7 1C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG 3D 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

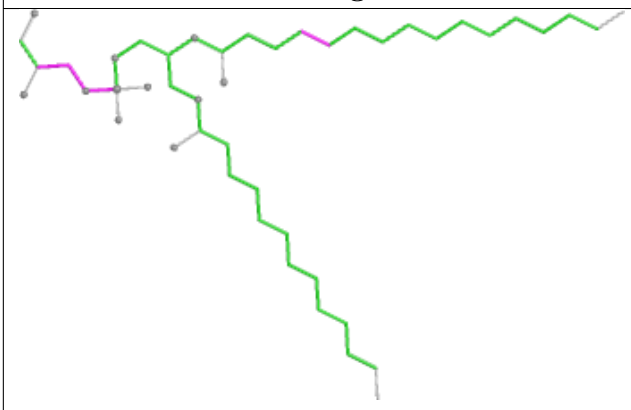
Ligand LHG 3A 408



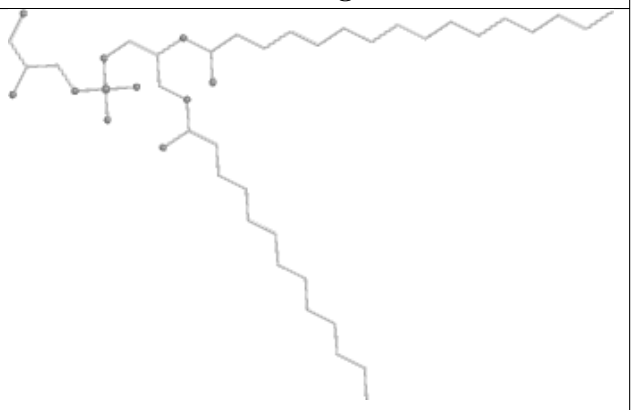
Bond lengths



Bond angles

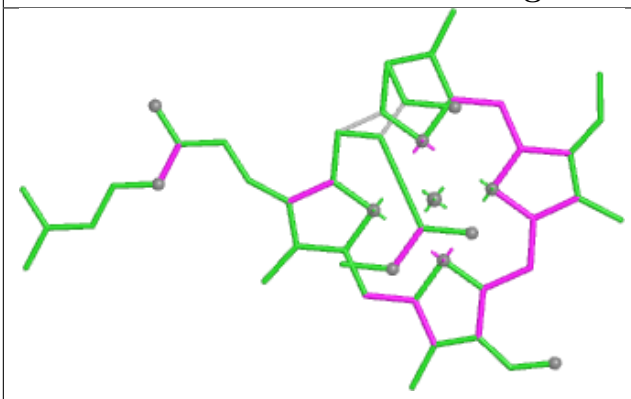


Torsions

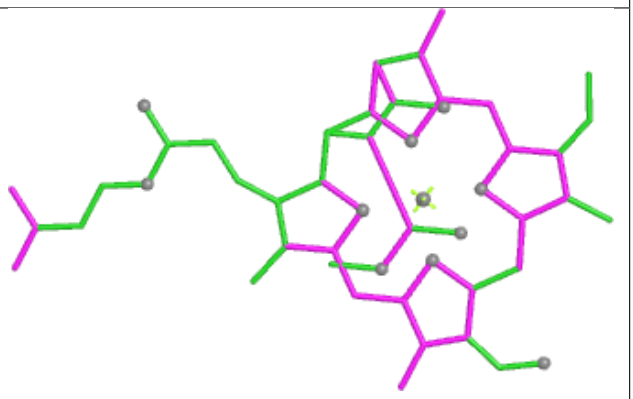


Rings

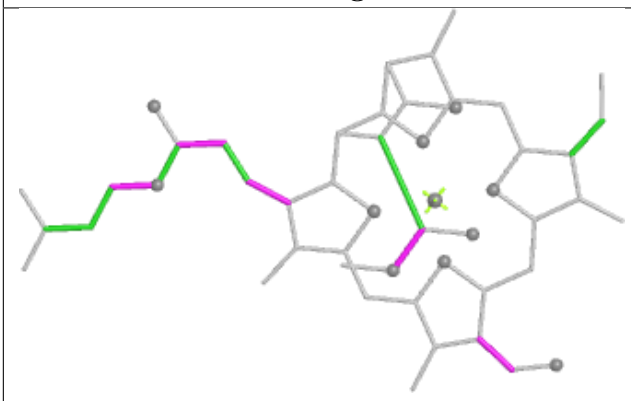
Ligand CL7 23 418



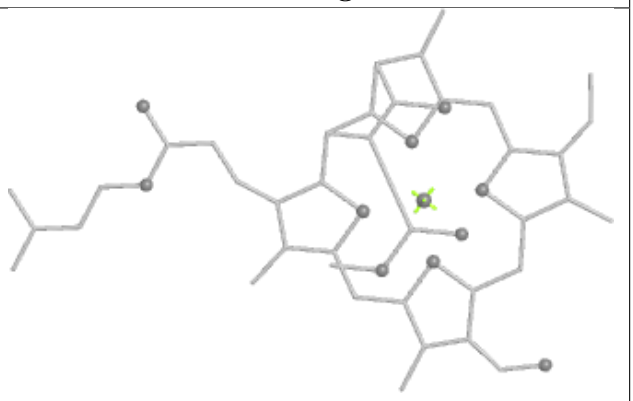
Bond lengths



Bond angles

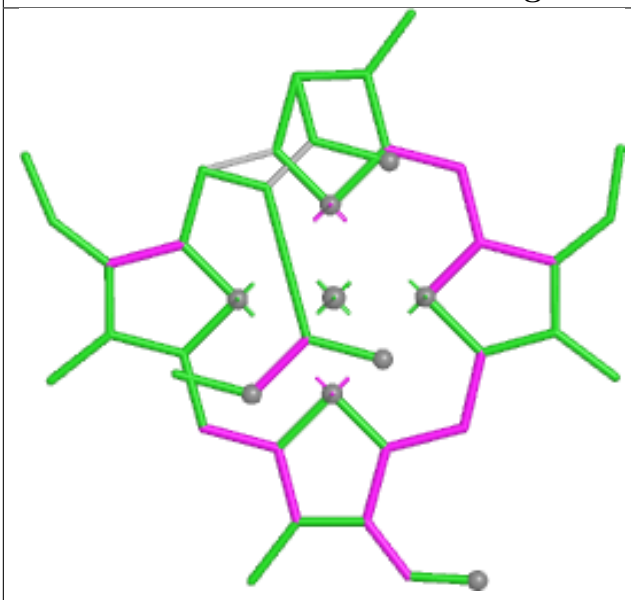


Torsions

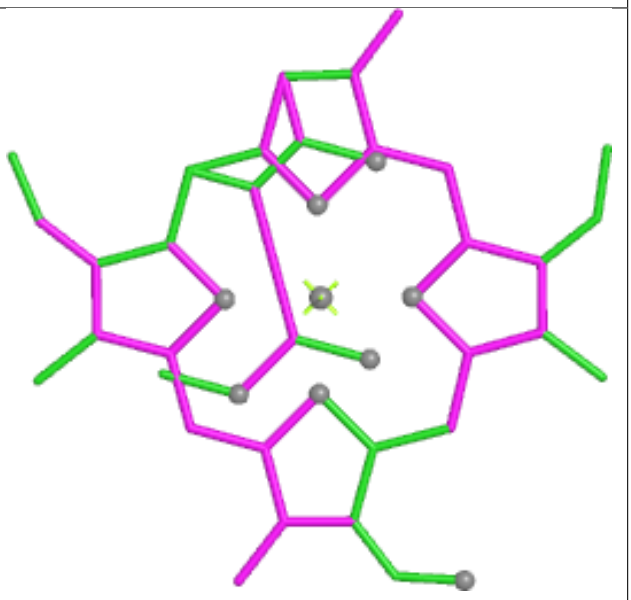


Rings

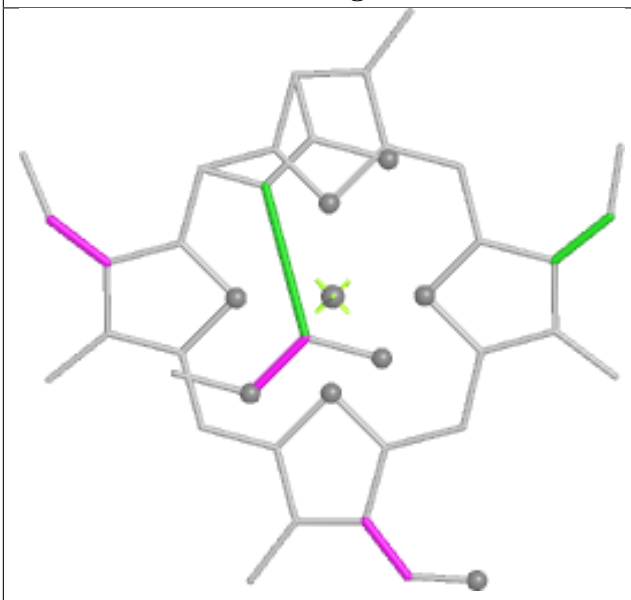
Ligand CL7 44 417



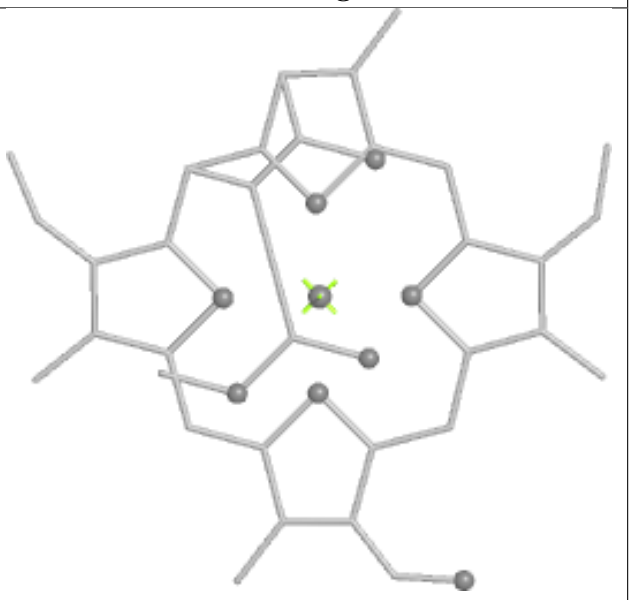
Bond lengths



Bond angles

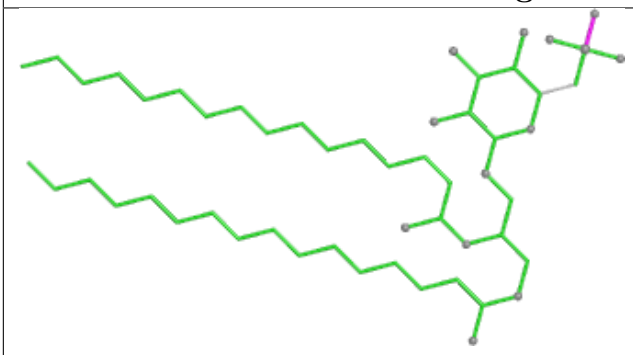


Torsions

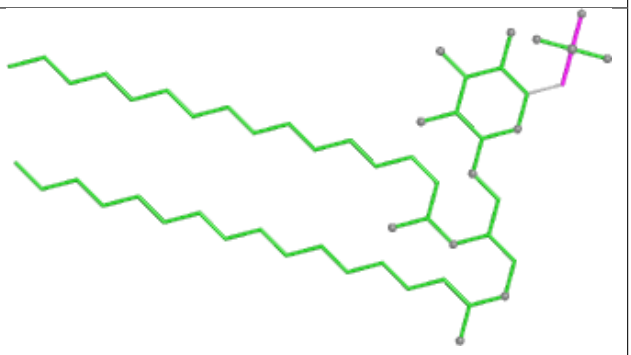


Rings

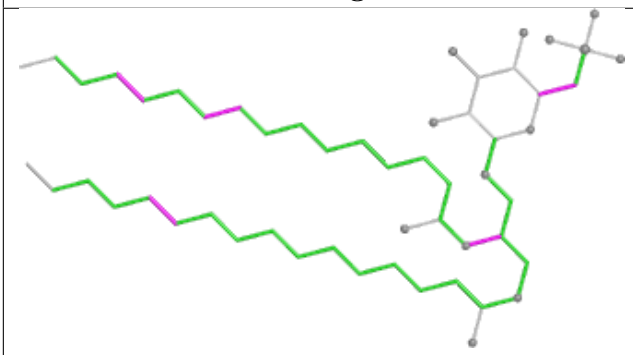
Ligand SQD 3B 620



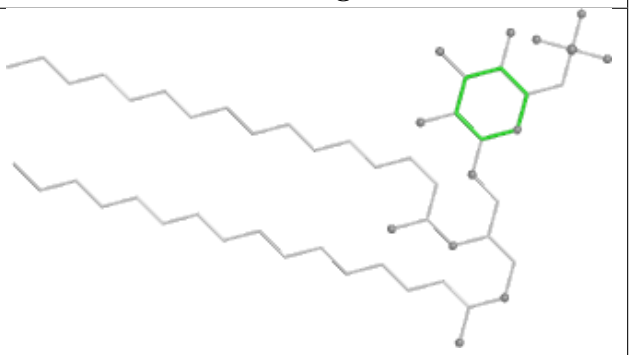
Bond lengths



Bond angles

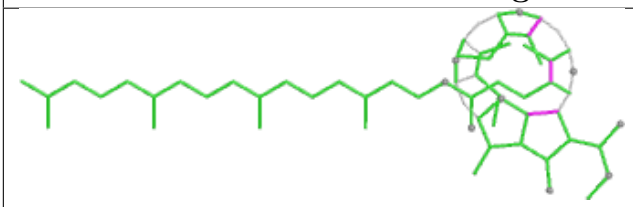


Torsions

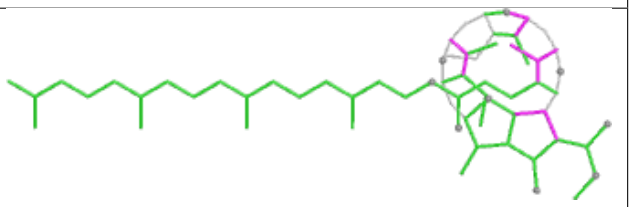


Rings

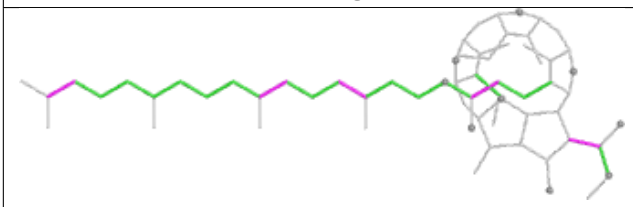
Ligand PHO 4D 408



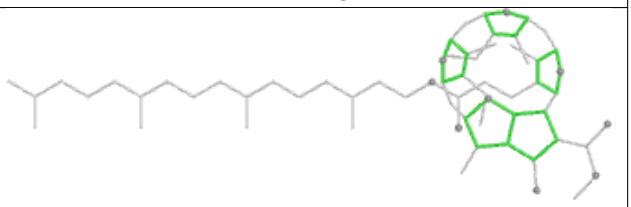
Bond lengths



Bond angles

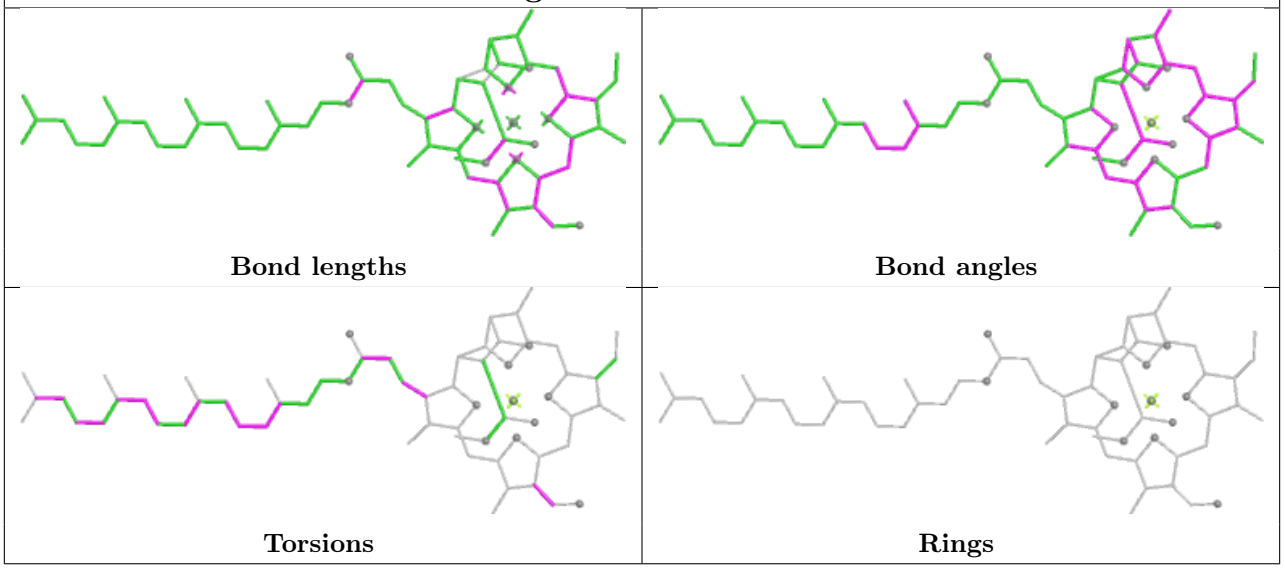


Torsions

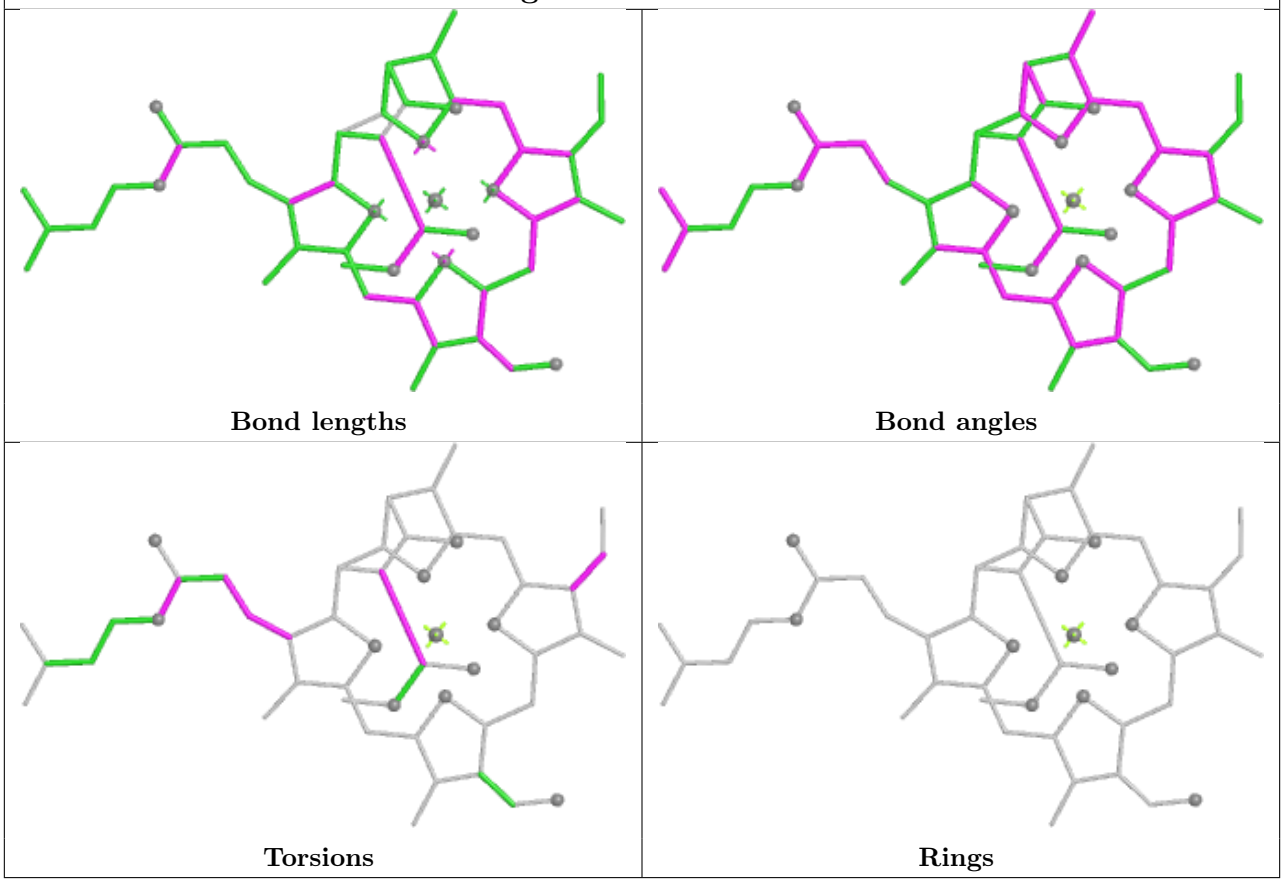


Rings

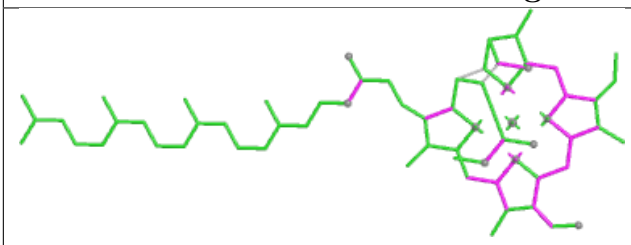
Ligand CL7 12 512



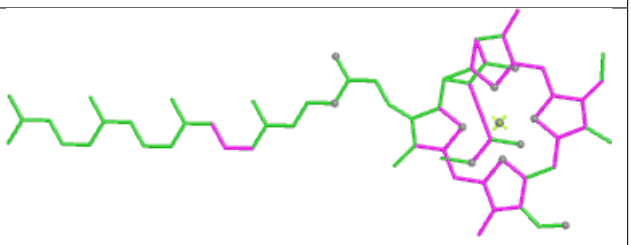
Ligand CL7 1B 615



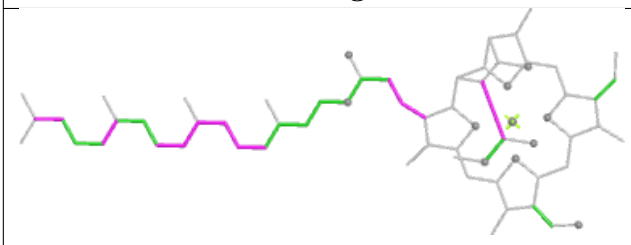
Ligand CL7 14 404



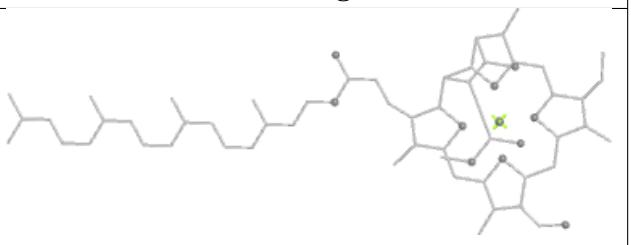
Bond lengths



Bond angles

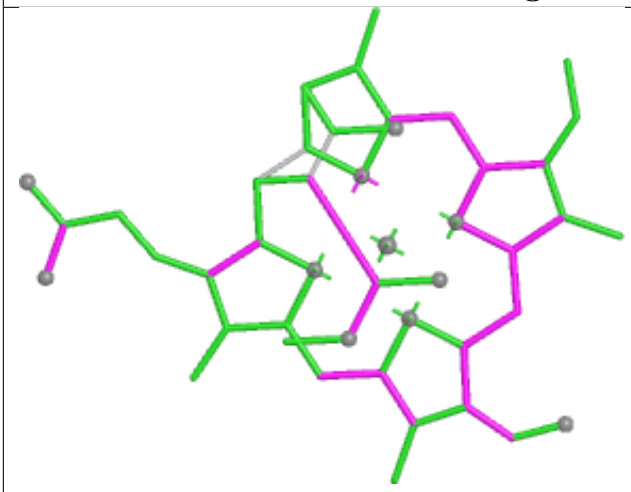


Torsions



Rings

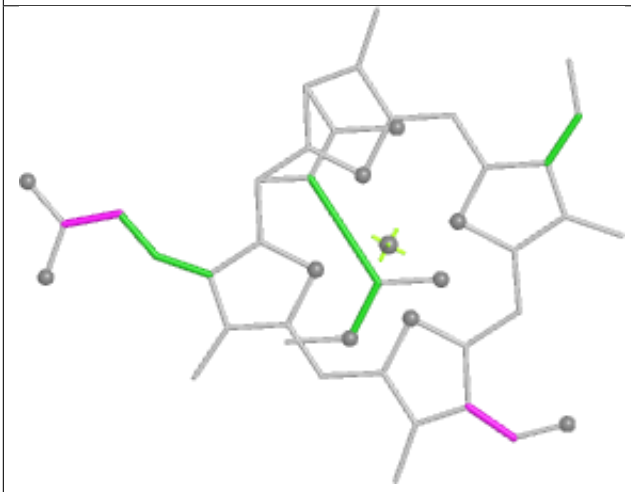
Ligand CL7 34 408



Bond lengths



Bond angles

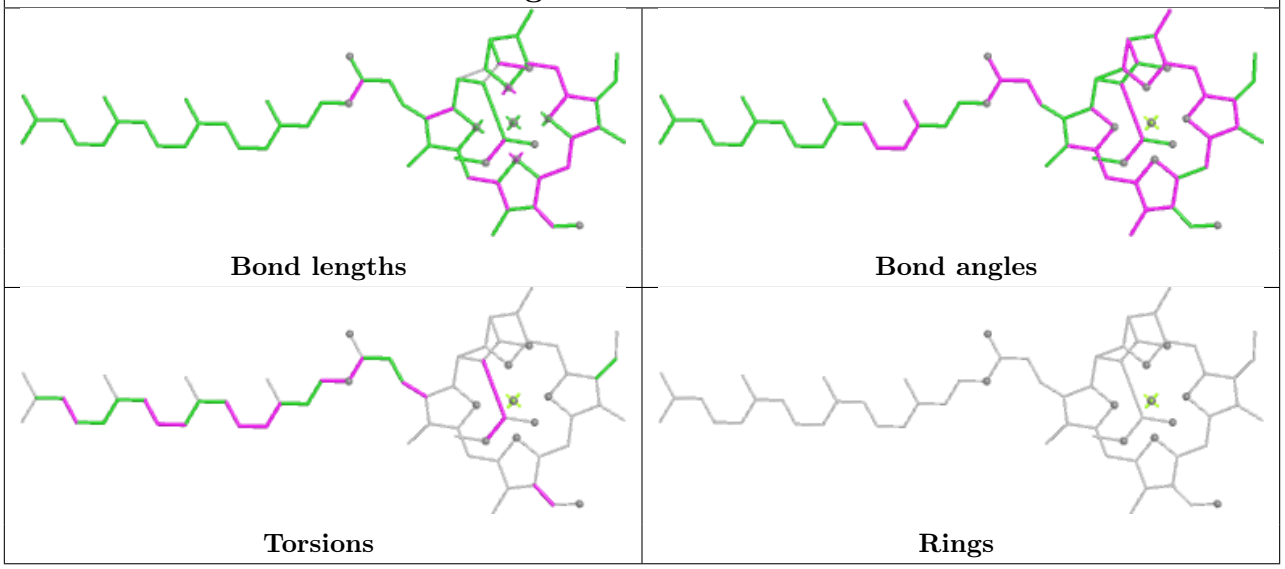


Torsions

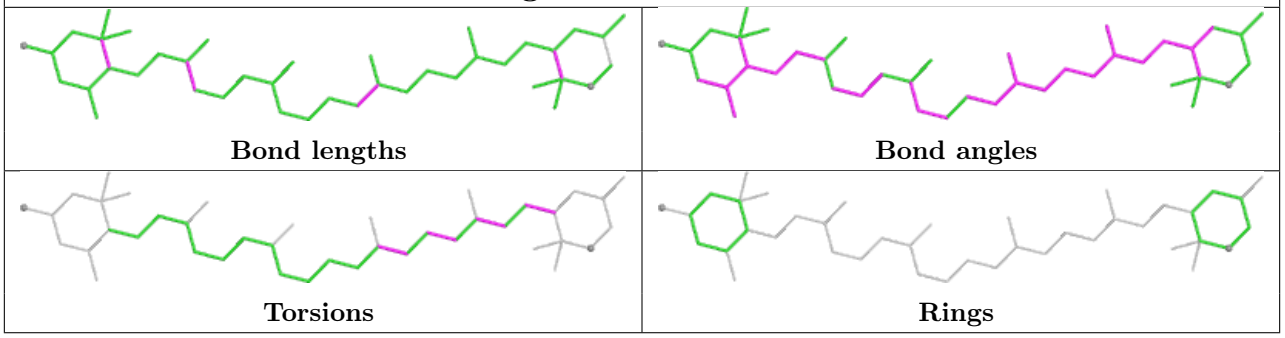


Rings

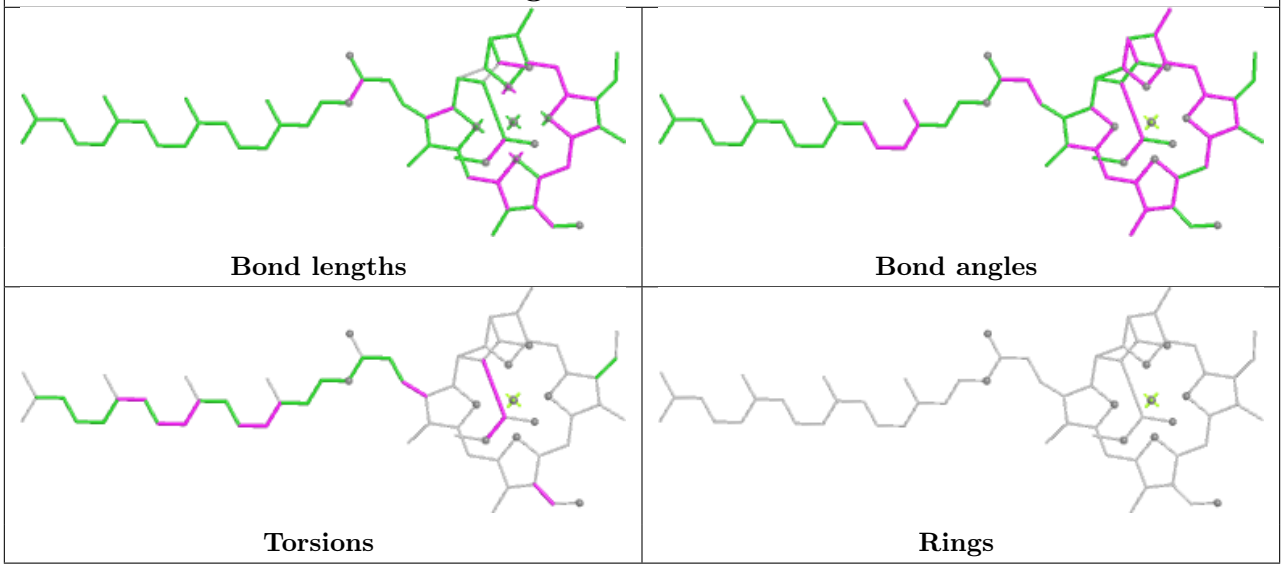
Ligand CL7 41 410



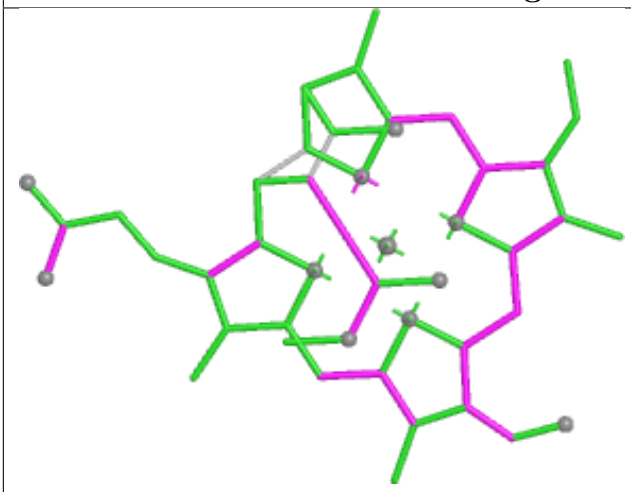
Ligand ZEX 12 522



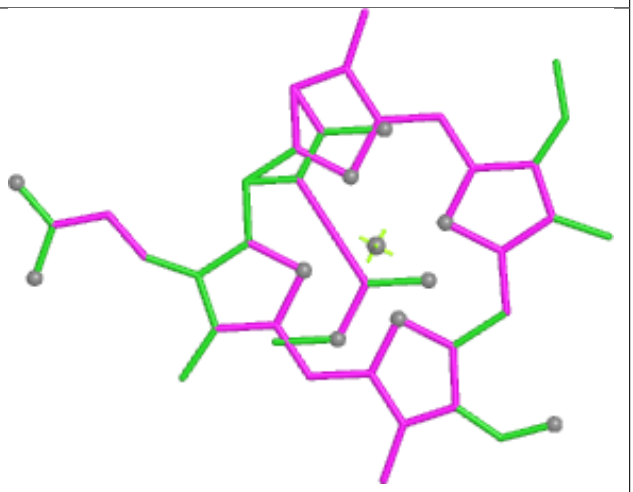
Ligand CL7 42 506



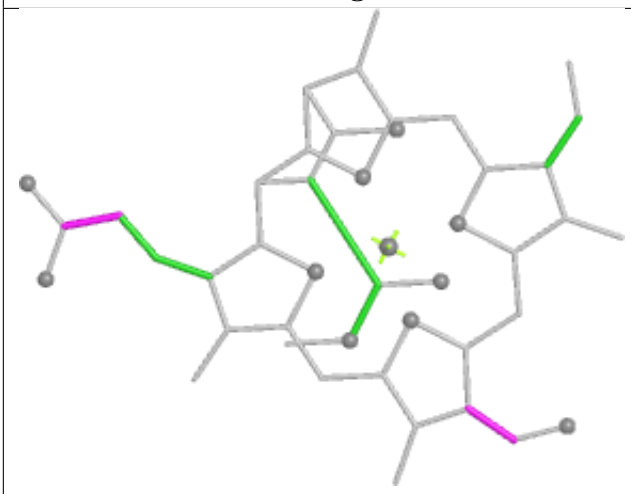
Ligand CL7 24 408



Bond lengths



Bond angles

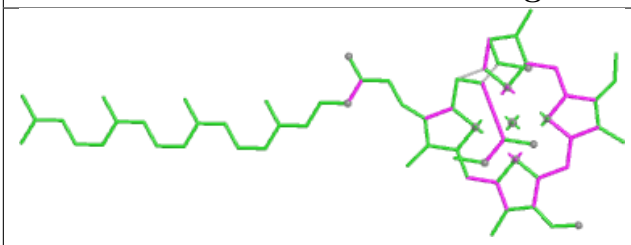


Torsions

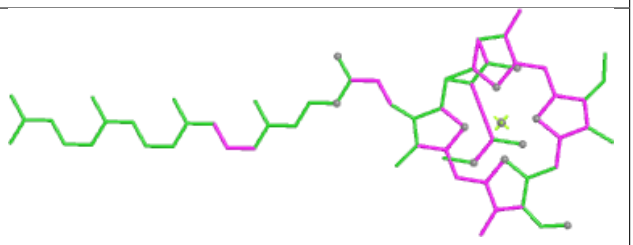


Rings

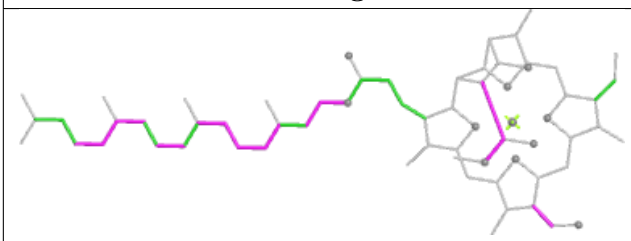
Ligand CL7 42 509



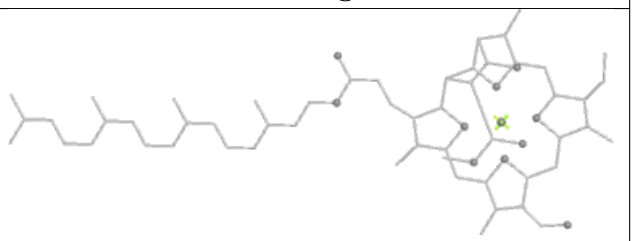
Bond lengths



Bond angles

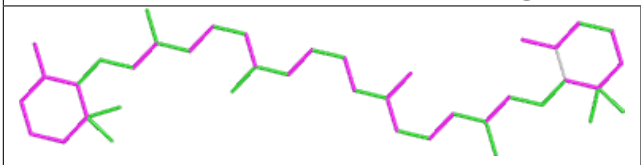


Torsions

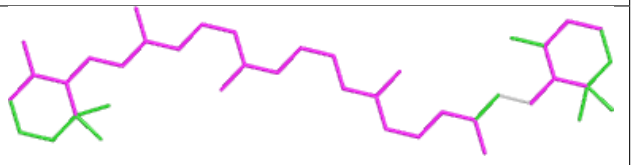


Rings

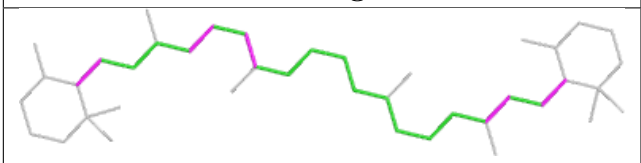
Ligand 8CT 3C 518



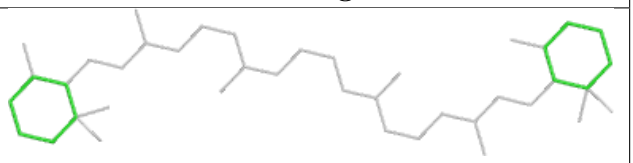
Bond lengths



Bond angles

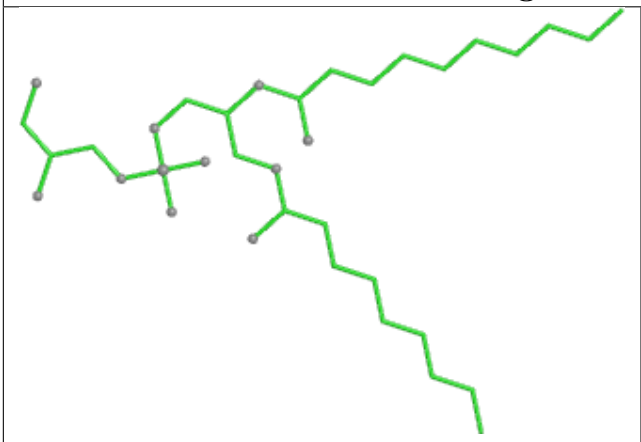


Torsions

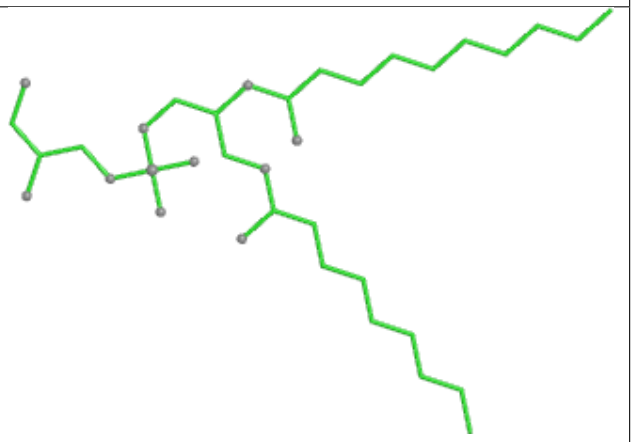


Rings

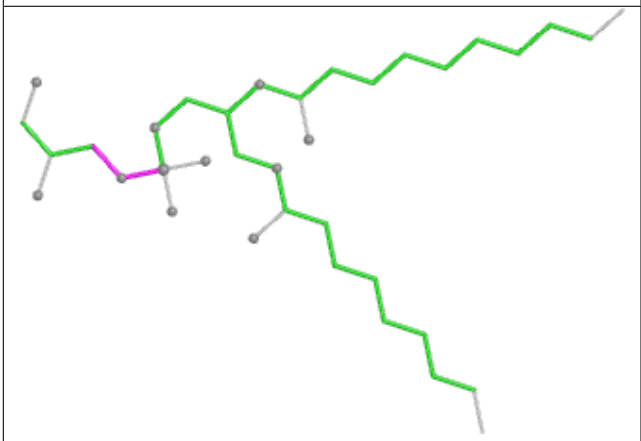
Ligand LHG 23 425



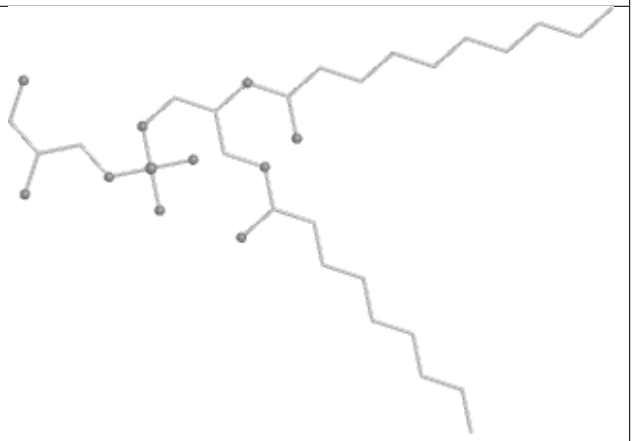
Bond lengths



Bond angles

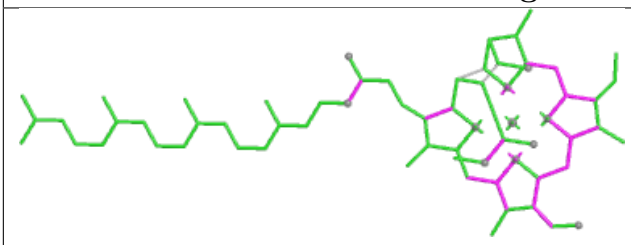


Torsions

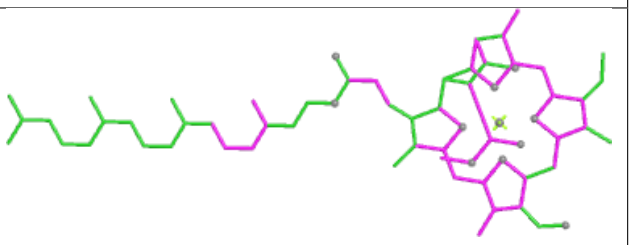


Rings

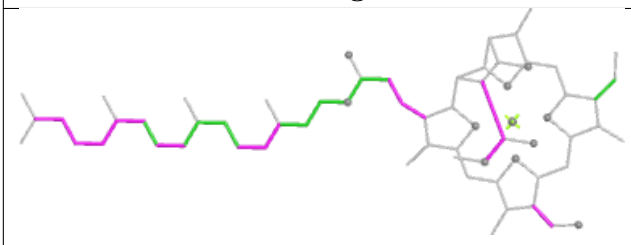
Ligand CL7 2B 605



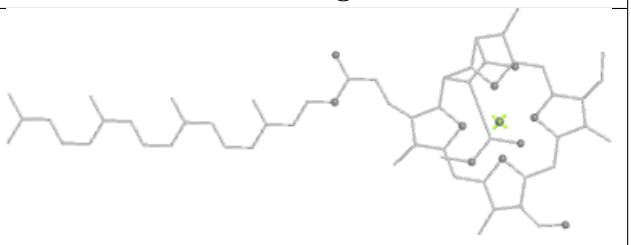
Bond lengths



Bond angles

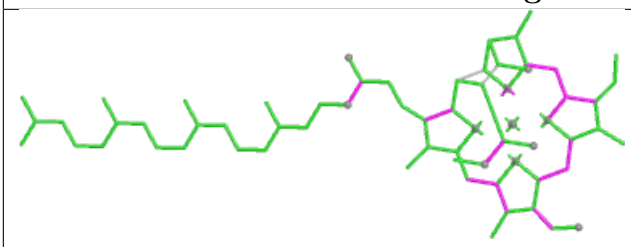


Torsions

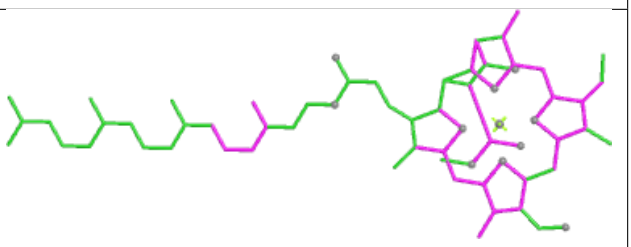


Rings

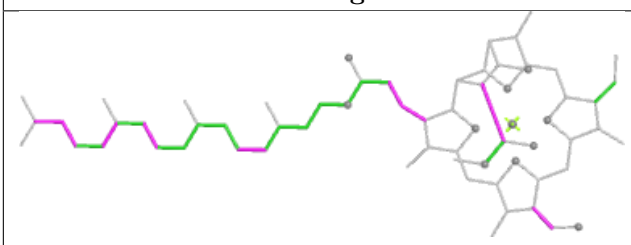
Ligand CL7 42 518



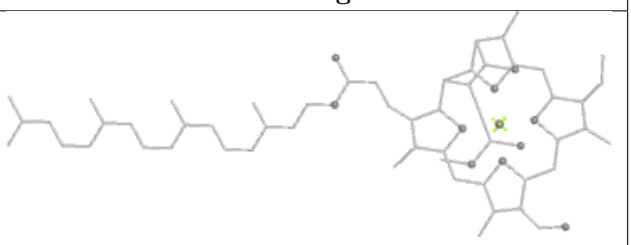
Bond lengths



Bond angles

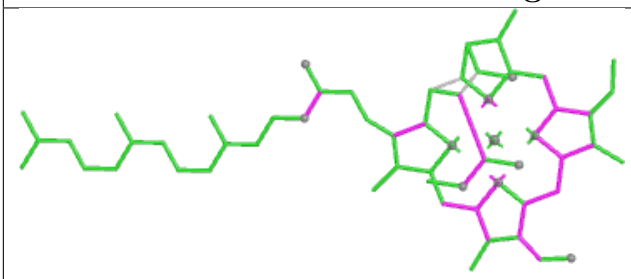


Torsions

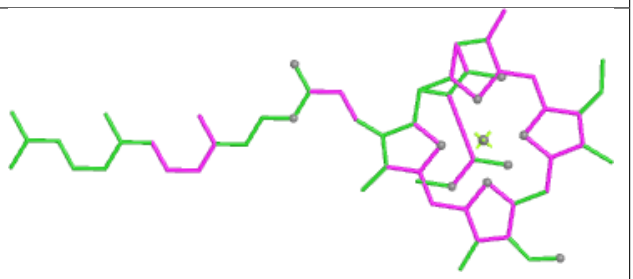


Rings

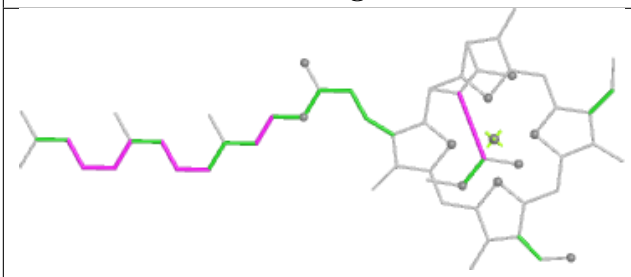
Ligand CL7 34 413



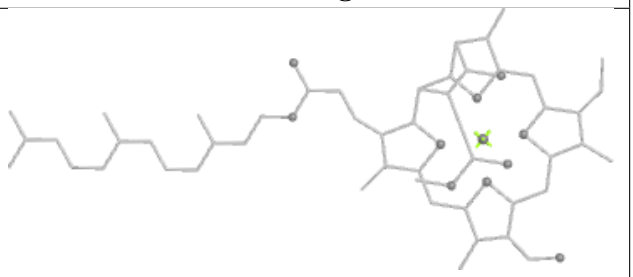
Bond lengths



Bond angles

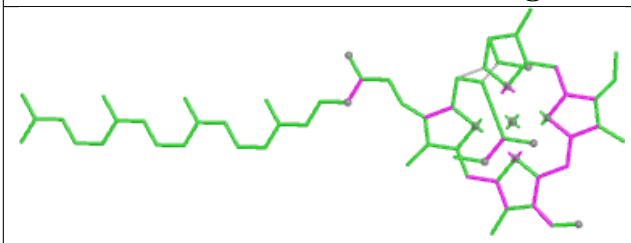


Torsions

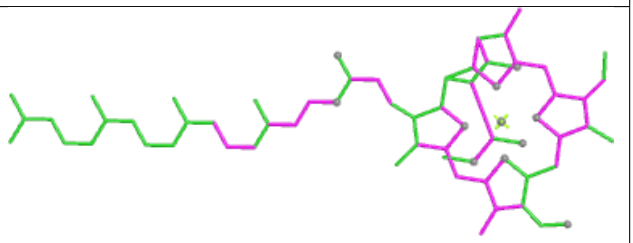


Rings

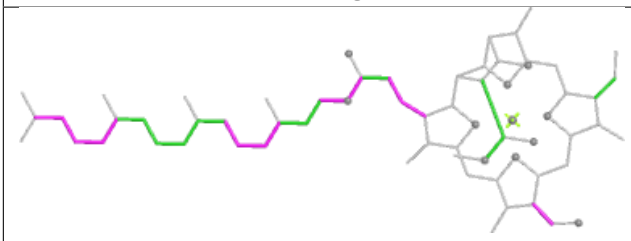
Ligand CL7 42 516



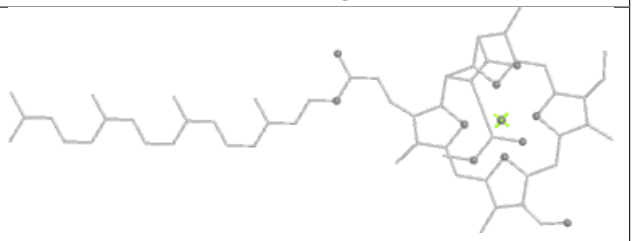
Bond lengths



Bond angles

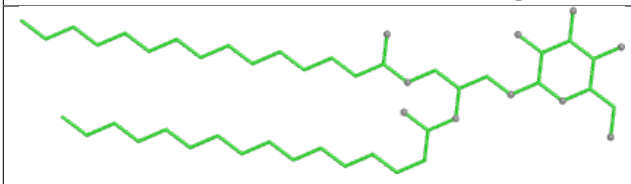


Torsions

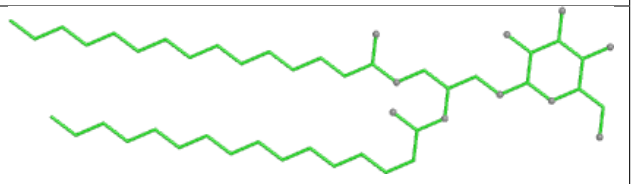


Rings

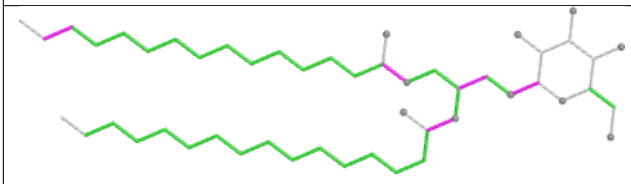
Ligand LMG 3A 405



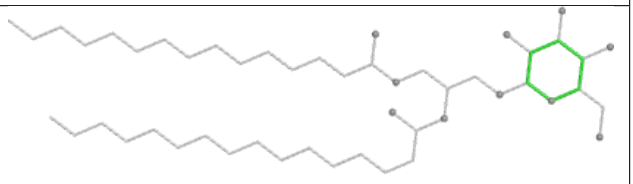
Bond lengths



Bond angles

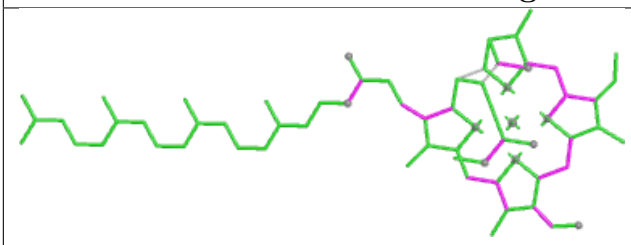


Torsions

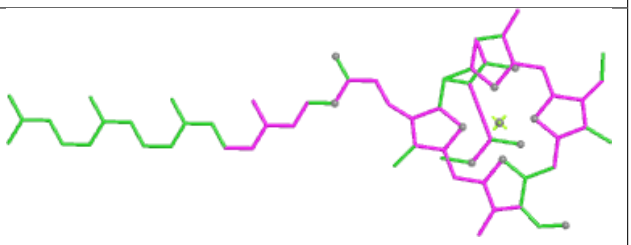


Rings

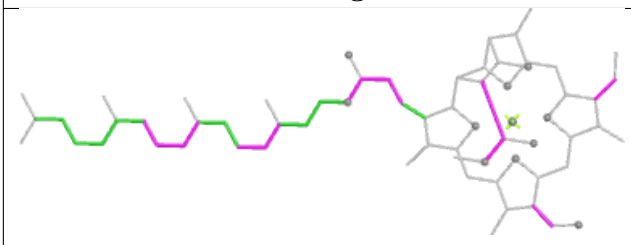
Ligand CL7 3A 401



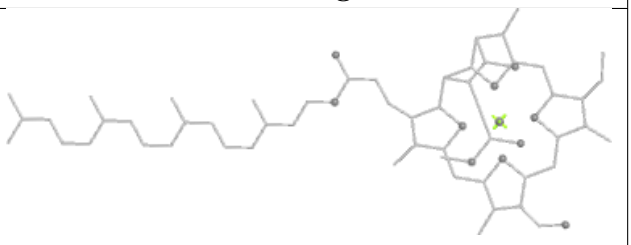
Bond lengths



Bond angles

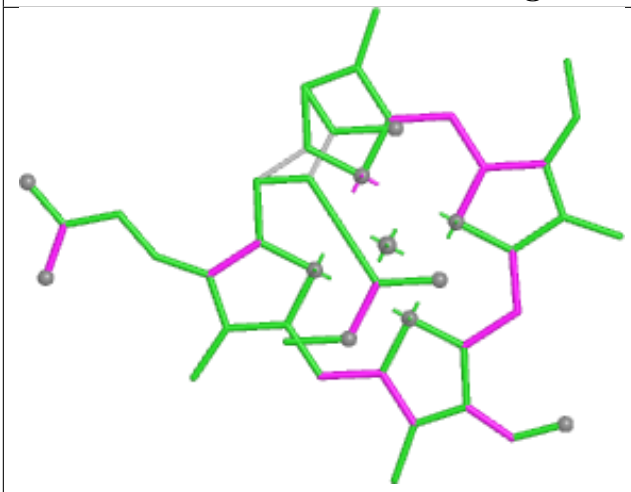


Torsions



Rings

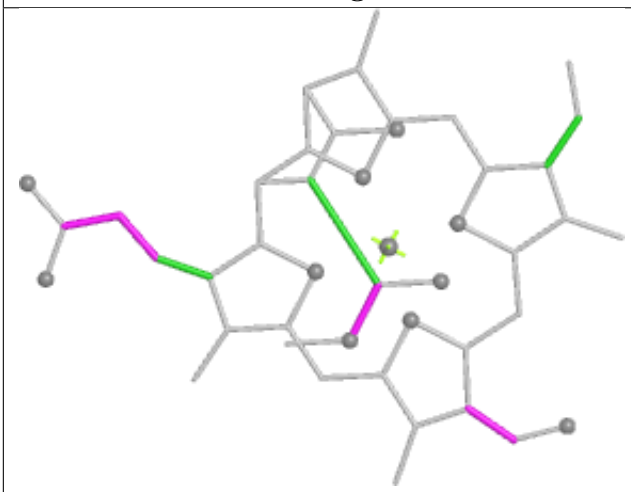
Ligand CL7 33 518



Bond lengths



Bond angles

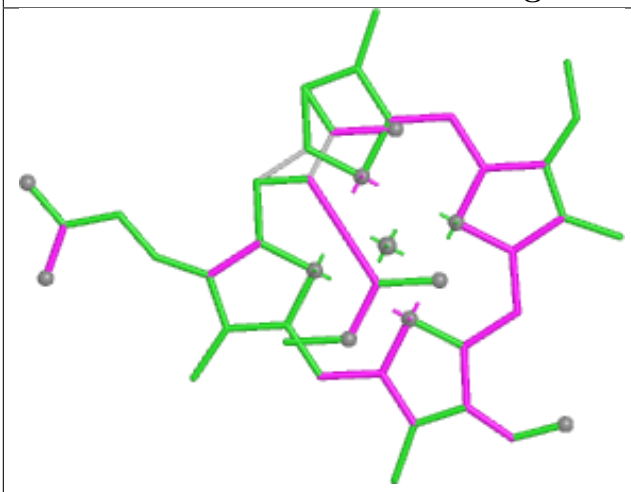


Torsions

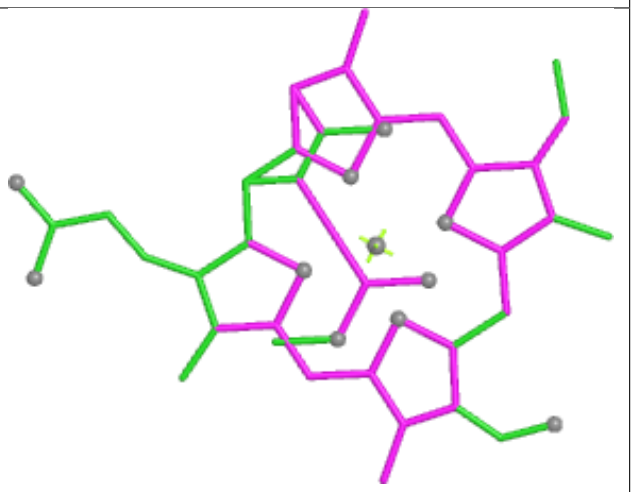


Rings

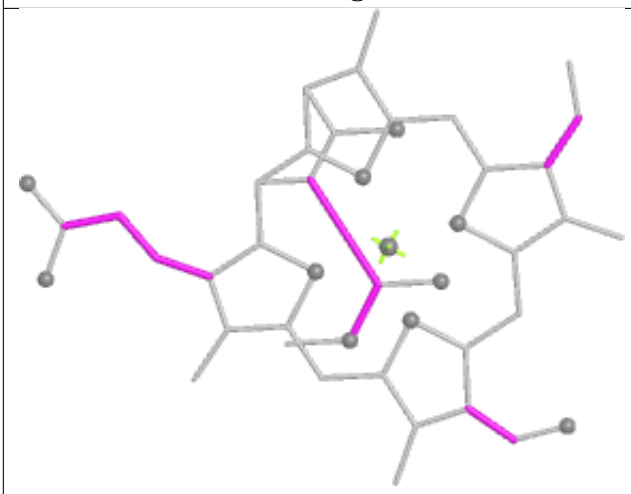
Ligand CL7 44 415



Bond lengths



Bond angles

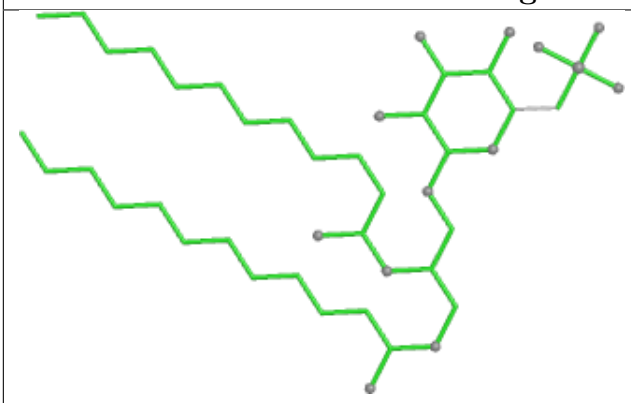


Torsions

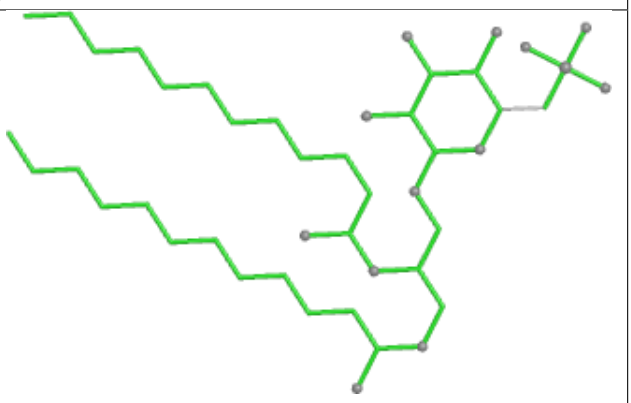


Rings

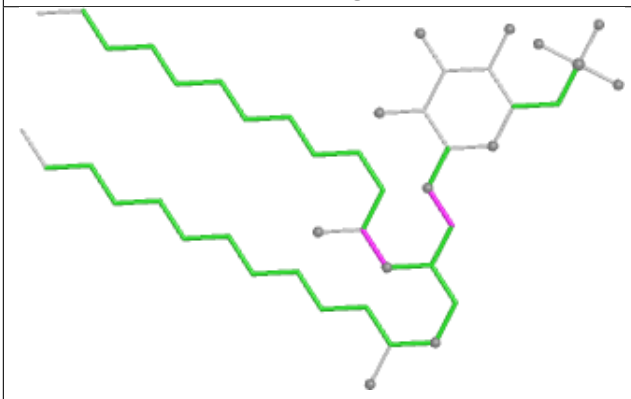
Ligand SQD 43 422



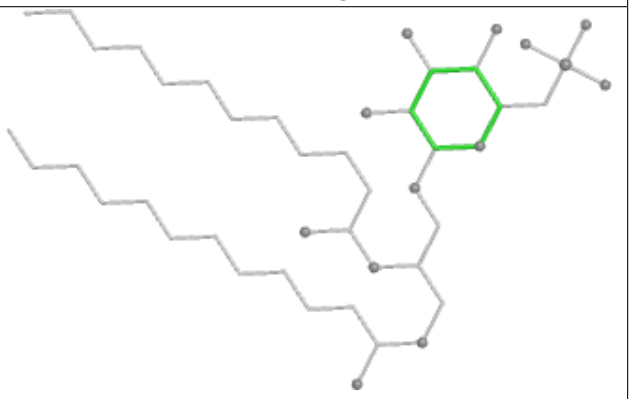
Bond lengths



Bond angles

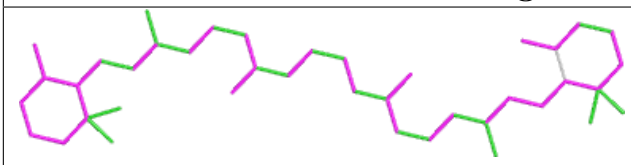


Torsions

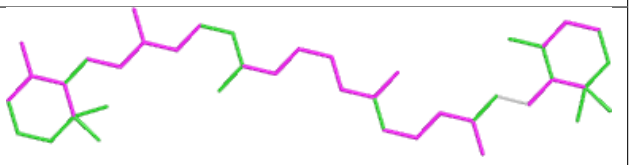


Rings

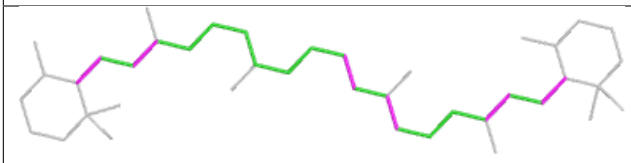
Ligand 8CT 2K 101



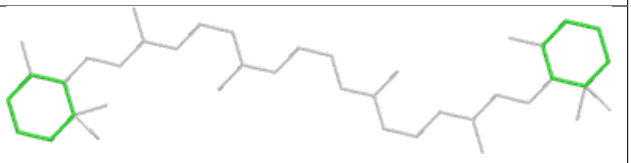
Bond lengths



Bond angles

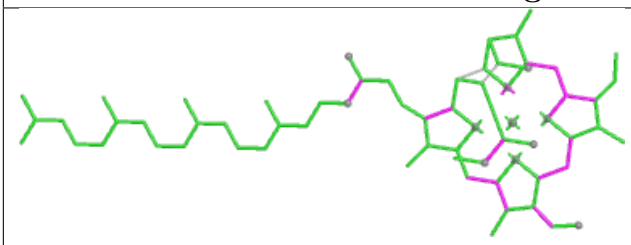


Torsions

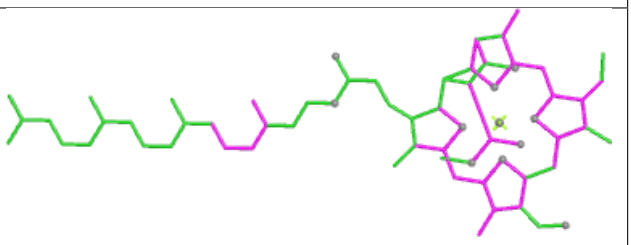


Rings

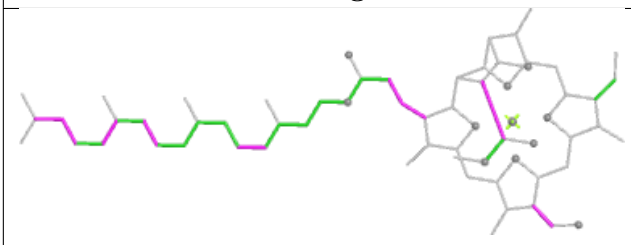
Ligand CL7 12 518



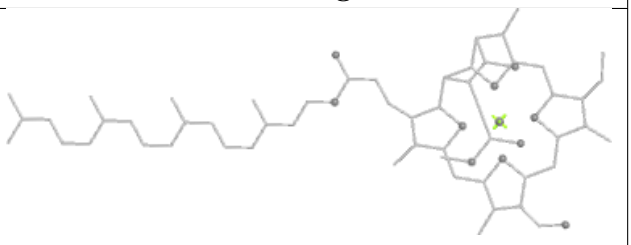
Bond lengths



Bond angles

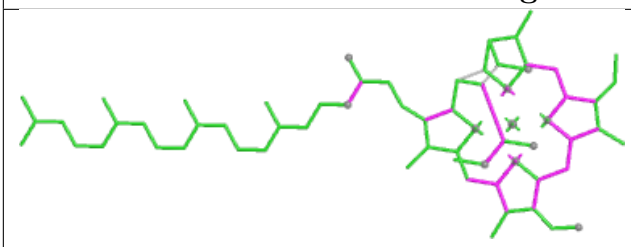


Torsions

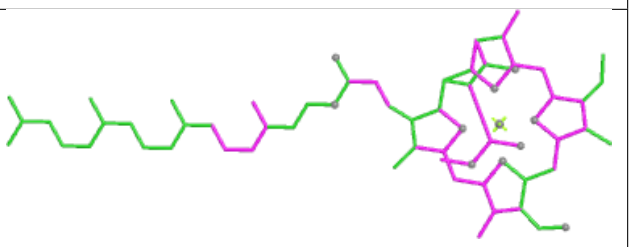


Rings

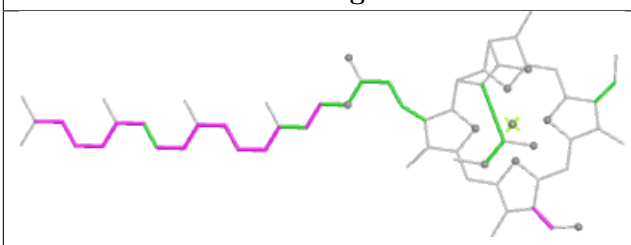
Ligand CL7 3C 507



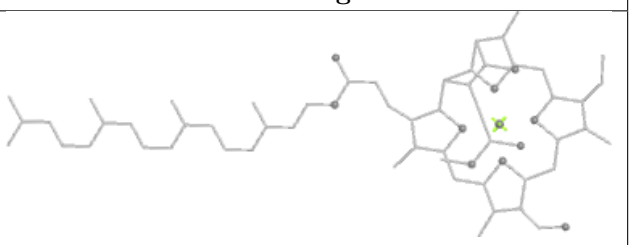
Bond lengths



Bond angles

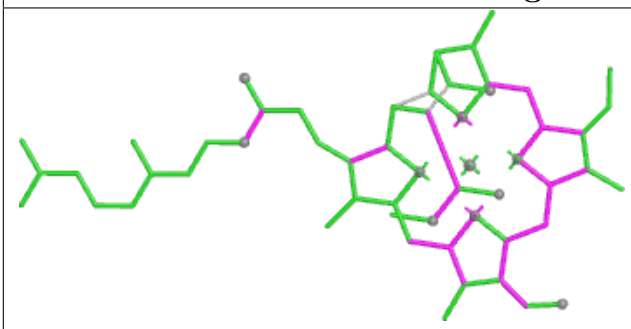


Torsions

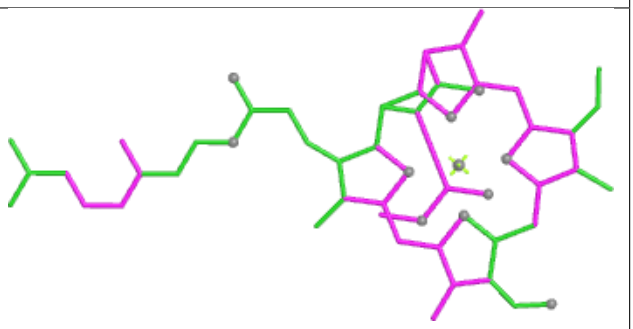


Rings

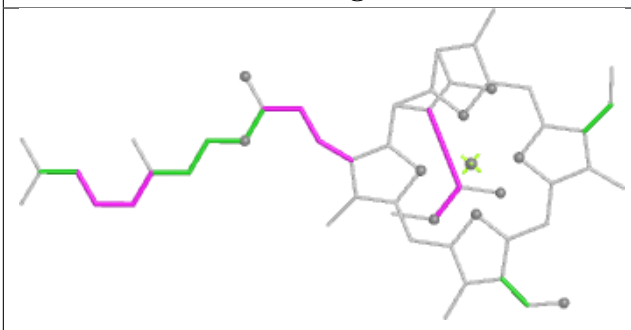
Ligand CL7 13 512



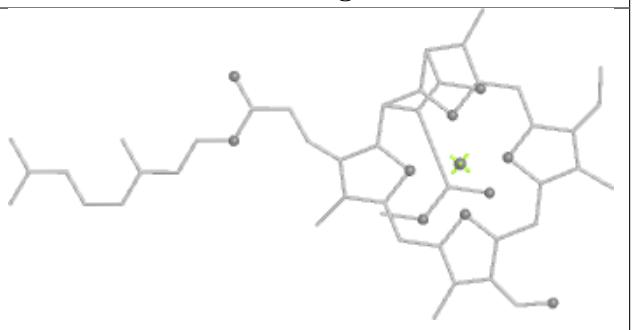
Bond lengths



Bond angles

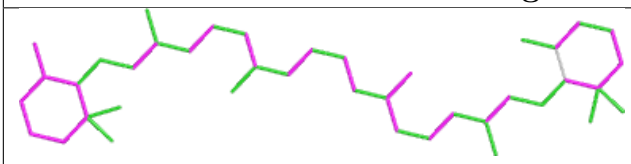


Torsions

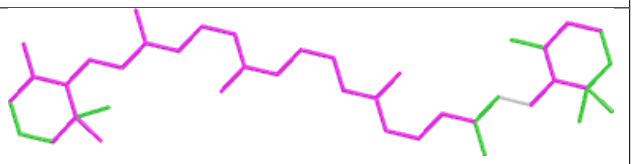


Rings

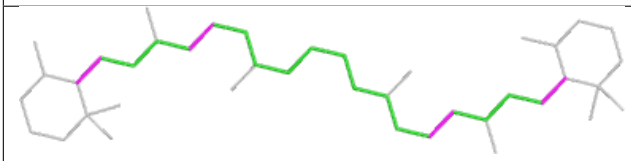
Ligand 8CT 44 402



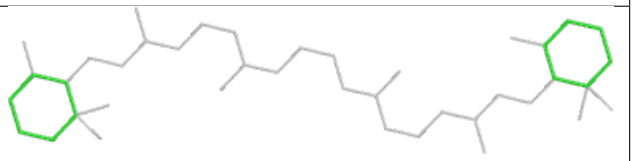
Bond lengths



Bond angles

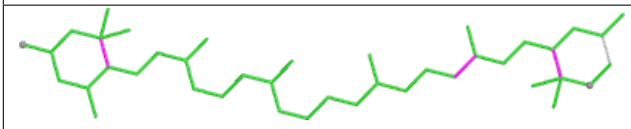


Torsions

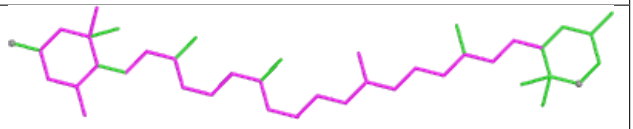


Rings

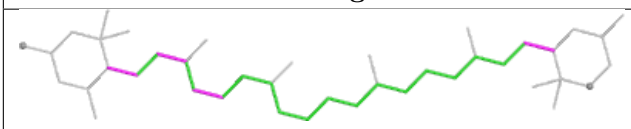
Ligand ZEX 22 520



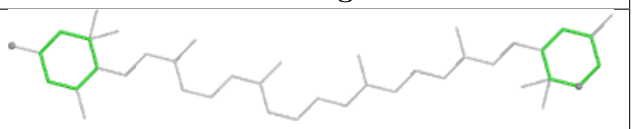
Bond lengths



Bond angles

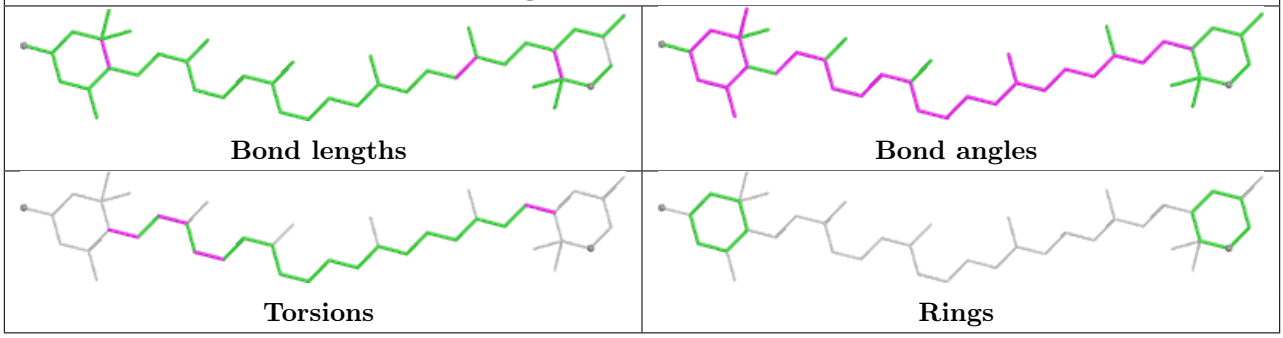


Torsions

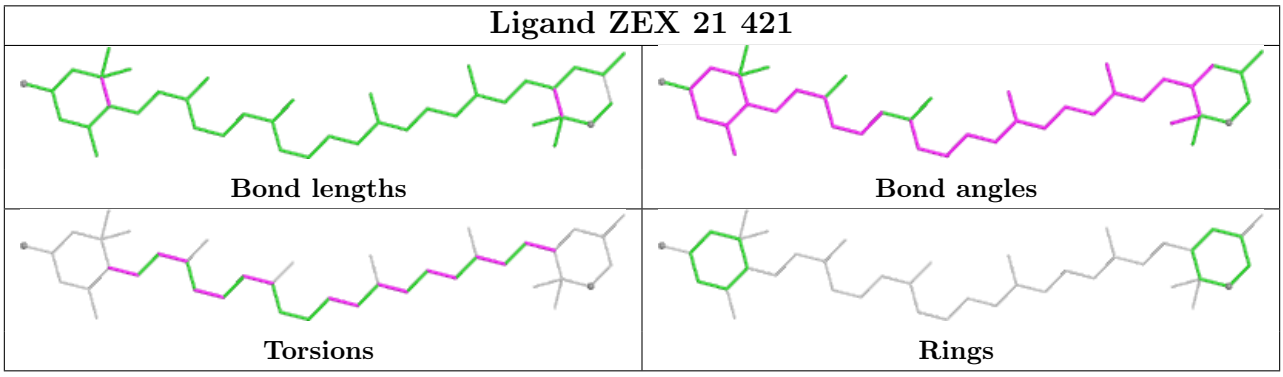


Rings

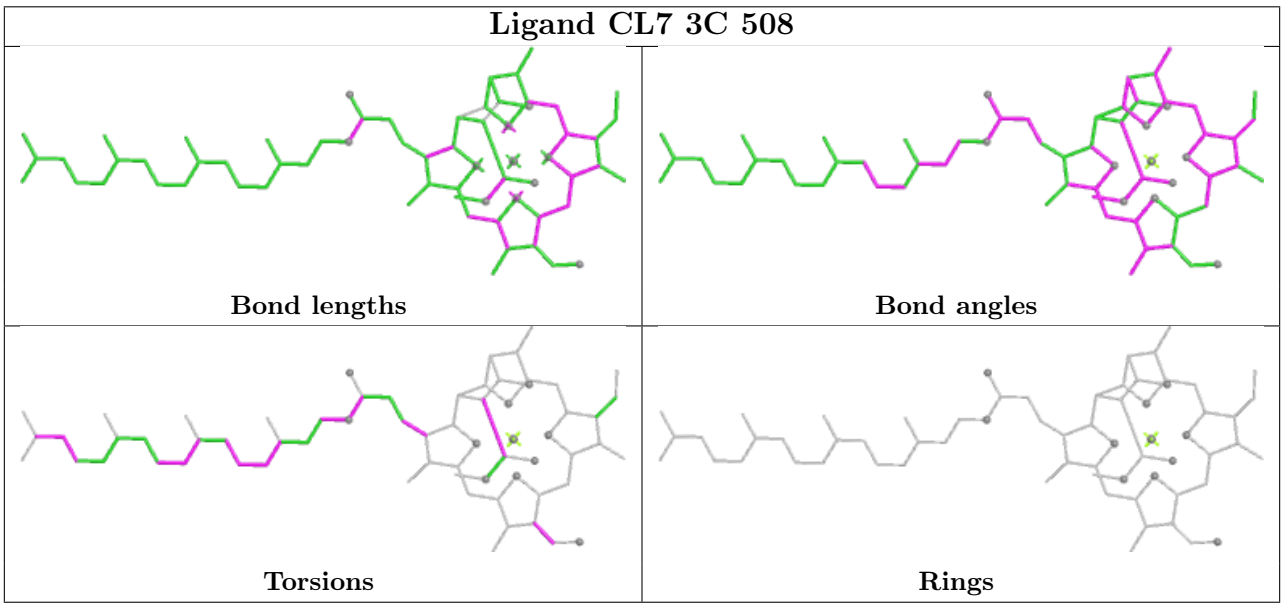
Ligand ZEX 32 520



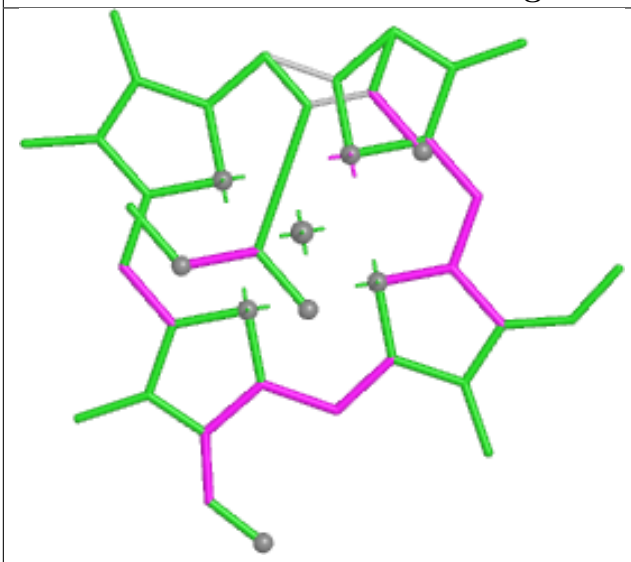
Ligand ZEX 21 421



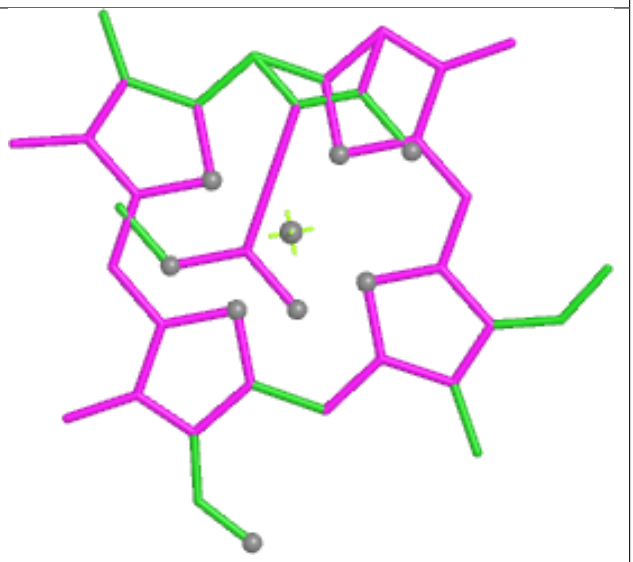
Ligand CL7 3C 508



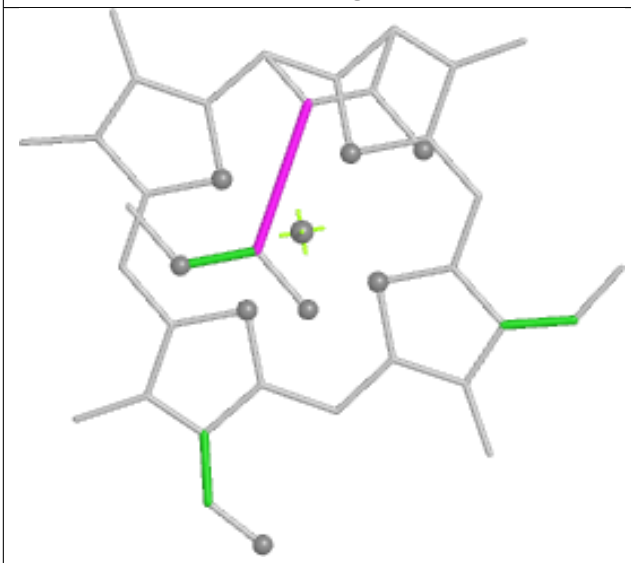
Ligand CL7 31 413



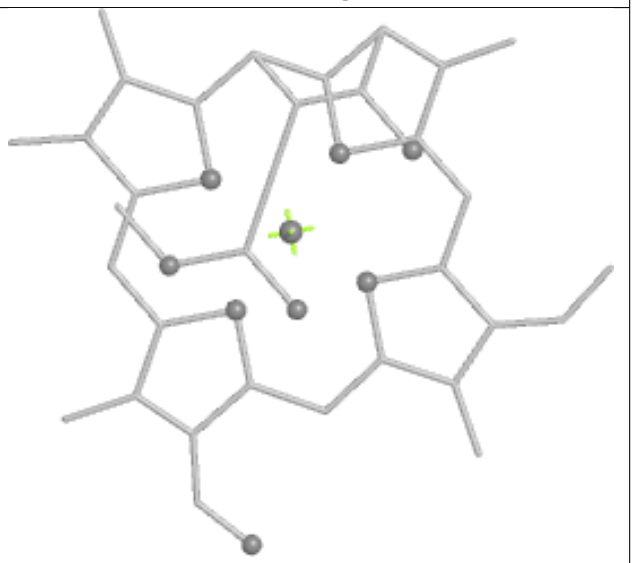
Bond lengths



Bond angles

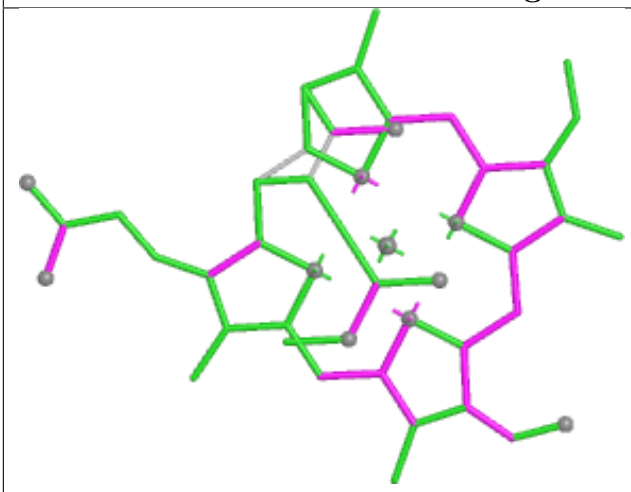


Torsions

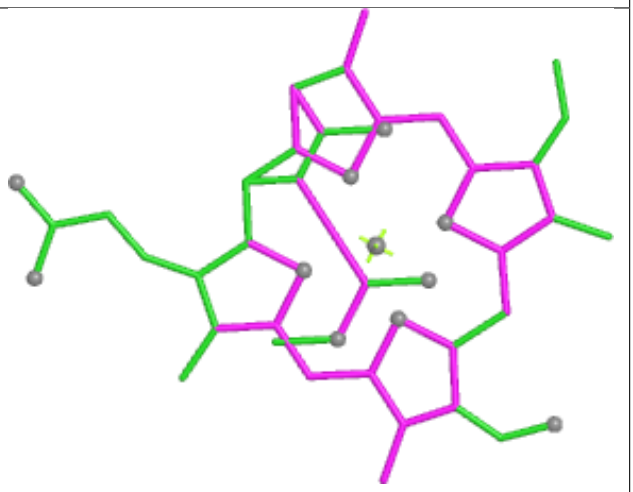


Rings

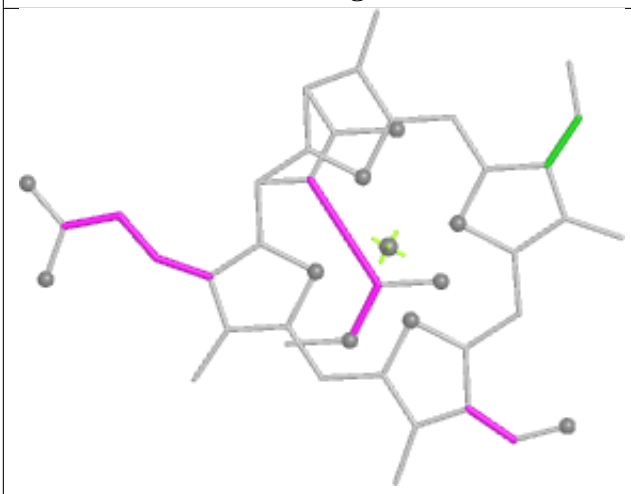
Ligand CL7 31 405



Bond lengths



Bond angles

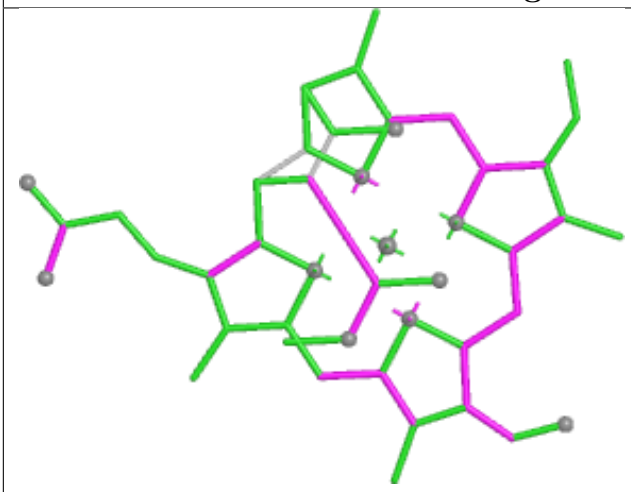


Torsions

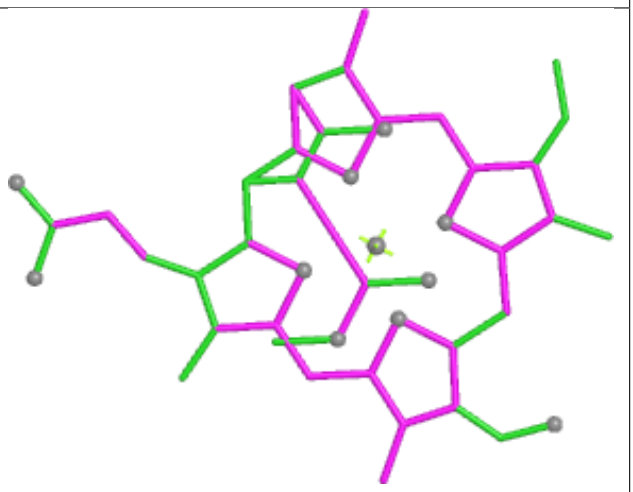


Rings

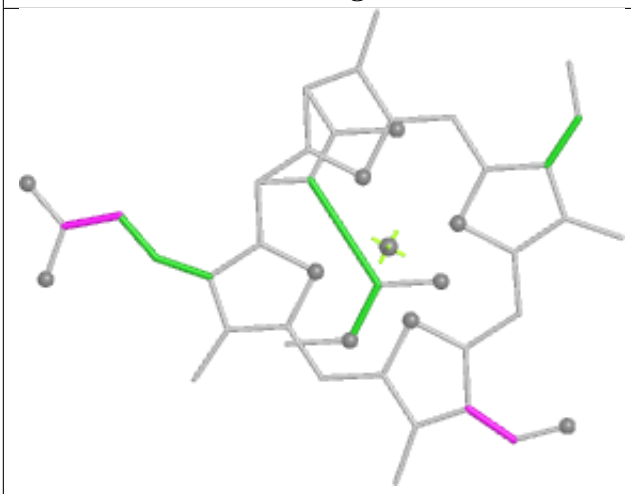
Ligand CL7 44 408



Bond lengths



Bond angles

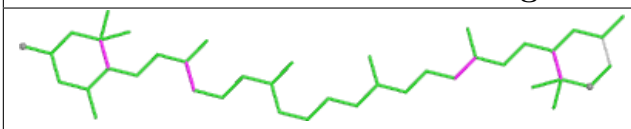


Torsions

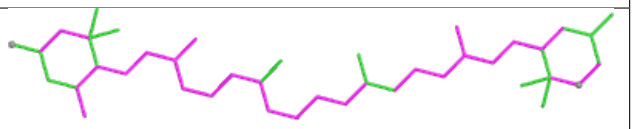


Rings

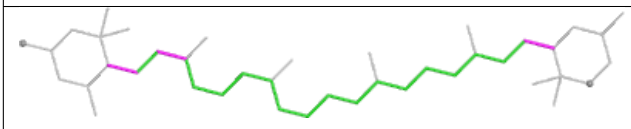
Ligand ZEX 23 423



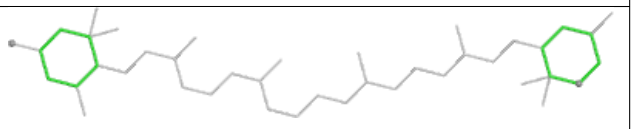
Bond lengths



Bond angles

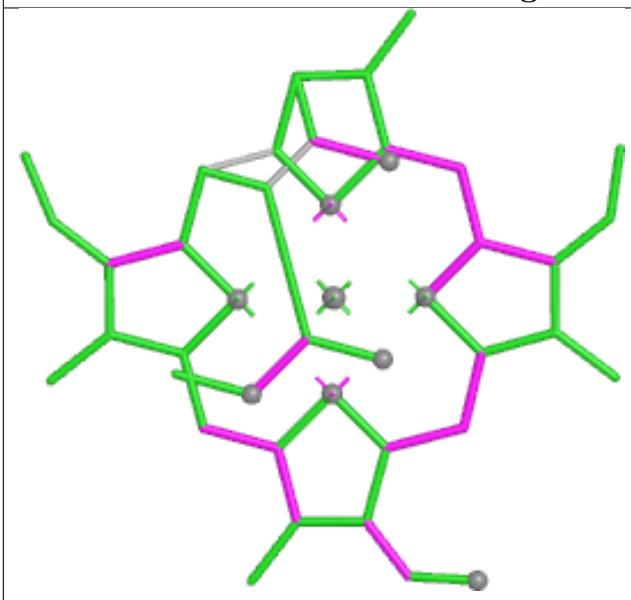


Torsions

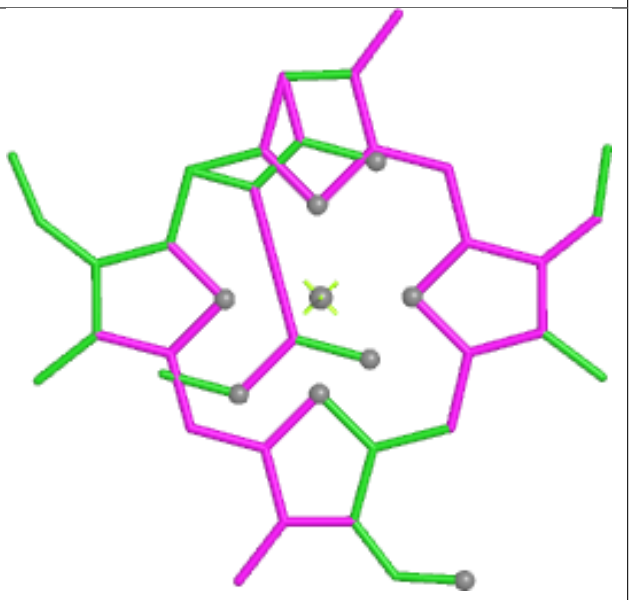


Rings

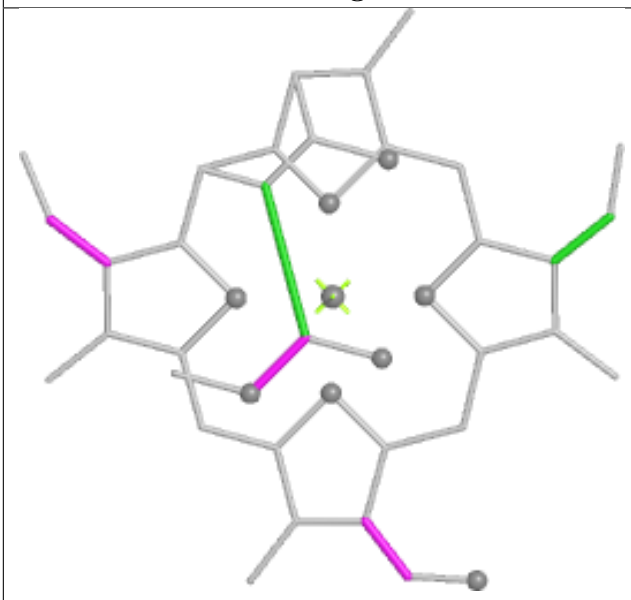
Ligand CL7 2C 511



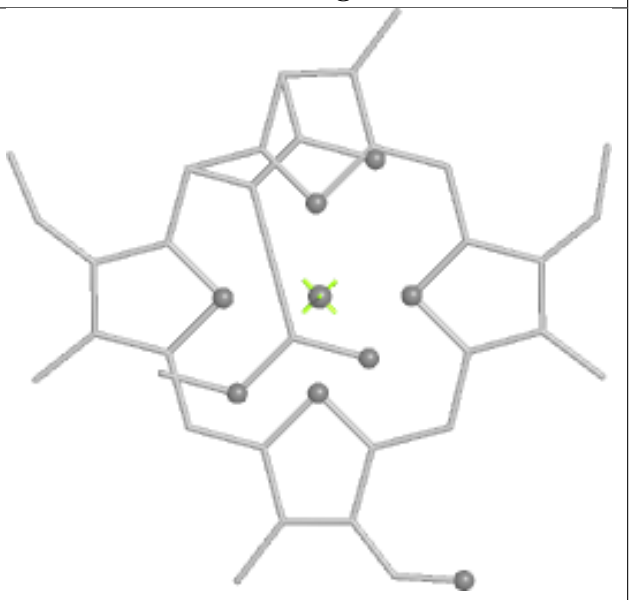
Bond lengths



Bond angles

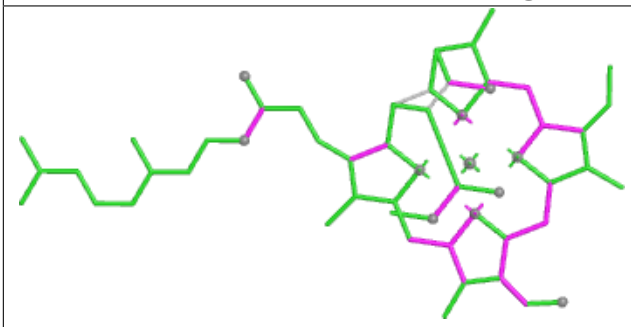


Torsions

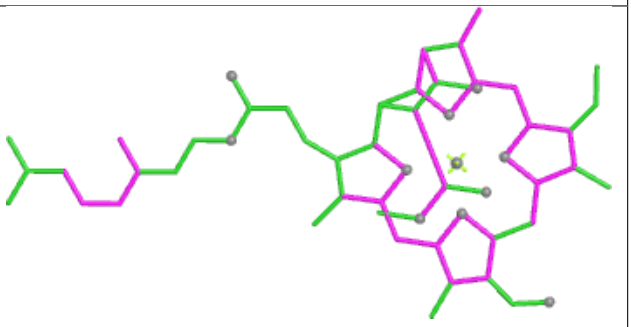


Rings

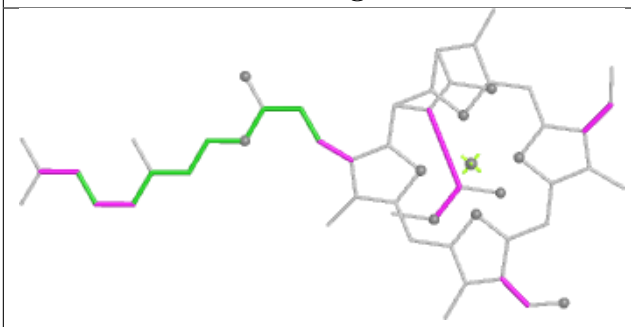
Ligand CL7 2C 504



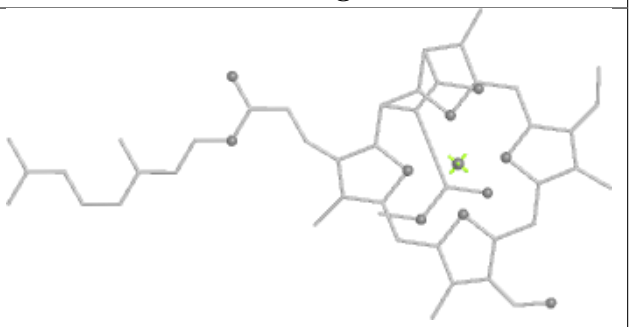
Bond lengths



Bond angles

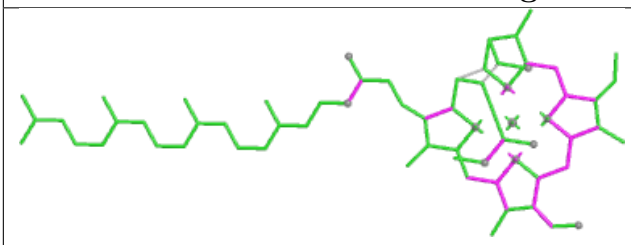


Torsions

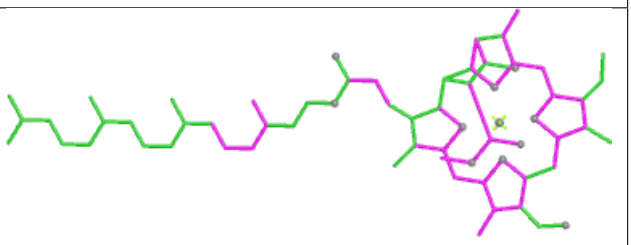


Rings

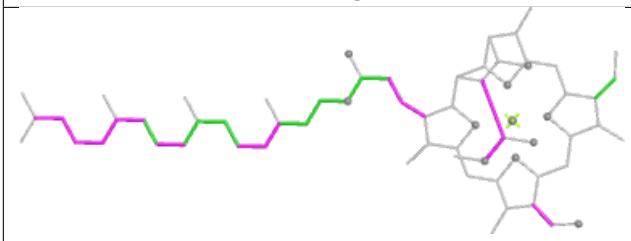
Ligand CL7 3B 604



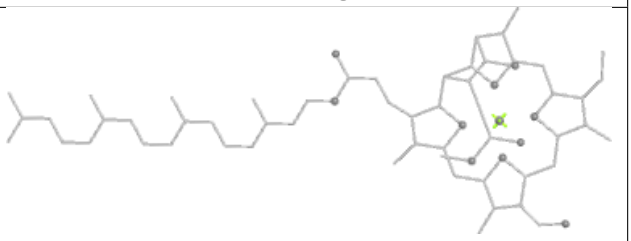
Bond lengths



Bond angles

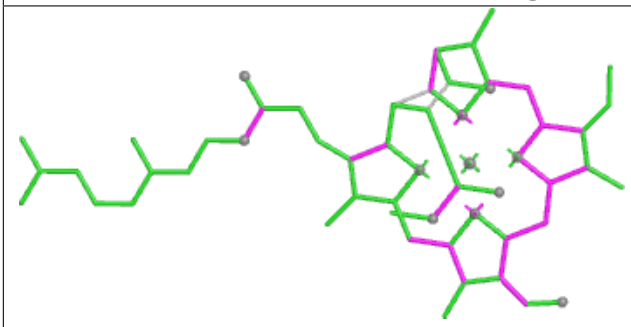


Torsions

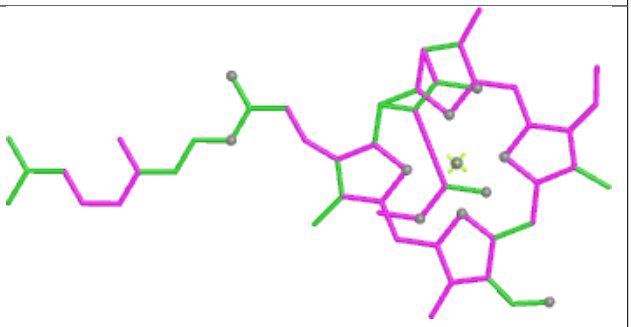


Rings

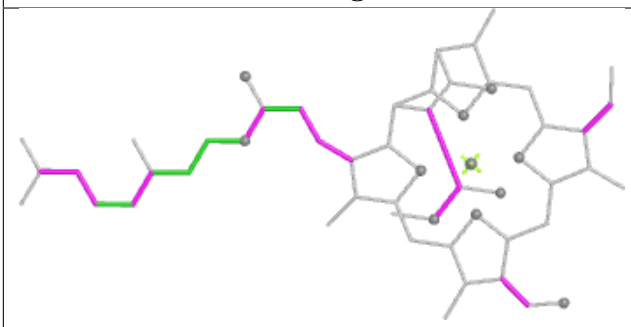
Ligand CL7 43 417



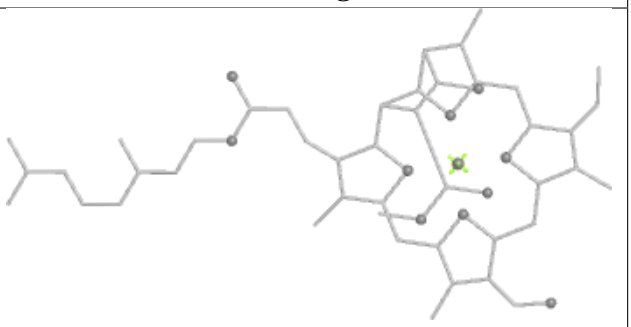
Bond lengths



Bond angles

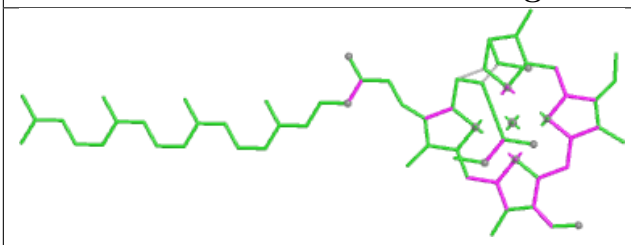


Torsions

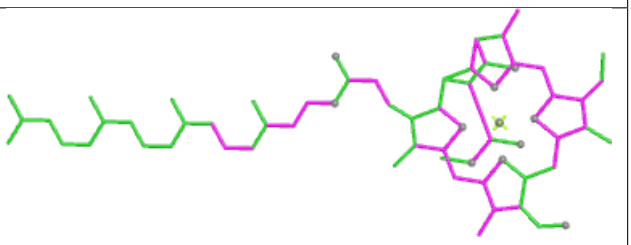


Rings

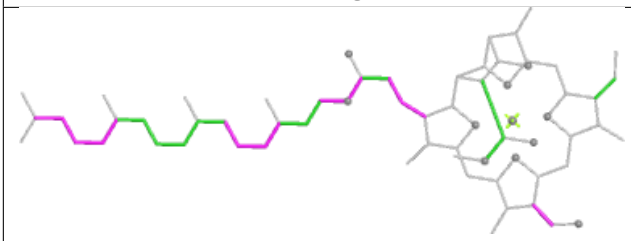
Ligand CL7 32 516



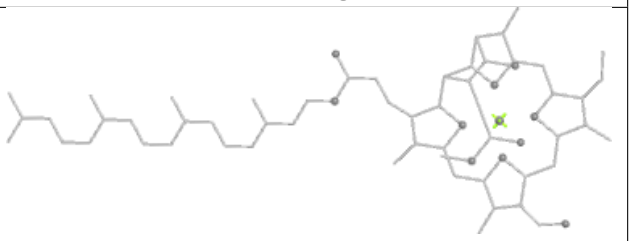
Bond lengths



Bond angles

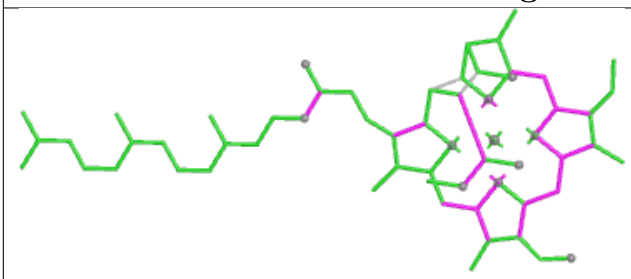


Torsions

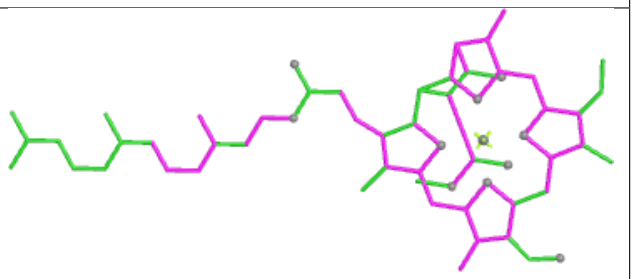


Rings

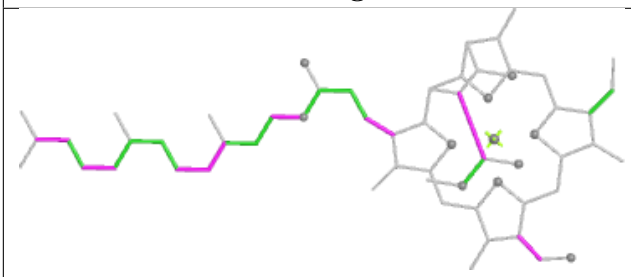
Ligand CL7 2B 615



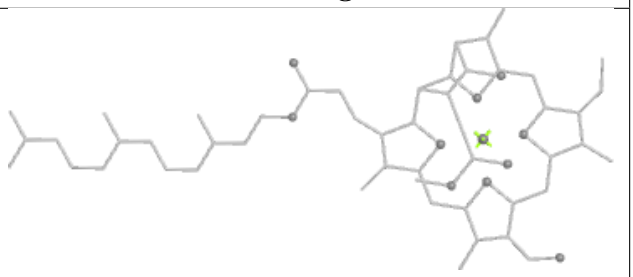
Bond lengths



Bond angles

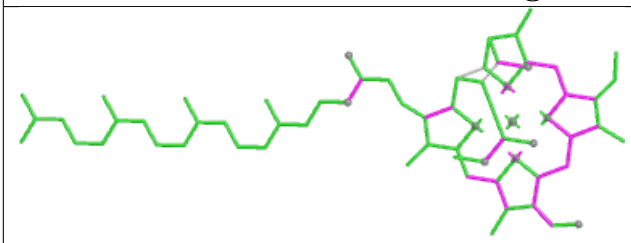


Torsions

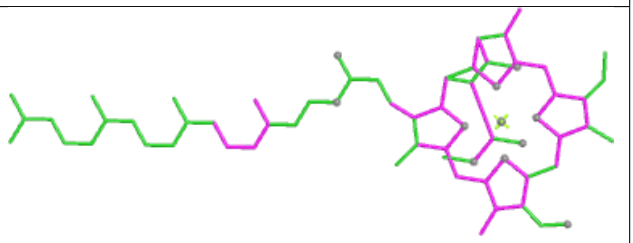


Rings

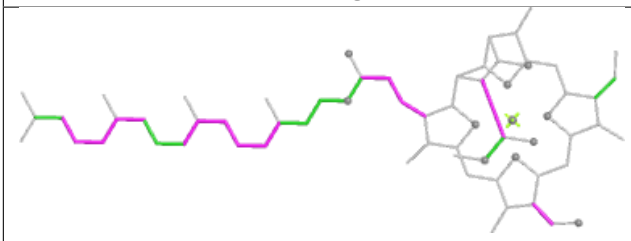
Ligand CL7 13 501



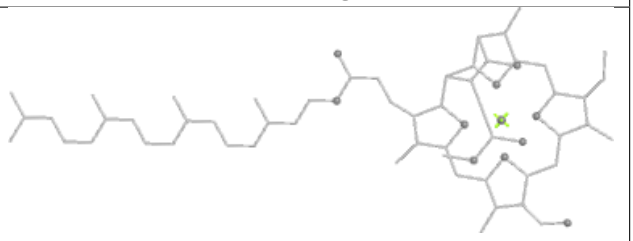
Bond lengths



Bond angles

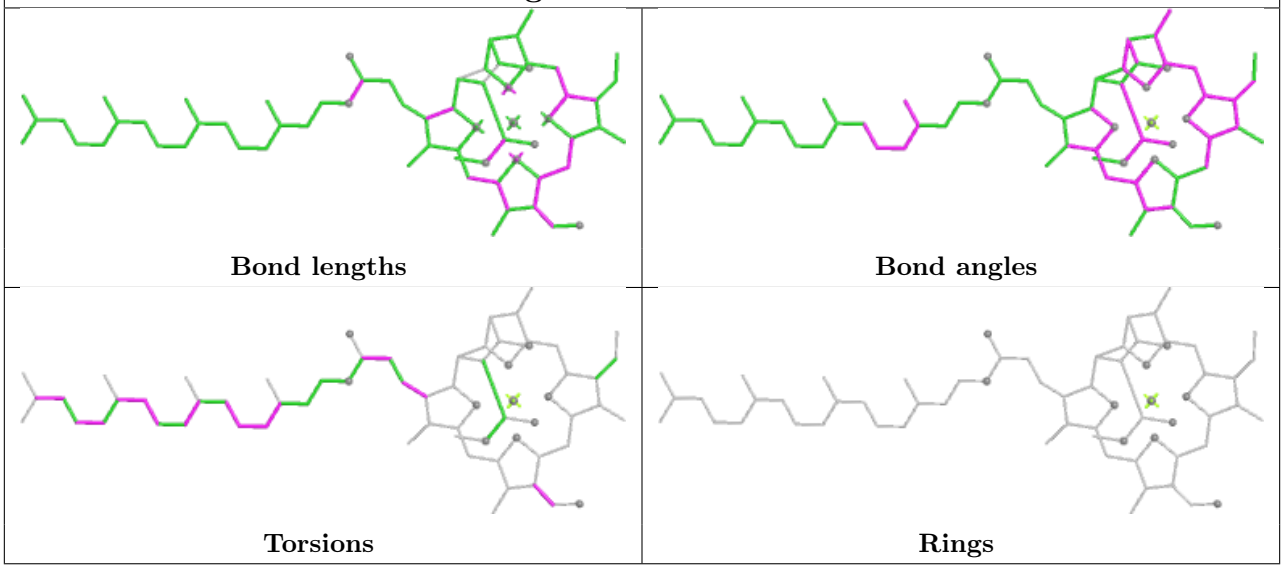


Torsions

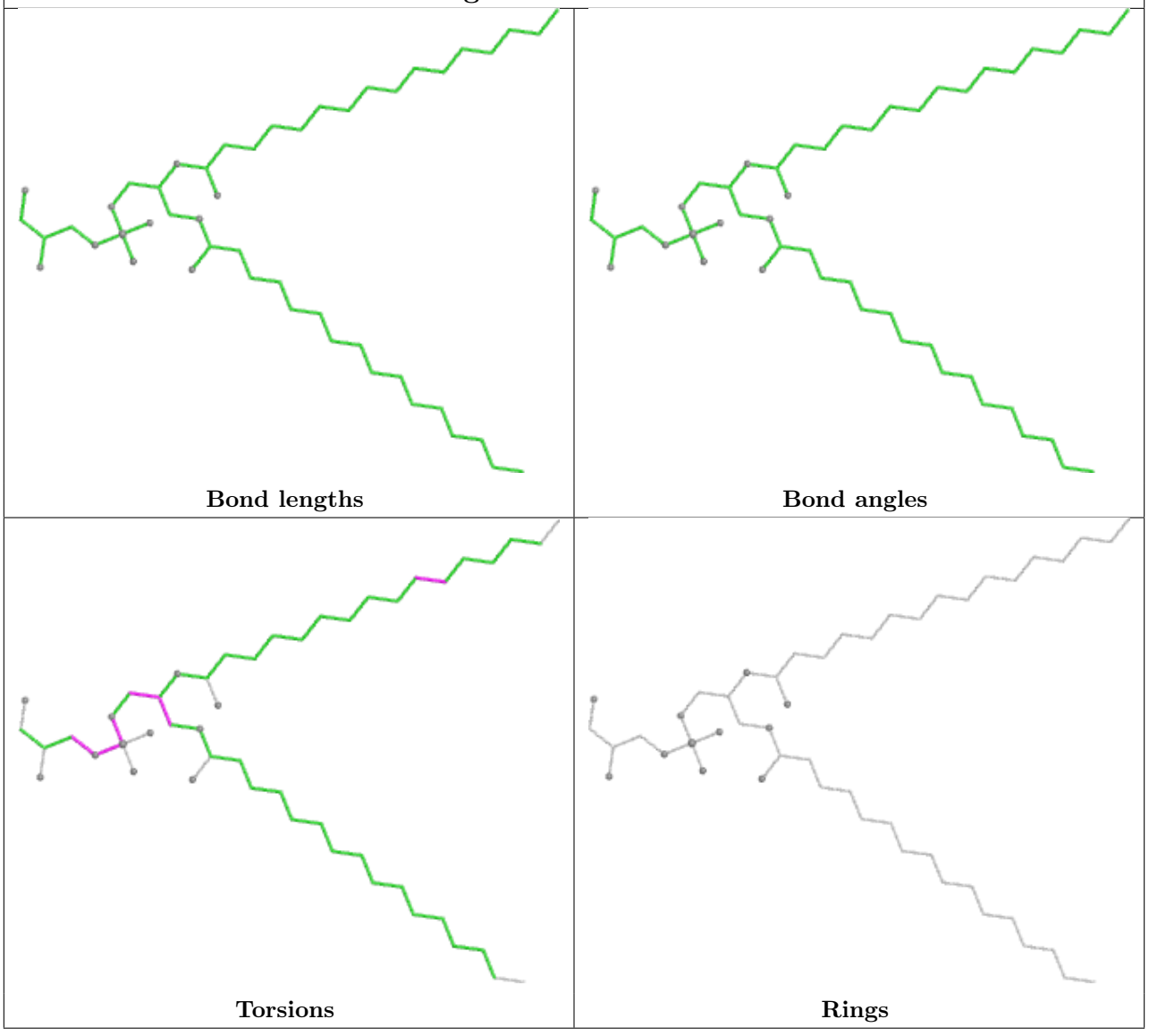


Rings

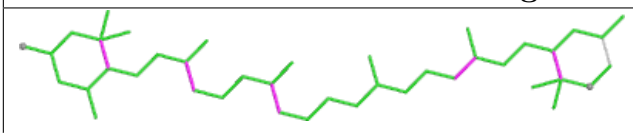
Ligand CL7 32 512



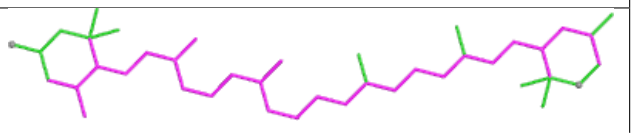
Ligand LHG 44 401



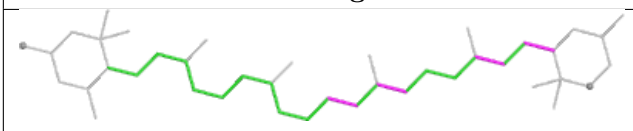
Ligand ZEX 43 401



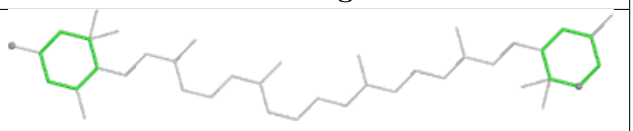
Bond lengths



Bond angles

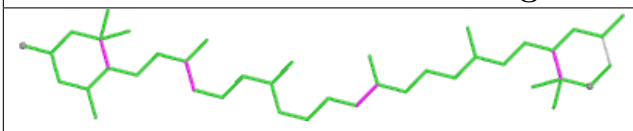


Torsions

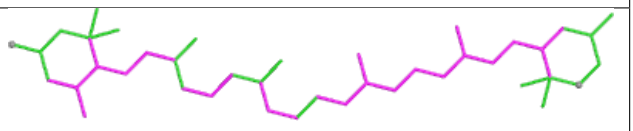


Rings

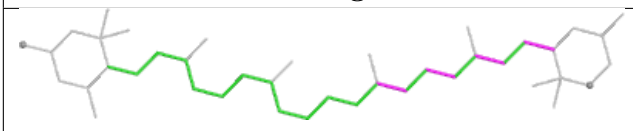
Ligand ZEX 32 522



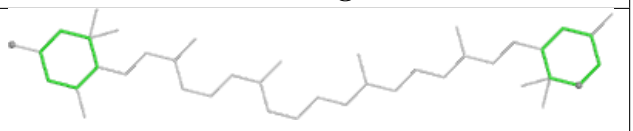
Bond lengths



Bond angles

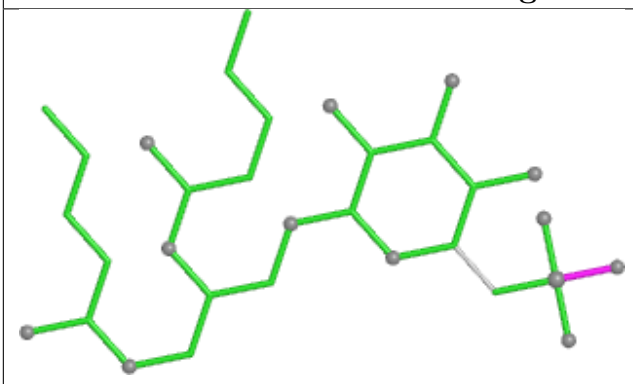


Torsions

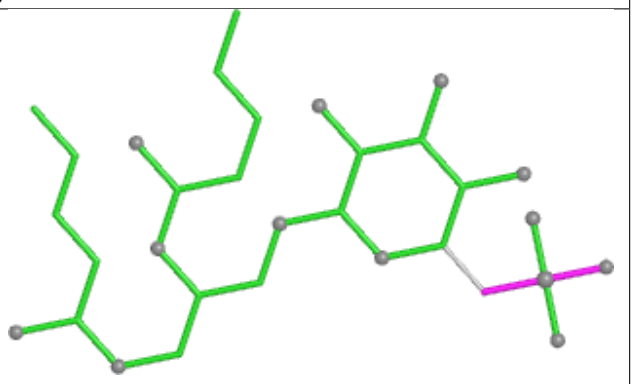


Rings

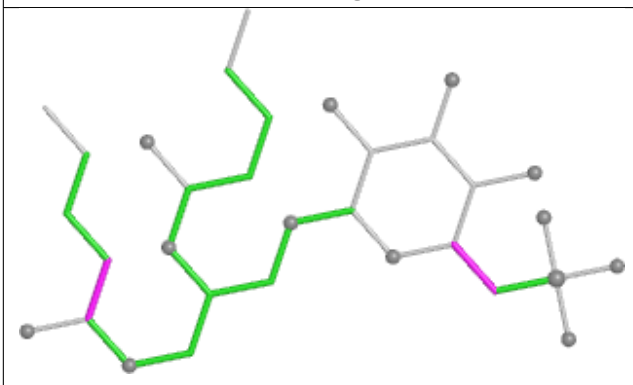
Ligand SQD 41 423



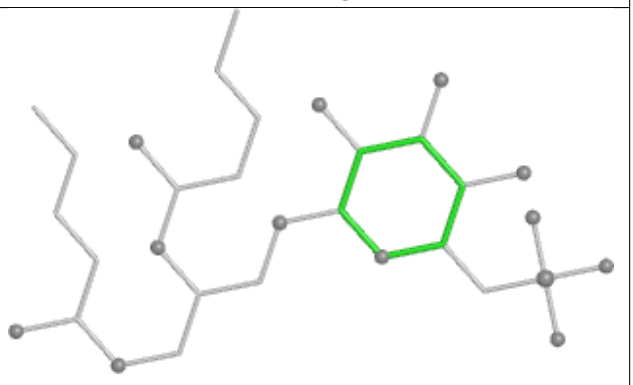
Bond lengths



Bond angles

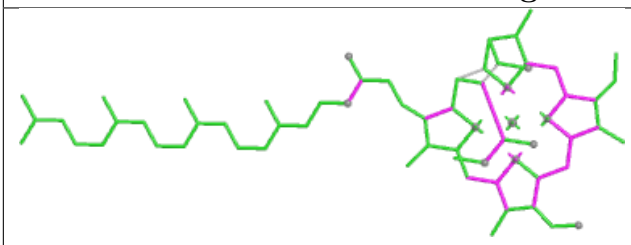


Torsions

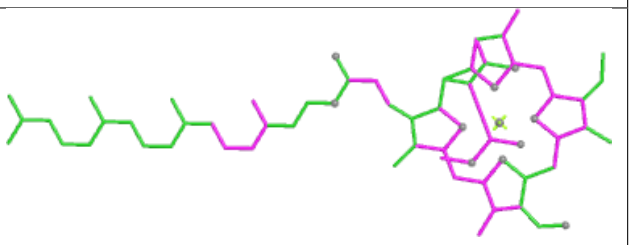


Rings

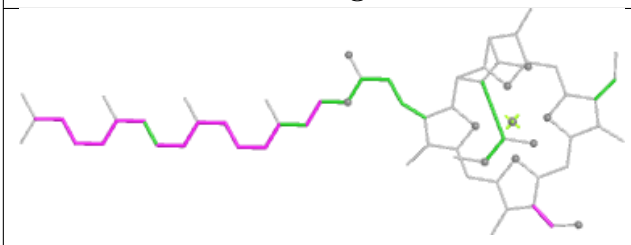
Ligand CL7 4C 507



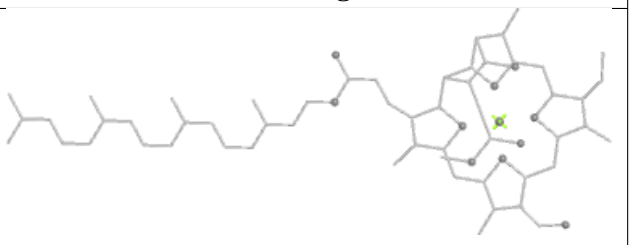
Bond lengths



Bond angles

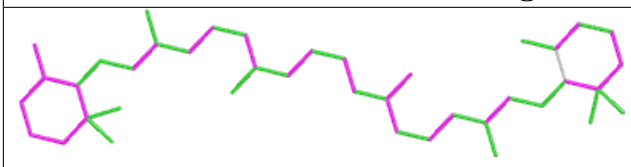


Torsions

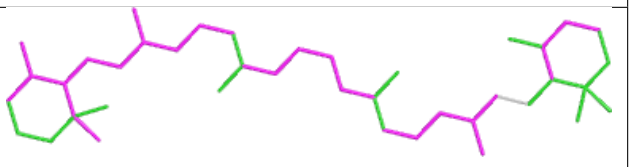


Rings

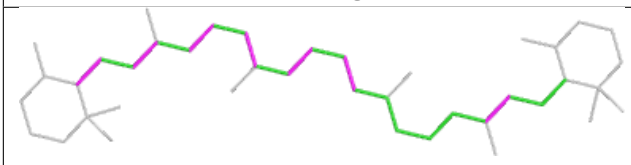
Ligand 8CT 2B 619



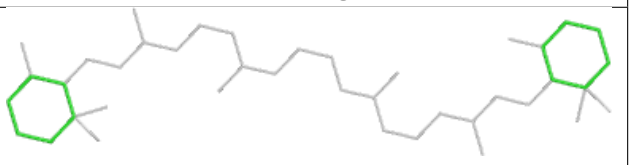
Bond lengths



Bond angles

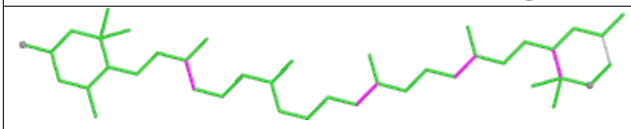


Torsions

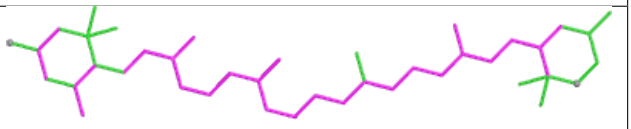


Rings

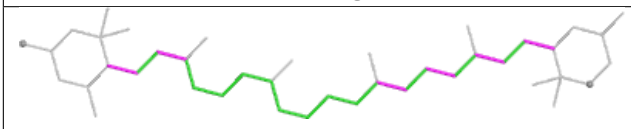
Ligand ZEX 23 420



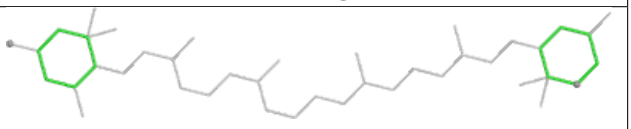
Bond lengths



Bond angles

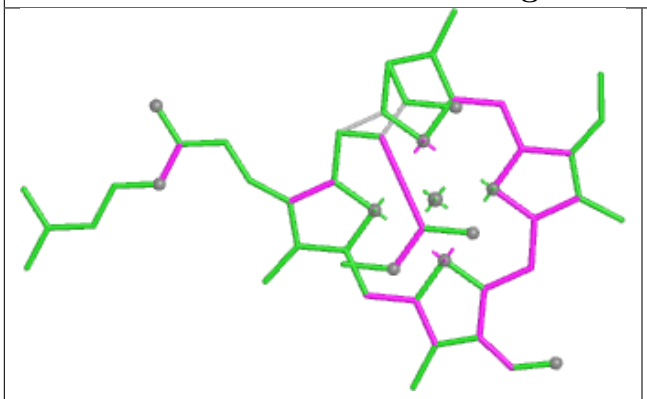


Torsions

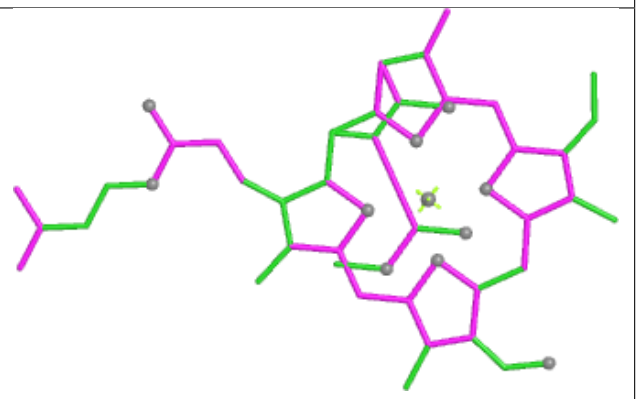


Rings

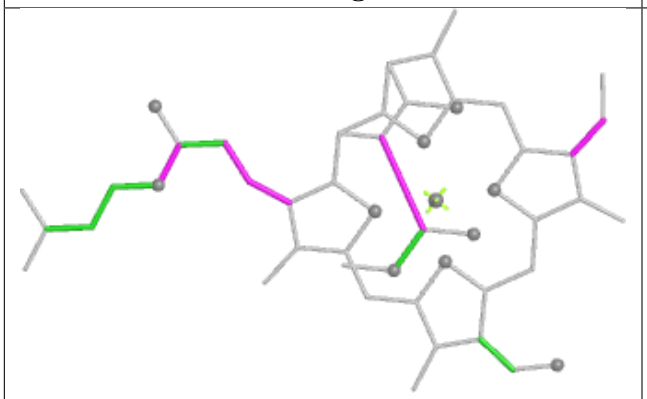
Ligand CL7 2B 616



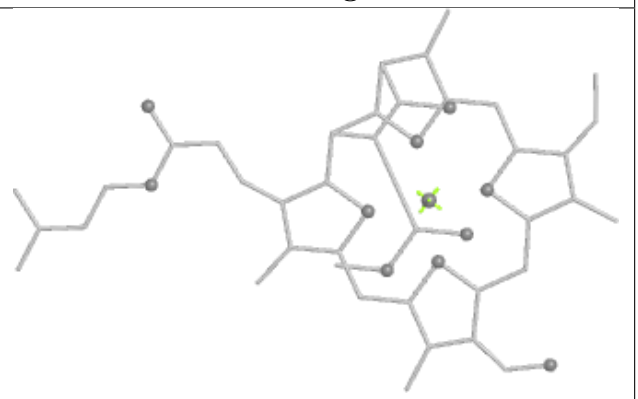
Bond lengths



Bond angles

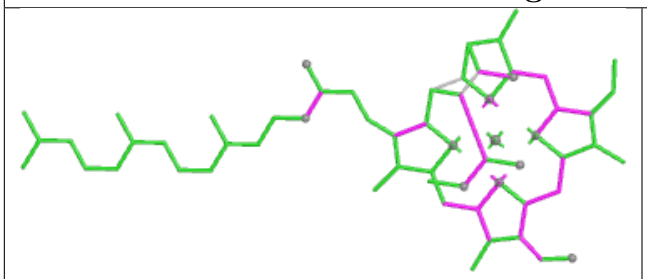


Torsions

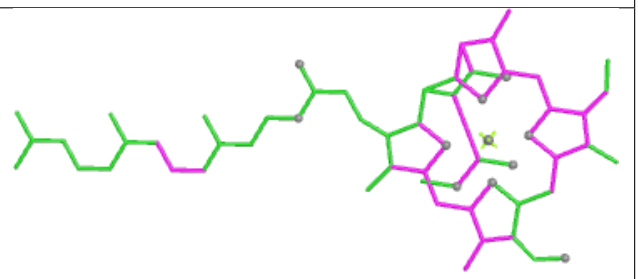


Rings

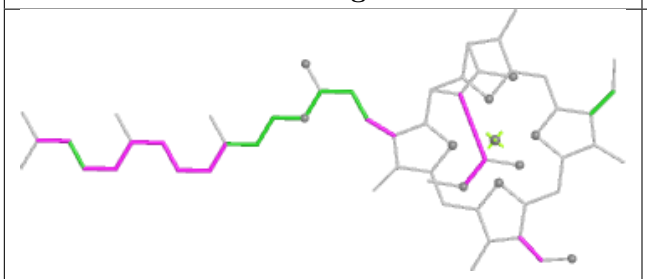
Ligand CL7 42 511



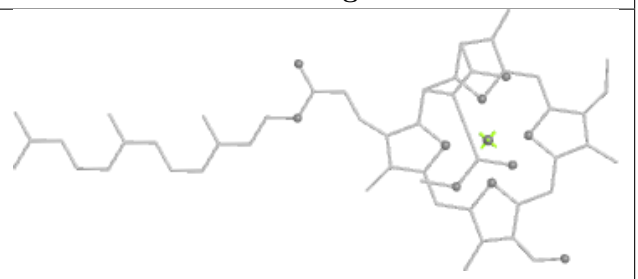
Bond lengths



Bond angles

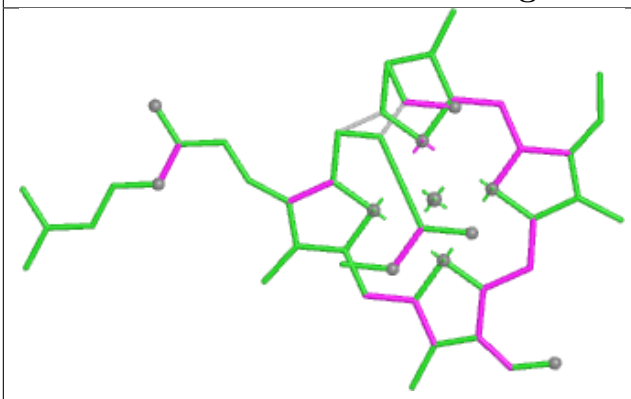


Torsions

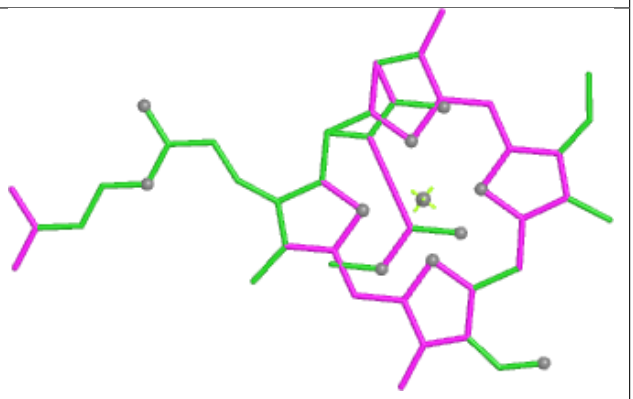


Rings

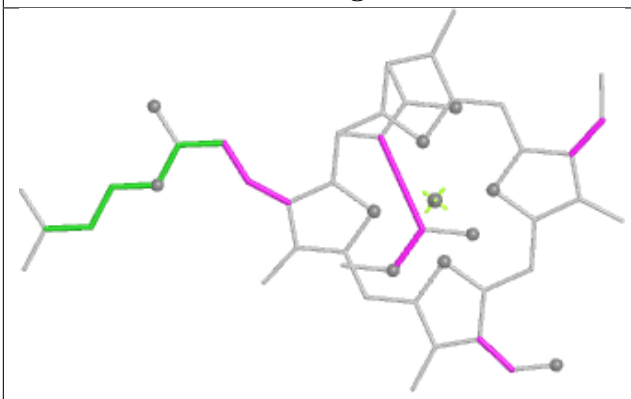
Ligand CL7 2D 402



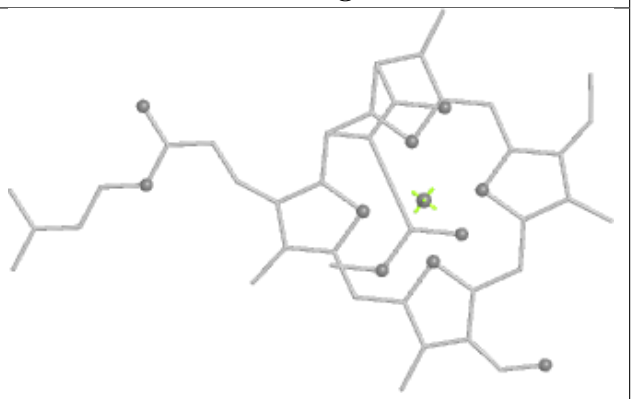
Bond lengths



Bond angles

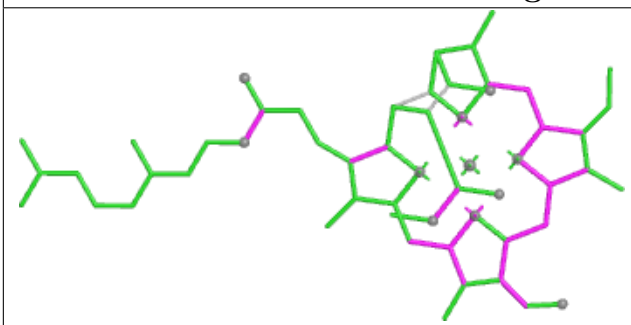


Torsions

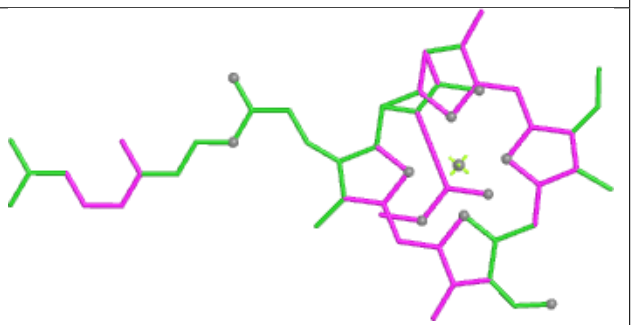


Rings

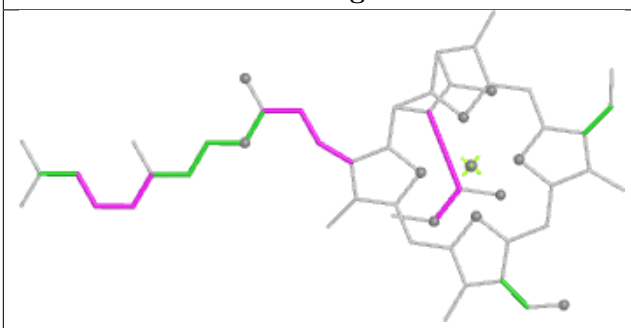
Ligand CL7 23 413



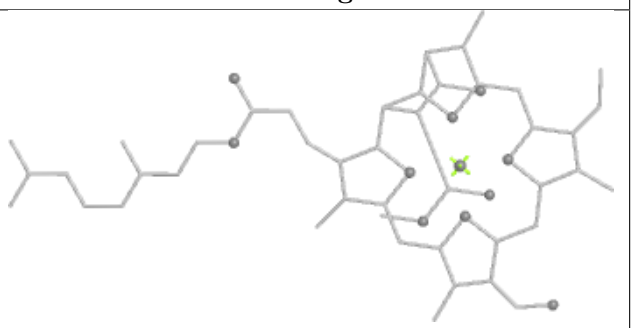
Bond lengths



Bond angles

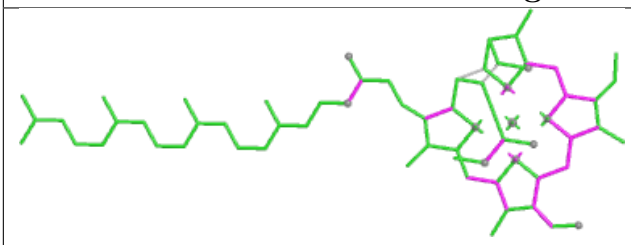


Torsions

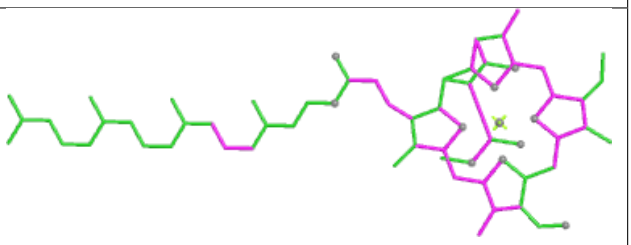


Rings

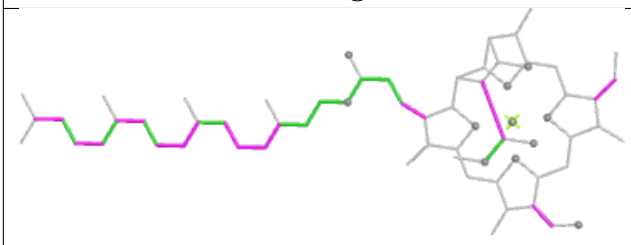
Ligand CL7 33 504



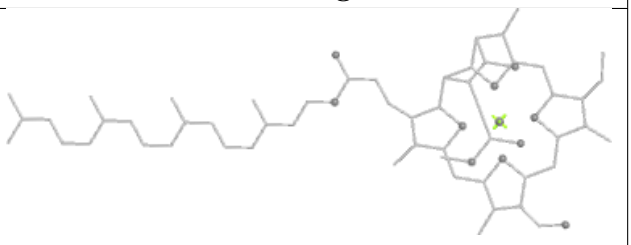
Bond lengths



Bond angles

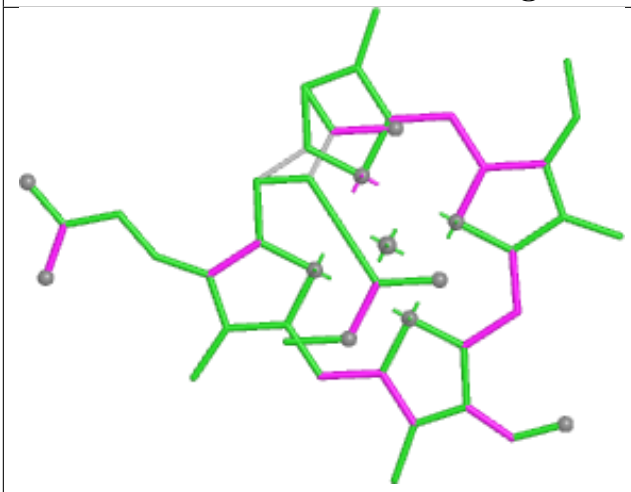


Torsions



Rings

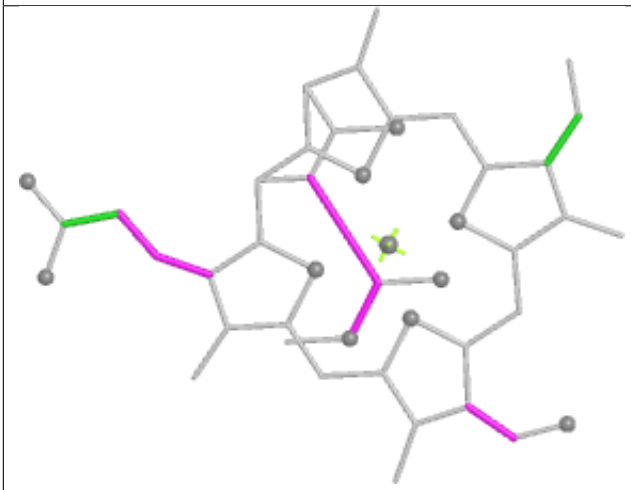
Ligand CL7 2C 513



Bond lengths



Bond angles

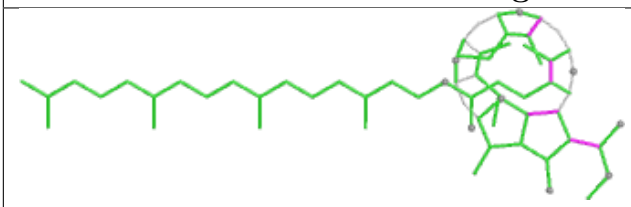


Torsions

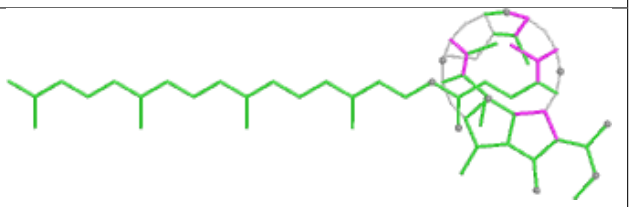


Rings

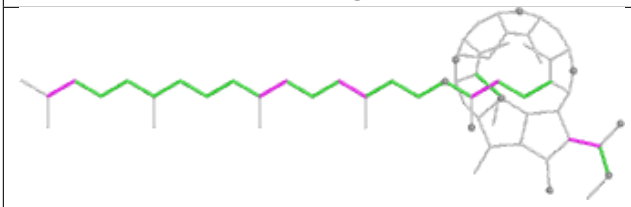
Ligand PHO 3D 408



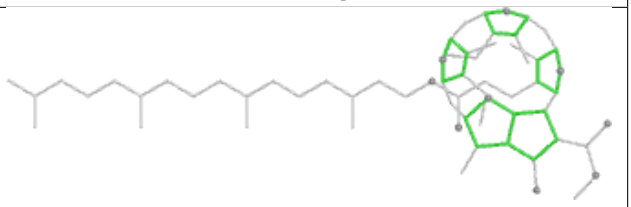
Bond lengths



Bond angles

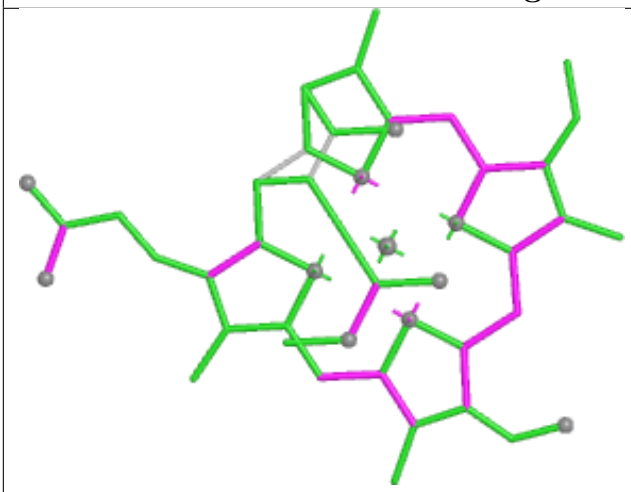


Torsions

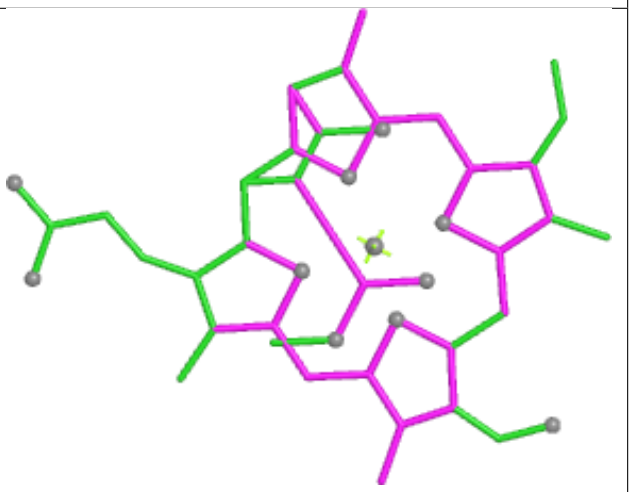


Rings

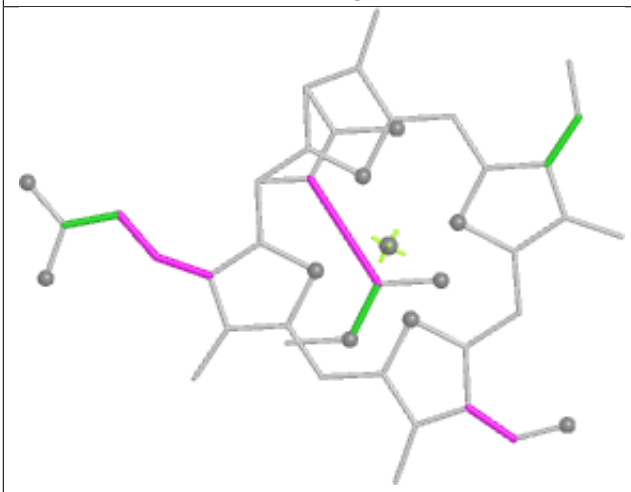
Ligand CL7 32 513



Bond lengths



Bond angles



Torsions

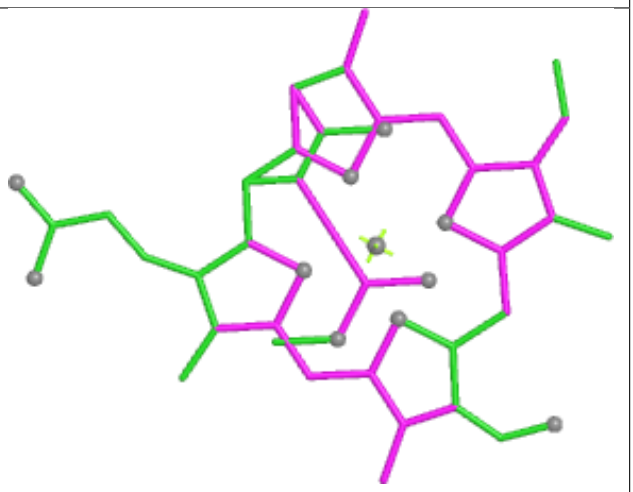


Rings

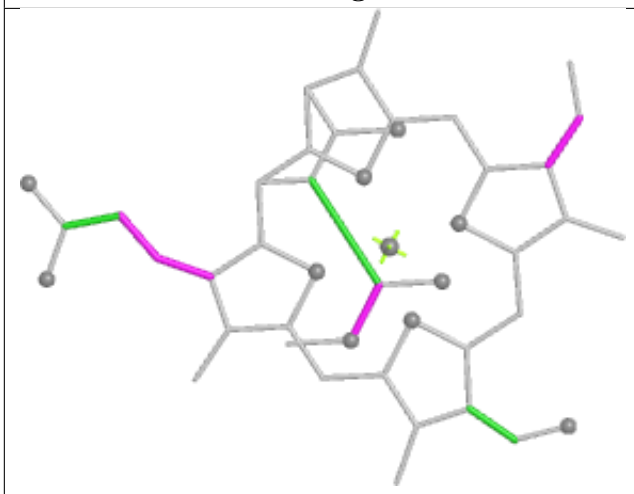
Ligand CL7 43 415



Bond lengths



Bond angles

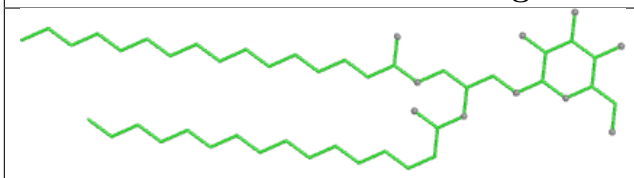


Torsions

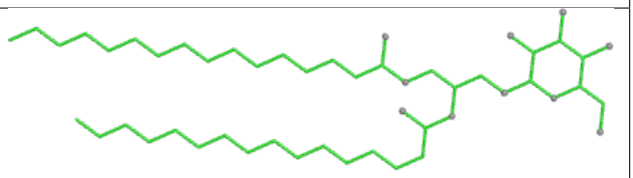


Rings

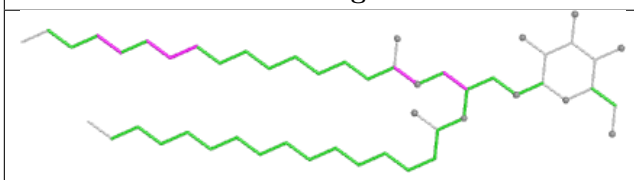
Ligand LMG 3B 621



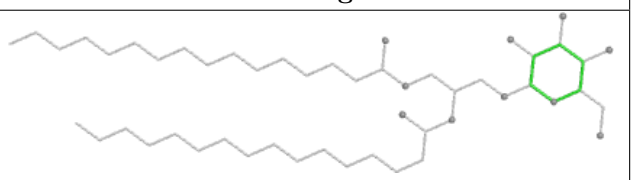
Bond lengths



Bond angles

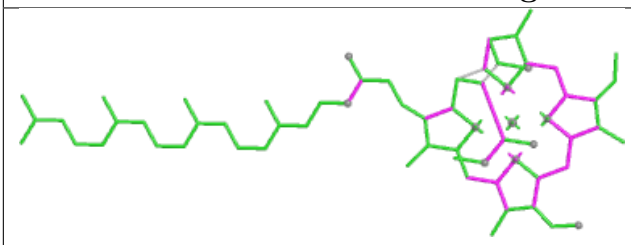


Torsions

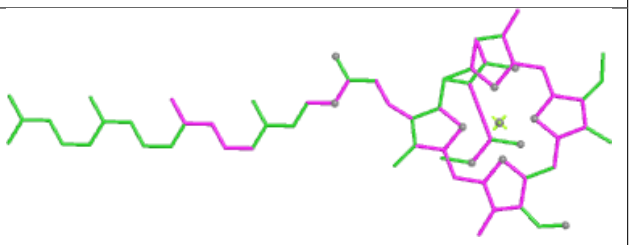


Rings

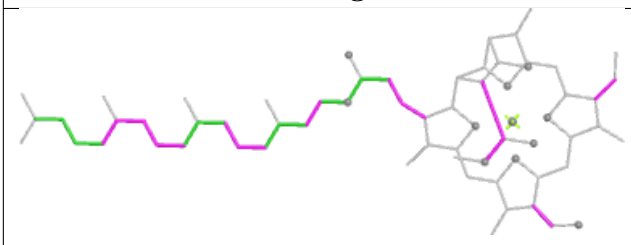
Ligand CL7 1C 505



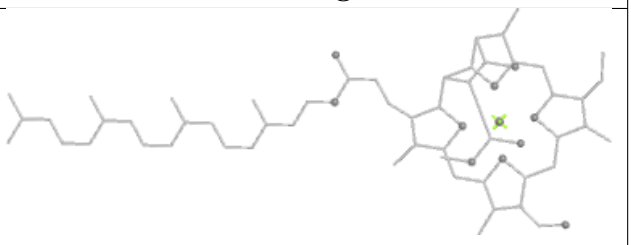
Bond lengths



Bond angles

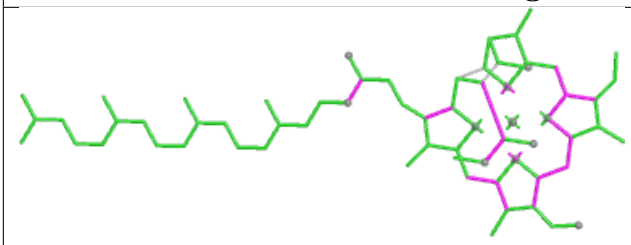


Torsions

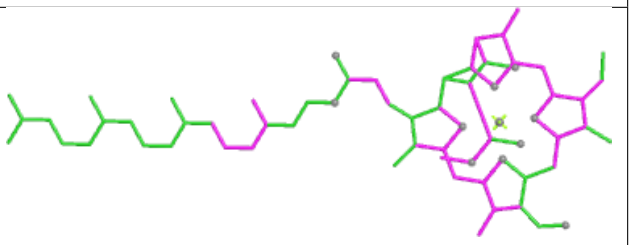


Rings

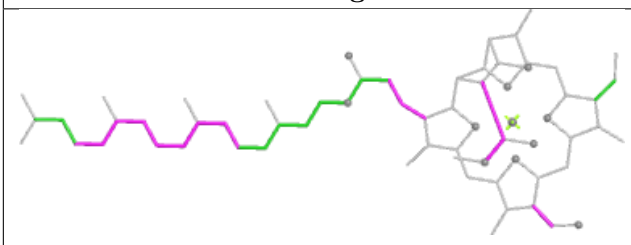
Ligand CL7 33 503



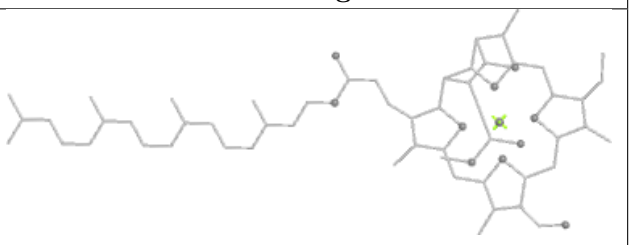
Bond lengths



Bond angles

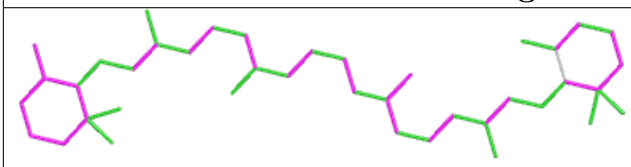


Torsions

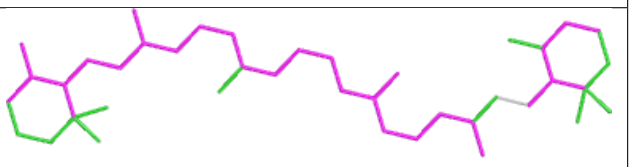


Rings

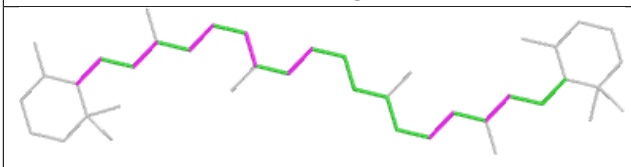
Ligand 8CT 1C 515



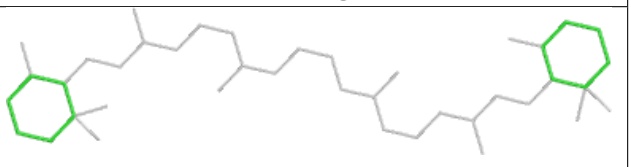
Bond lengths



Bond angles

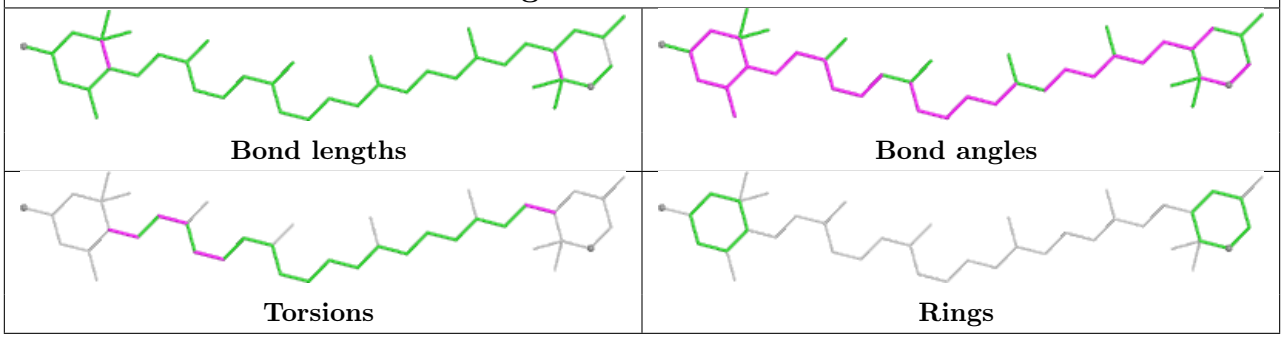


Torsions

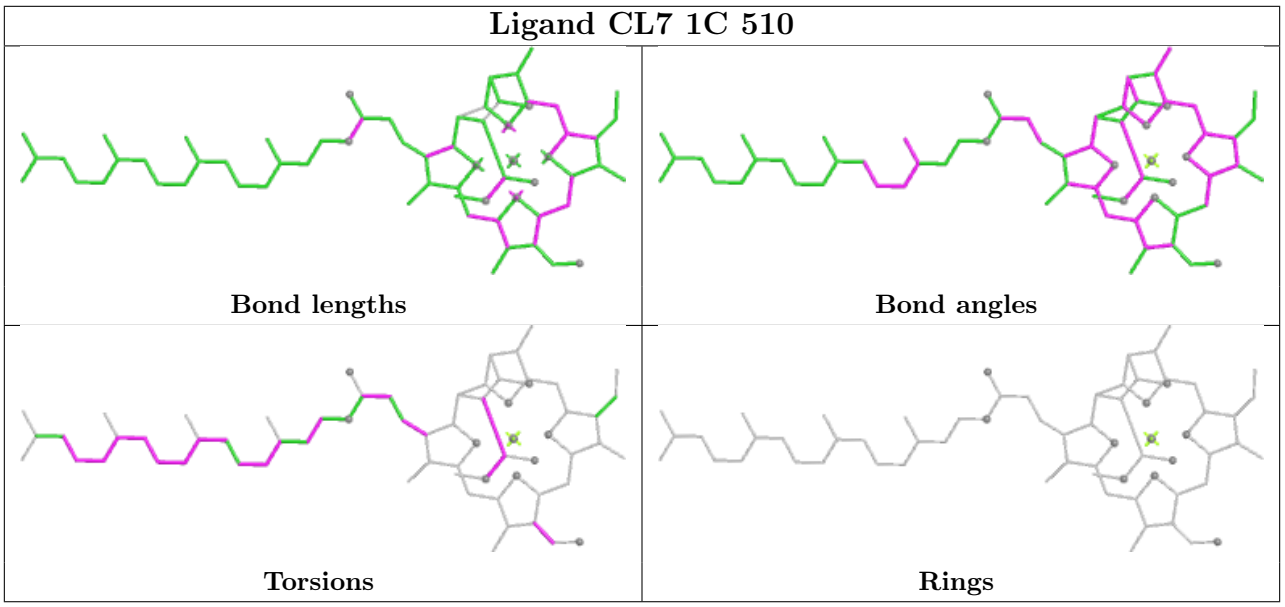


Rings

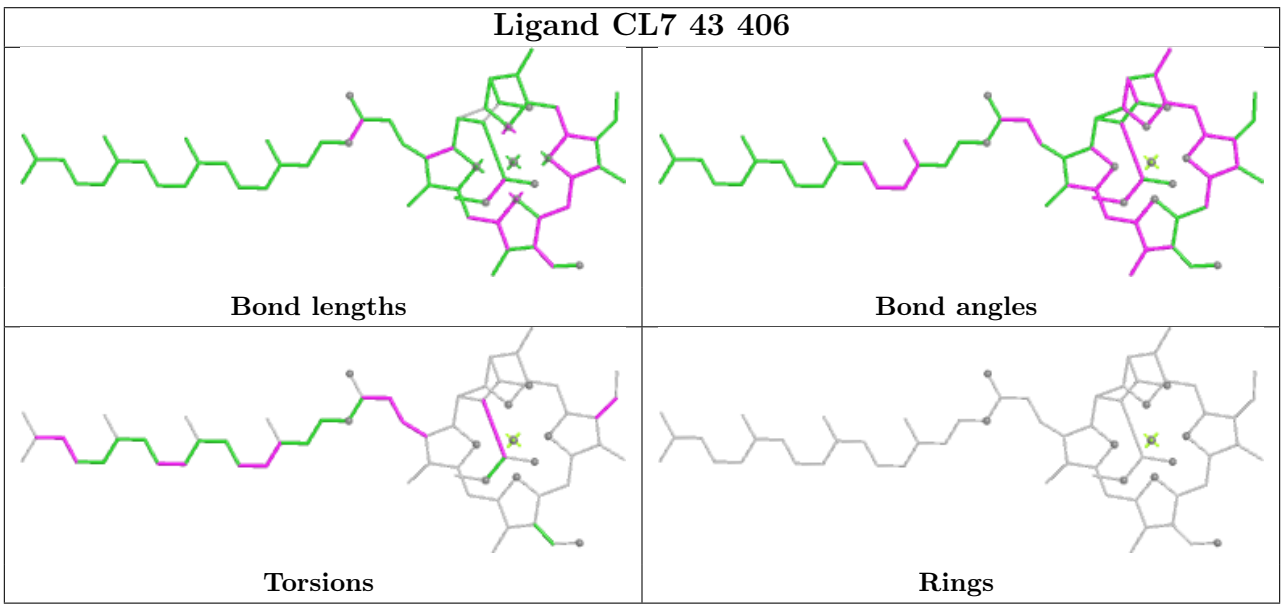
Ligand ZEX 41 422



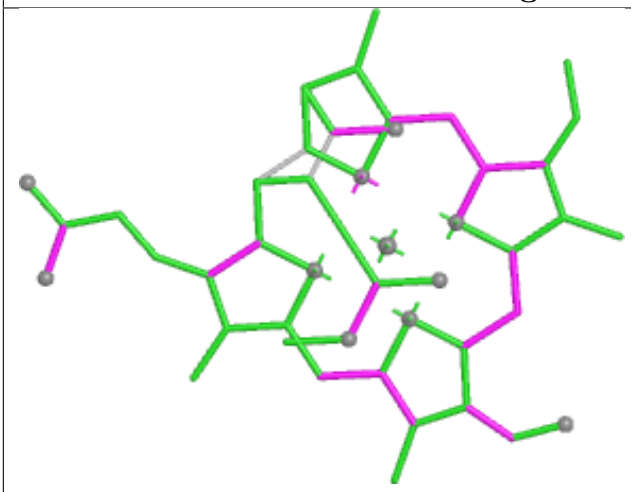
Ligand CL7 1C 510



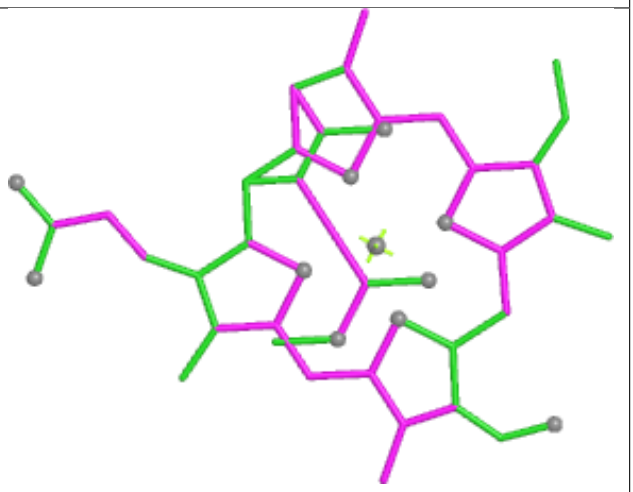
Ligand CL7 43 406



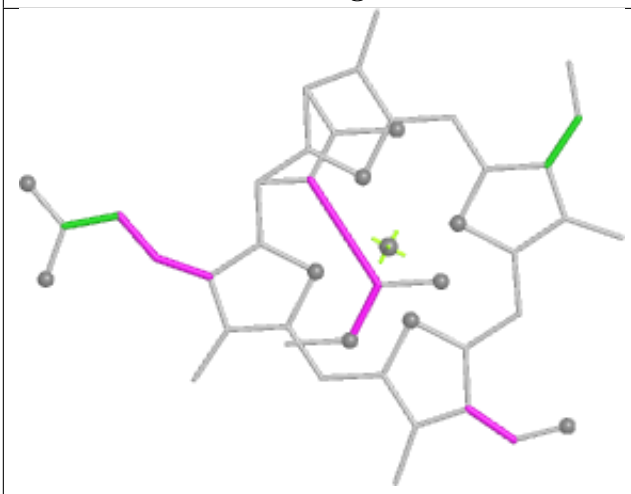
Ligand CL7 3C 513



Bond lengths



Bond angles

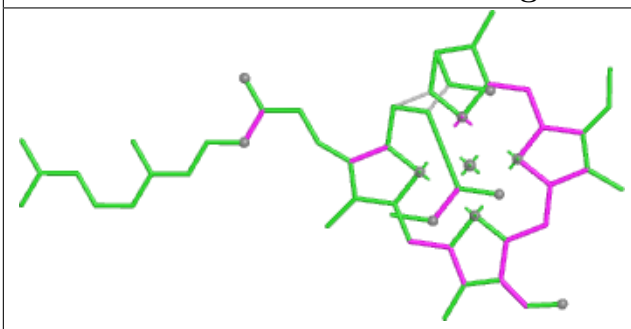


Torsions

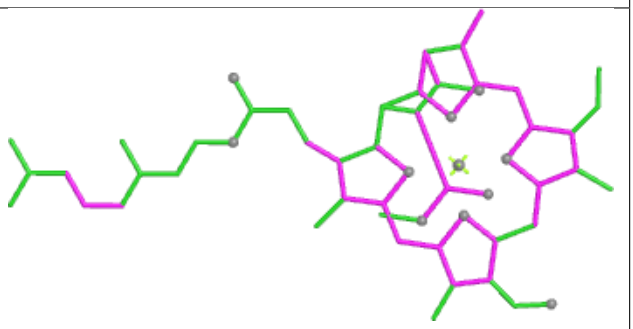


Rings

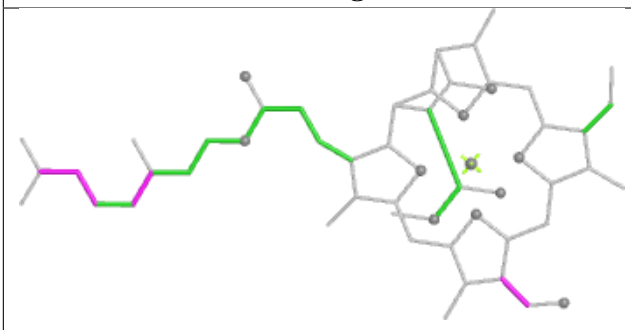
Ligand CL7 3B 606



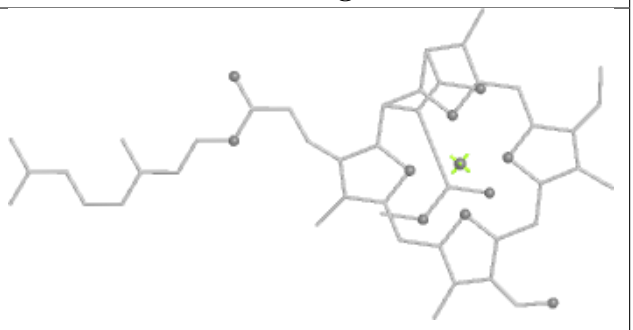
Bond lengths



Bond angles

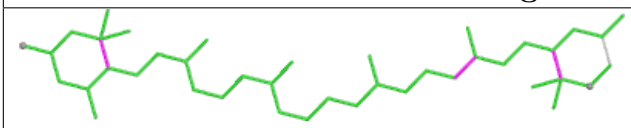


Torsions

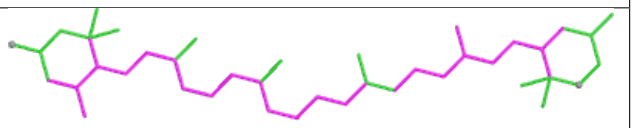


Rings

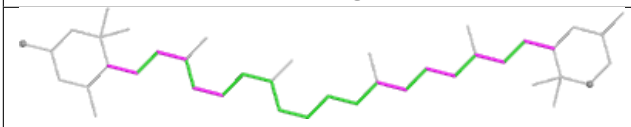
Ligand ZEX 32 524



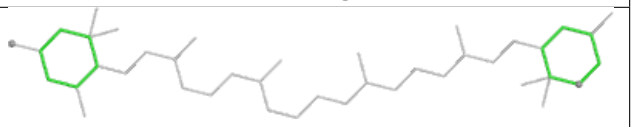
Bond lengths



Bond angles

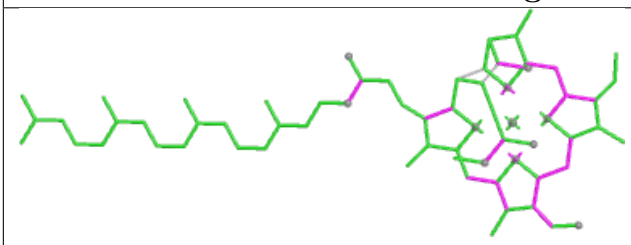


Torsions

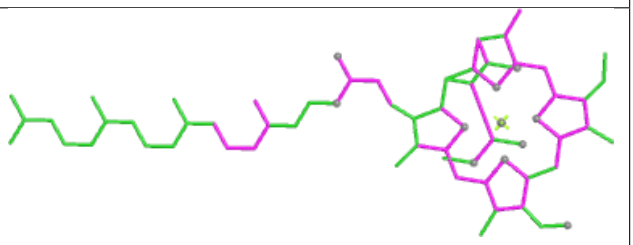


Rings

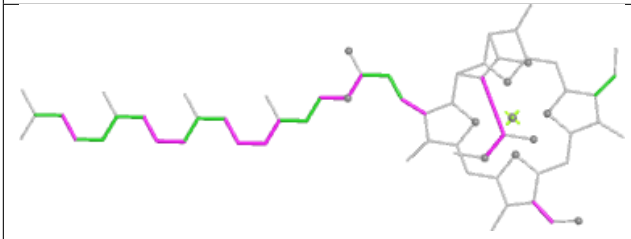
Ligand CL7 21 410



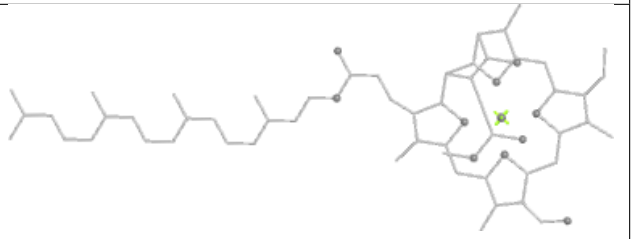
Bond lengths



Bond angles

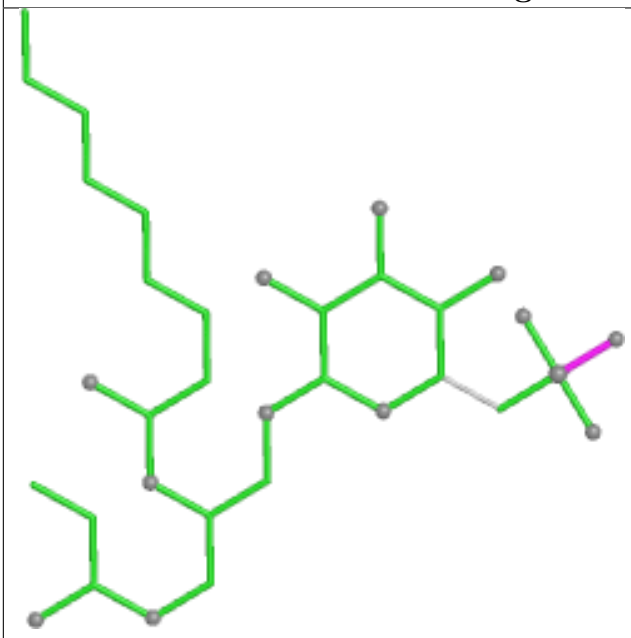


Torsions

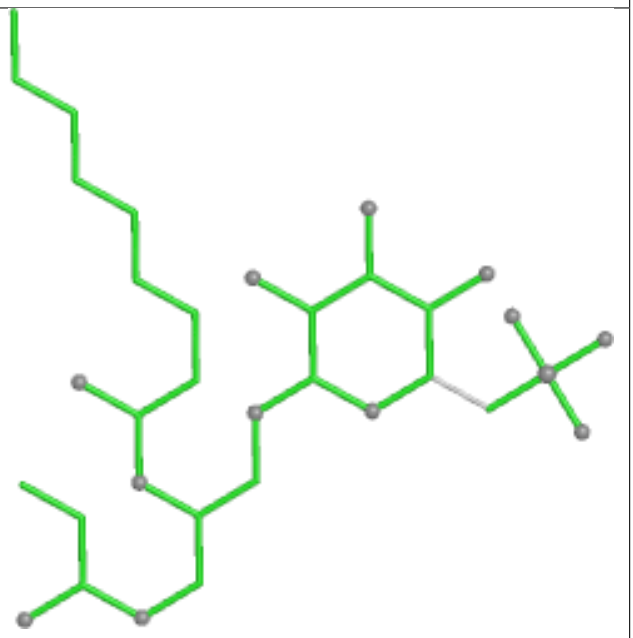


Rings

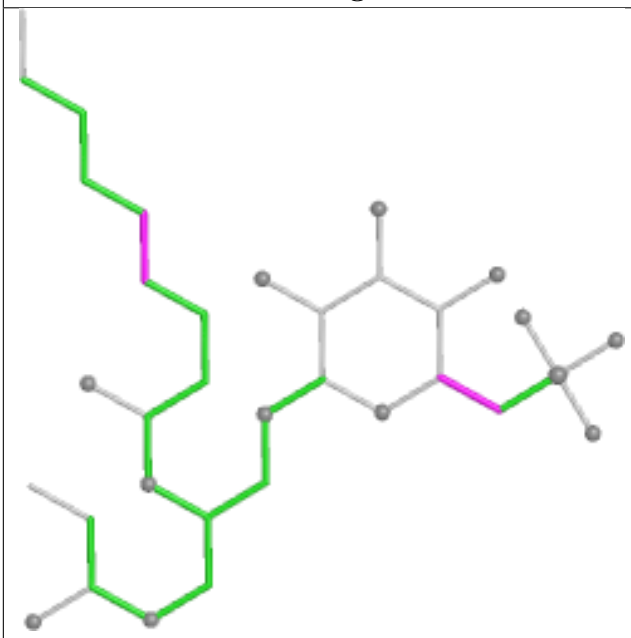
Ligand SQD 4A 406



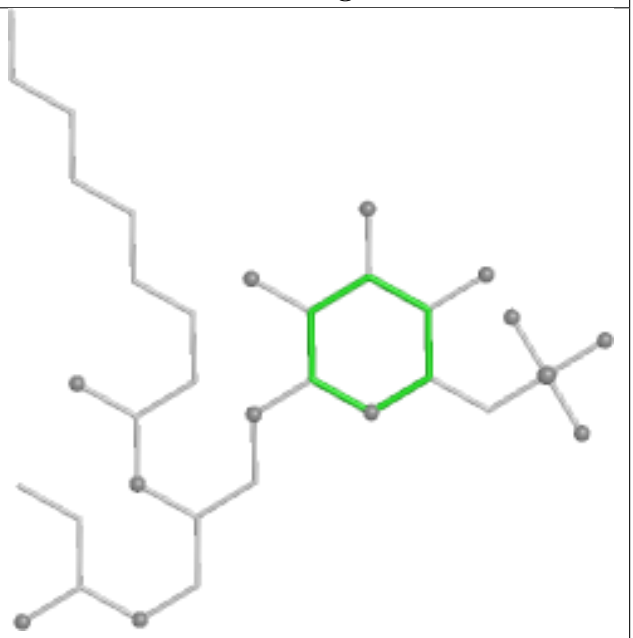
Bond lengths



Bond angles

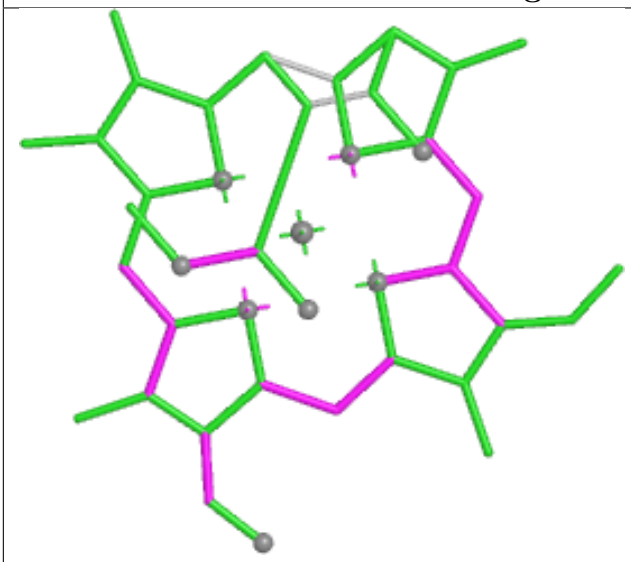


Torsions

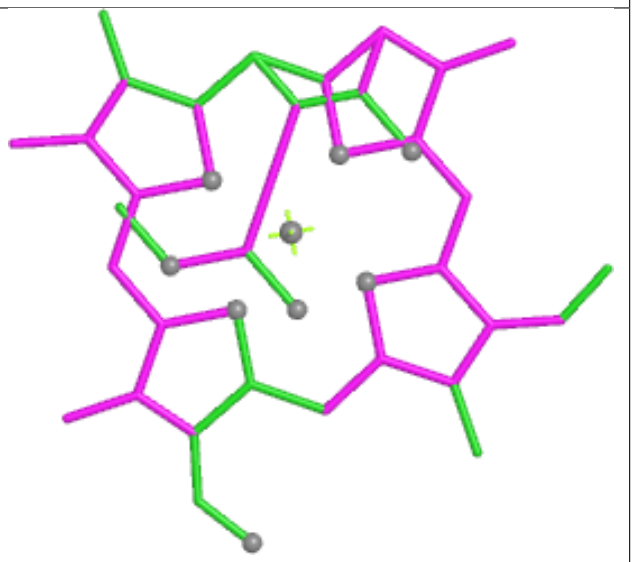


Rings

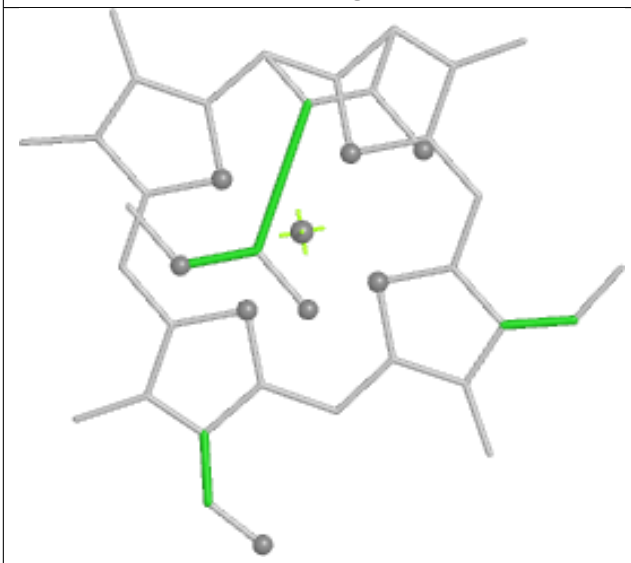
Ligand CL7 23 416



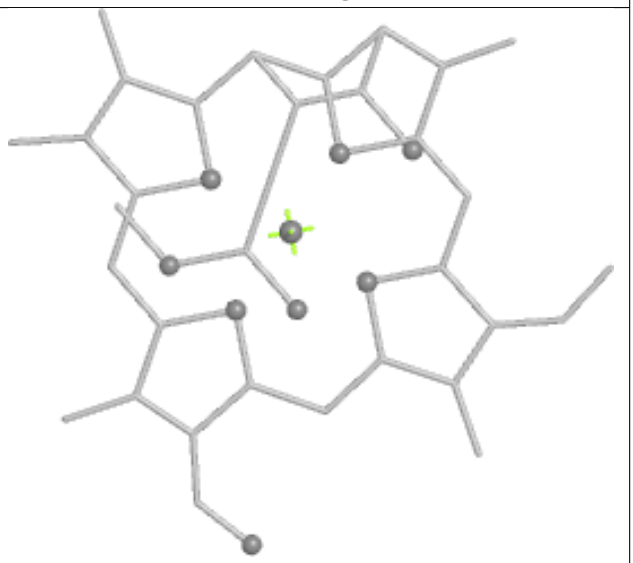
Bond lengths



Bond angles

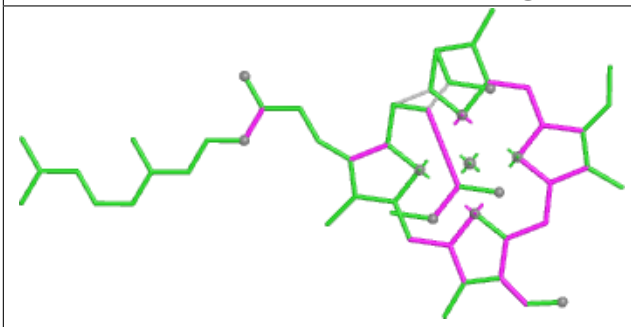


Torsions

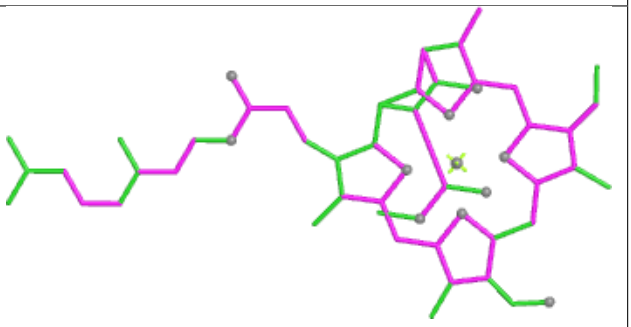


Rings

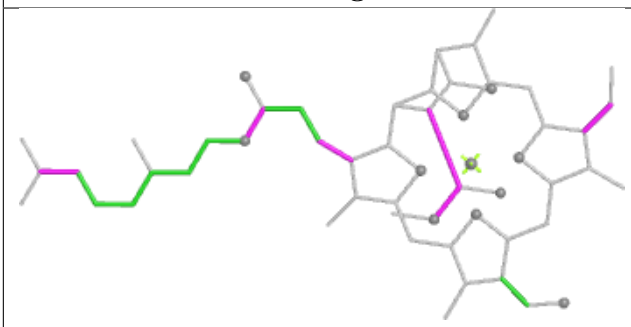
Ligand CL7 3A 403



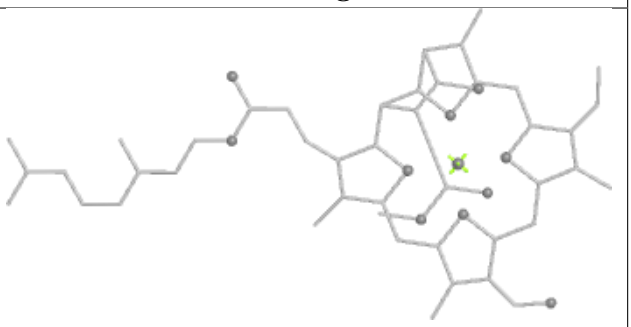
Bond lengths



Bond angles

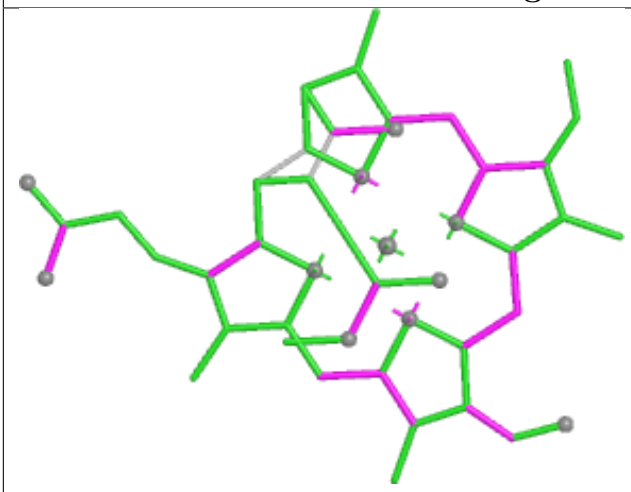


Torsions

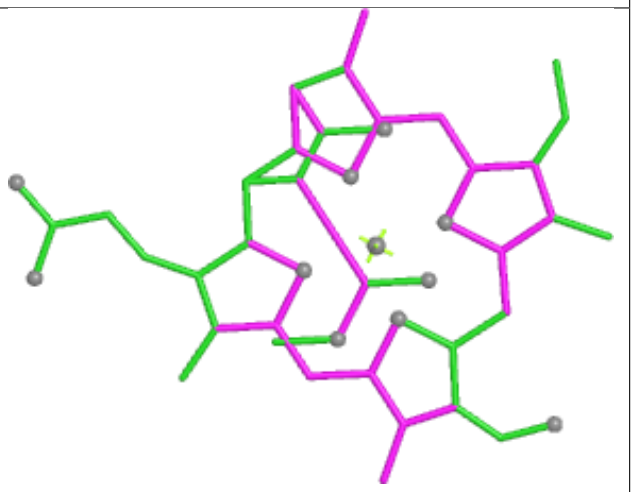


Rings

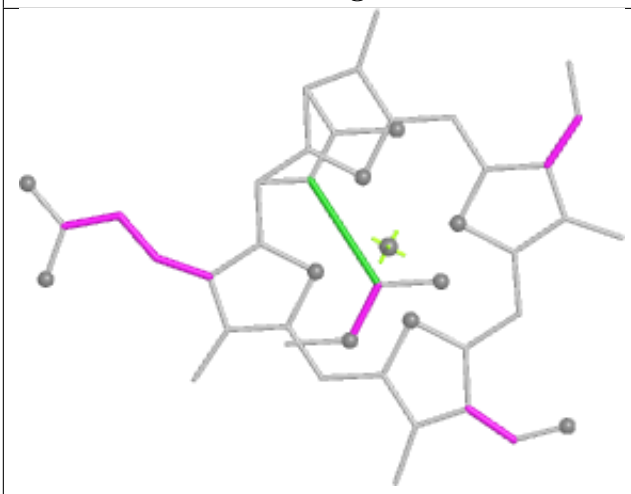
Ligand CL7 11 419



Bond lengths



Bond angles

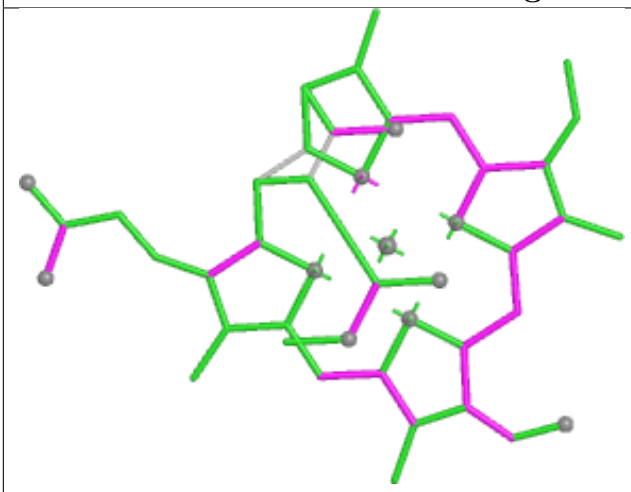


Torsions

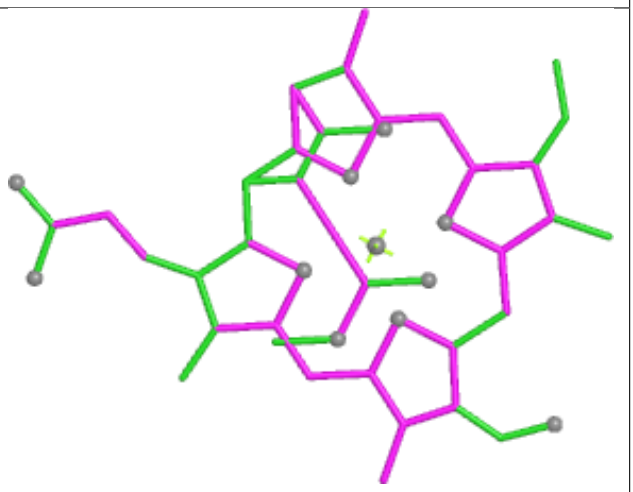


Rings

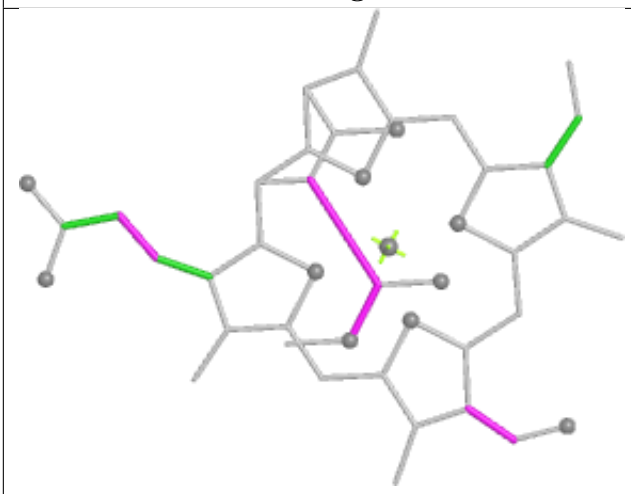
Ligand CL7 31 409



Bond lengths



Bond angles

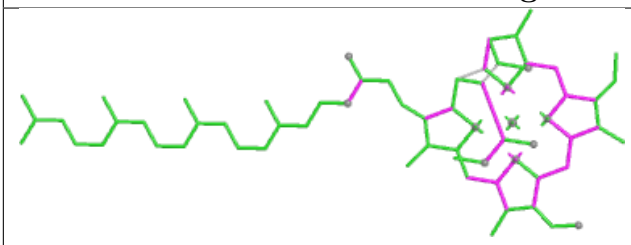


Torsions

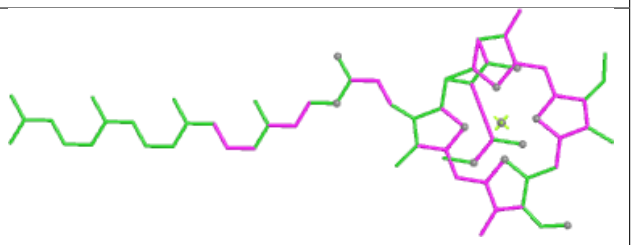


Rings

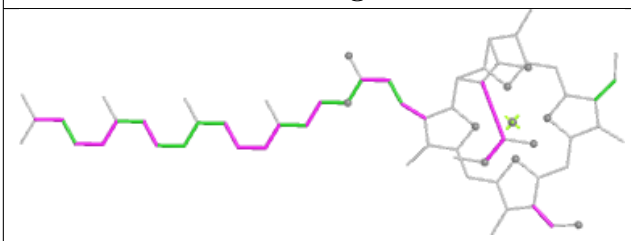
Ligand CL7 3C 509



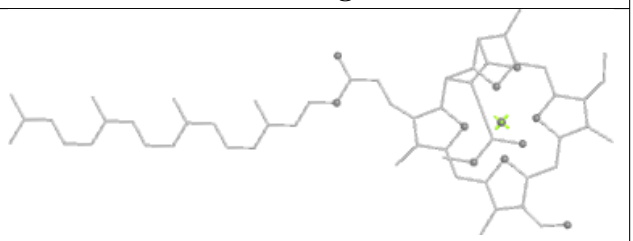
Bond lengths



Bond angles

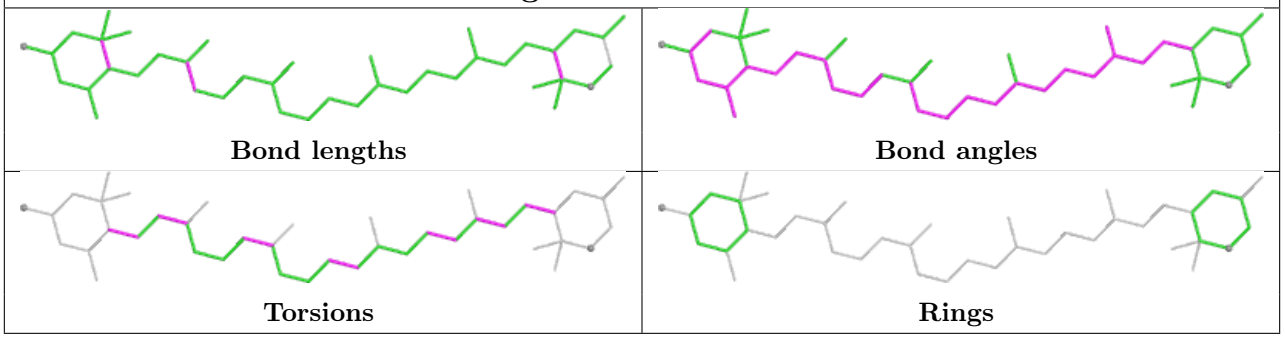


Torsions

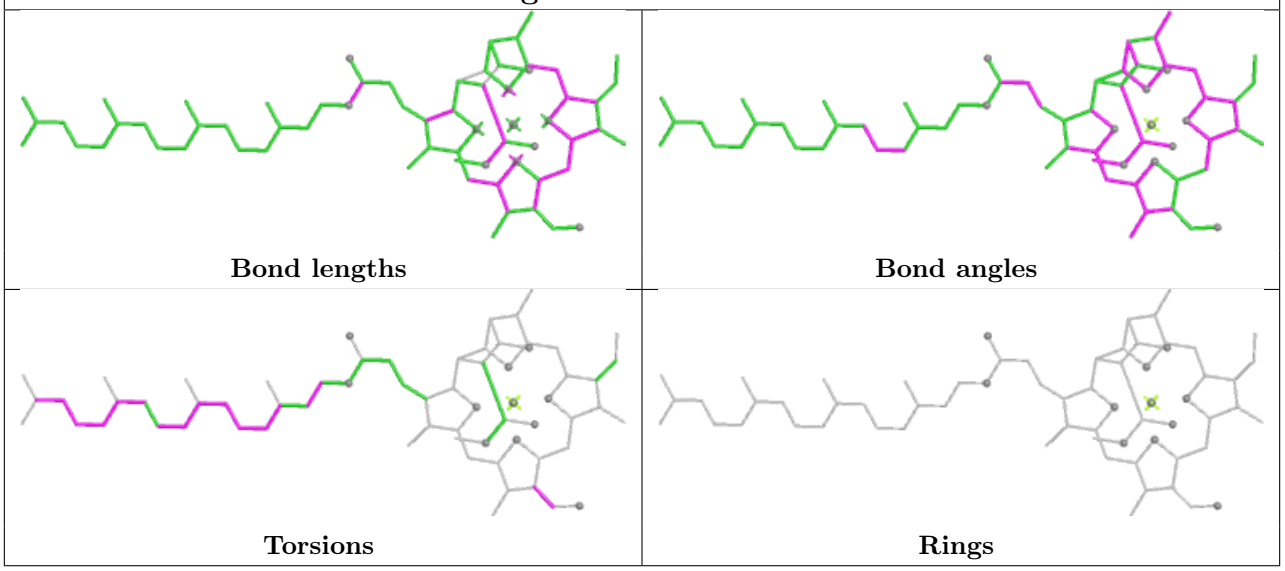


Rings

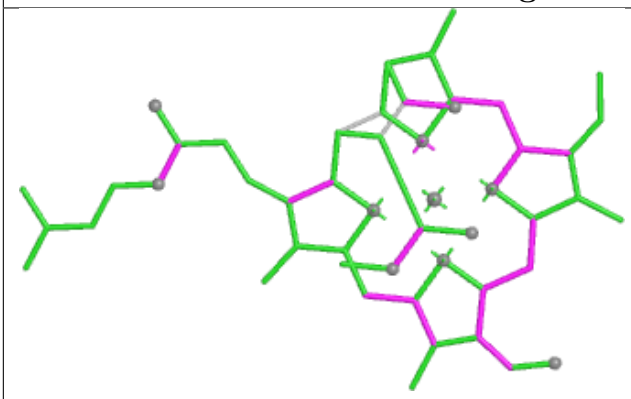
Ligand ZEX 12 519



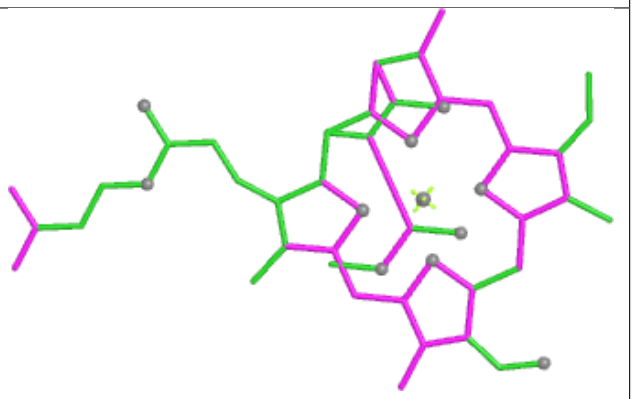
Ligand CL7 2C 507



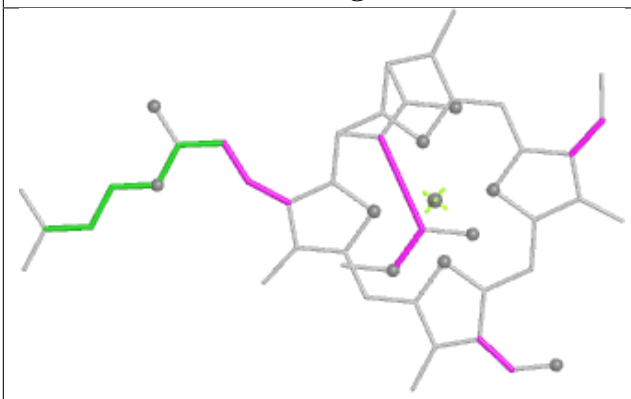
Ligand CL7 3D 402



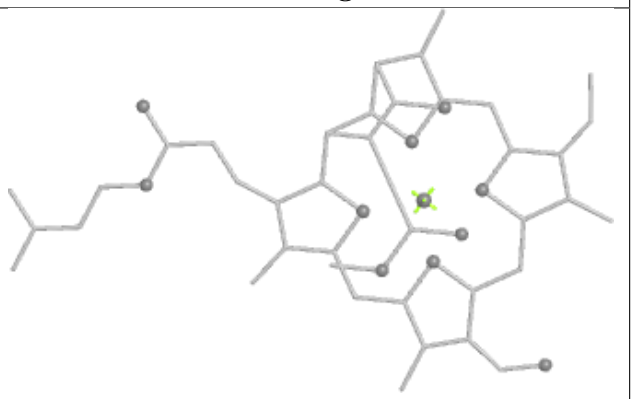
Bond lengths



Bond angles

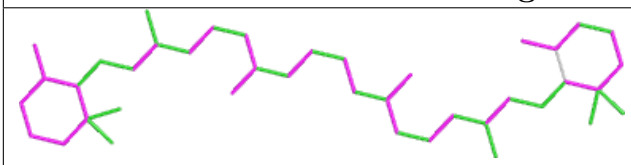


Torsions

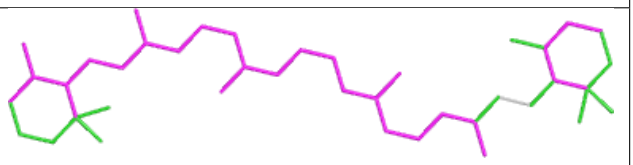


Rings

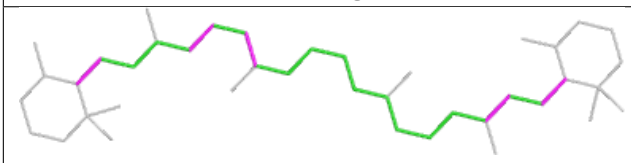
Ligand 8CT 4C 518



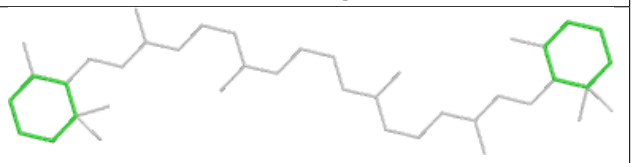
Bond lengths



Bond angles

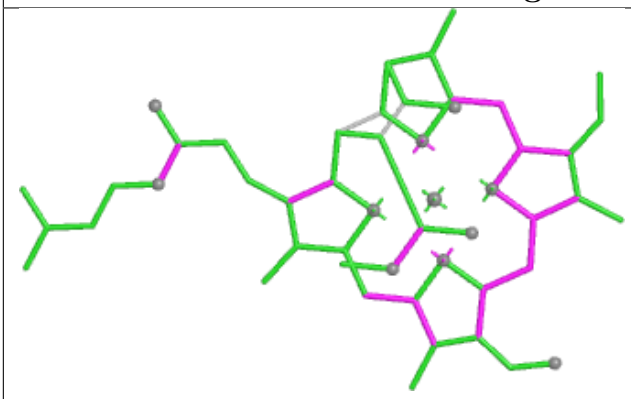


Torsions

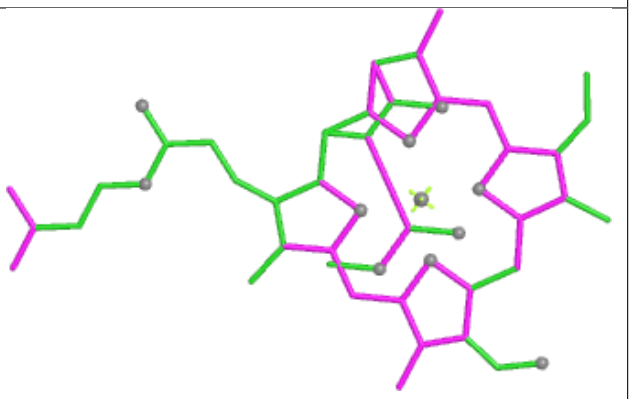


Rings

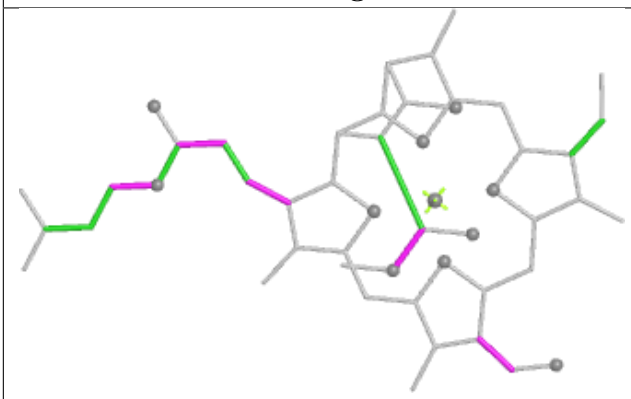
Ligand CL7 13 517



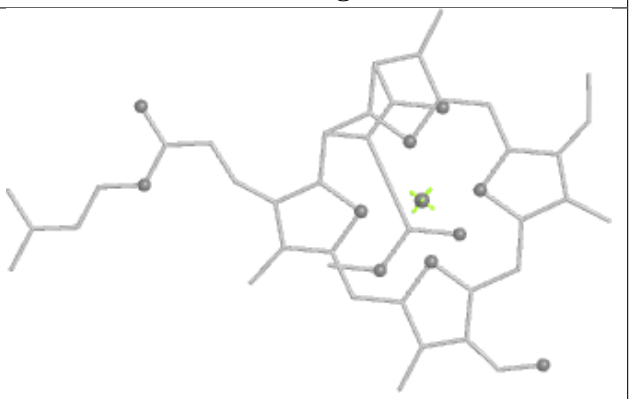
Bond lengths



Bond angles

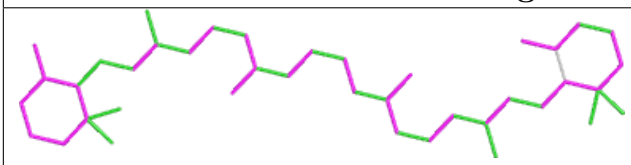


Torsions

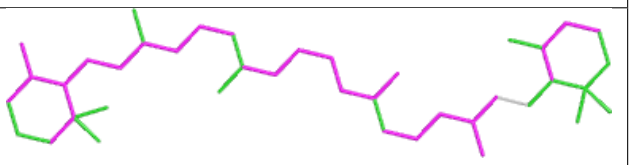


Rings

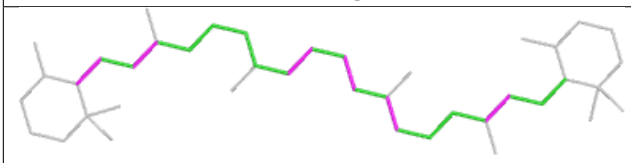
Ligand 8CT 1D 406



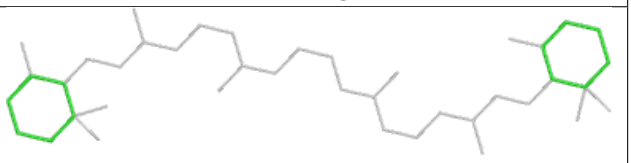
Bond lengths



Bond angles

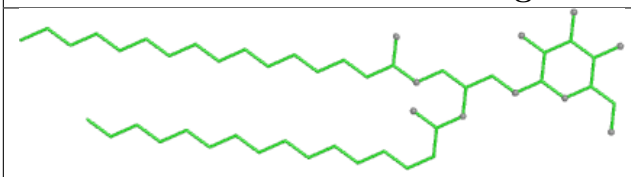


Torsions

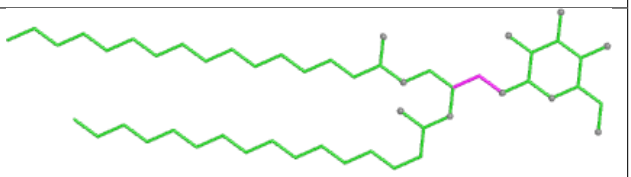


Rings

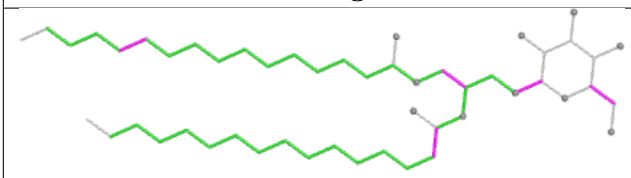
Ligand LMG 21 401



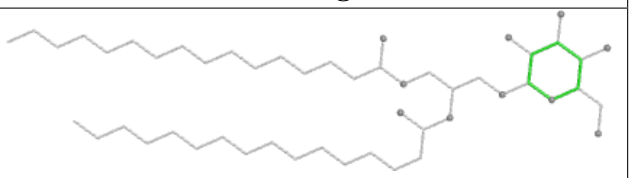
Bond lengths



Bond angles

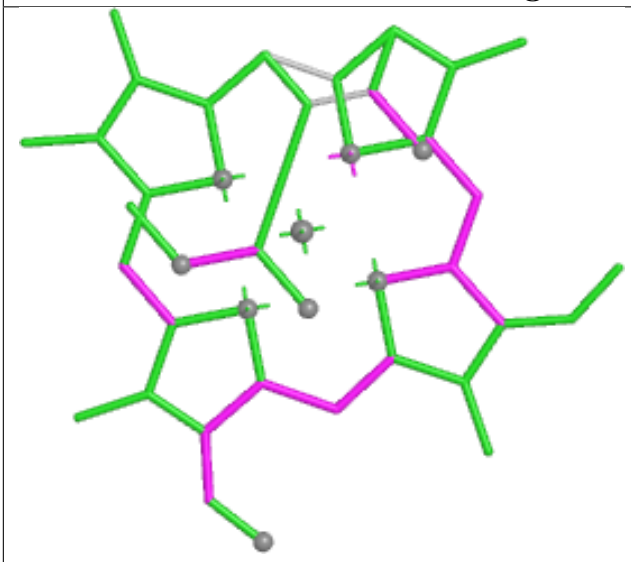


Torsions

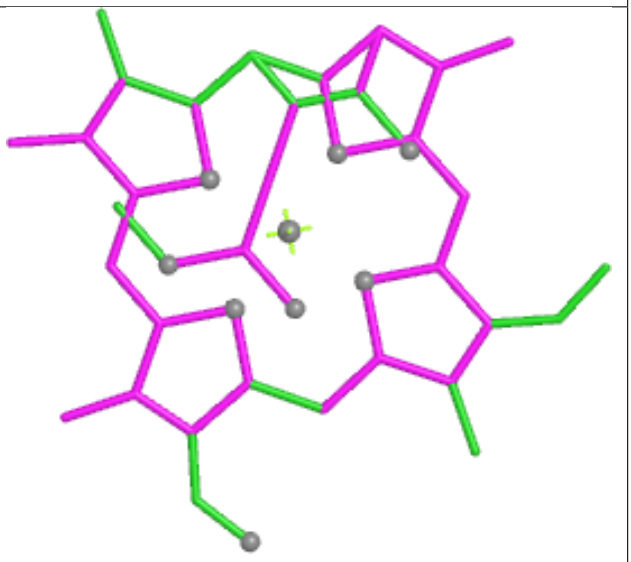


Rings

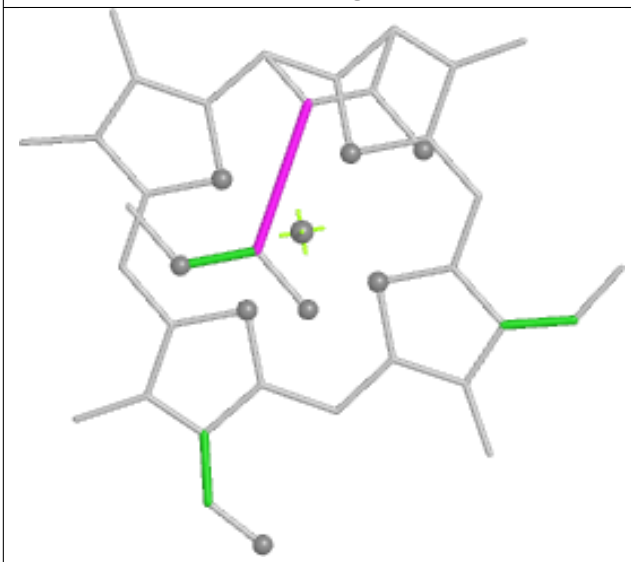
Ligand CL7 41 413



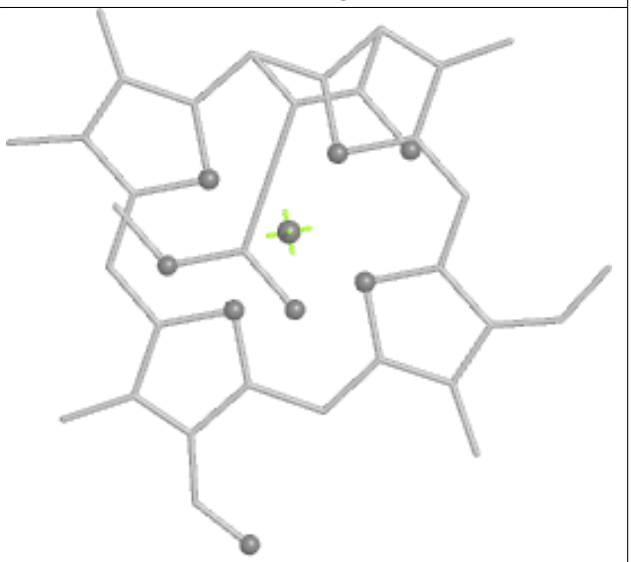
Bond lengths



Bond angles

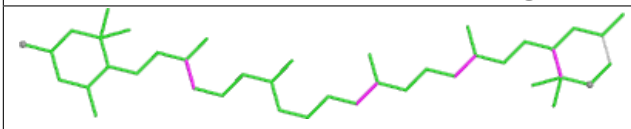


Torsions

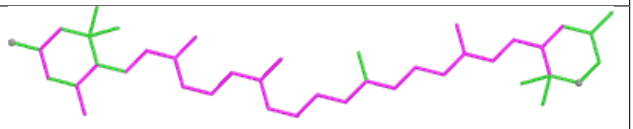


Rings

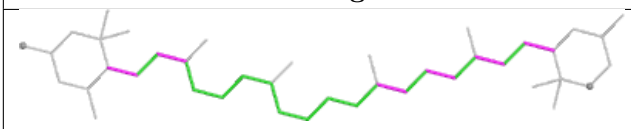
Ligand ZEX 43 420



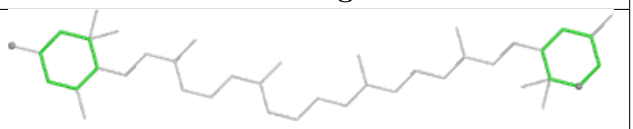
Bond lengths



Bond angles

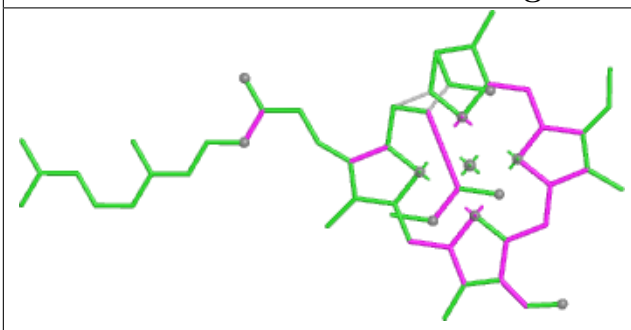


Torsions

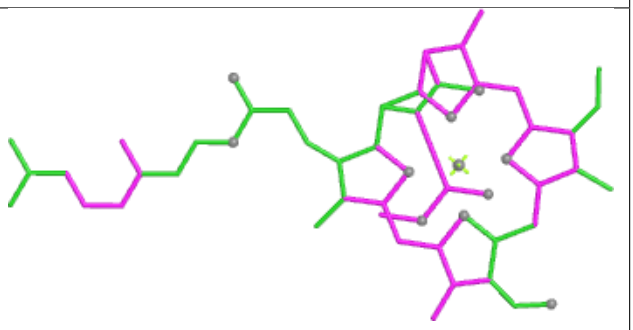


Rings

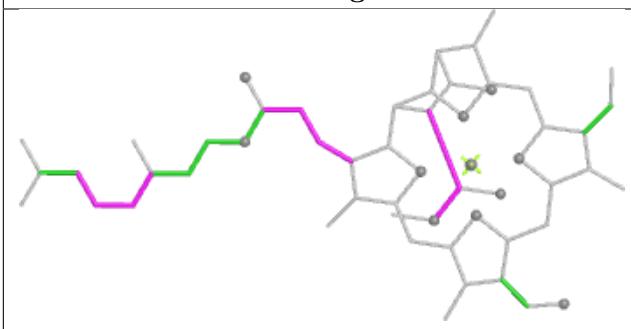
Ligand CL7 43 413



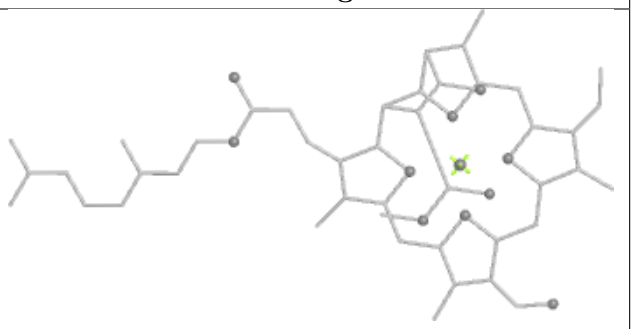
Bond lengths



Bond angles

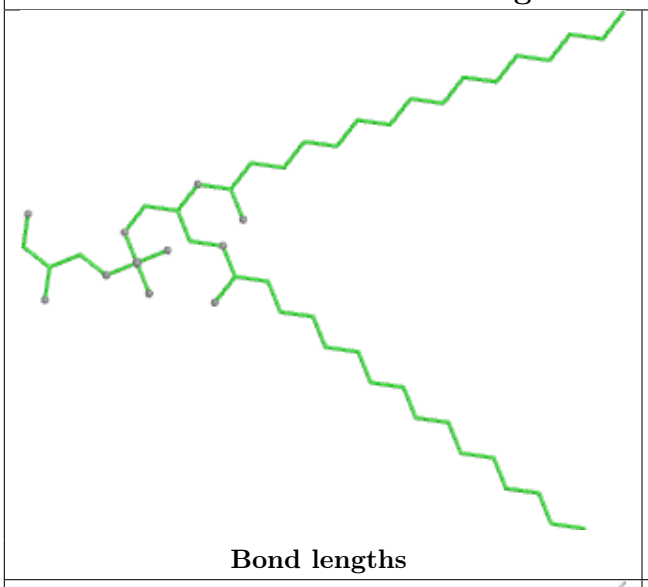


Torsions

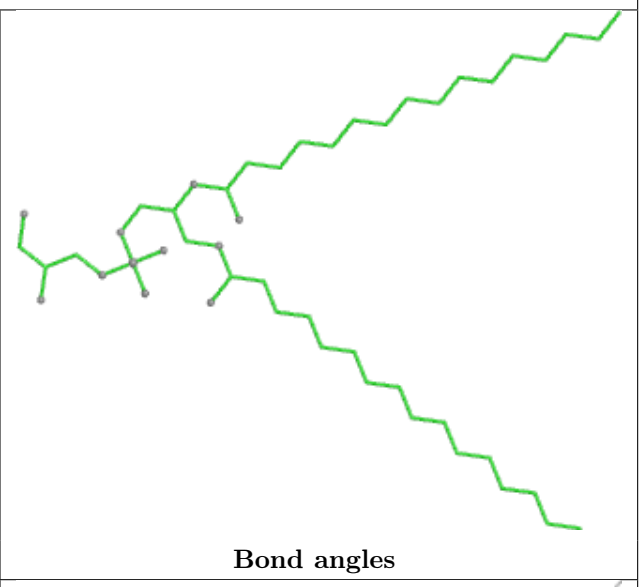


Rings

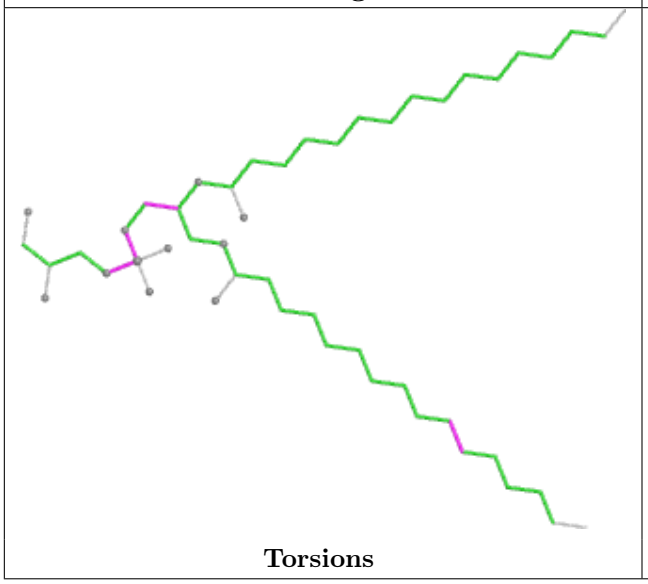
Ligand LHG 3D 409



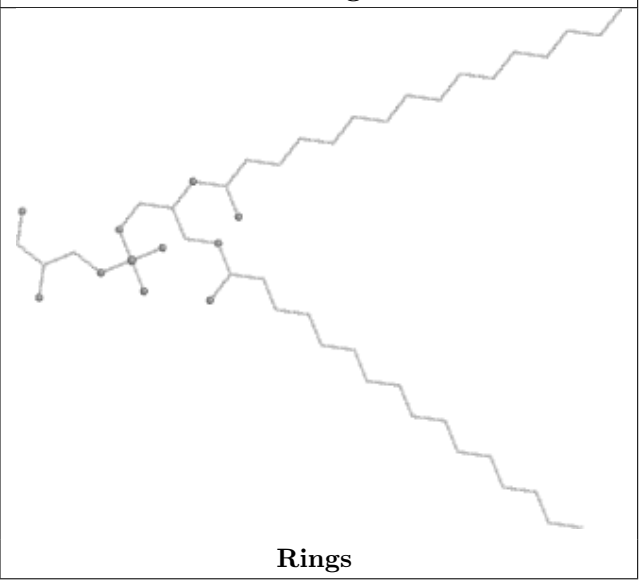
Bond lengths



Bond angles

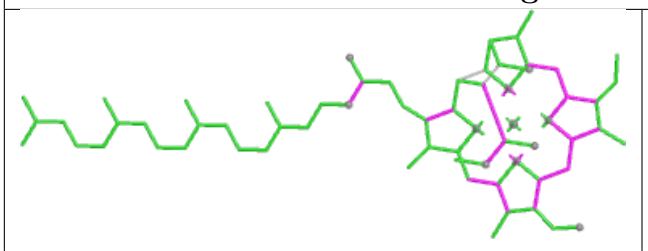


Torsions

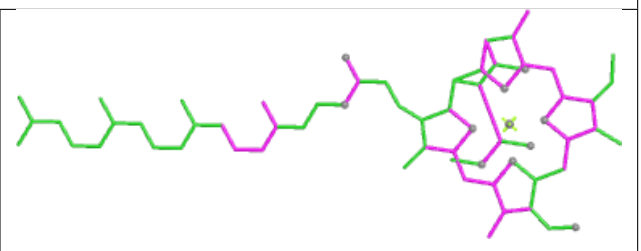


Rings

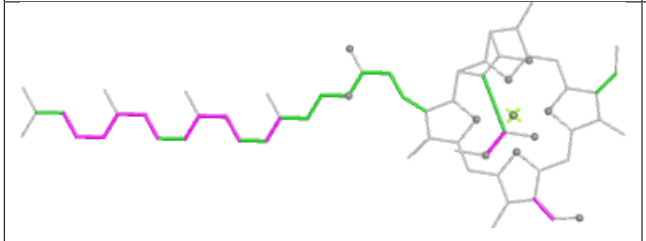
Ligand CL7 1B 611



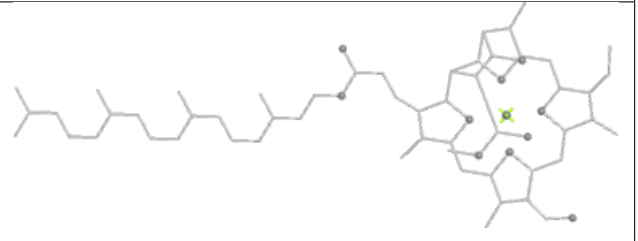
Bond lengths



Bond angles

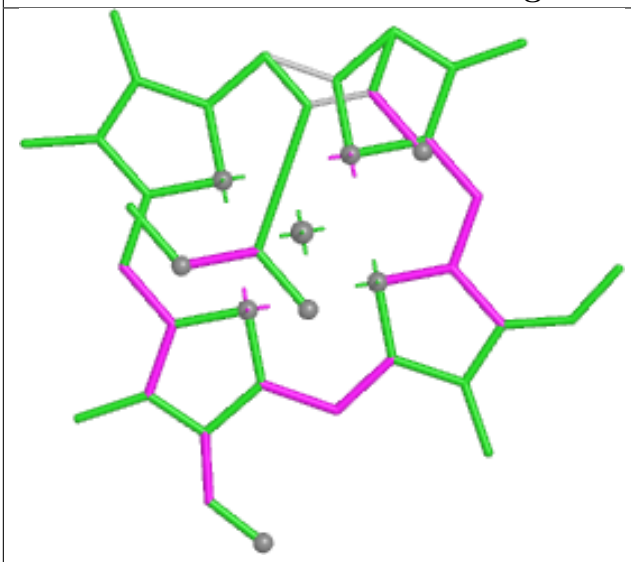


Torsions

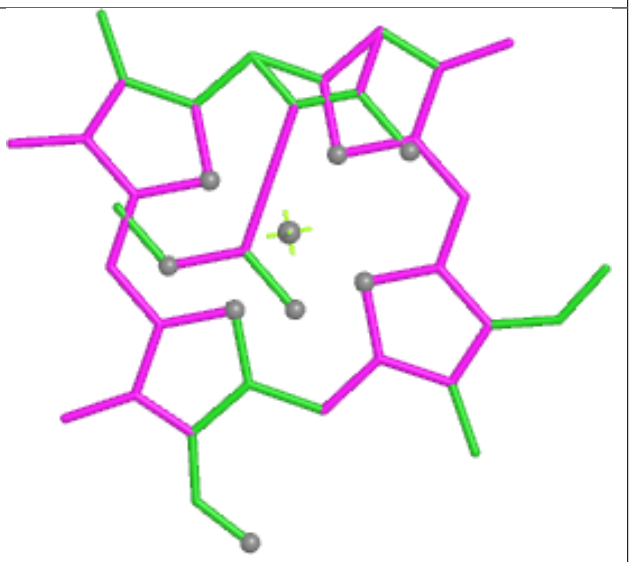


Rings

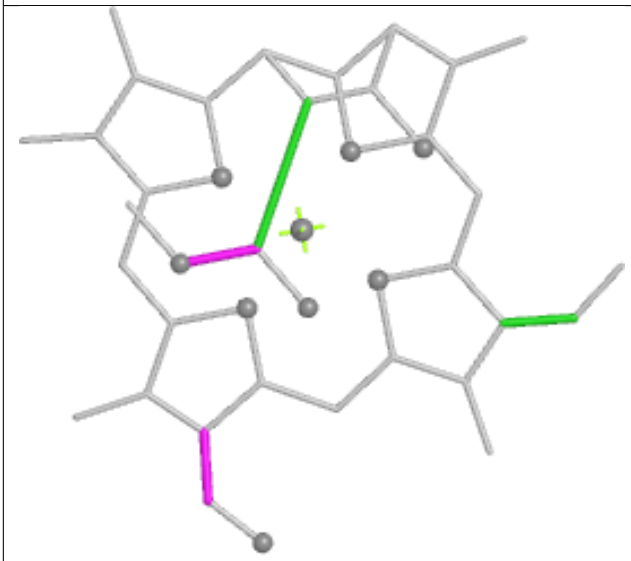
Ligand CL7 11 416



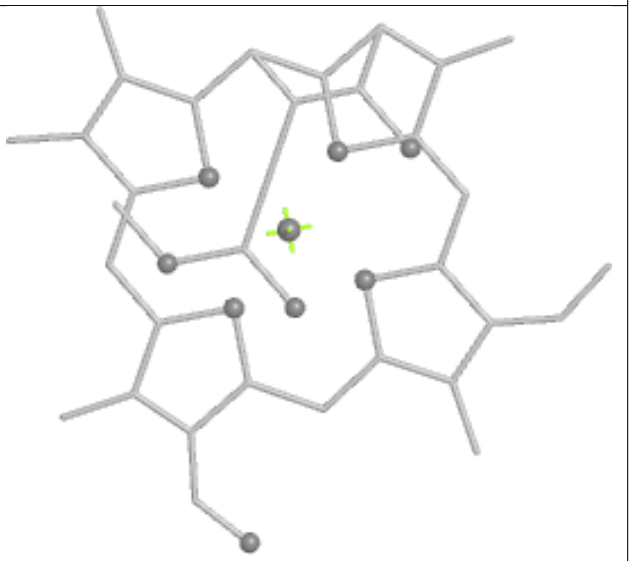
Bond lengths



Bond angles

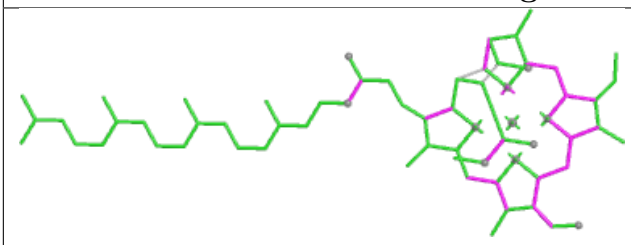


Torsions

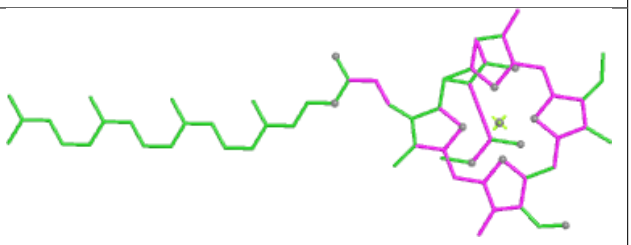


Rings

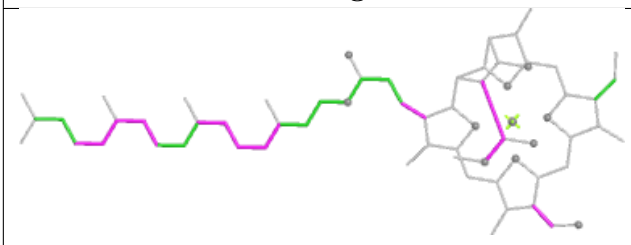
Ligand CL7 1B 605



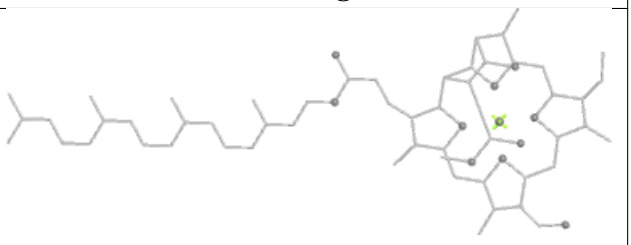
Bond lengths



Bond angles

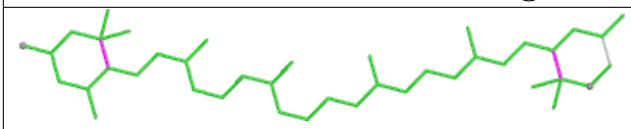


Torsions

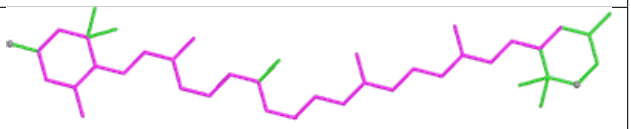


Rings

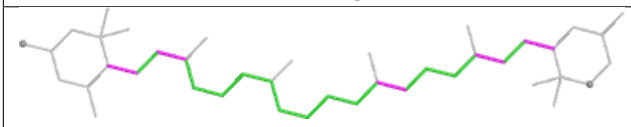
Ligand ZEX 23 421



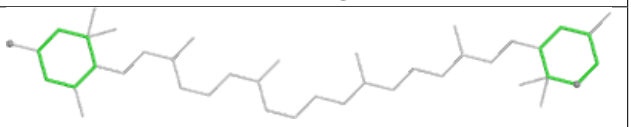
Bond lengths



Bond angles

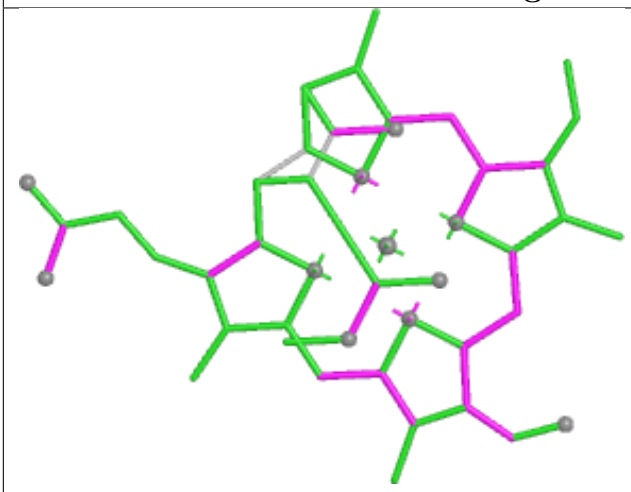


Torsions

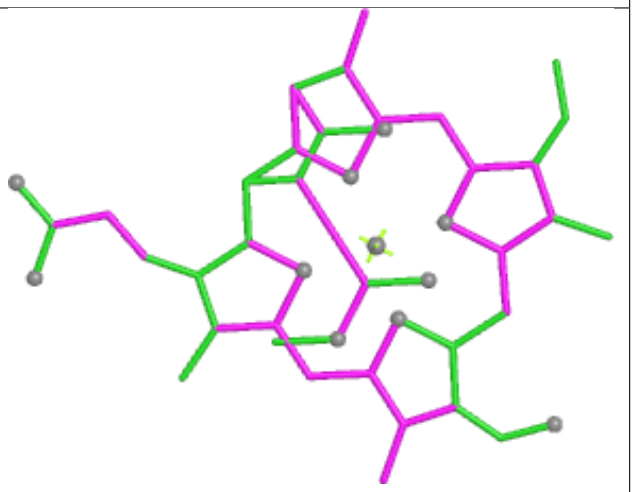


Rings

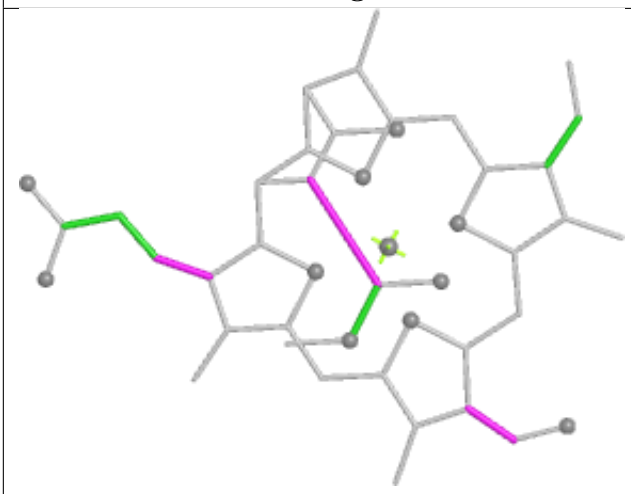
Ligand CL7 32 515



Bond lengths



Bond angles

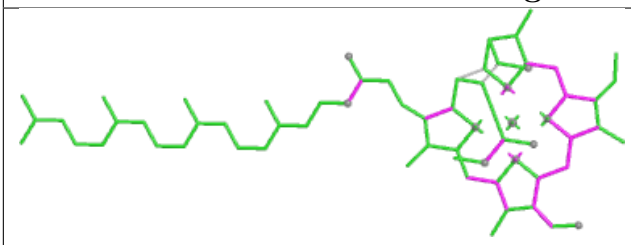


Torsions

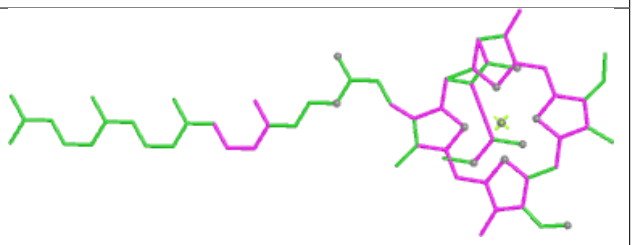


Rings

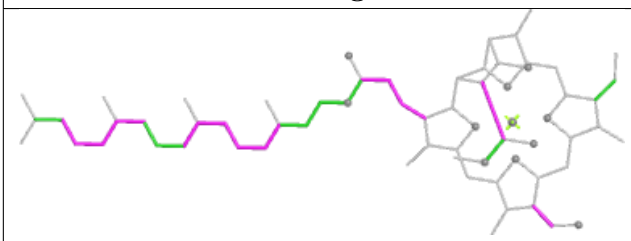
Ligand CL7 23 402



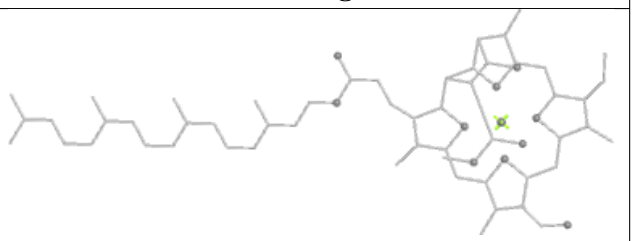
Bond lengths



Bond angles

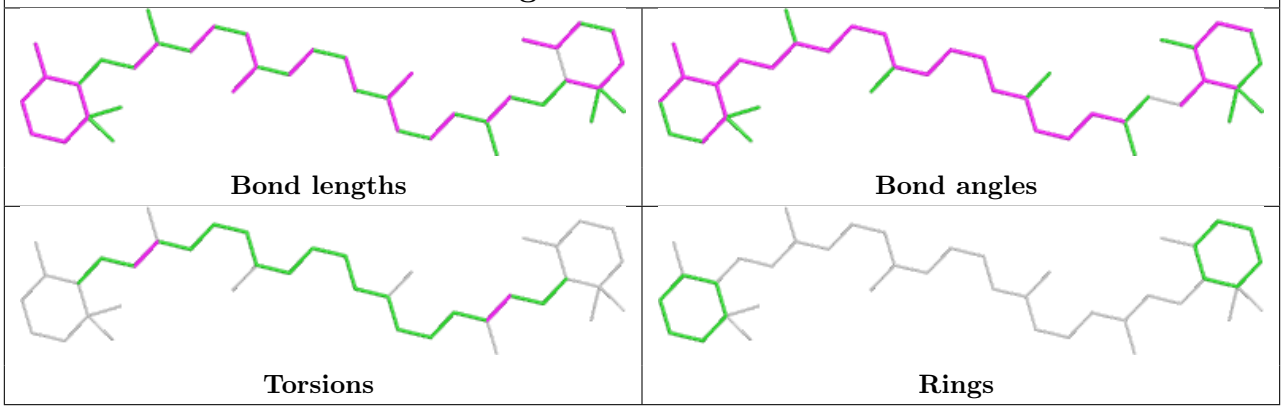


Torsions

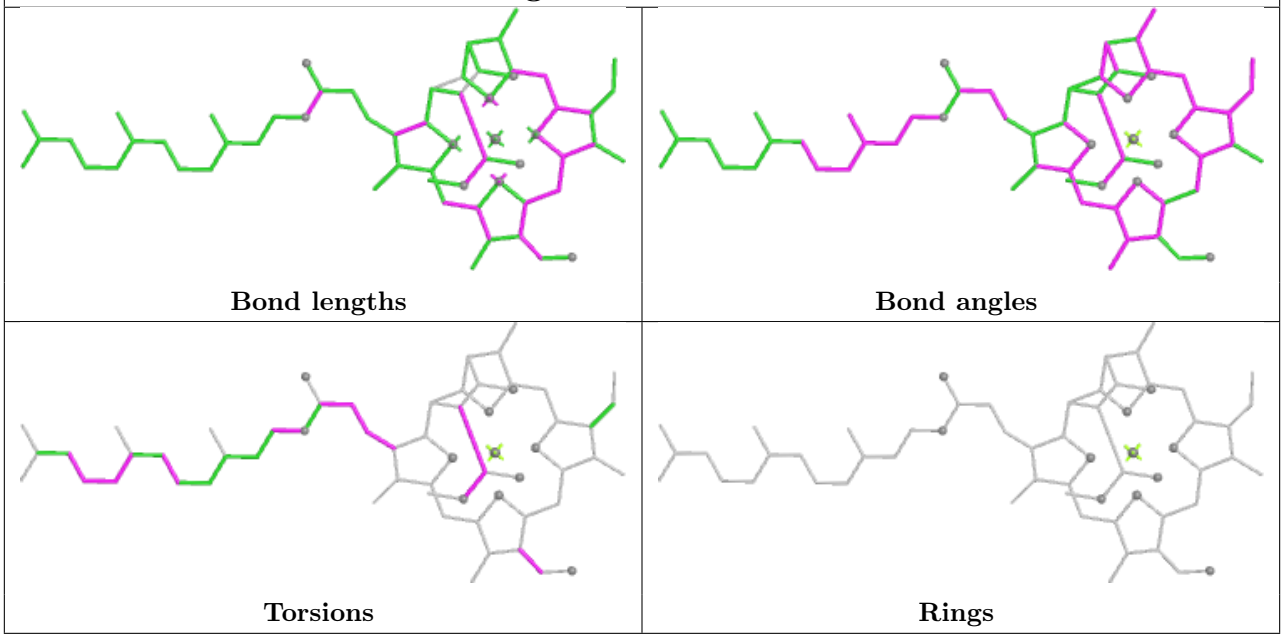


Rings

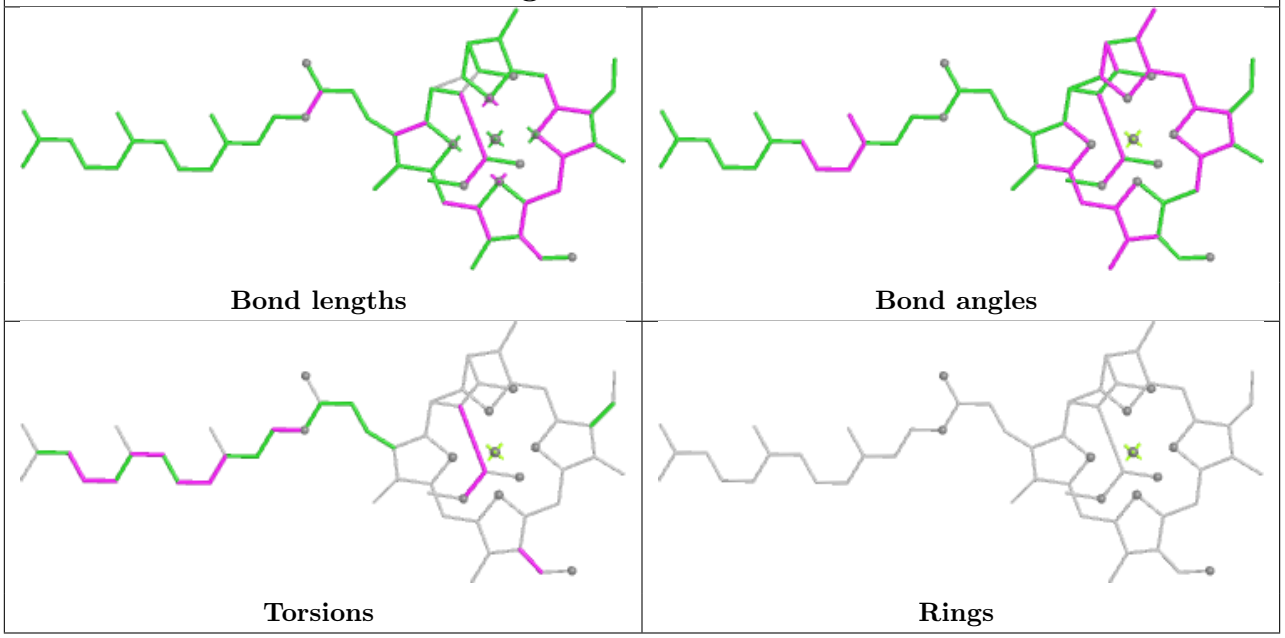
Ligand 8CT 3B 619



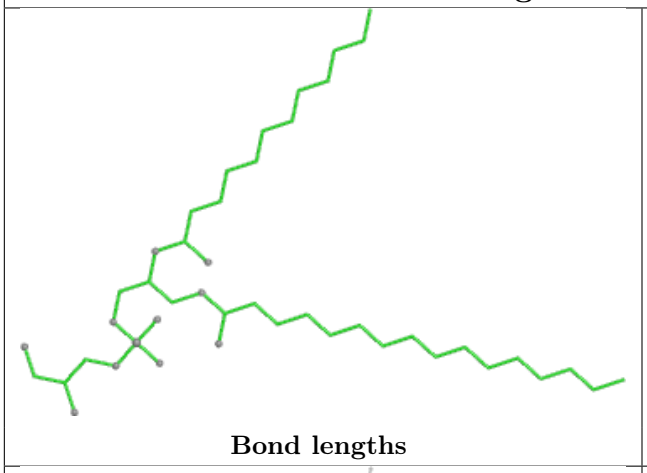
Ligand CL7 14 409



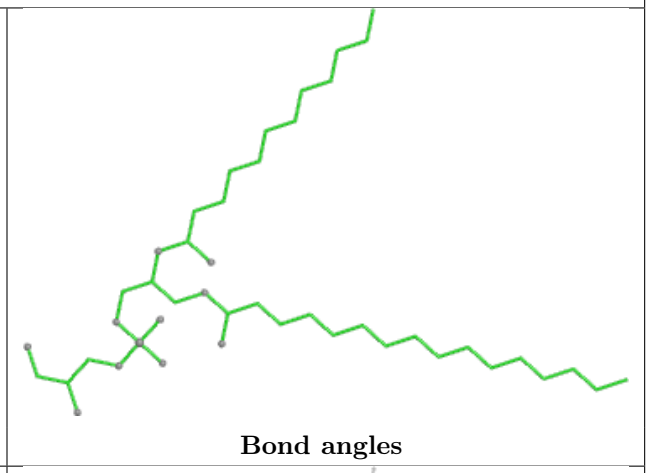
Ligand CL7 2C 502



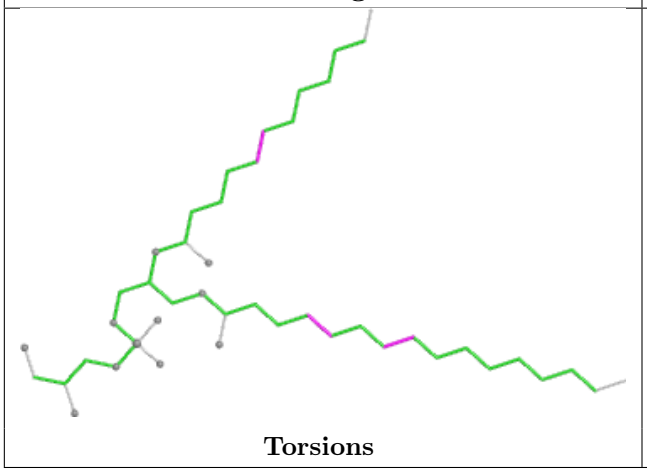
Ligand LHG 1B 623



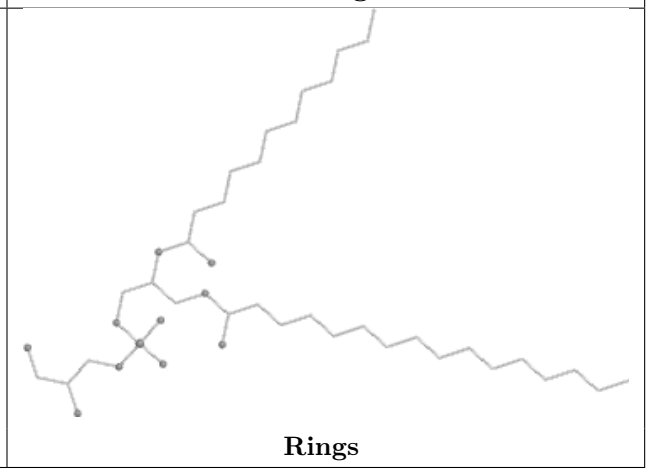
Bond lengths



Bond angles

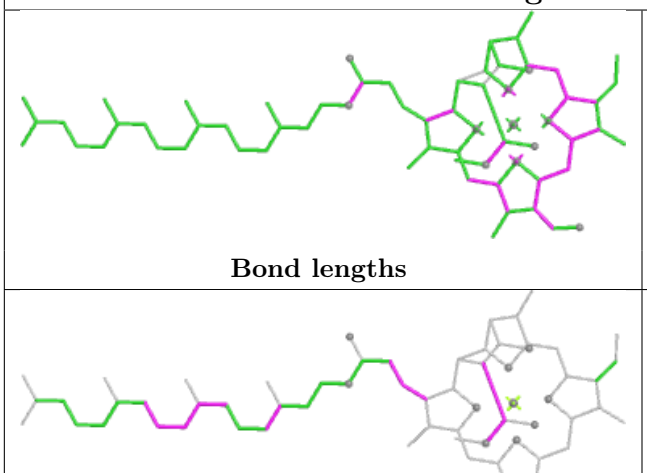


Torsions

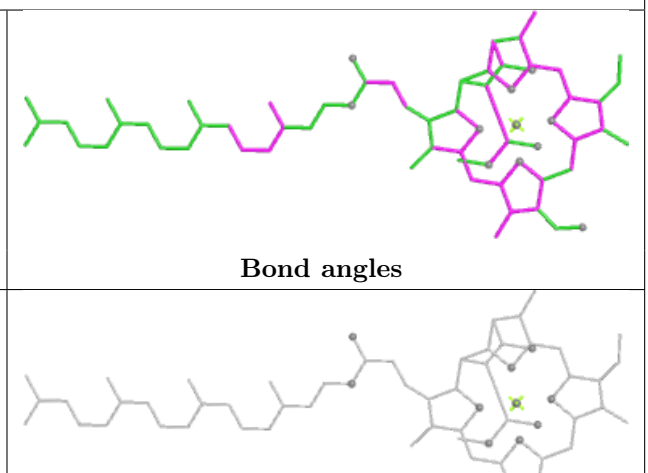


Rings

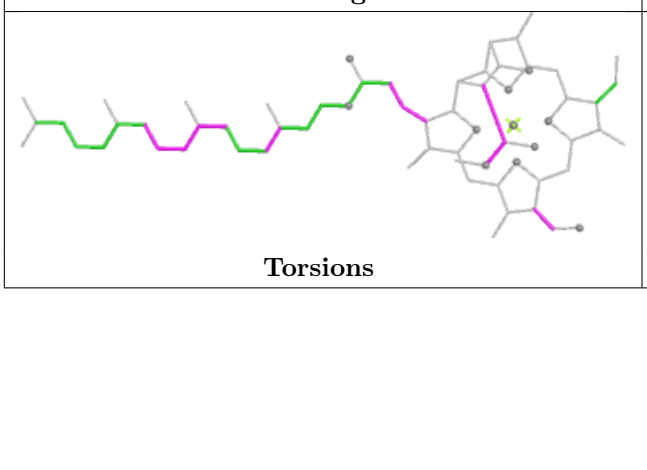
Ligand CL7 32 502



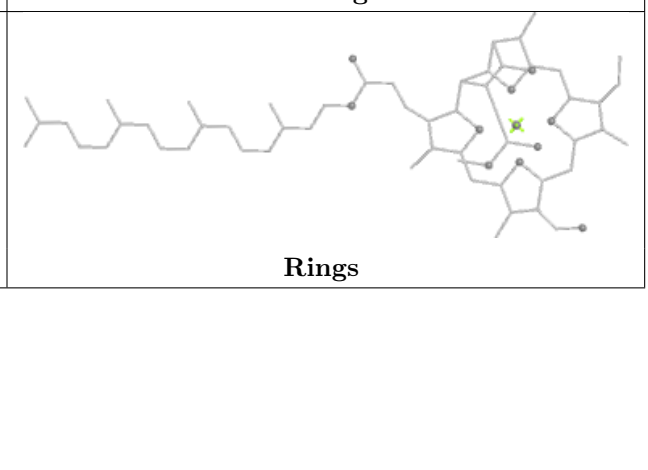
Bond lengths



Bond angles

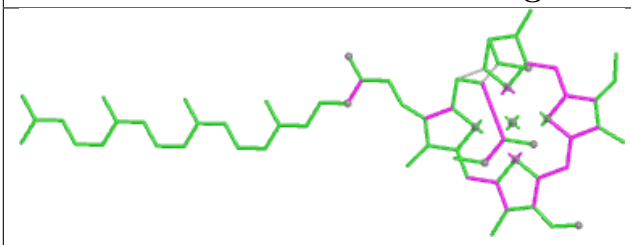


Torsions

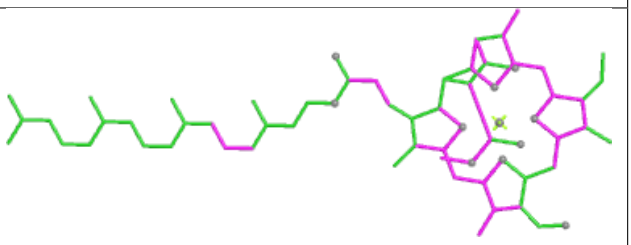


Rings

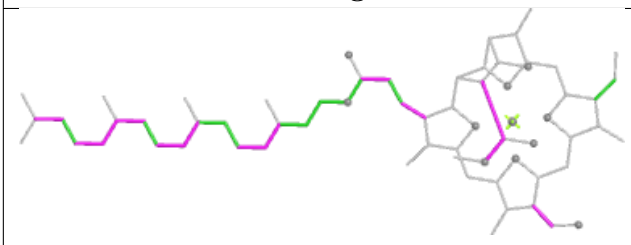
Ligand CL7 42 507



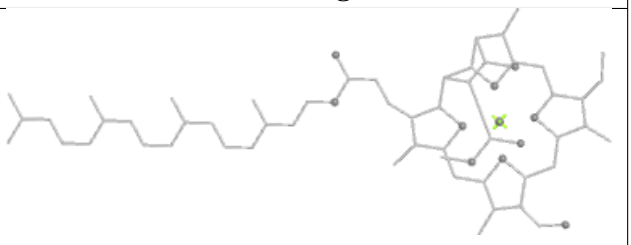
Bond lengths



Bond angles

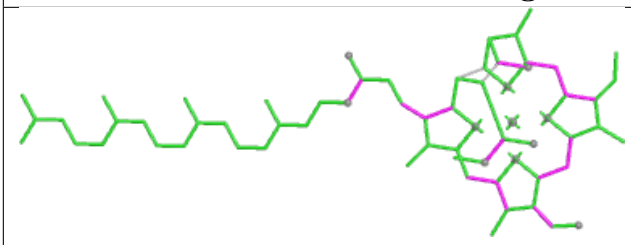


Torsions

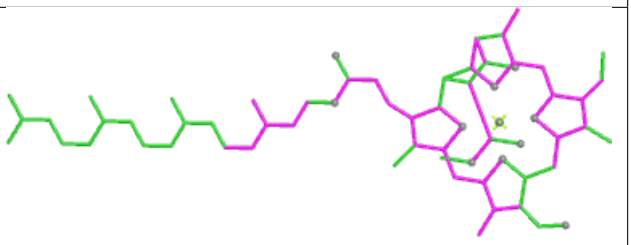


Rings

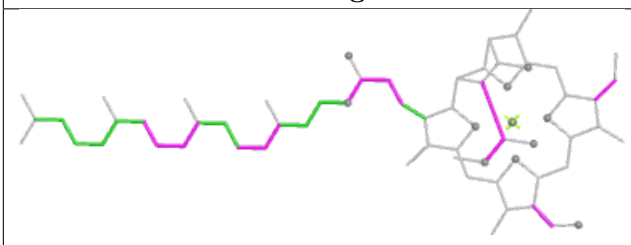
Ligand CL7 2A 401



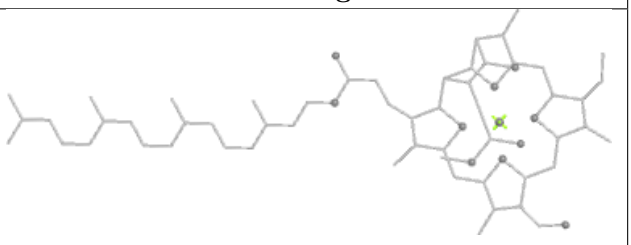
Bond lengths



Bond angles

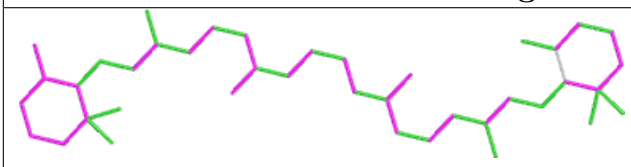


Torsions

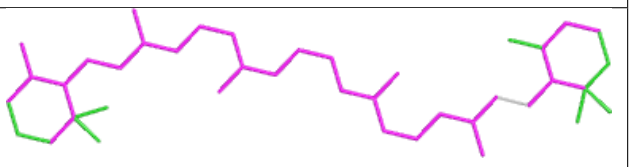


Rings

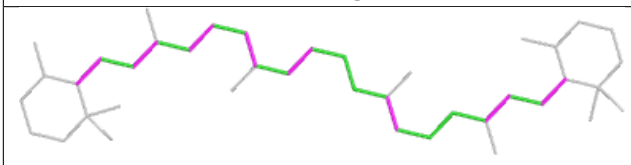
Ligand 8CT 1C 514



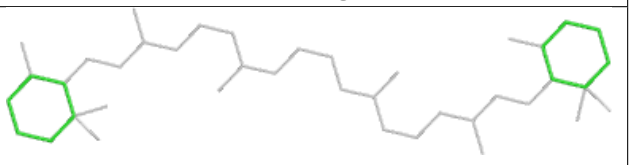
Bond lengths



Bond angles

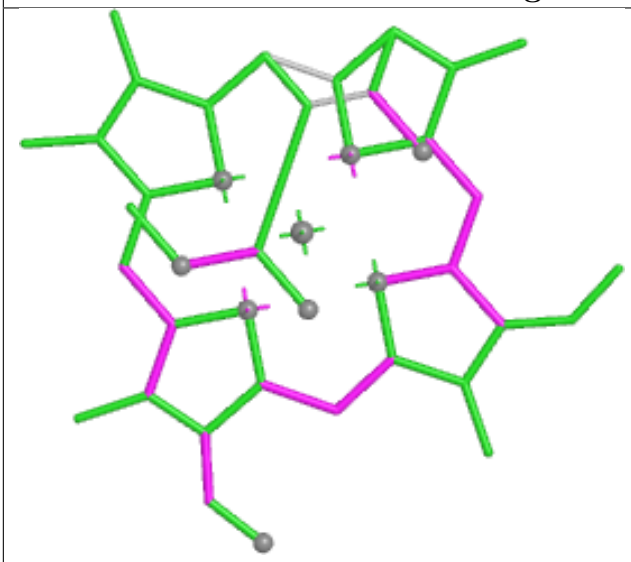


Torsions

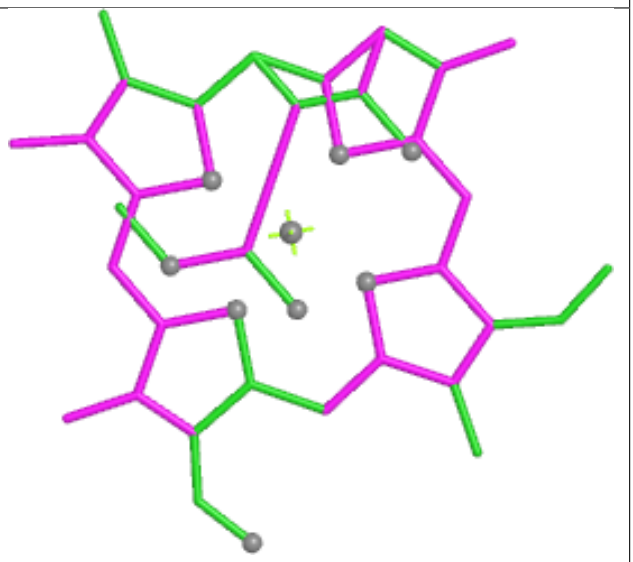


Rings

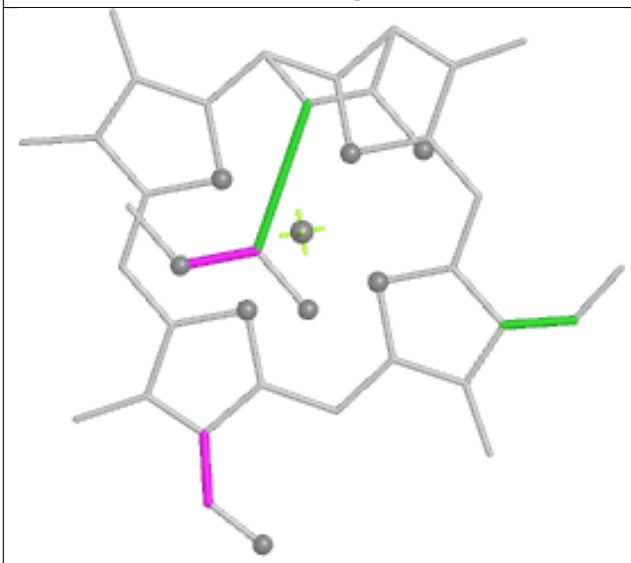
Ligand CL7 41 416



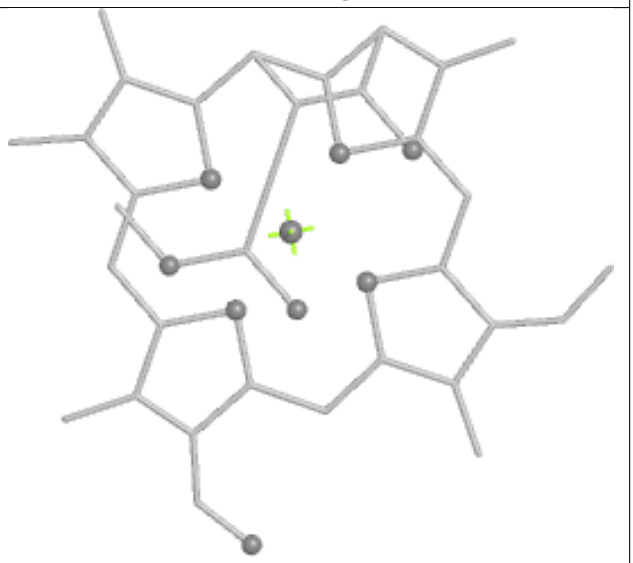
Bond lengths



Bond angles

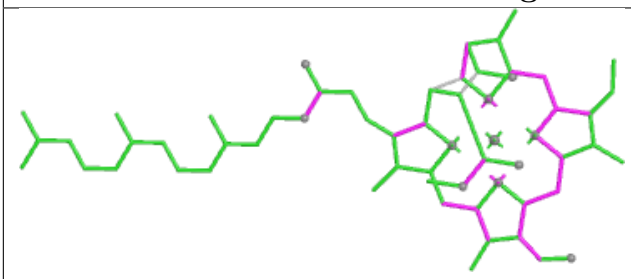


Torsions

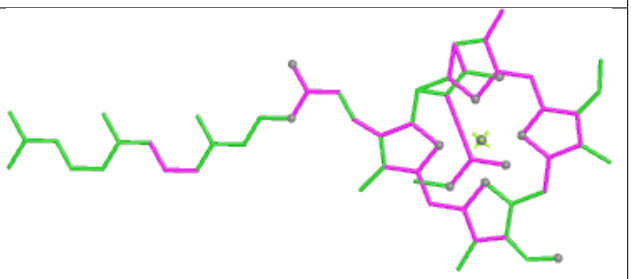


Rings

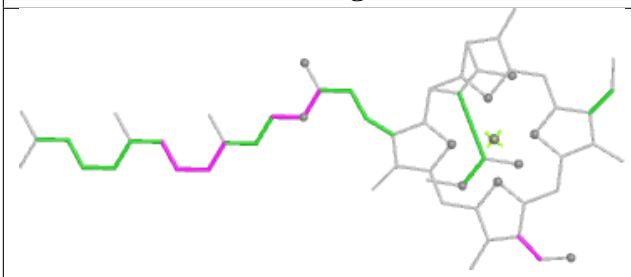
Ligand CL7 3B 602



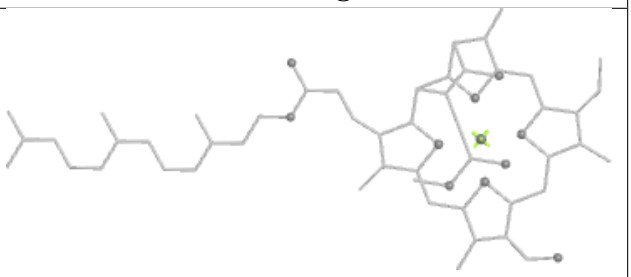
Bond lengths



Bond angles

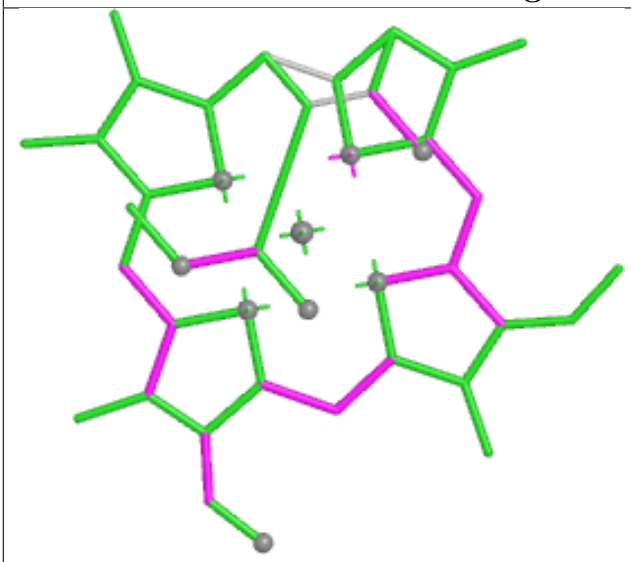


Torsions

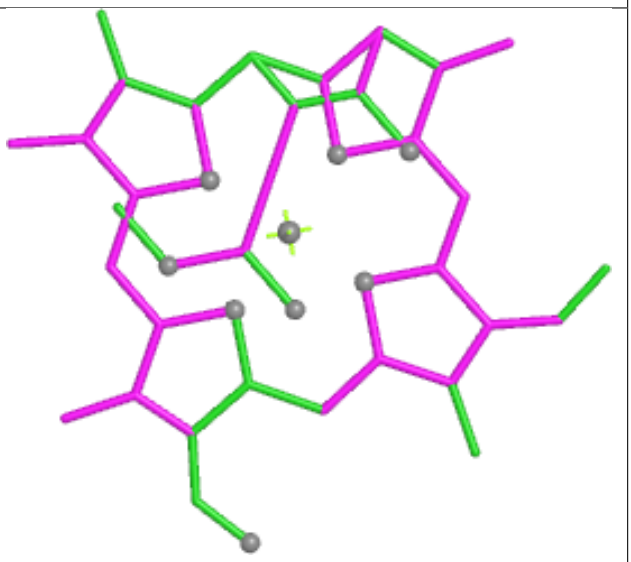


Rings

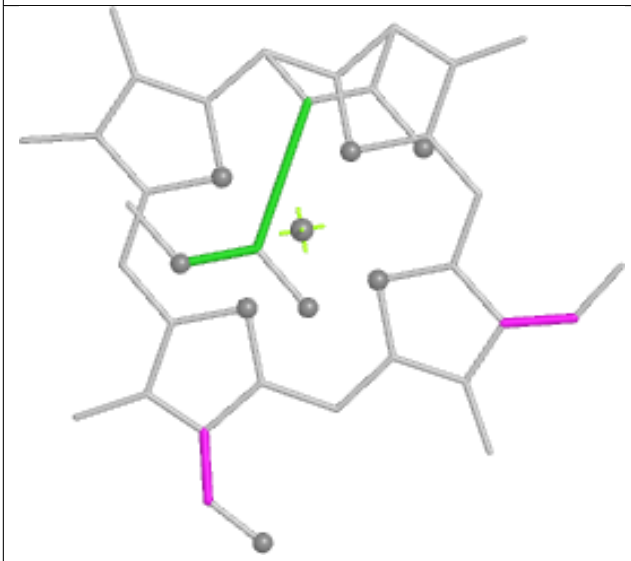
Ligand CL7 41 414



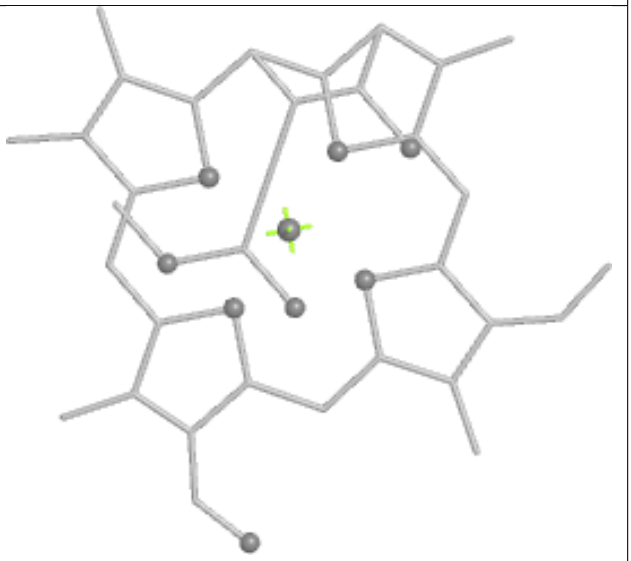
Bond lengths



Bond angles

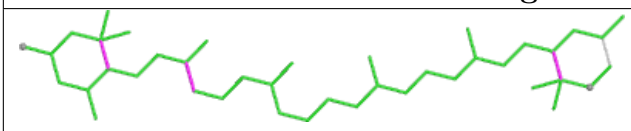


Torsions

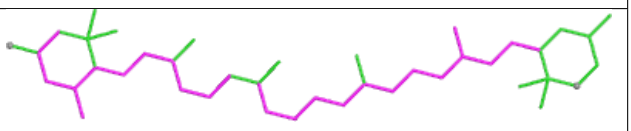


Rings

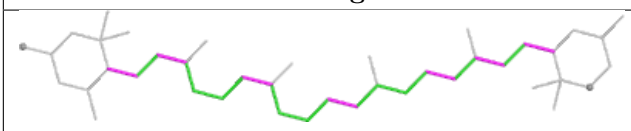
Ligand ZEX 42 519



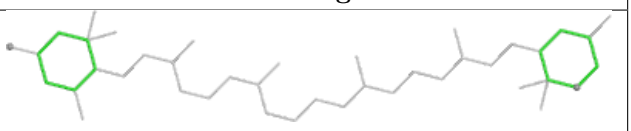
Bond lengths



Bond angles

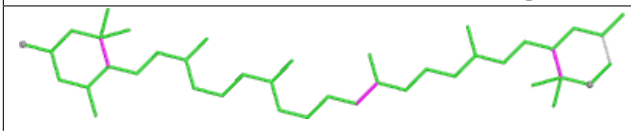


Torsions

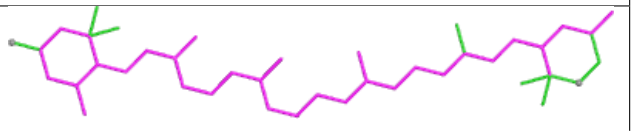


Rings

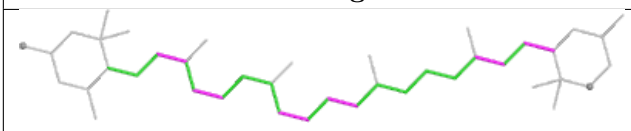
Ligand ZEX 24 419



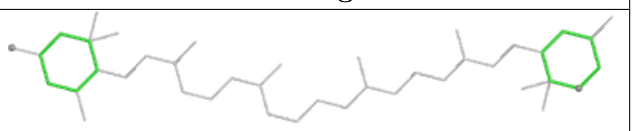
Bond lengths



Bond angles

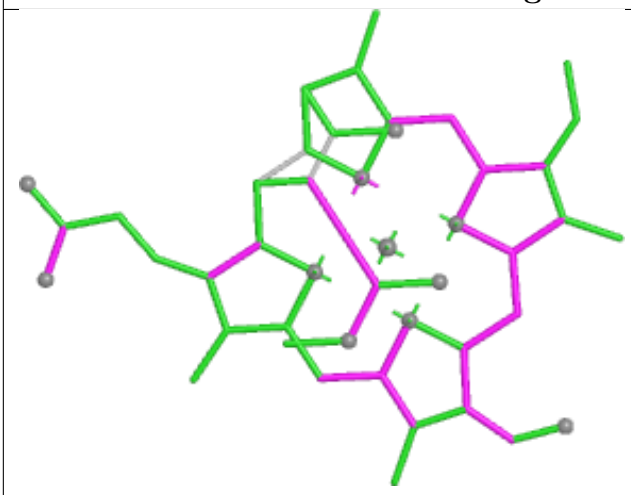


Torsions

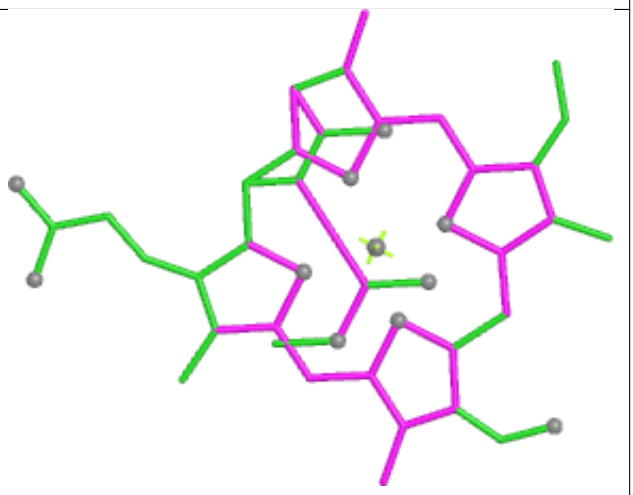


Rings

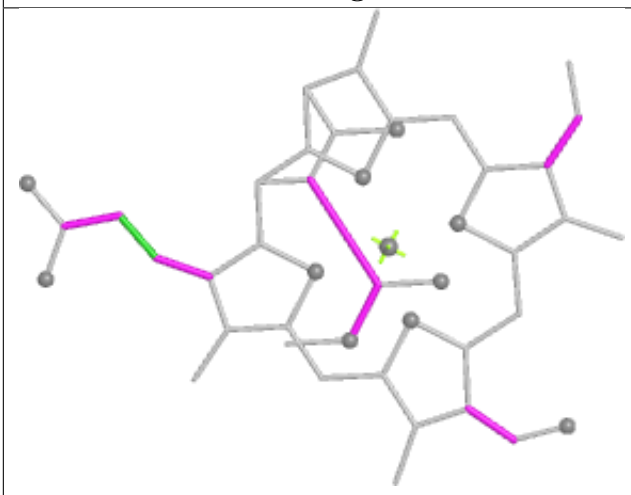
Ligand CL7 13 506



Bond lengths



Bond angles

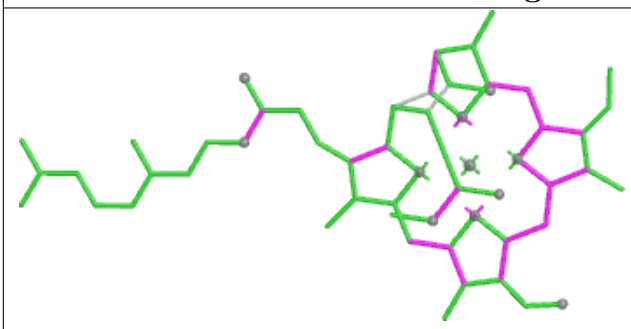


Torsions

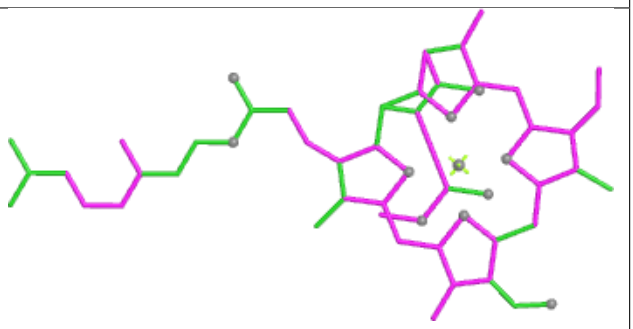


Rings

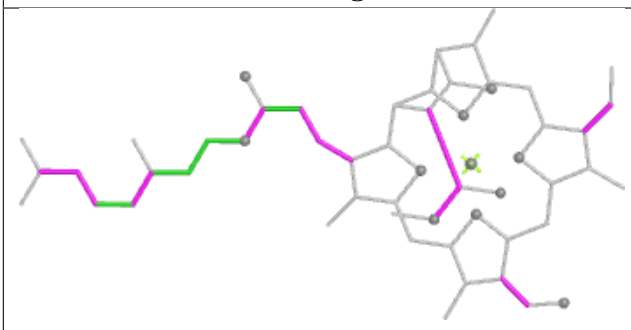
Ligand CL7 33 516



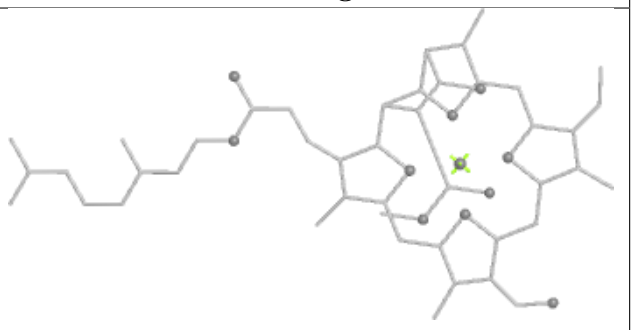
Bond lengths



Bond angles

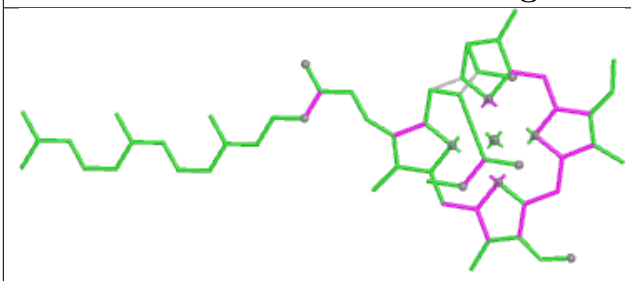


Torsions

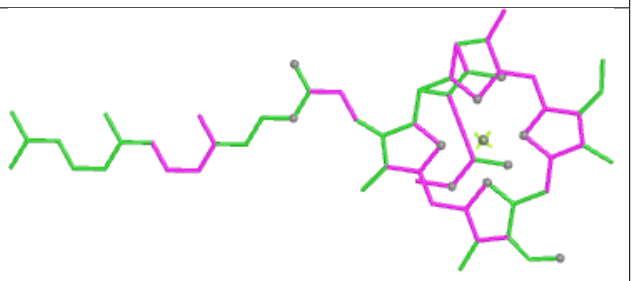


Rings

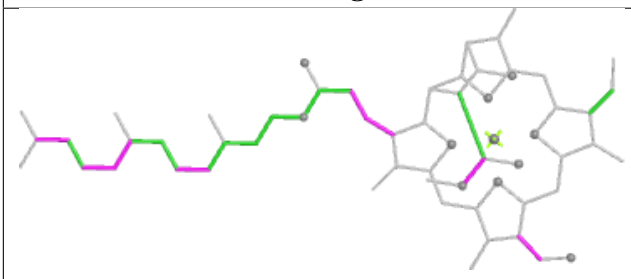
Ligand CL7 4B 608



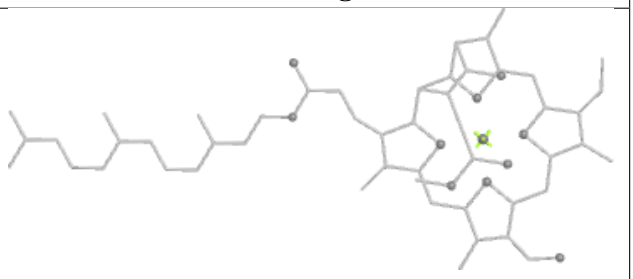
Bond lengths



Bond angles

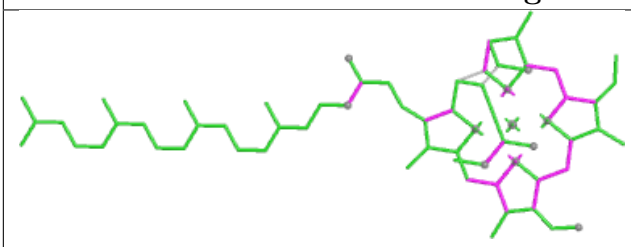


Torsions

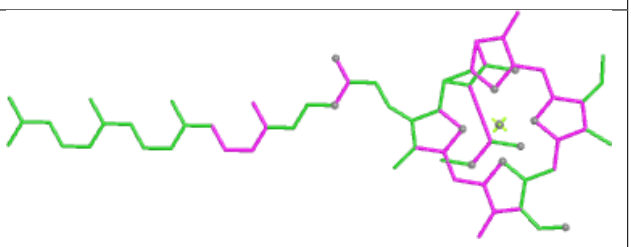


Rings

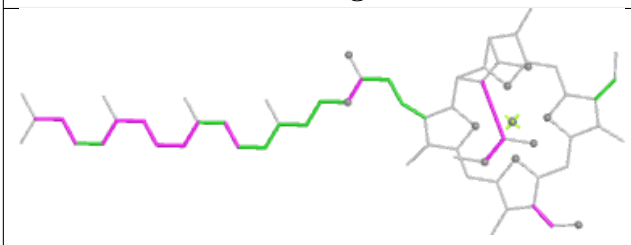
Ligand CL7 13 509



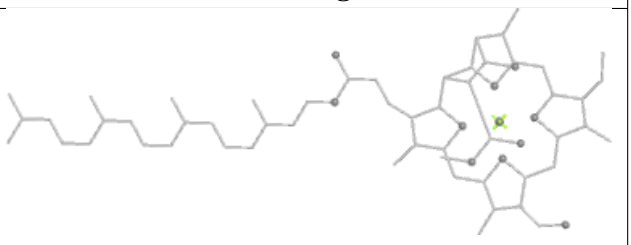
Bond lengths



Bond angles

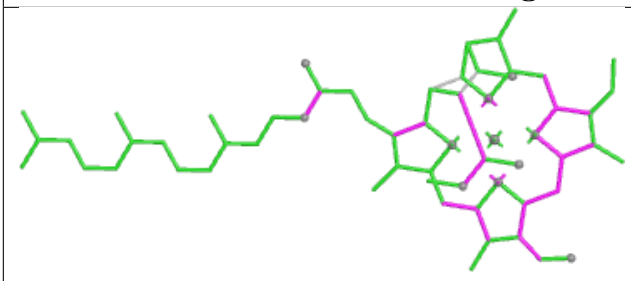


Torsions

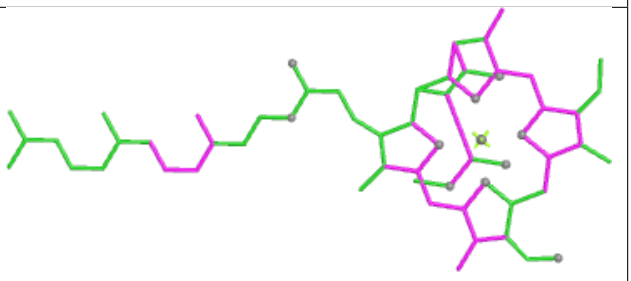


Rings

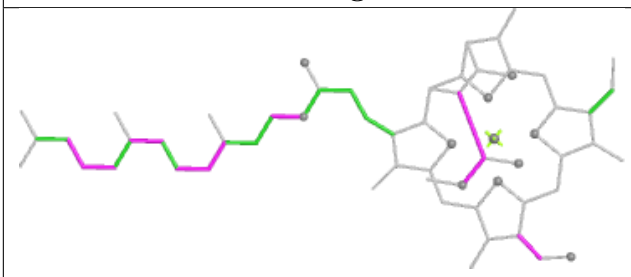
Ligand CL7 3C 502



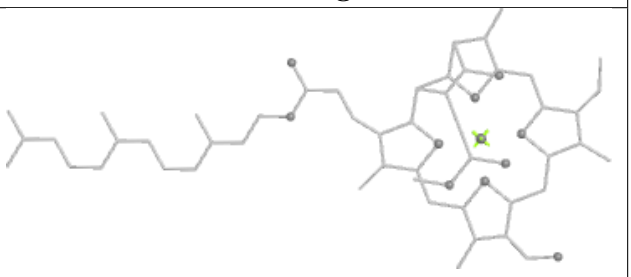
Bond lengths



Bond angles

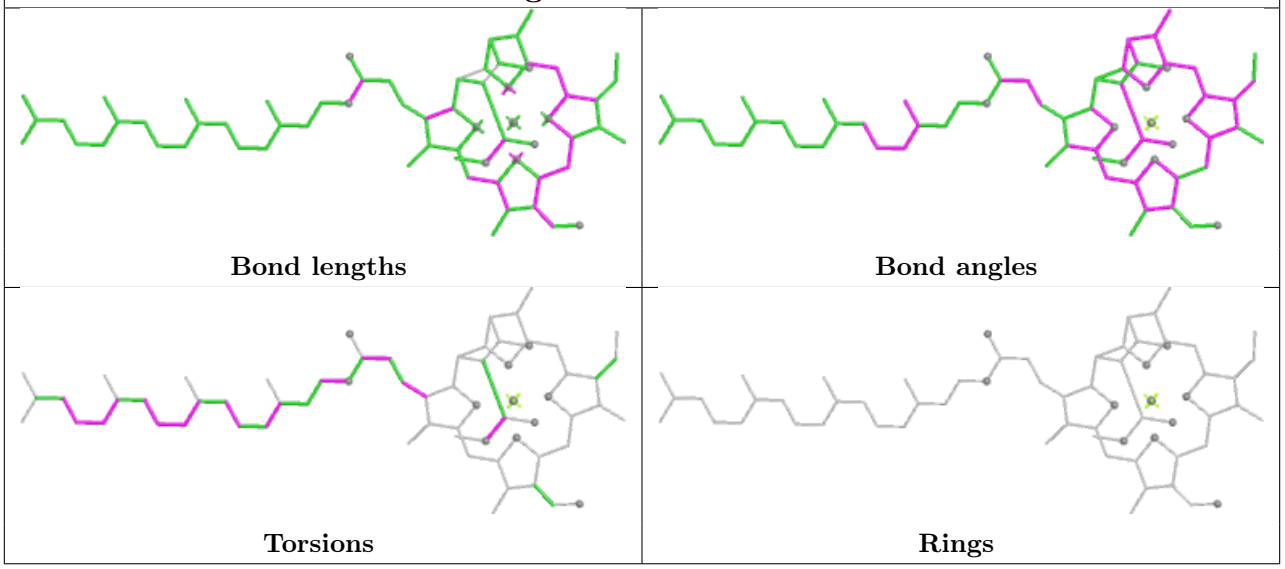


Torsions

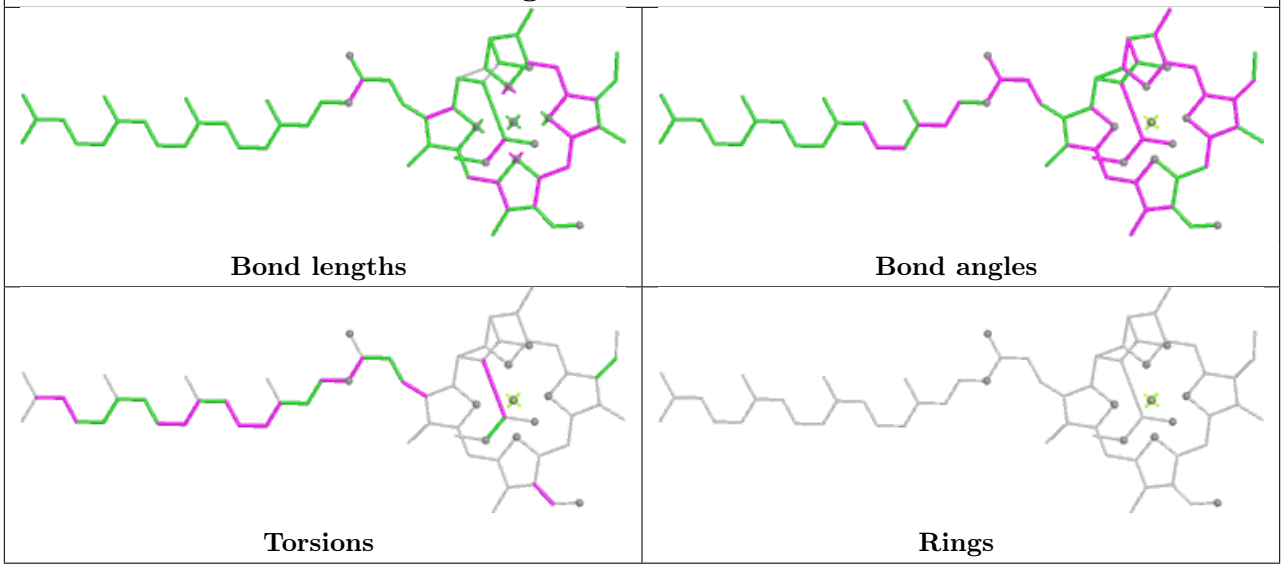


Rings

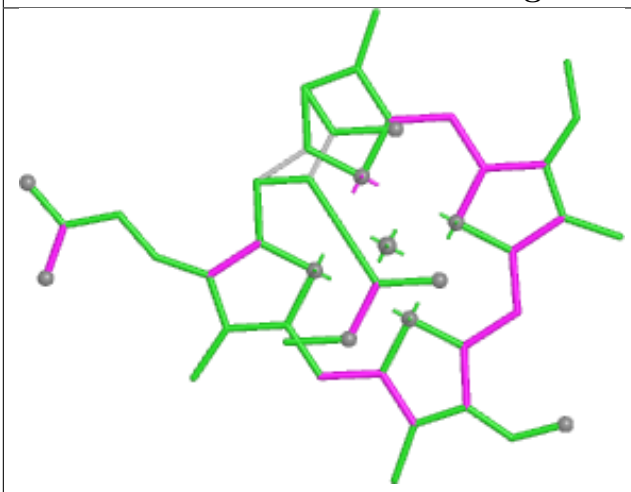
Ligand CL7 44 412



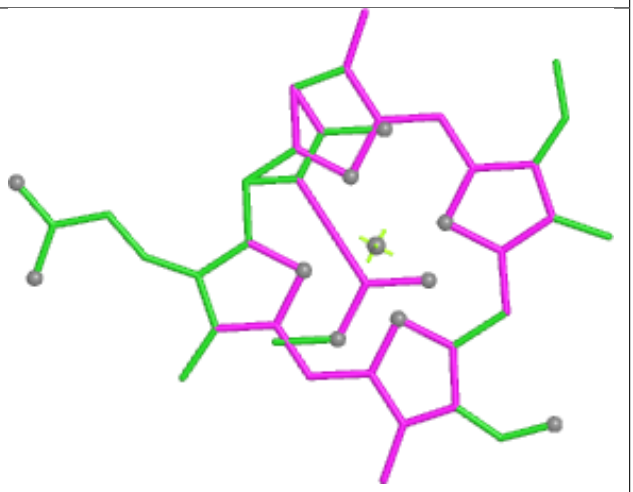
Ligand CL7 1C 508



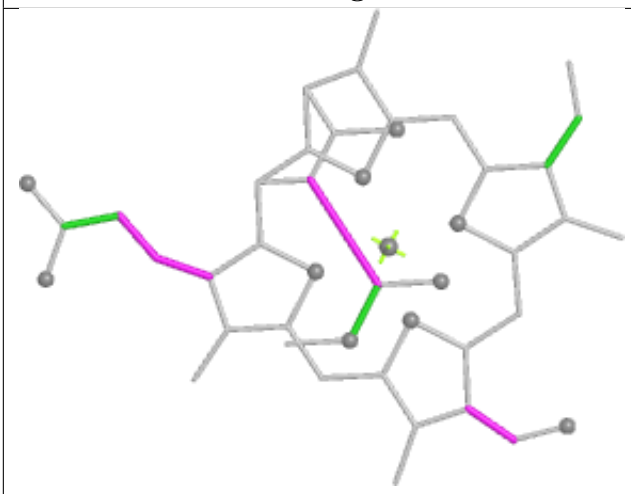
Ligand CL7 22 513



Bond lengths



Bond angles

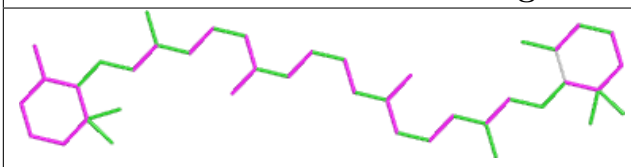


Torsions

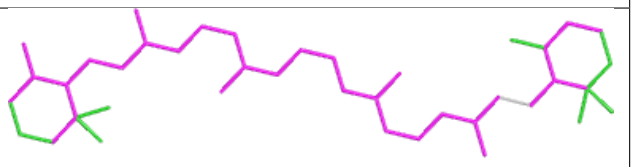


Rings

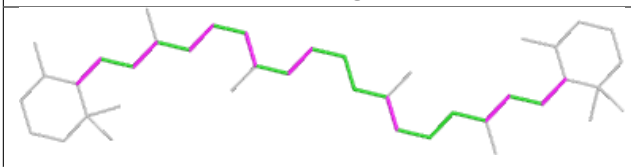
Ligand 8CT 2C 514



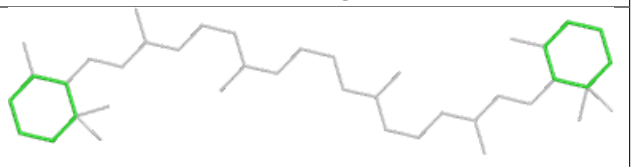
Bond lengths



Bond angles

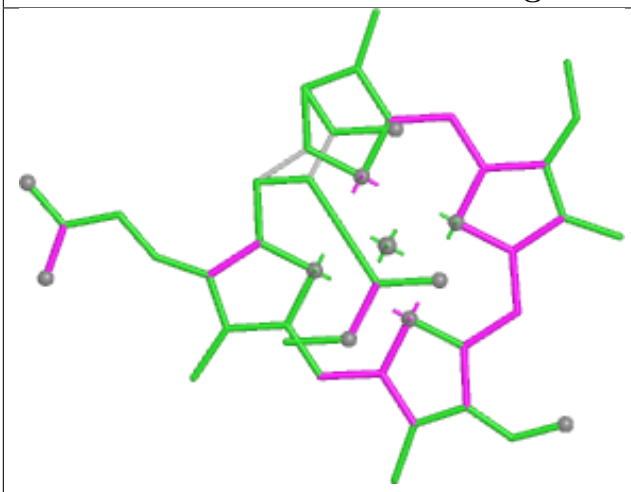


Torsions

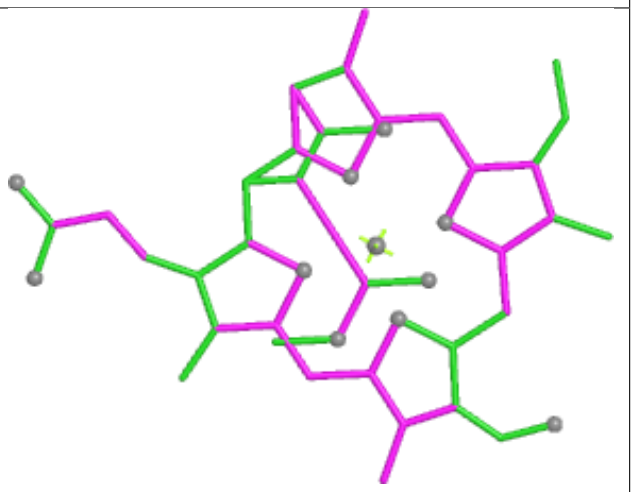


Rings

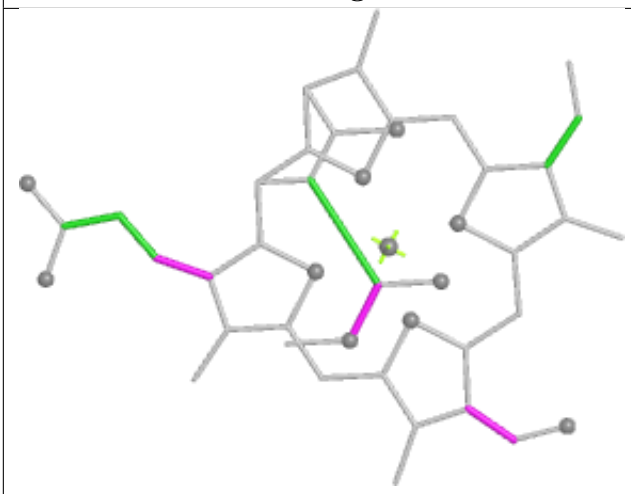
Ligand CL7 32 504



Bond lengths



Bond angles

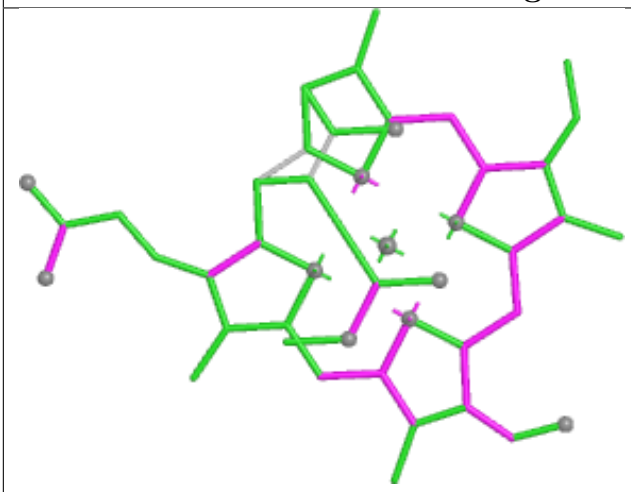


Torsions

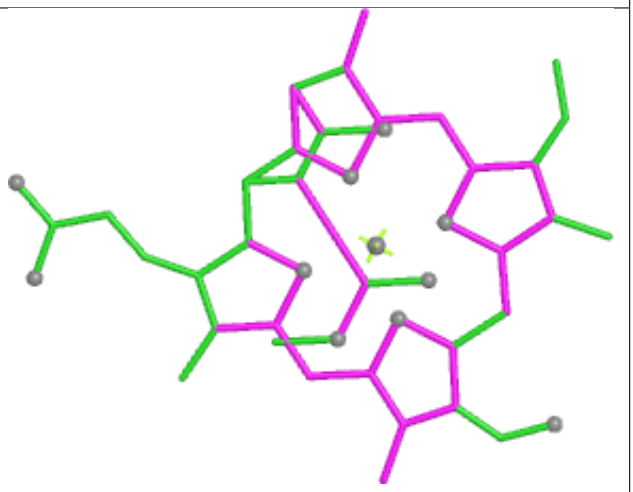


Rings

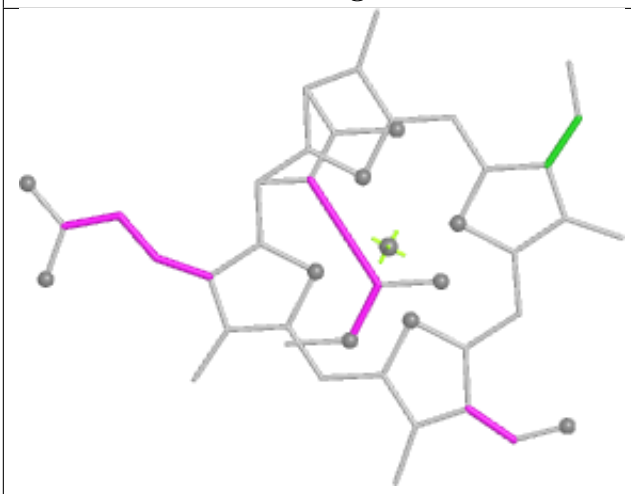
Ligand CL7 14 410



Bond lengths



Bond angles

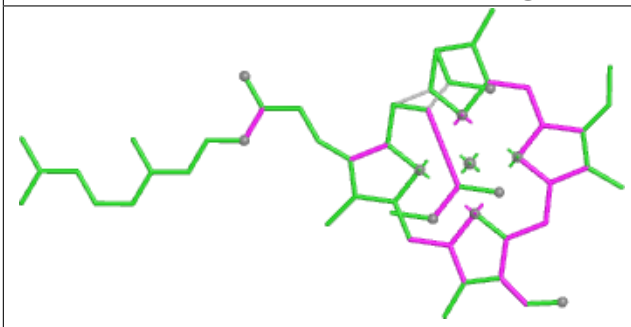


Torsions

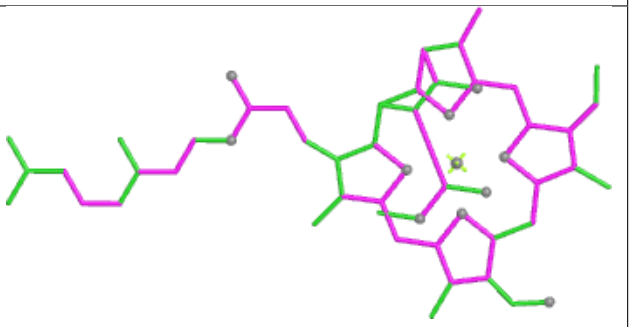


Rings

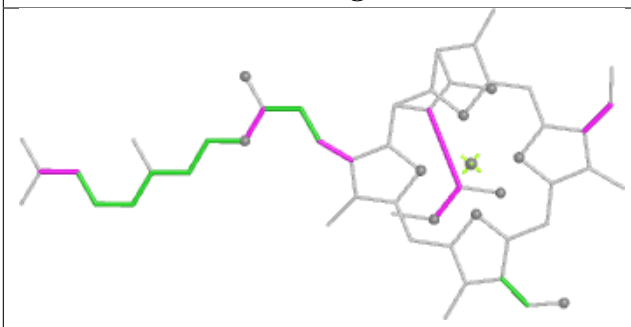
Ligand CL7 4A 403



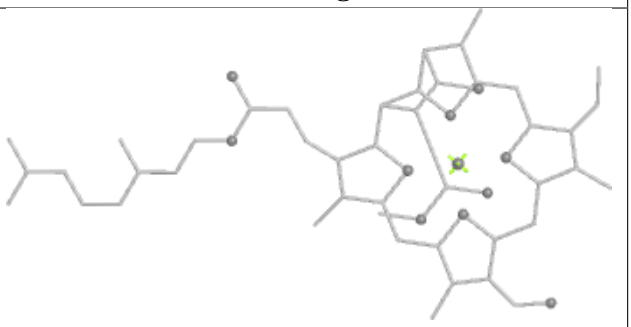
Bond lengths



Bond angles

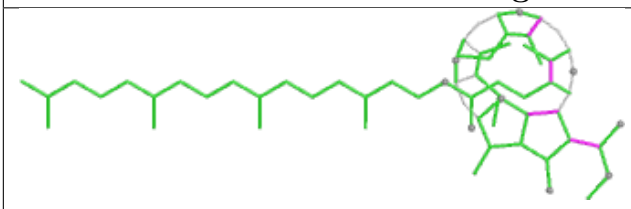


Torsions

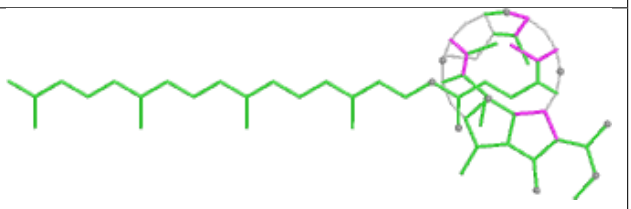


Rings

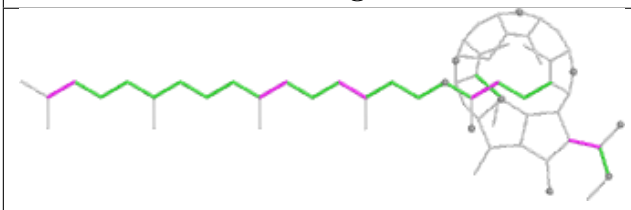
Ligand PHO 2D 408



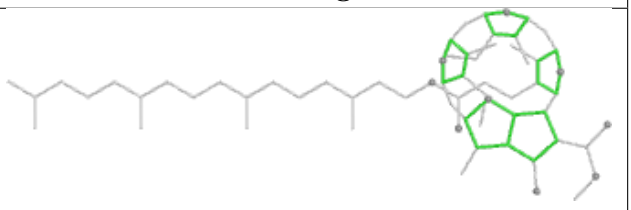
Bond lengths



Bond angles

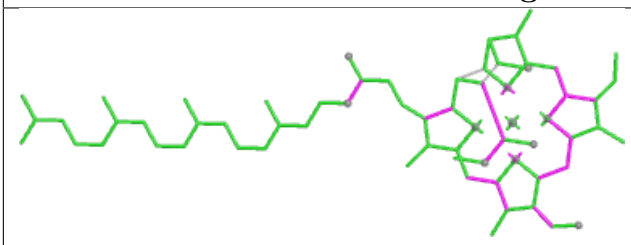


Torsions

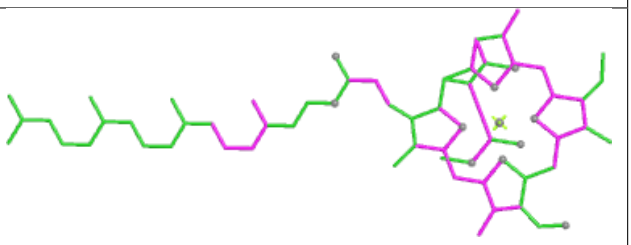


Rings

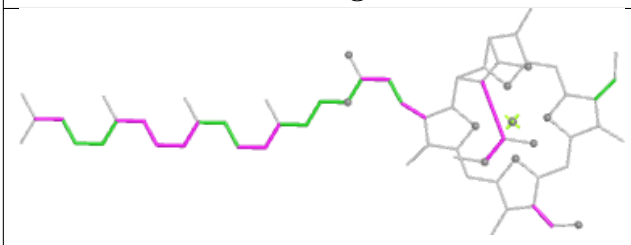
Ligand CL7 1C 503



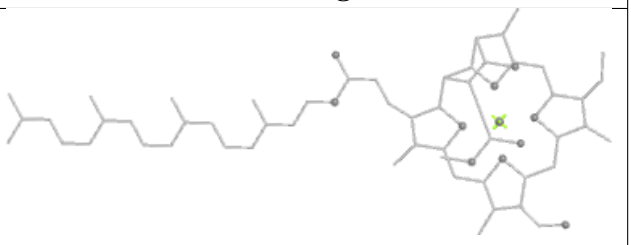
Bond lengths



Bond angles

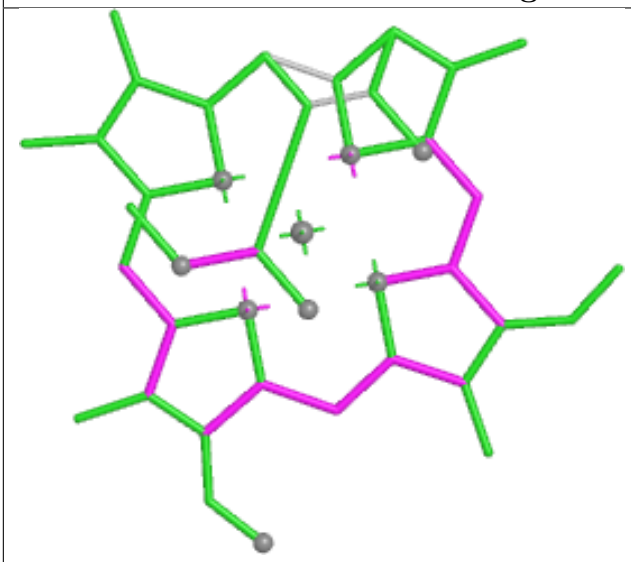


Torsions

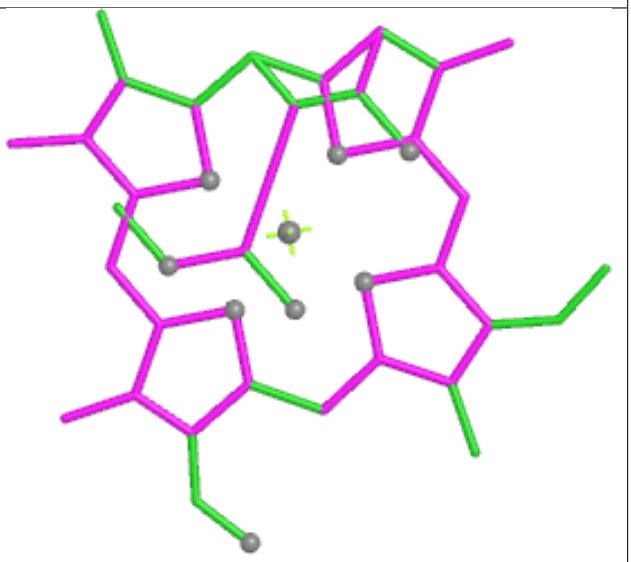


Rings

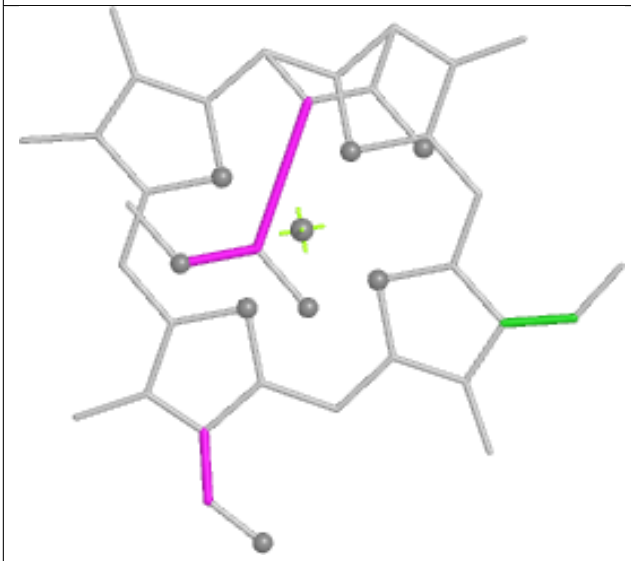
Ligand CL7 3C 517



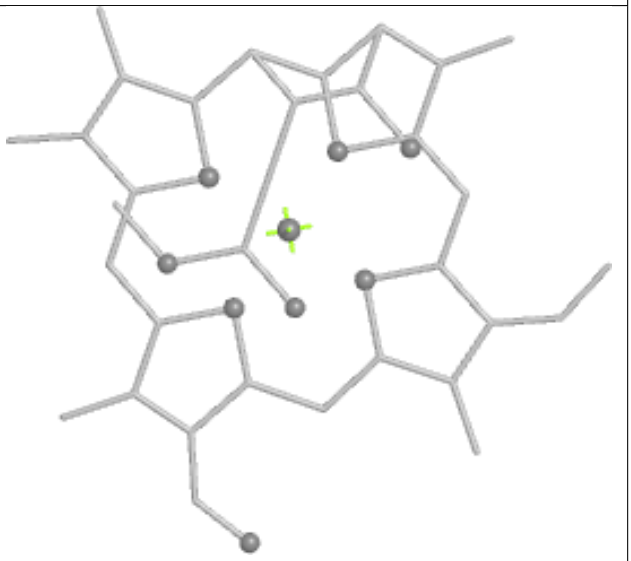
Bond lengths



Bond angles

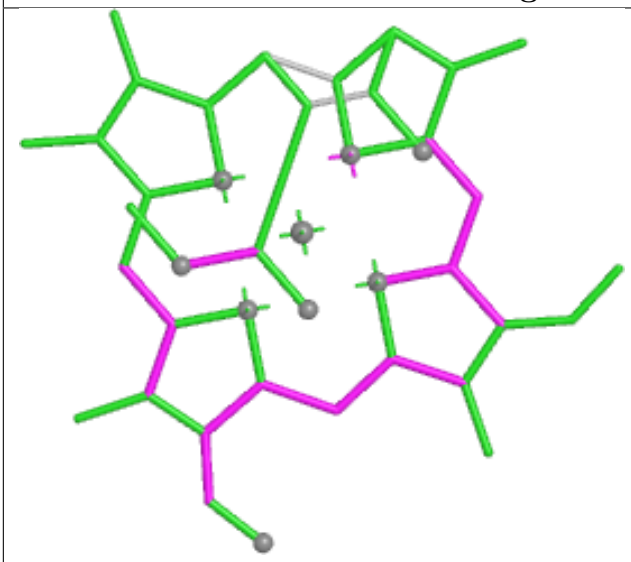


Torsions

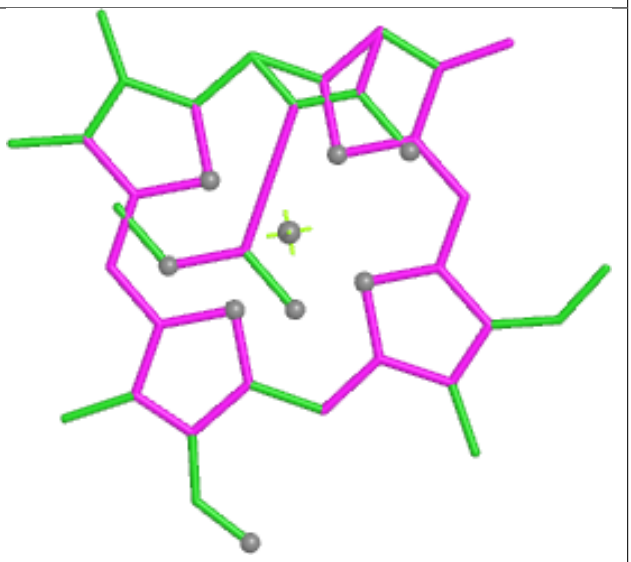


Rings

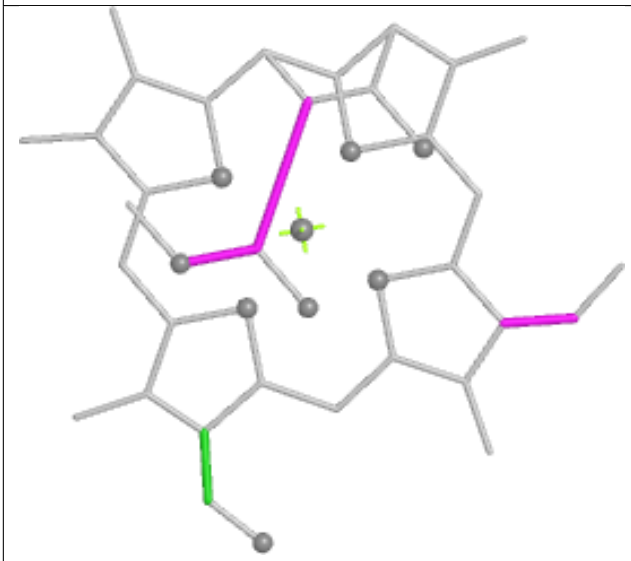
Ligand CL7 4B 602



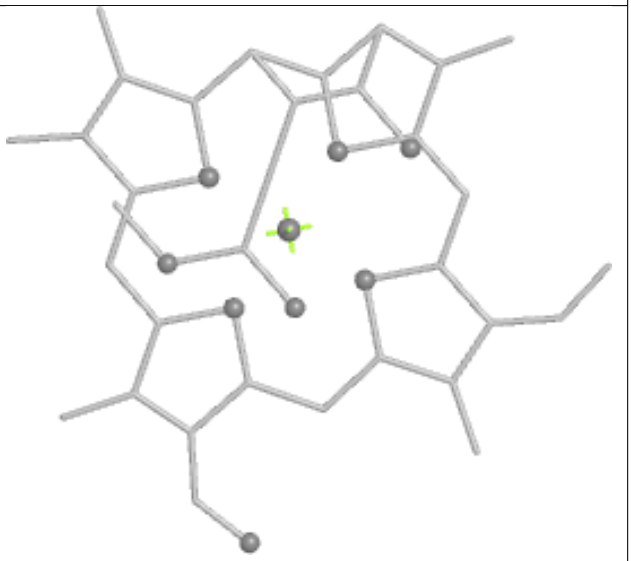
Bond lengths



Bond angles

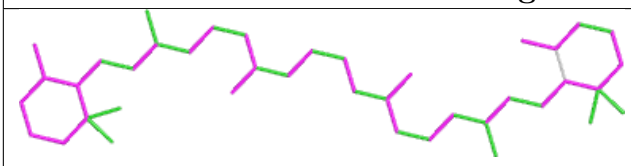


Torsions

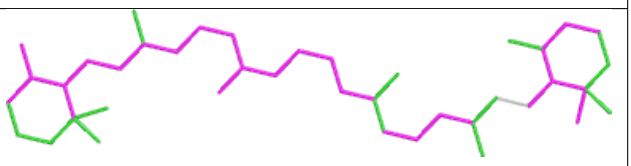


Rings

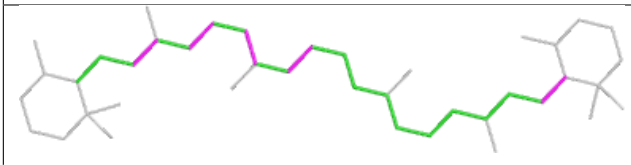
Ligand 8CT 4B 618



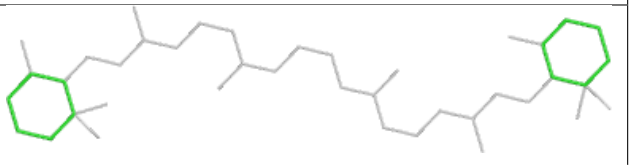
Bond lengths



Bond angles

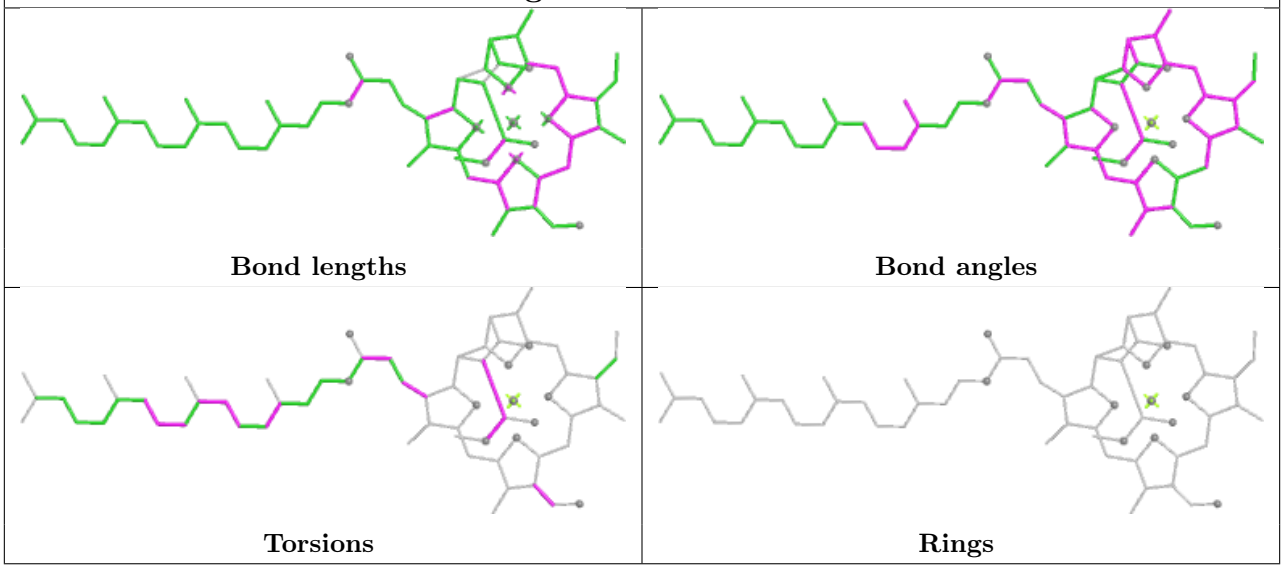


Torsions

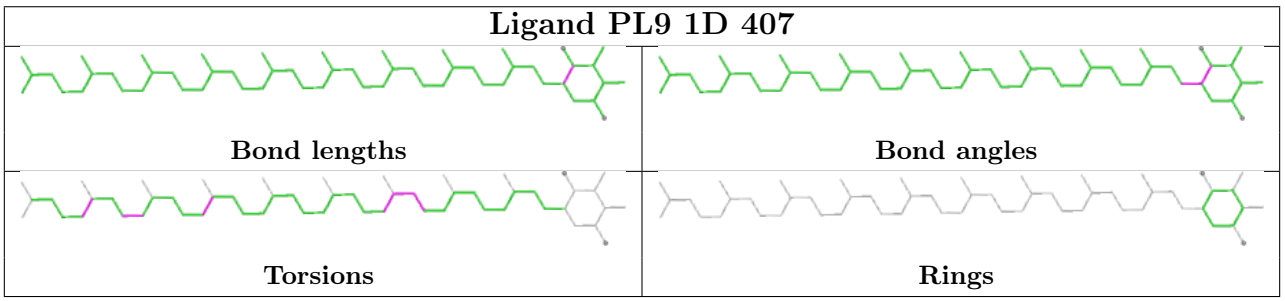


Rings

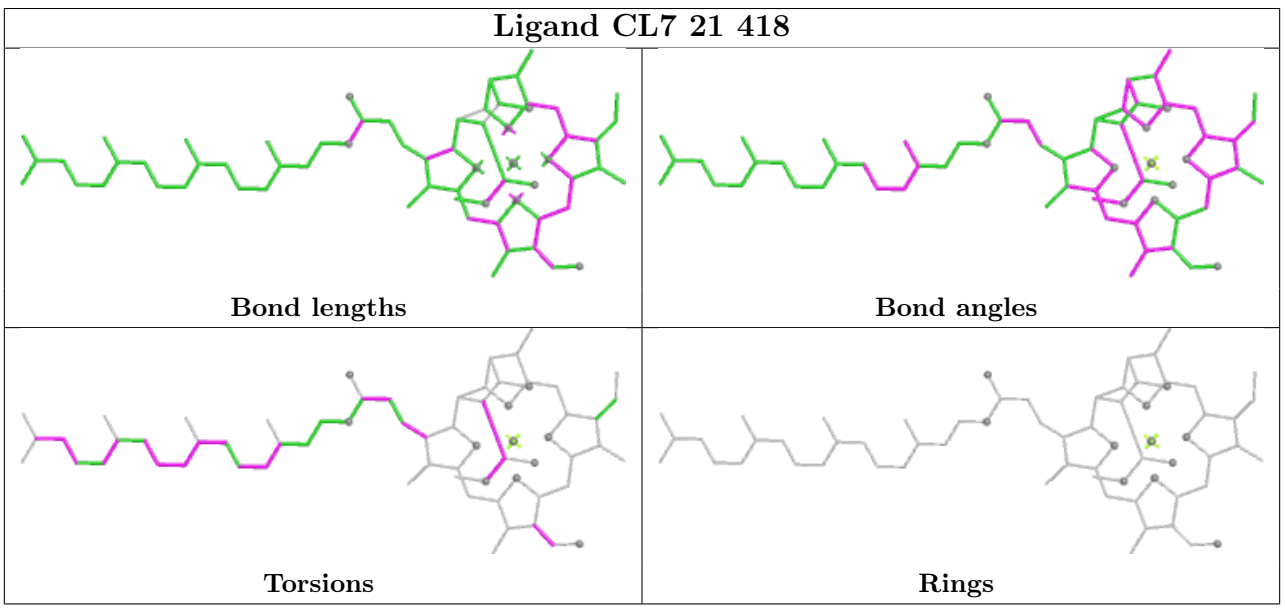
Ligand CL7 23 411



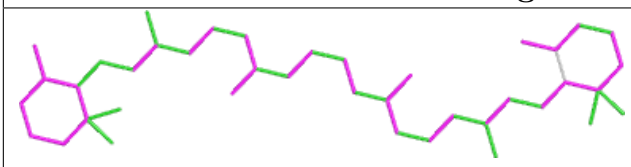
Ligand PL9 1D 407



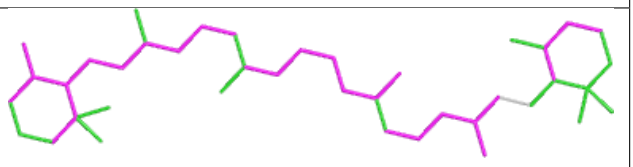
Ligand CL7 21 418



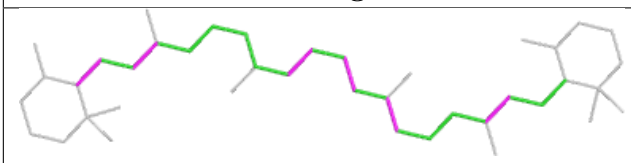
Ligand 8CT 2D 406



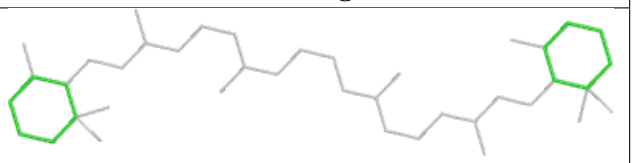
Bond lengths



Bond angles

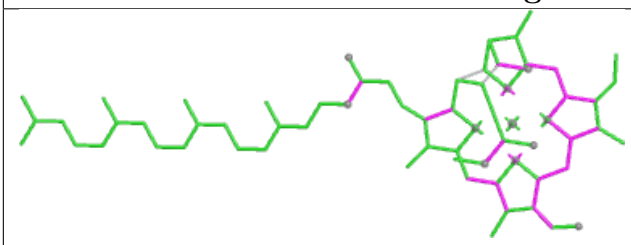


Torsions

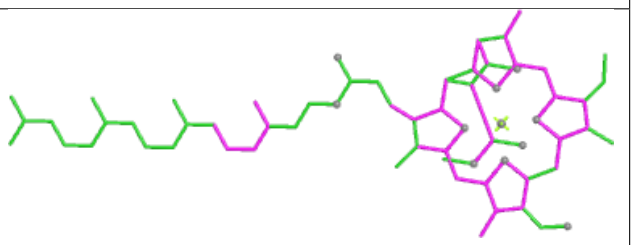


Rings

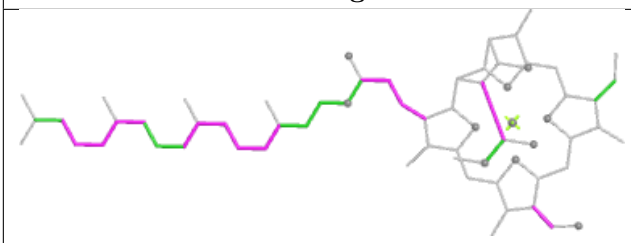
Ligand CL7 43 402



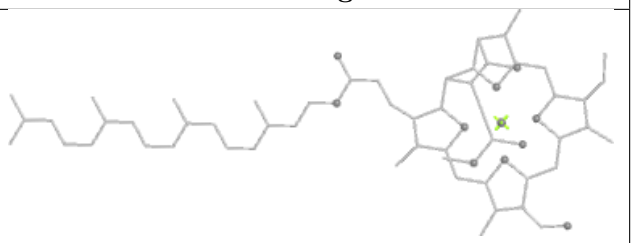
Bond lengths



Bond angles

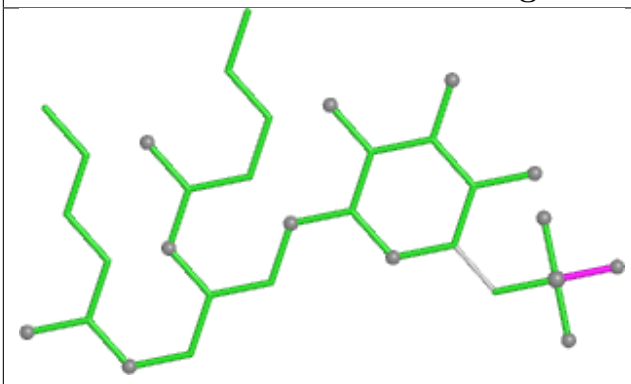


Torsions

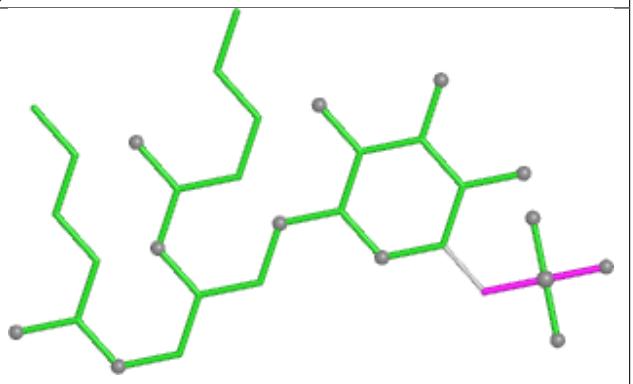


Rings

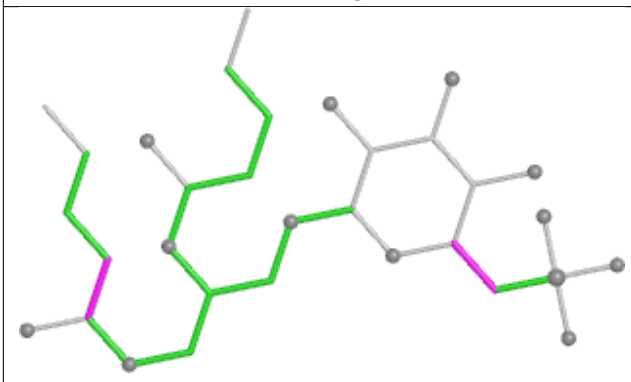
Ligand SQD 21 423



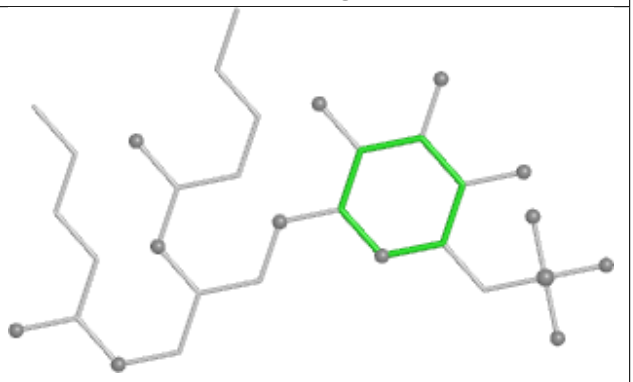
Bond lengths



Bond angles

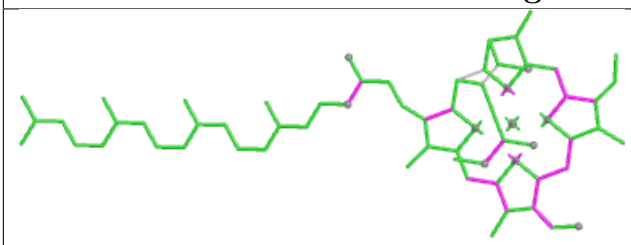


Torsions

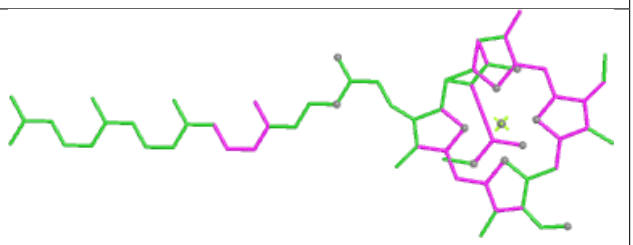


Rings

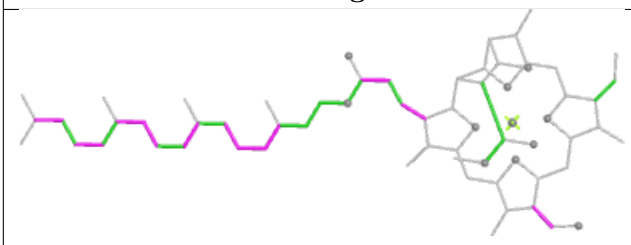
Ligand CL7 42 512



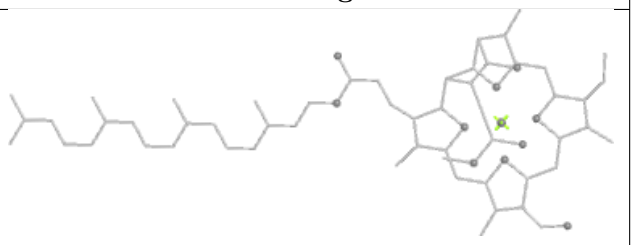
Bond lengths



Bond angles

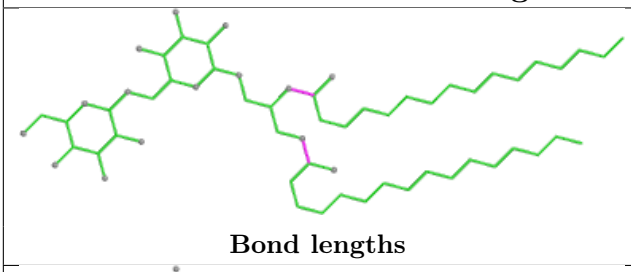


Torsions

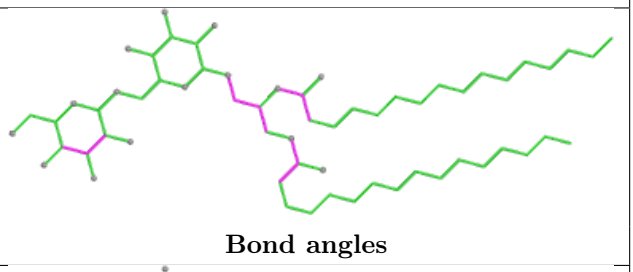


Rings

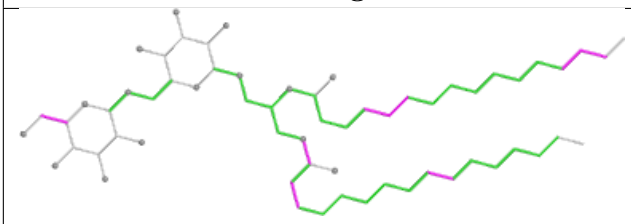
Ligand DGD 2C 516



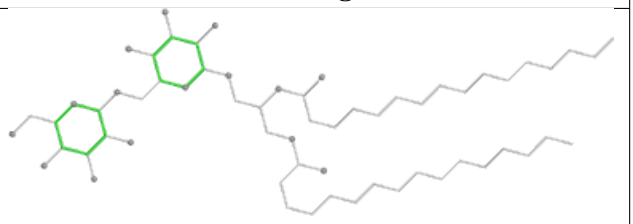
Bond lengths



Bond angles

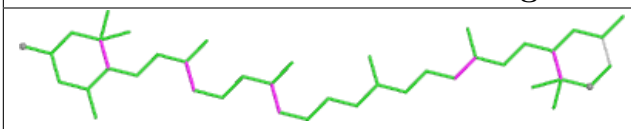


Torsions

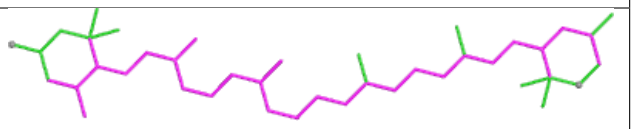


Rings

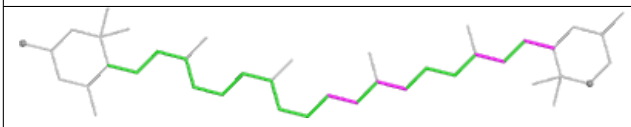
Ligand ZEX 33 525



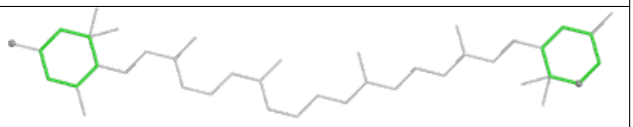
Bond lengths



Bond angles

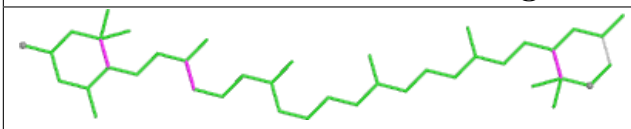


Torsions

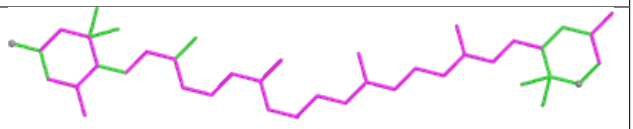


Rings

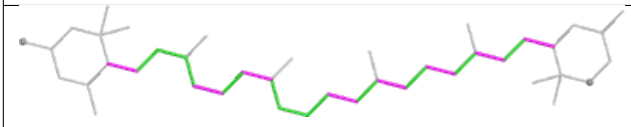
Ligand ZEX 44 420



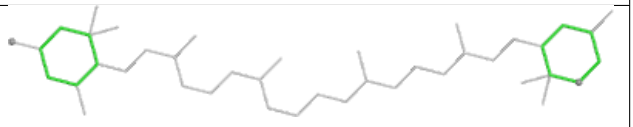
Bond lengths



Bond angles

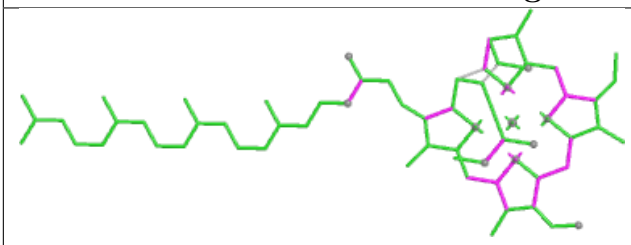


Torsions

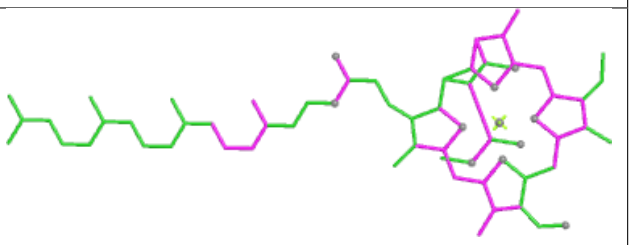


Rings

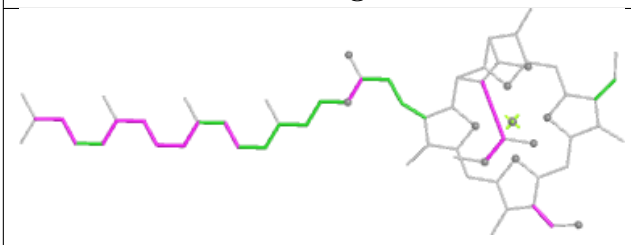
Ligand CL7 33 509



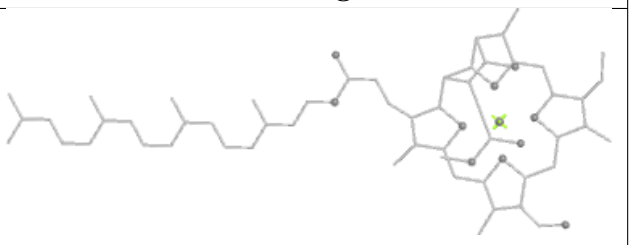
Bond lengths



Bond angles

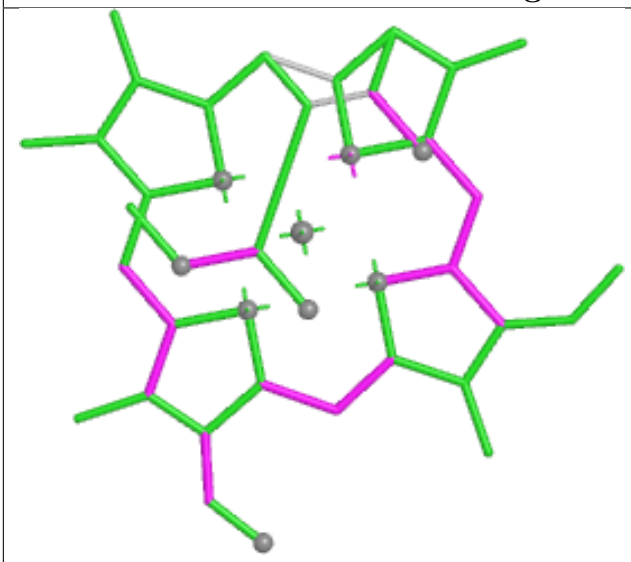


Torsions

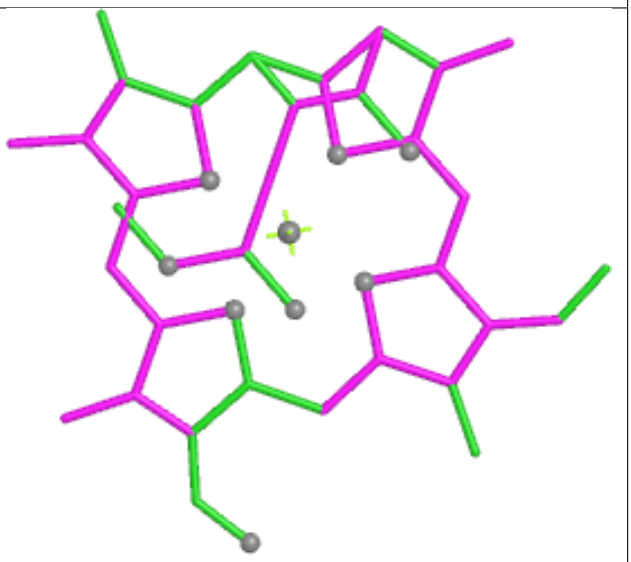


Rings

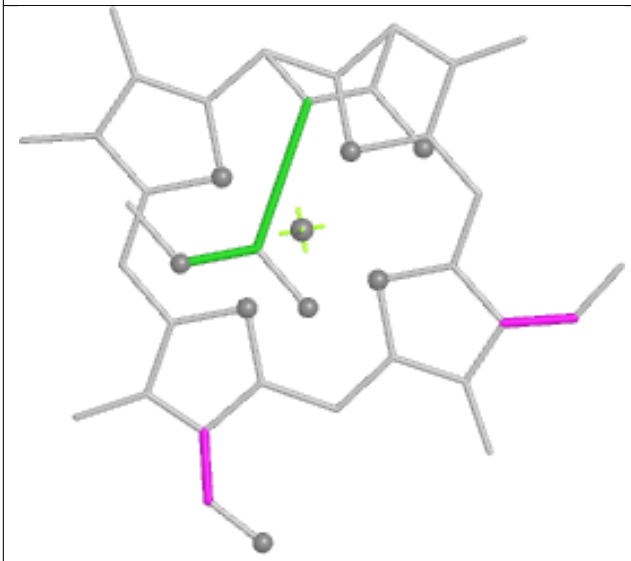
Ligand CL7 11 414



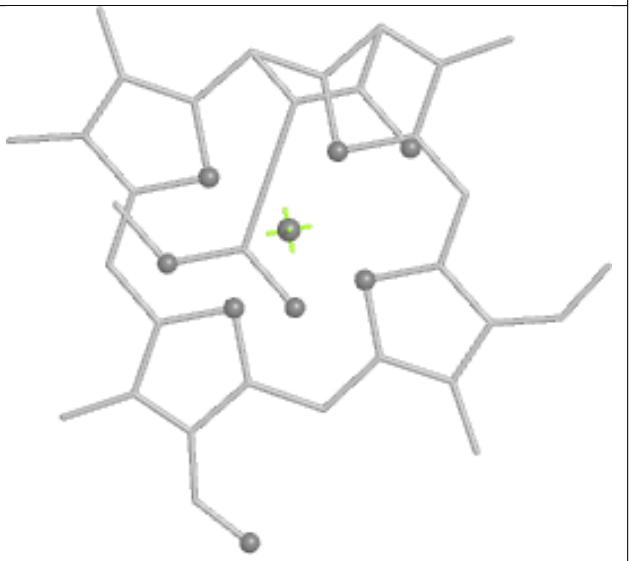
Bond lengths



Bond angles

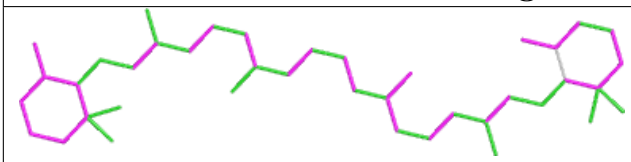


Torsions

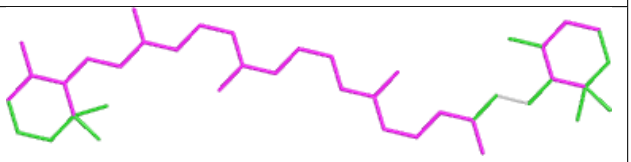


Rings

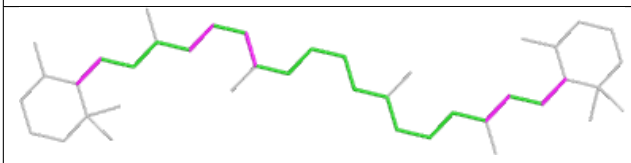
Ligand 8CT 1C 518



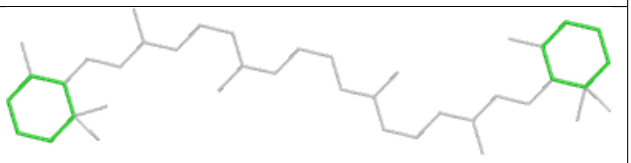
Bond lengths



Bond angles

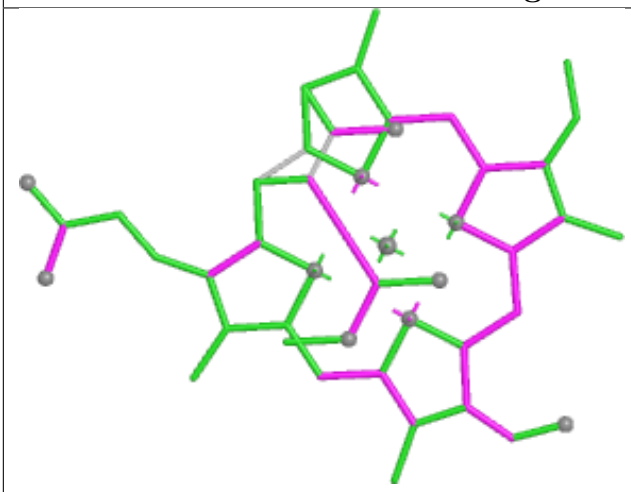


Torsions

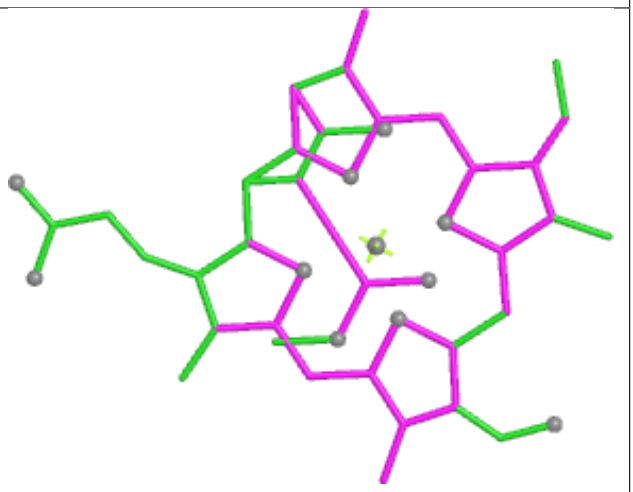


Rings

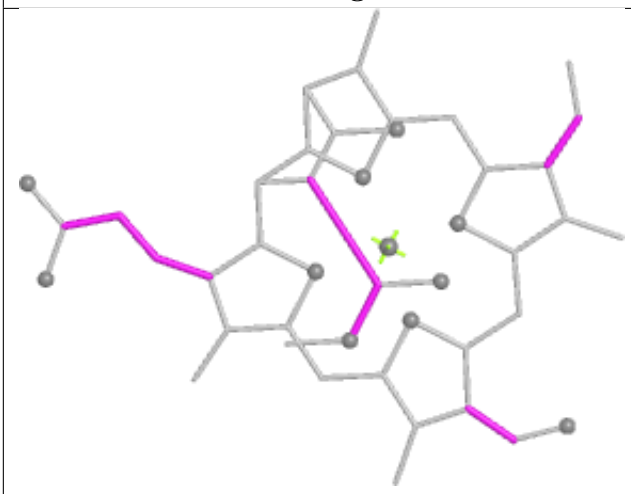
Ligand CL7 34 415



Bond lengths



Bond angles

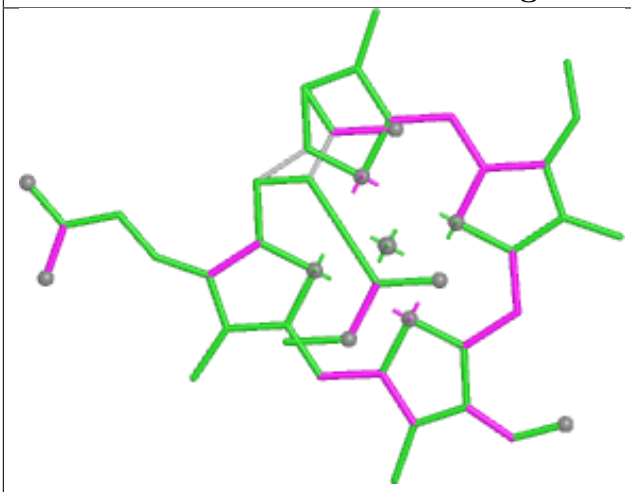


Torsions

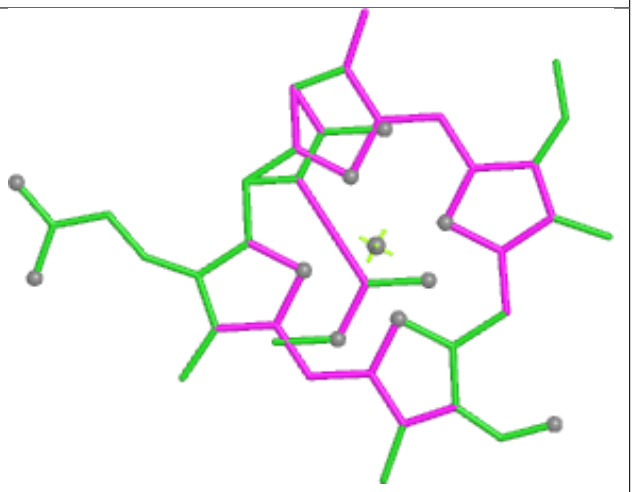


Rings

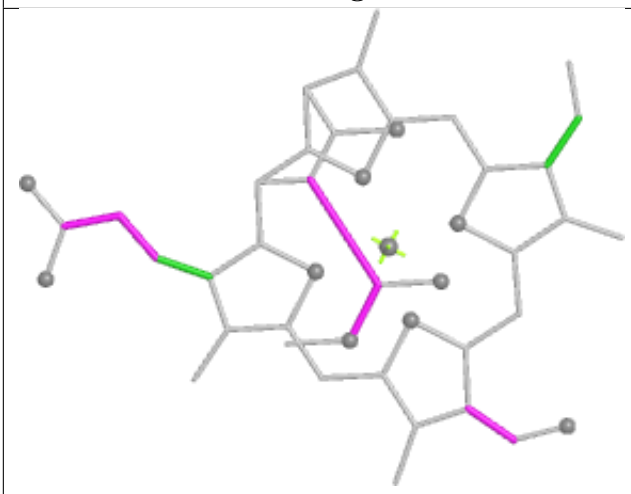
Ligand CL7 2B 623



Bond lengths



Bond angles



Torsions

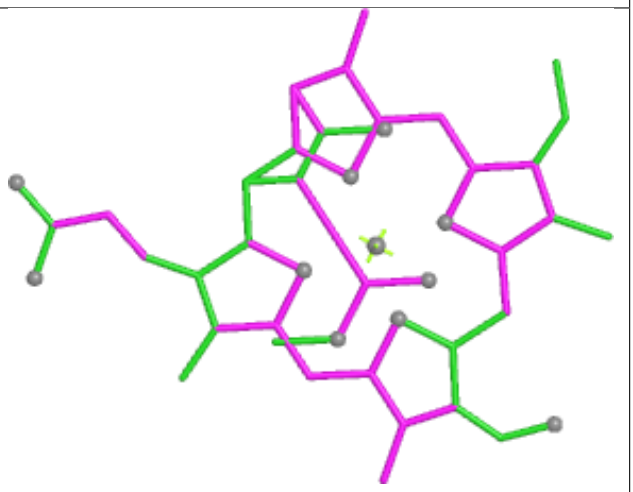


Rings

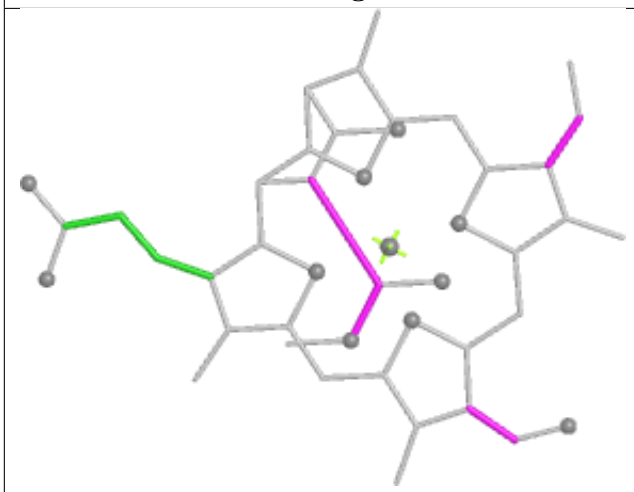
Ligand CL7 31 420



Bond lengths



Bond angles

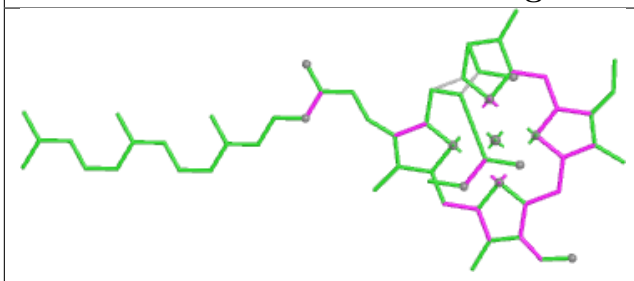


Torsions

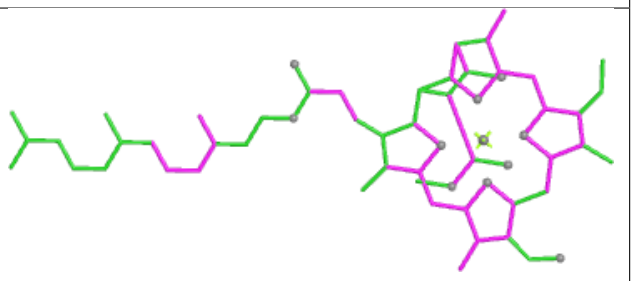


Rings

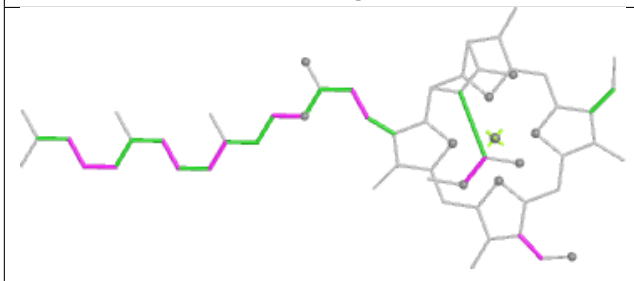
Ligand CL7 21 403



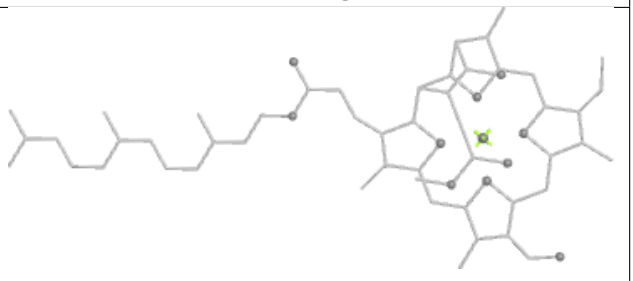
Bond lengths



Bond angles

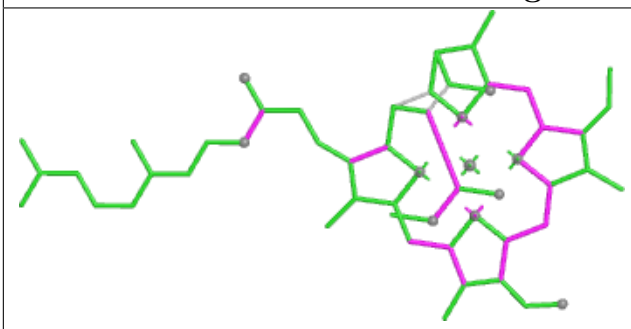


Torsions

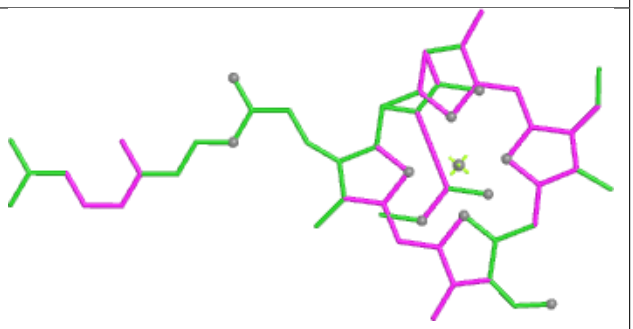


Rings

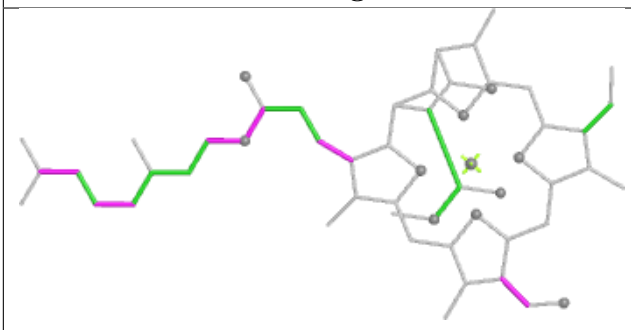
Ligand CL7 21 417



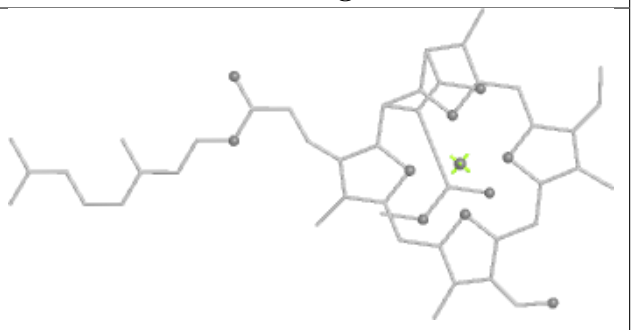
Bond lengths



Bond angles

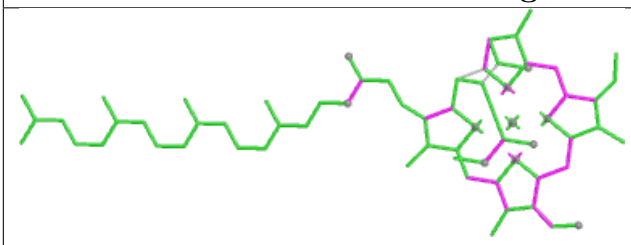


Torsions

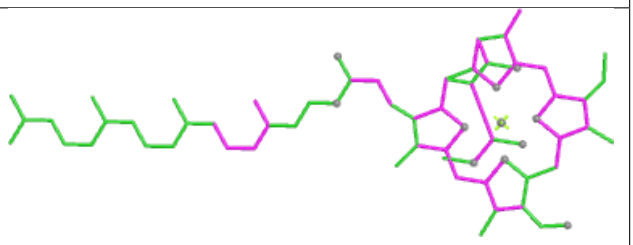


Rings

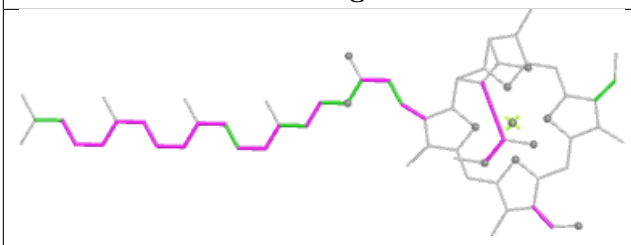
Ligand CL7 3C 510



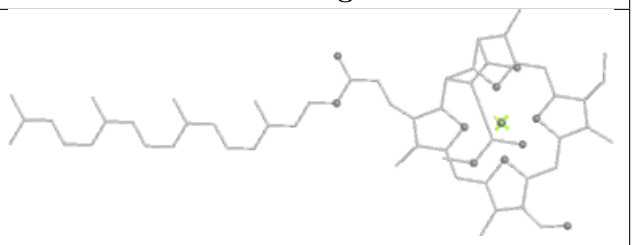
Bond lengths



Bond angles

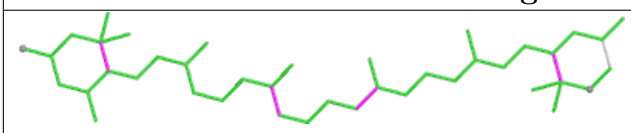


Torsions

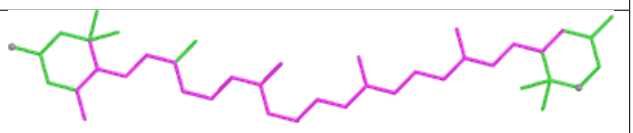


Rings

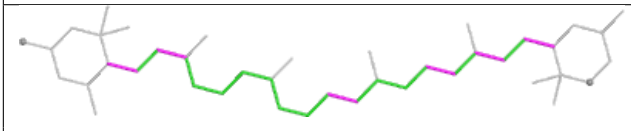
Ligand ZEX 34 403



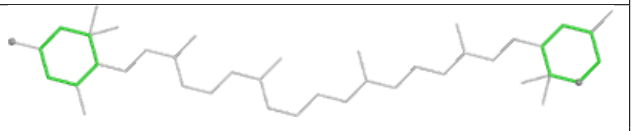
Bond lengths



Bond angles

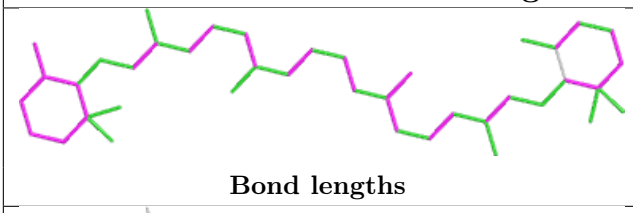


Torsions

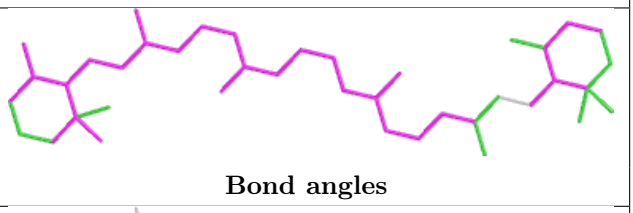


Rings

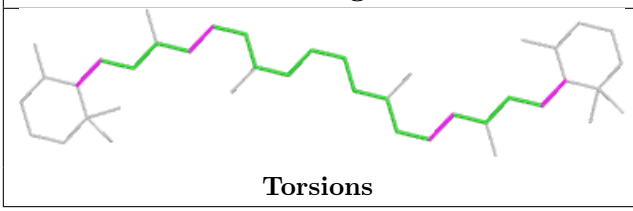
Ligand 8CT 34 402



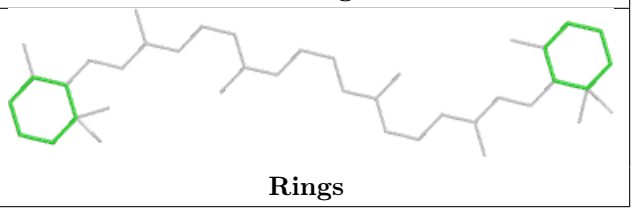
Bond lengths



Bond angles

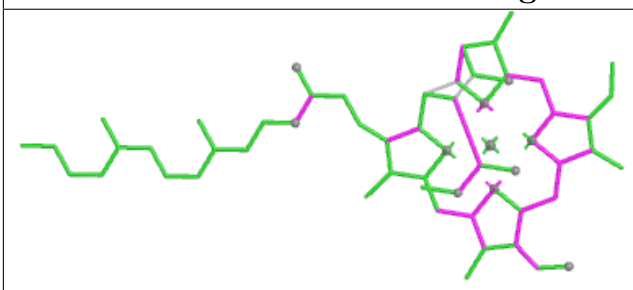


Torsions

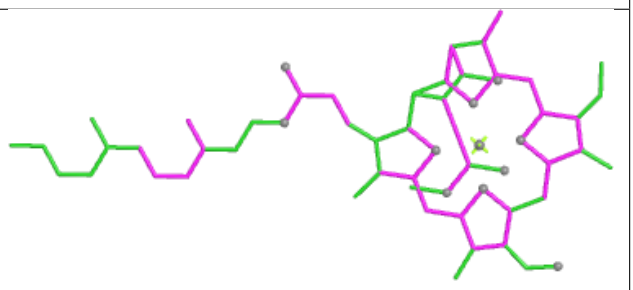


Rings

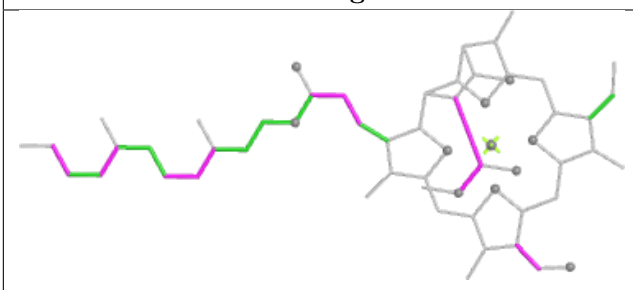
Ligand CL7 4D 404



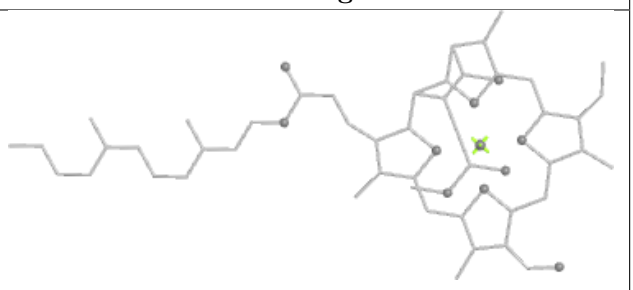
Bond lengths



Bond angles

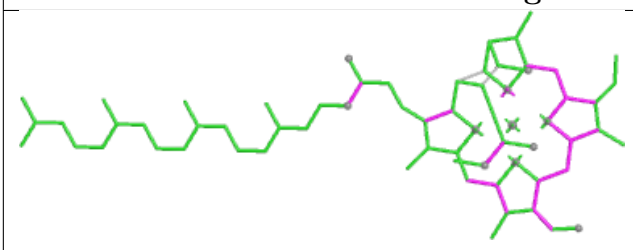


Torsions

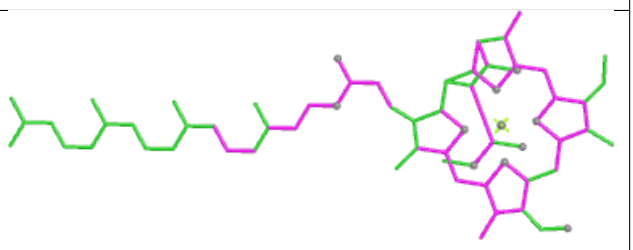


Rings

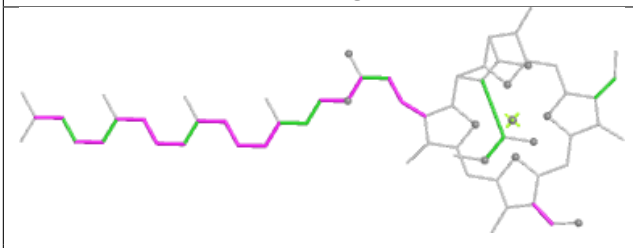
Ligand CL7 34 405



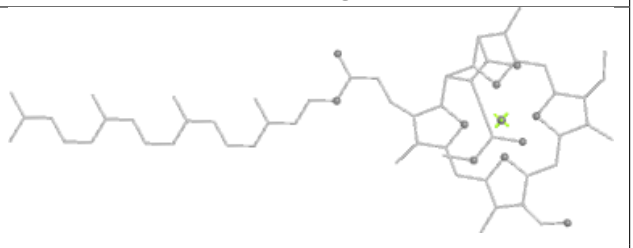
Bond lengths



Bond angles

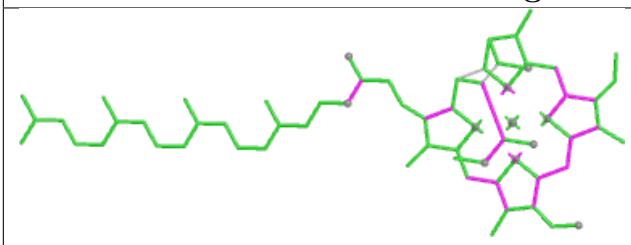


Torsions

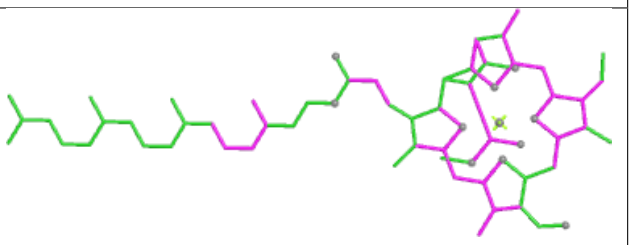


Rings

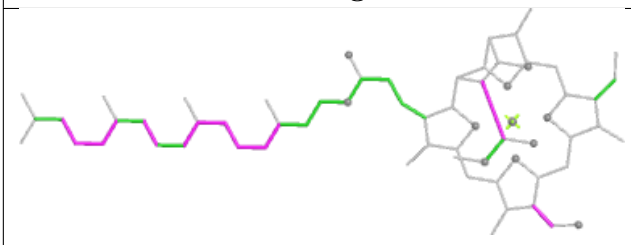
Ligand CL7 23 408



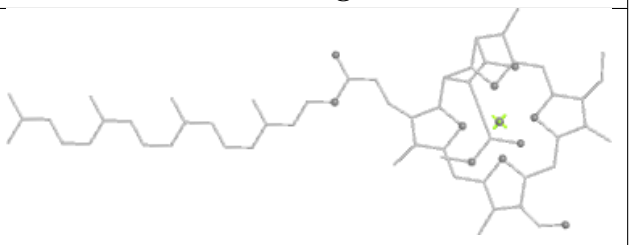
Bond lengths



Bond angles

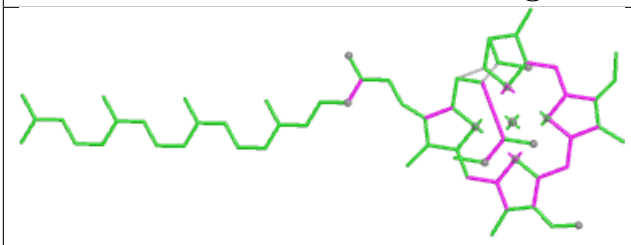


Torsions

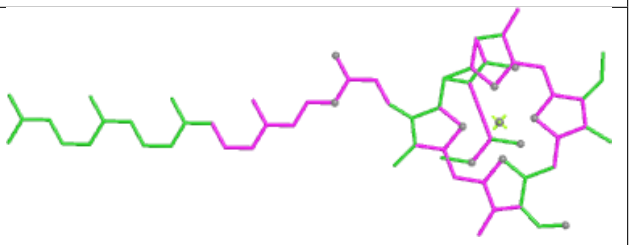


Rings

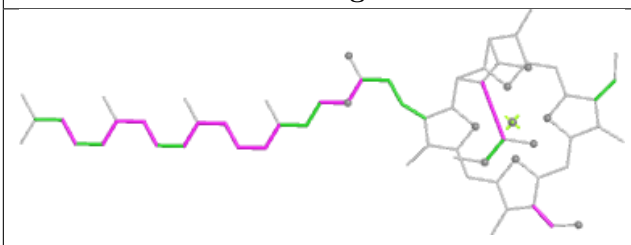
Ligand CL7 43 412



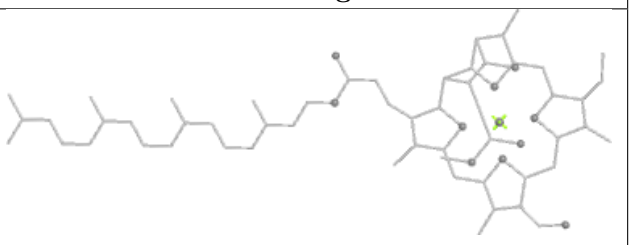
Bond lengths



Bond angles

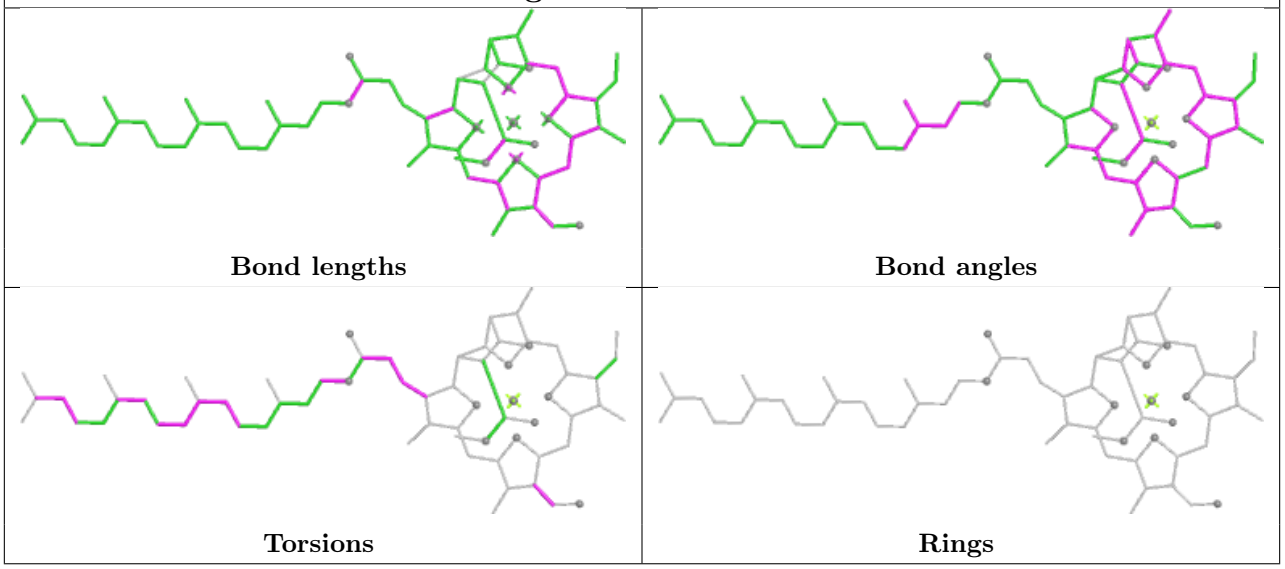


Torsions

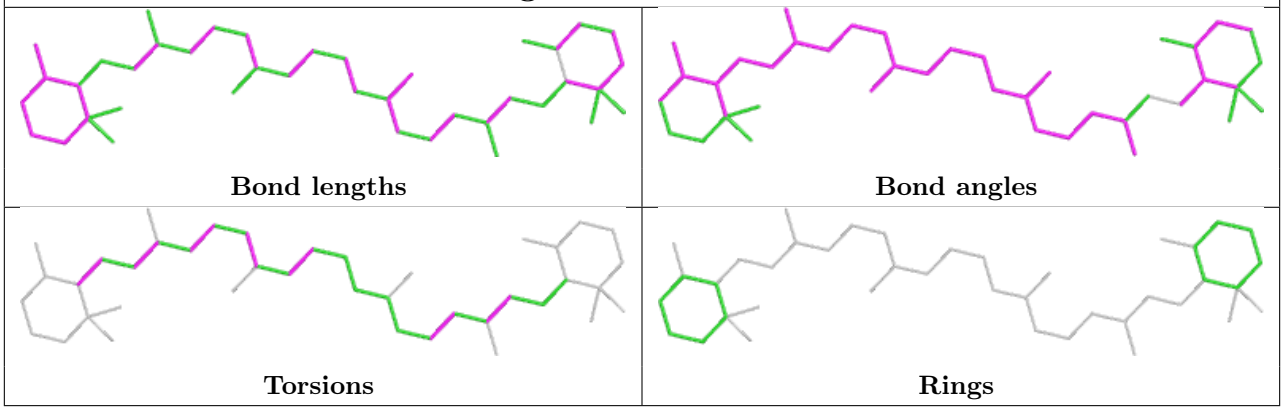


Rings

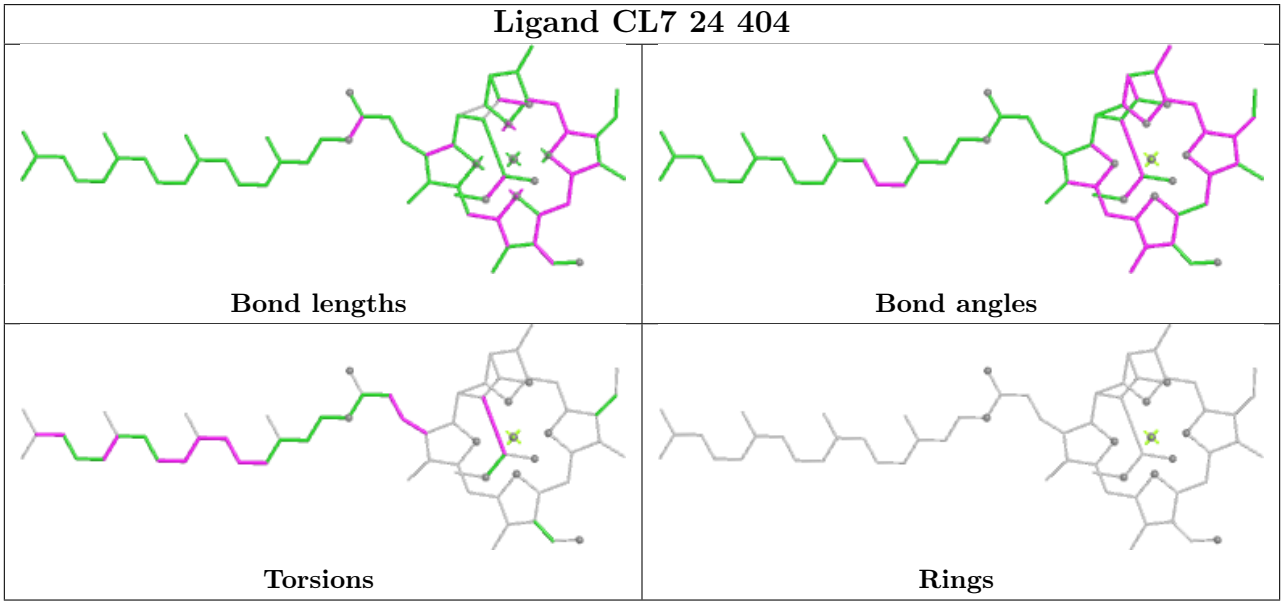
Ligand CL7 42 501



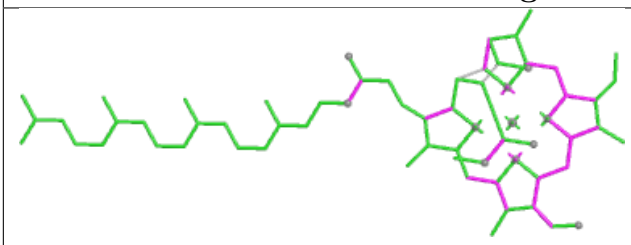
Ligand 8CT 3C 515



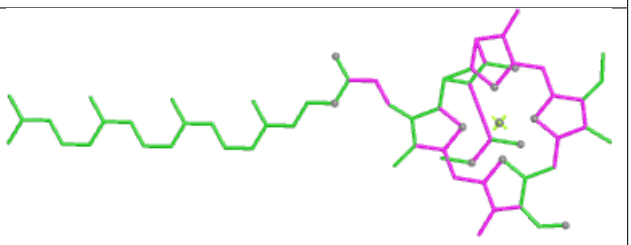
Ligand CL7 24 404



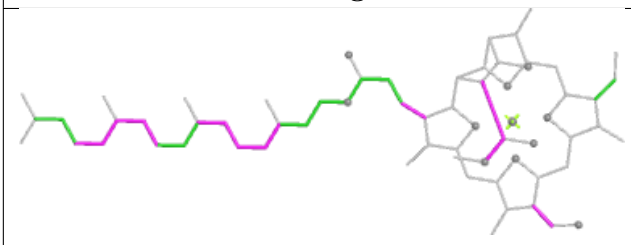
Ligand CL7 2B 606



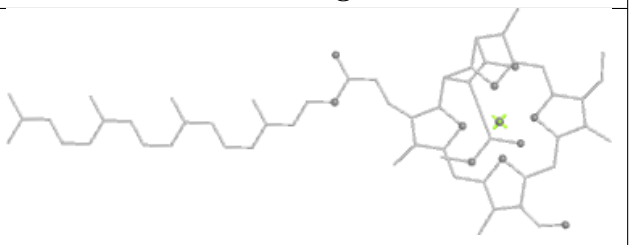
Bond lengths



Bond angles

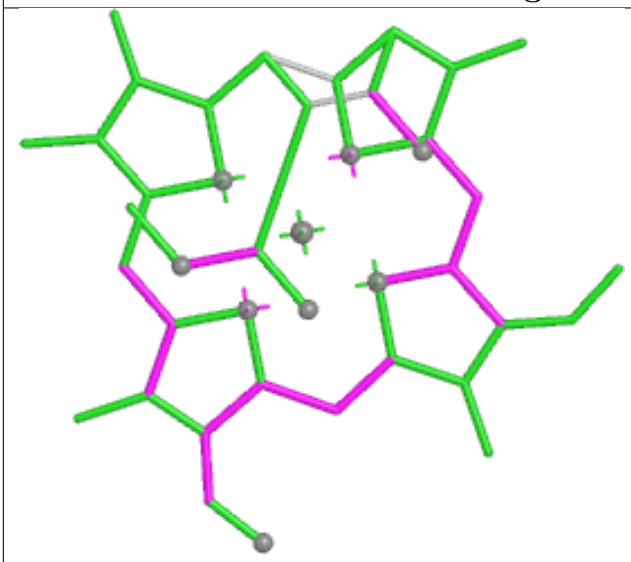


Torsions

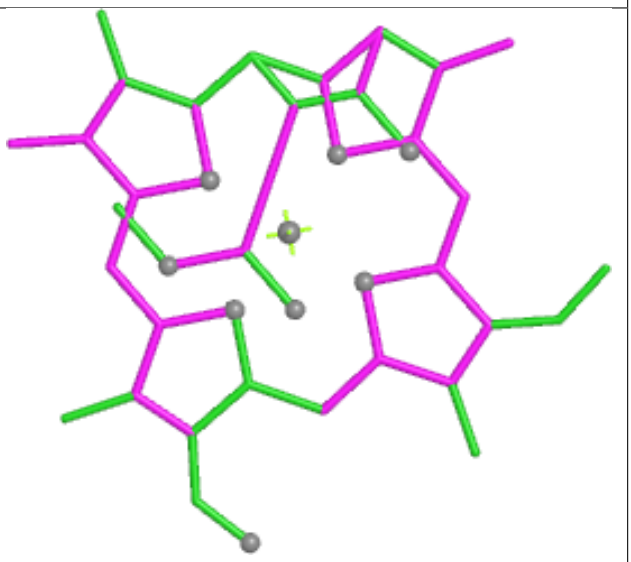


Rings

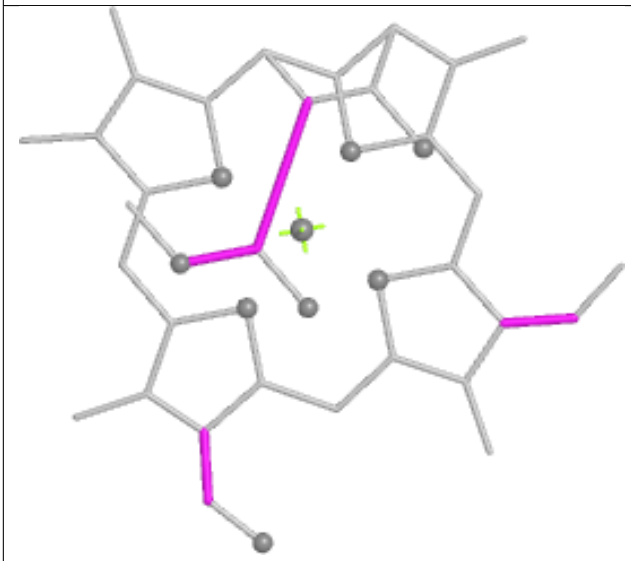
Ligand CL7 14 416



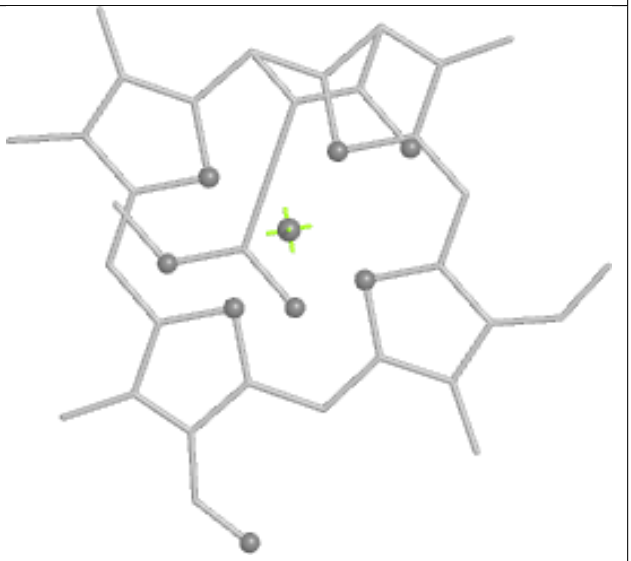
Bond lengths



Bond angles

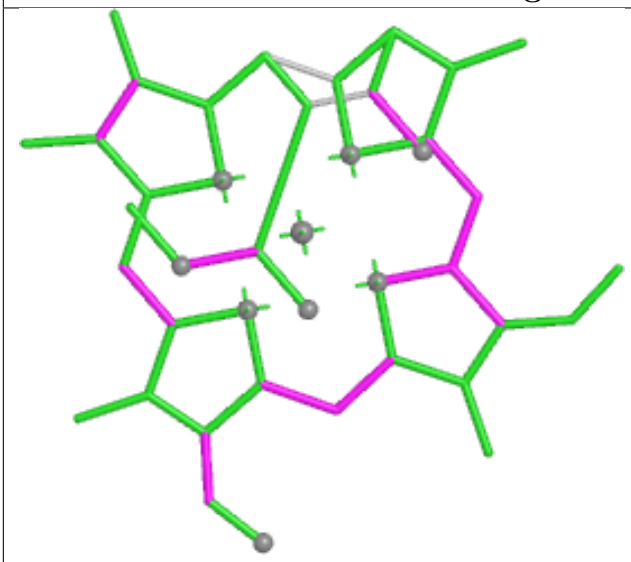


Torsions

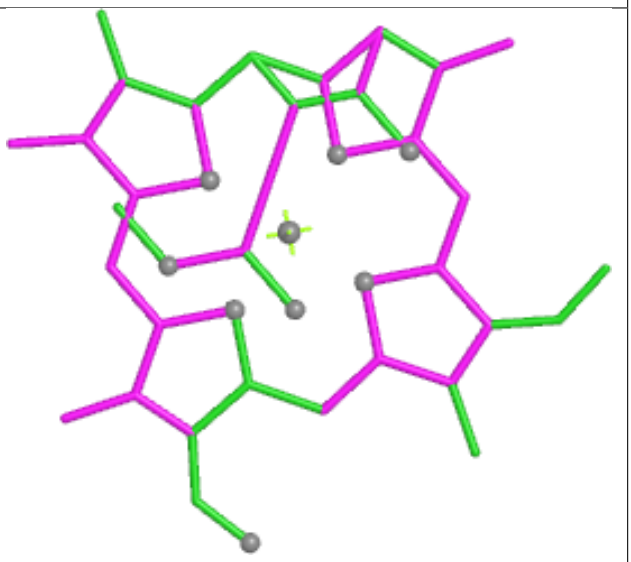


Rings

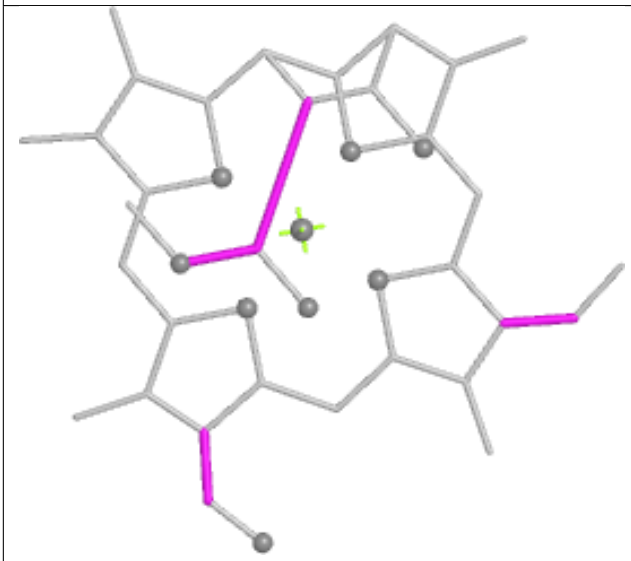
Ligand CL7 31 415



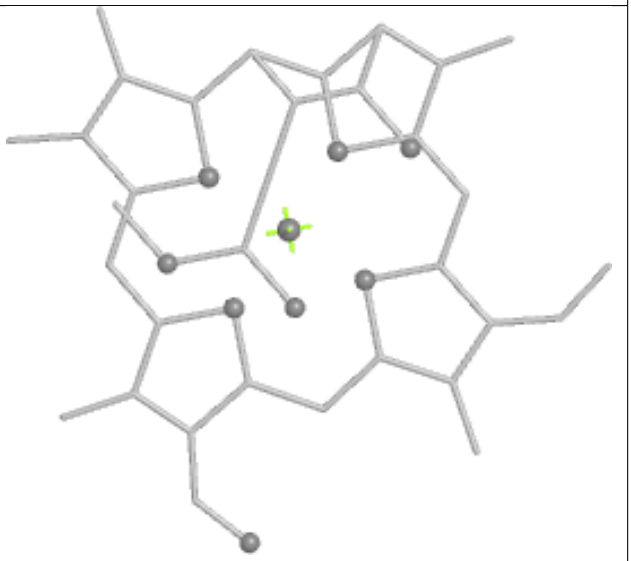
Bond lengths



Bond angles

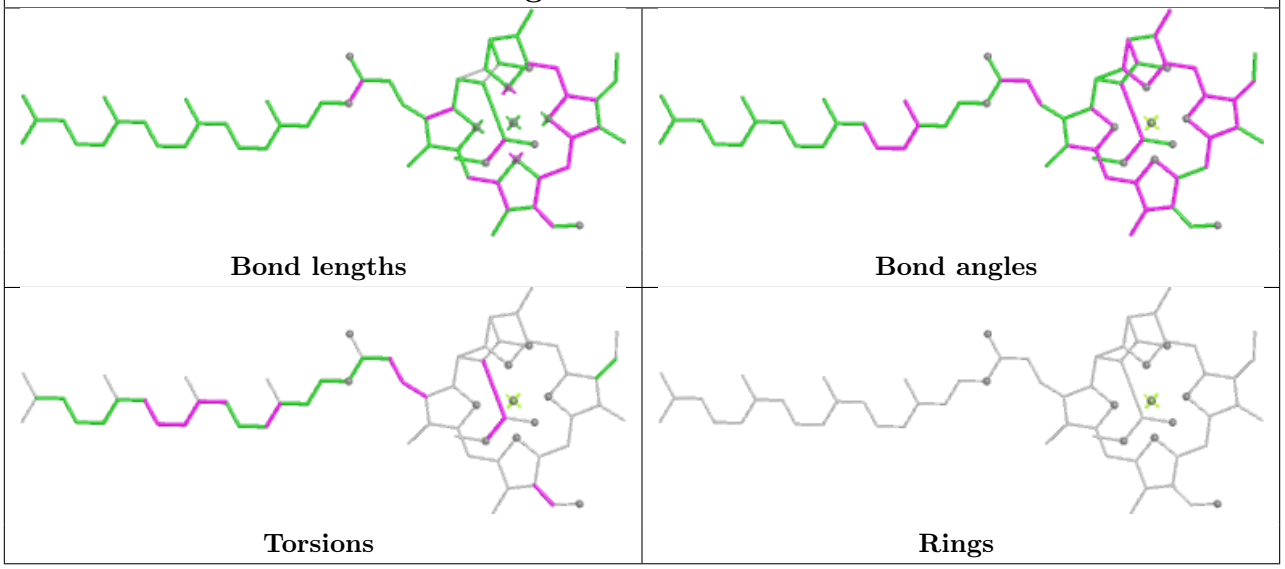


Torsions

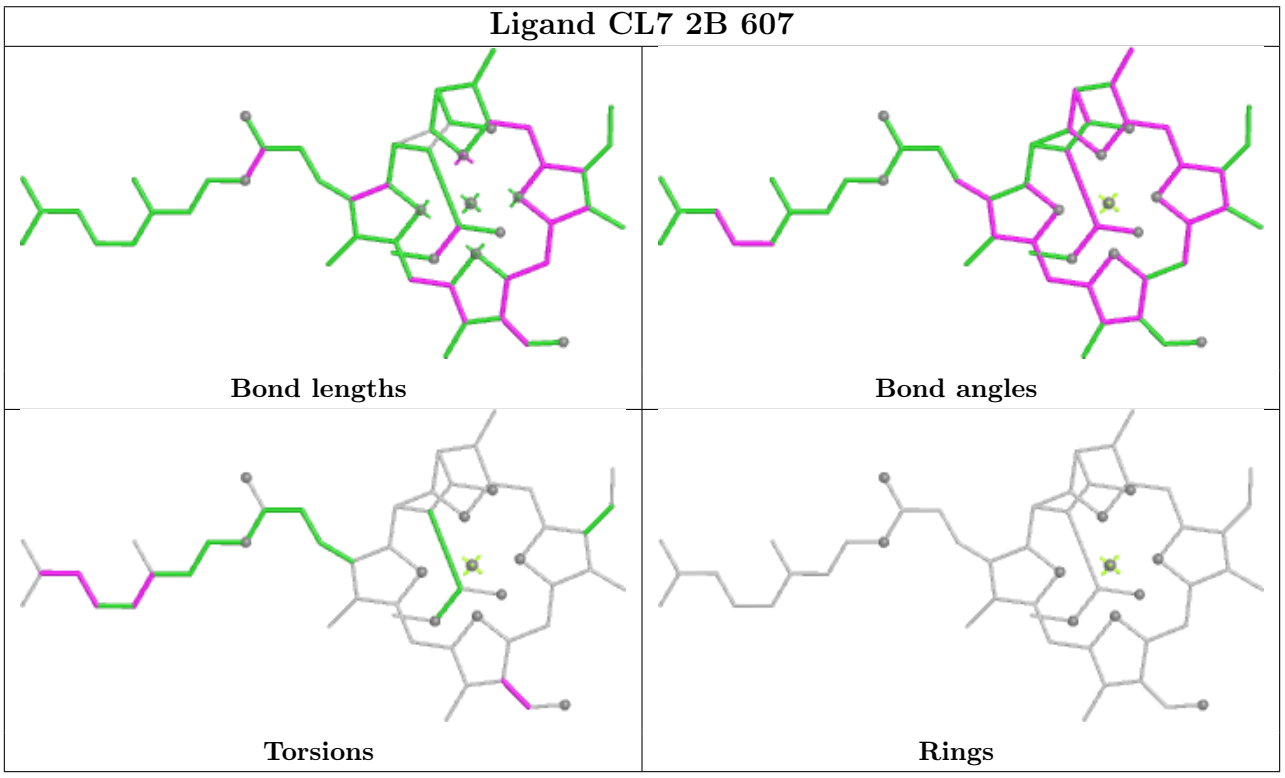


Rings

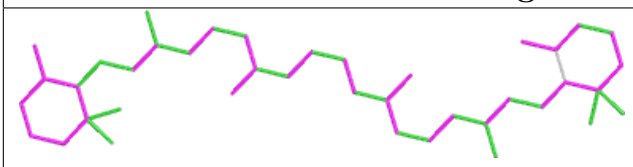
Ligand CL7 22 502



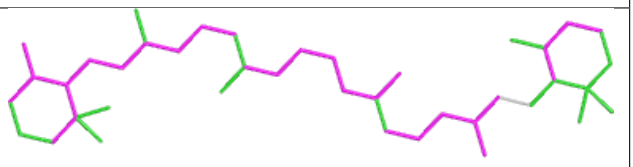
Ligand CL7 2B 607



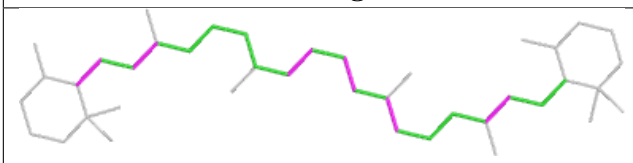
Ligand 8CT 3D 406



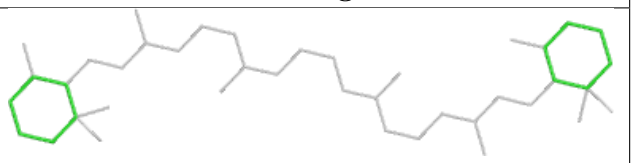
Bond lengths



Bond angles

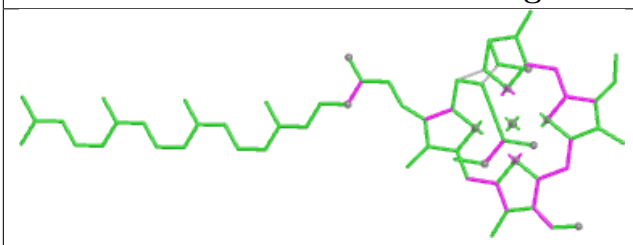


Torsions

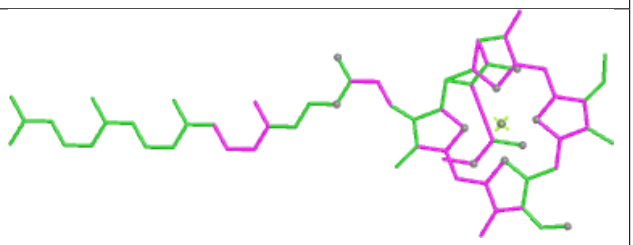


Rings

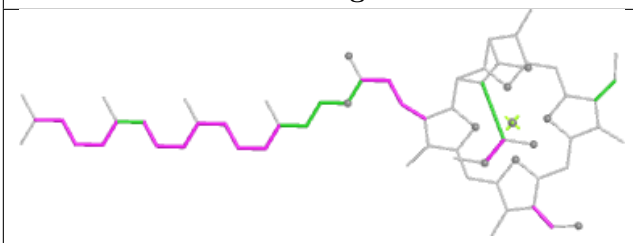
Ligand CL7 44 406



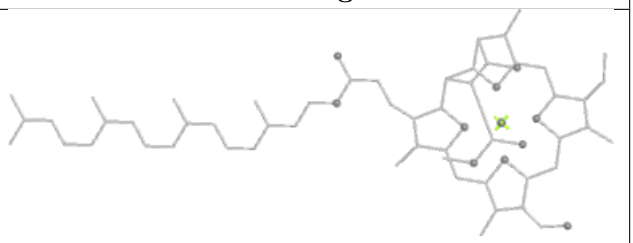
Bond lengths



Bond angles

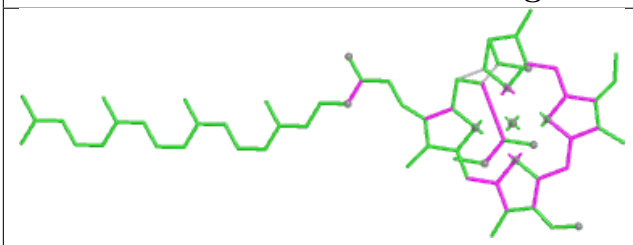


Torsions

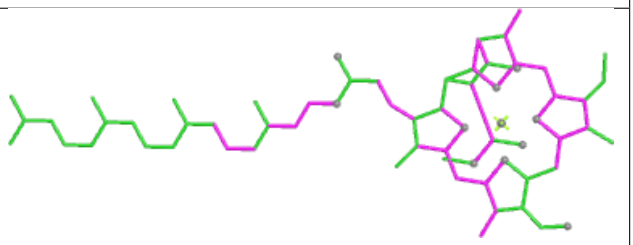


Rings

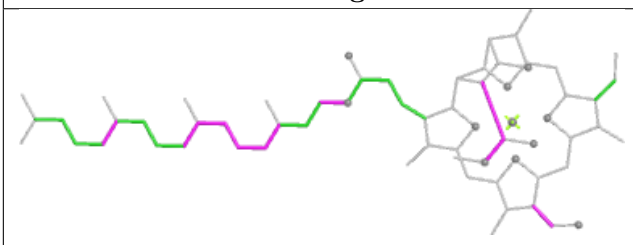
Ligand CL7 33 508



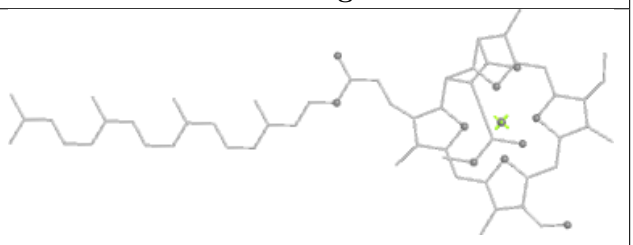
Bond lengths



Bond angles

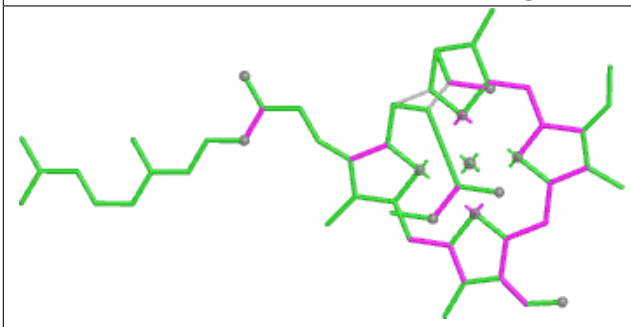


Torsions

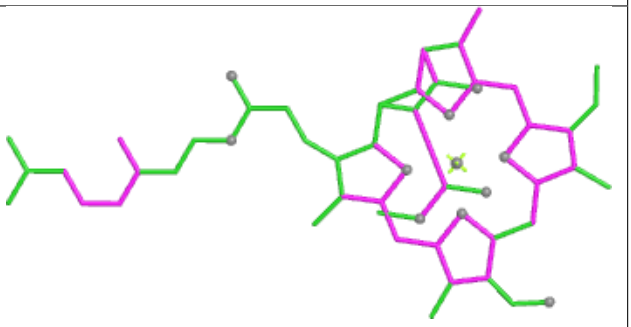


Rings

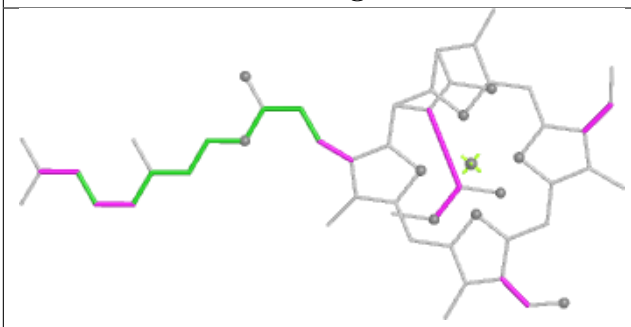
Ligand CL7 3C 504



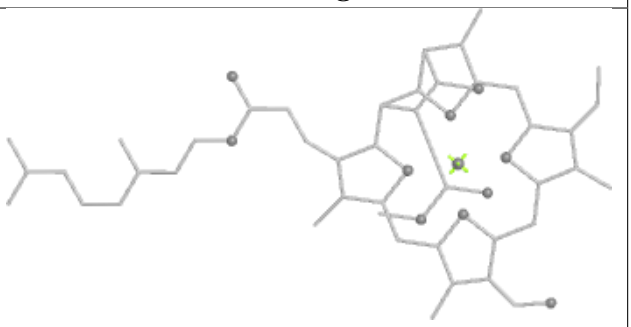
Bond lengths



Bond angles

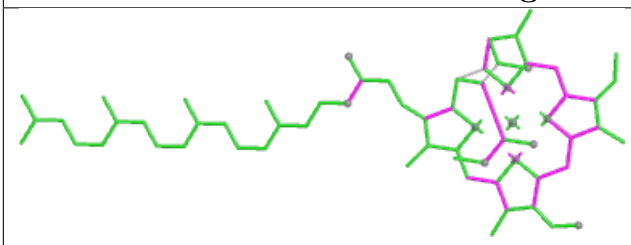


Torsions

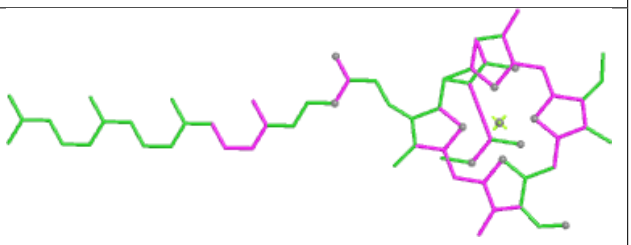


Rings

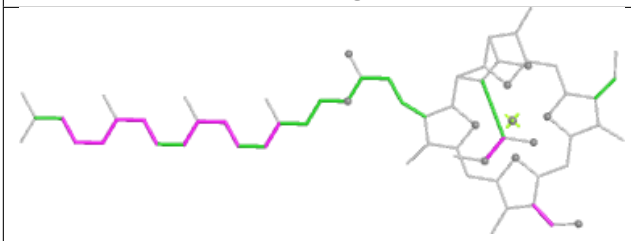
Ligand CL7 2B 612



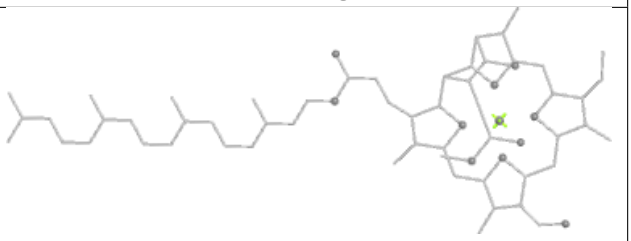
Bond lengths



Bond angles

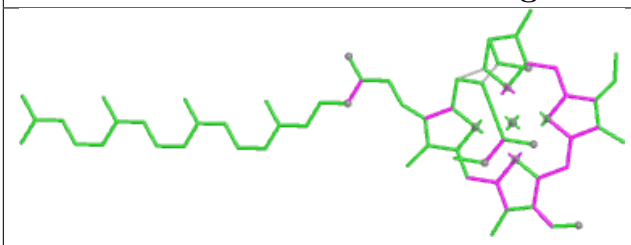


Torsions

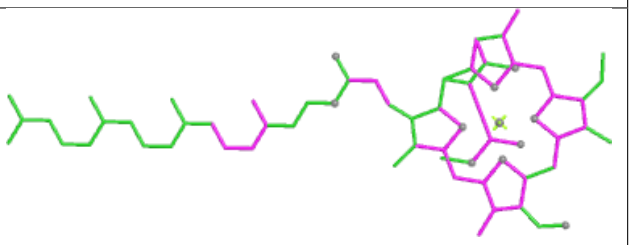


Rings

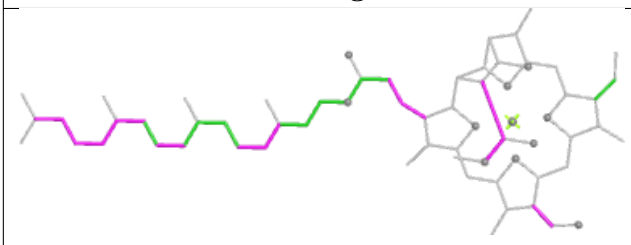
Ligand CL7 4B 605



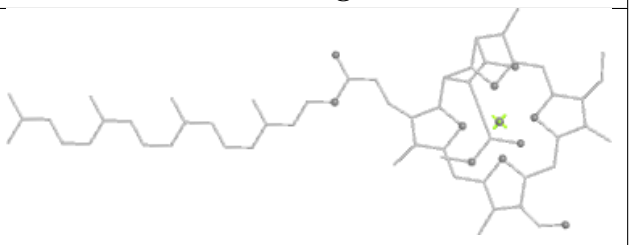
Bond lengths



Bond angles

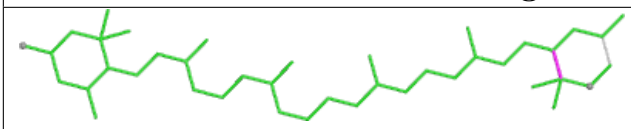


Torsions

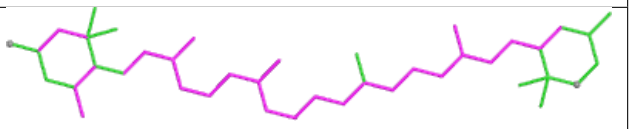


Rings

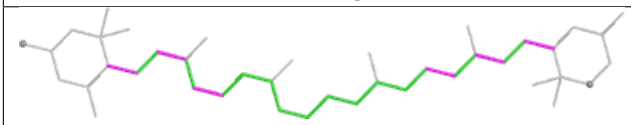
Ligand ZEX 24 418



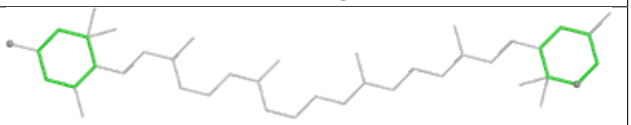
Bond lengths



Bond angles

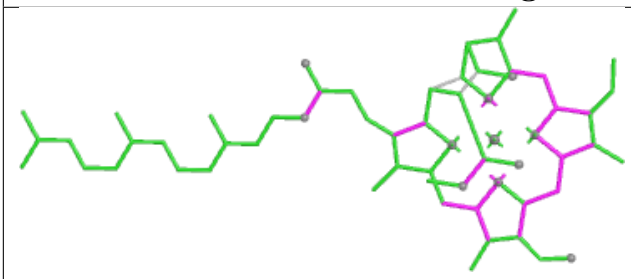


Torsions

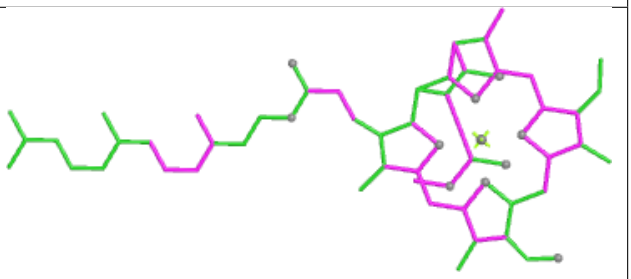


Rings

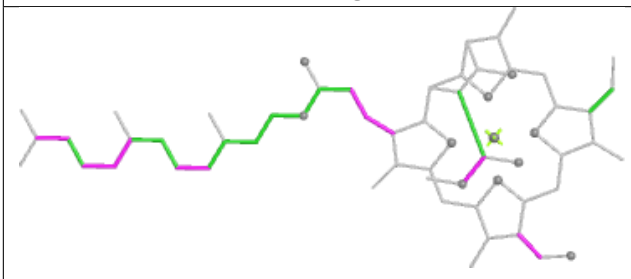
Ligand CL7 3B 607



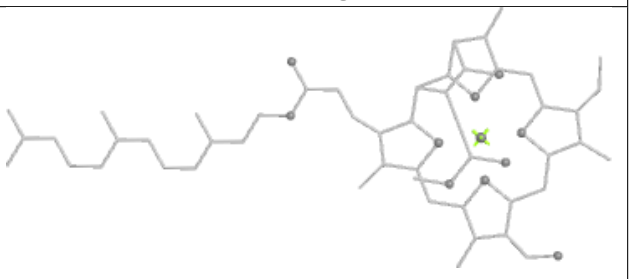
Bond lengths



Bond angles

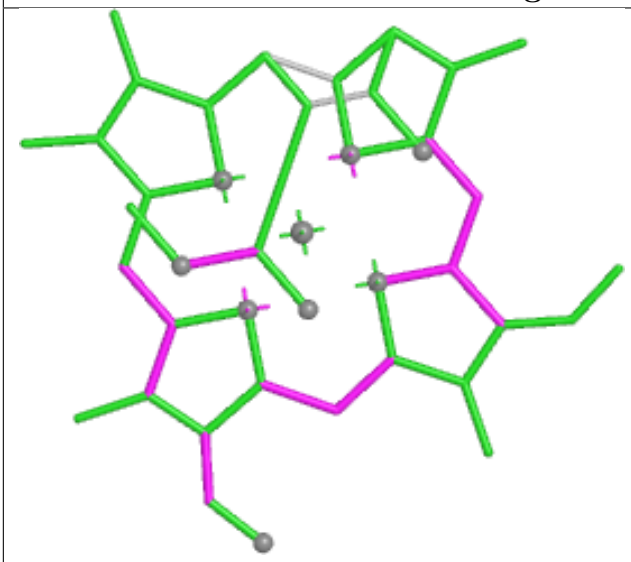


Torsions

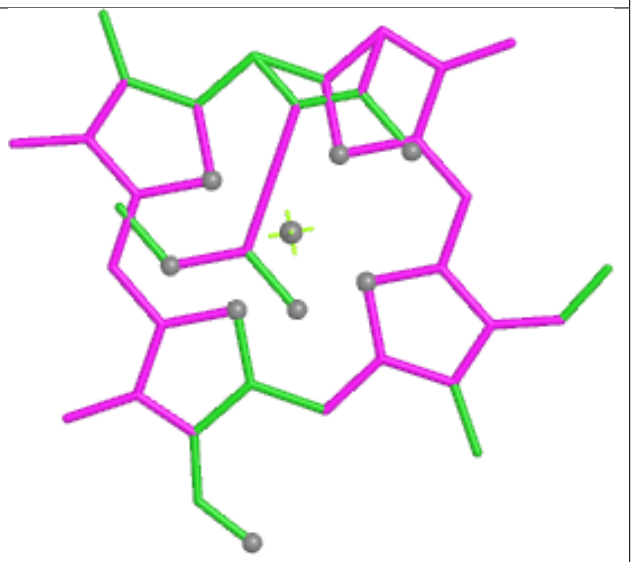


Rings

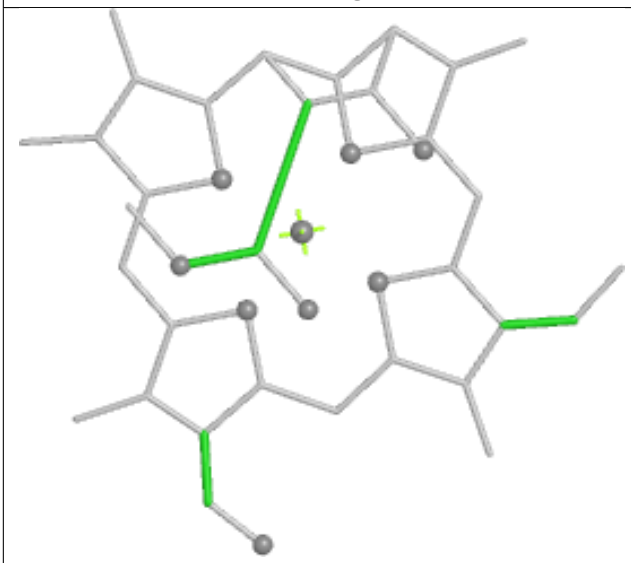
Ligand CL7 33 515



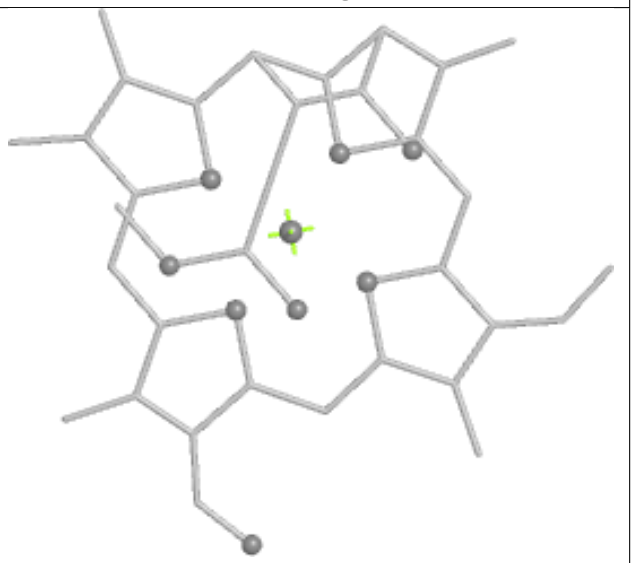
Bond lengths



Bond angles

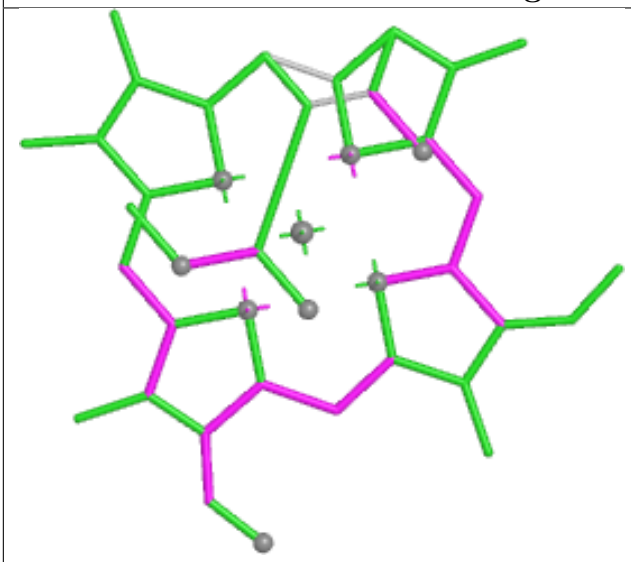


Torsions

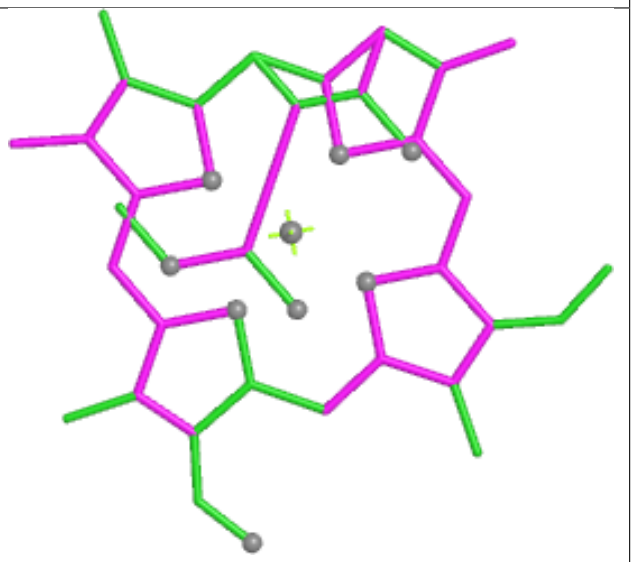


Rings

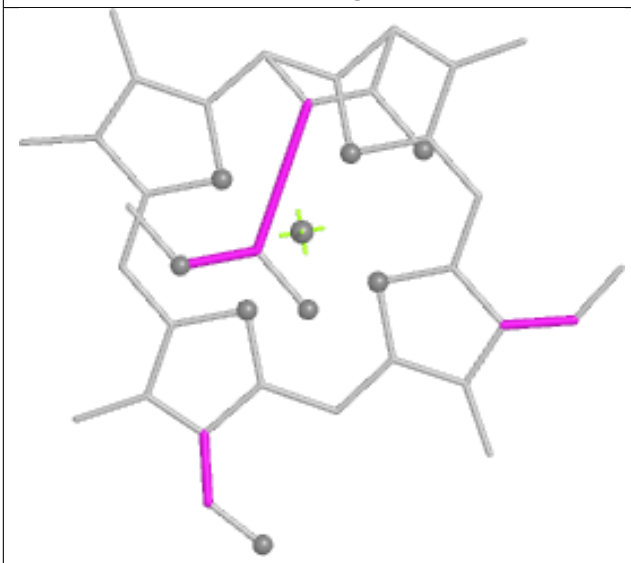
Ligand CL7 34 416



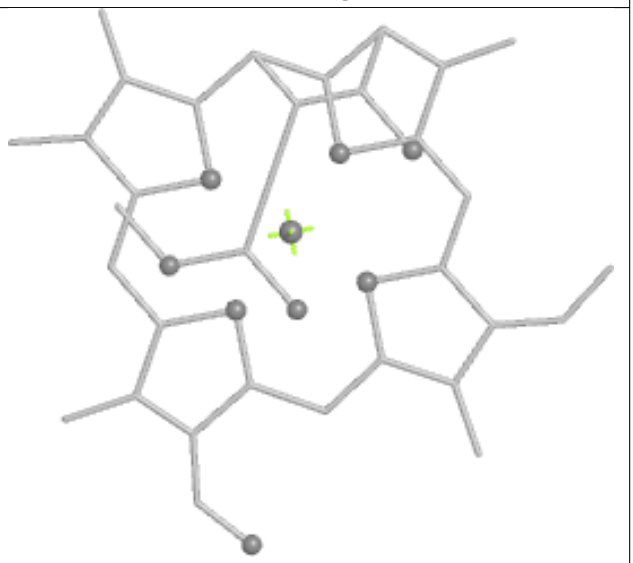
Bond lengths



Bond angles

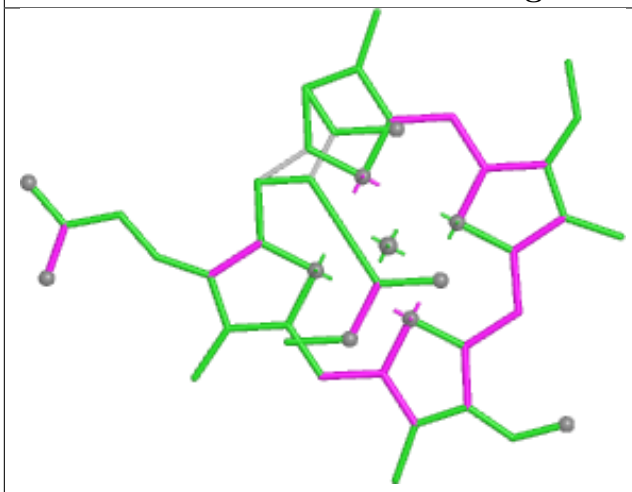


Torsions

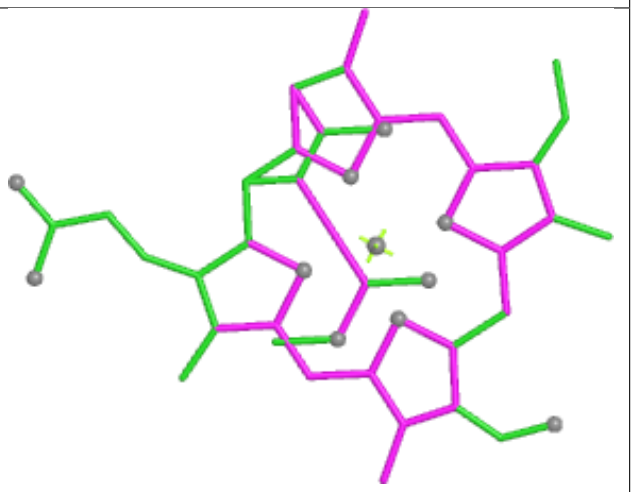


Rings

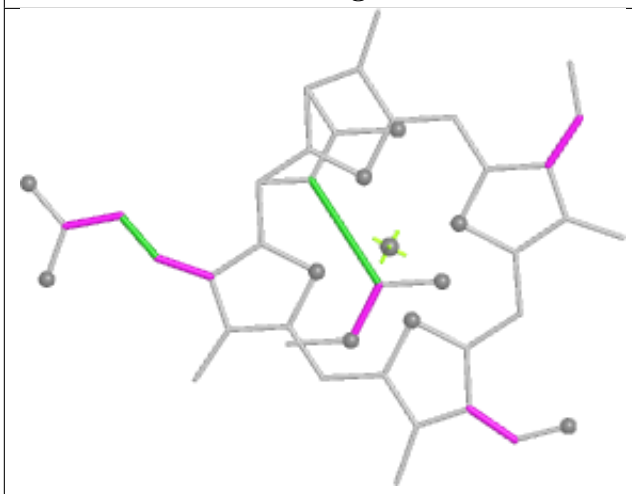
Ligand CL7 42 514



Bond lengths



Bond angles

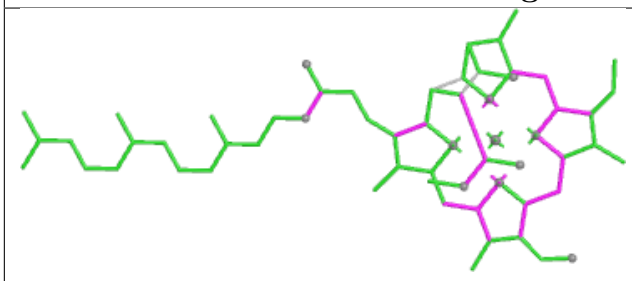


Torsions

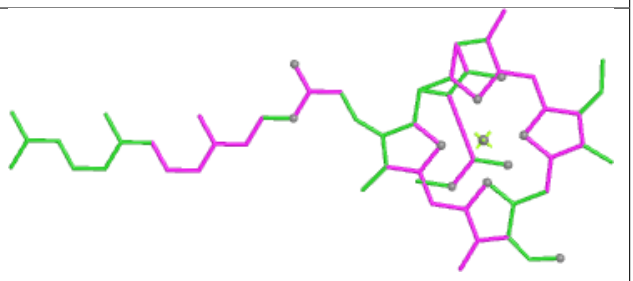


Rings

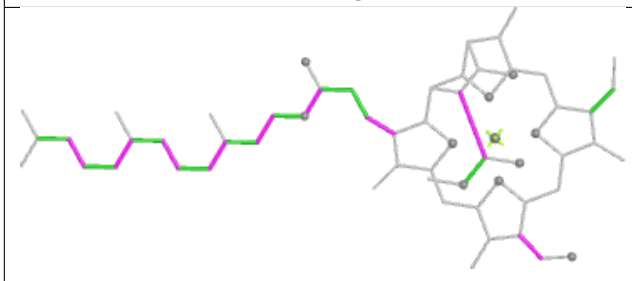
Ligand CL7 4C 506



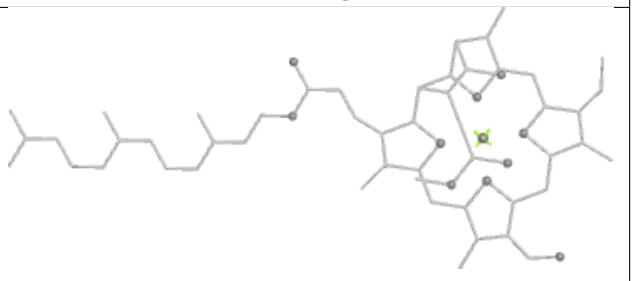
Bond lengths



Bond angles

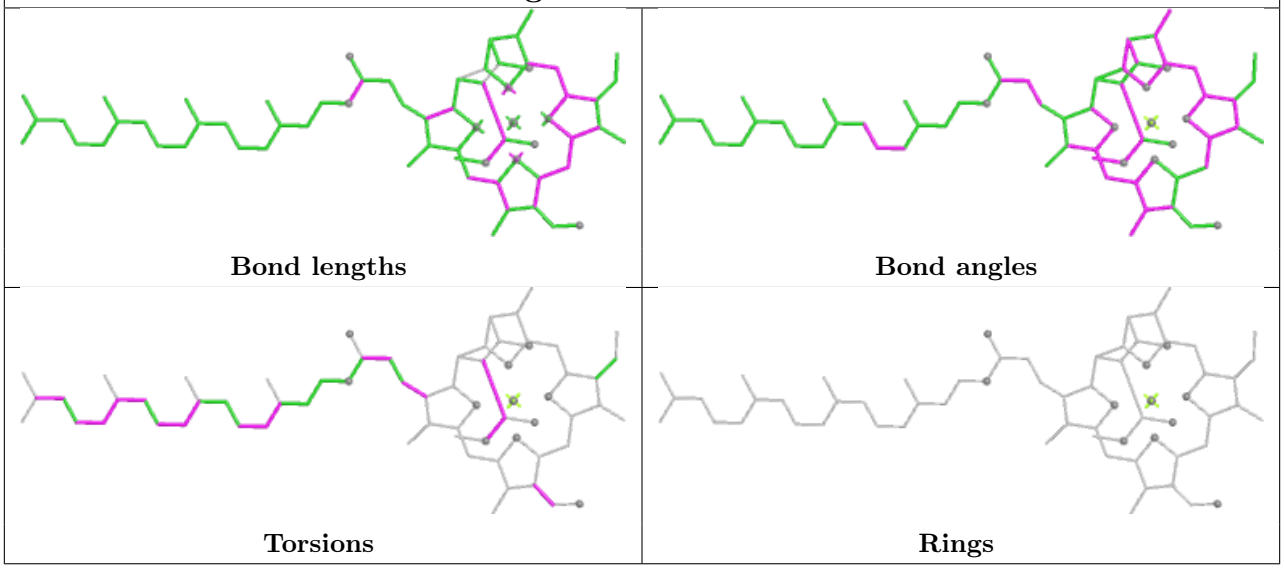


Torsions

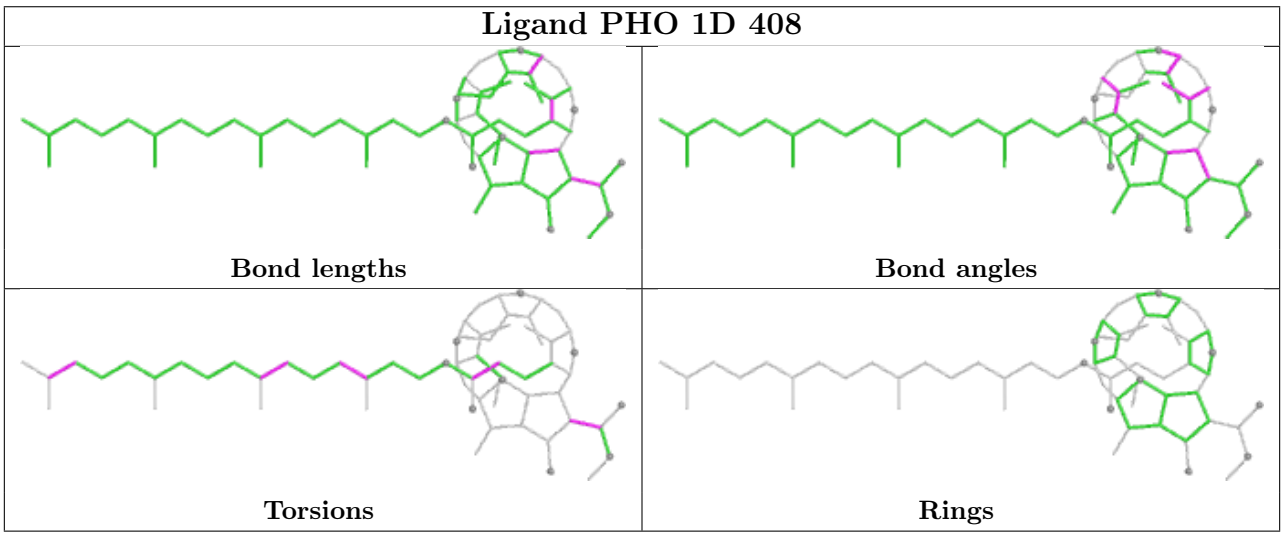


Rings

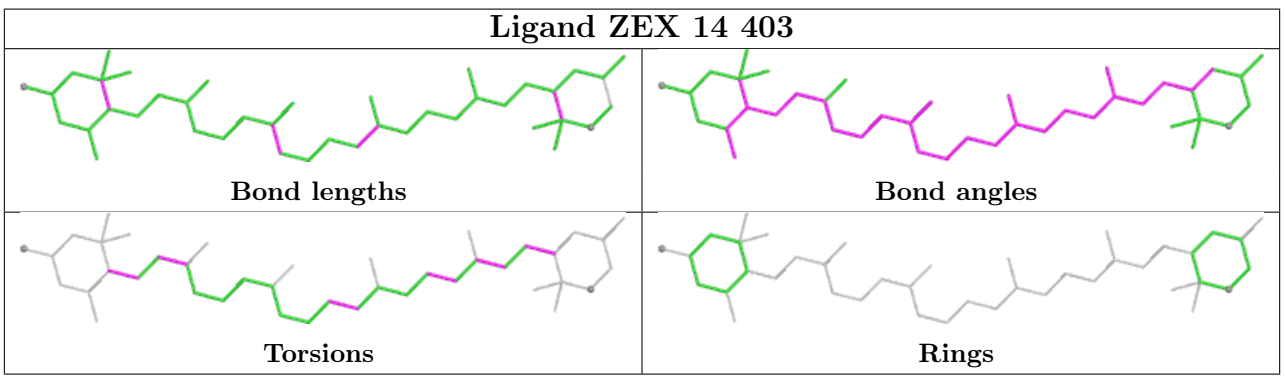
Ligand CL7 32 507



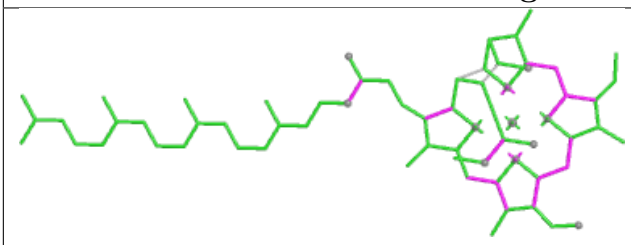
Ligand PHO 1D 408



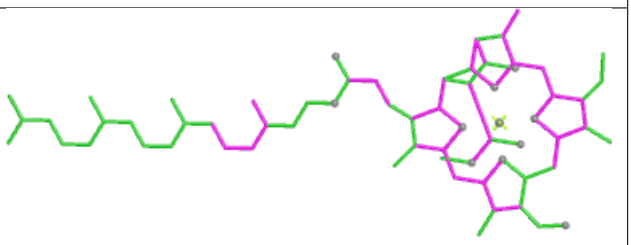
Ligand ZEX 14 403



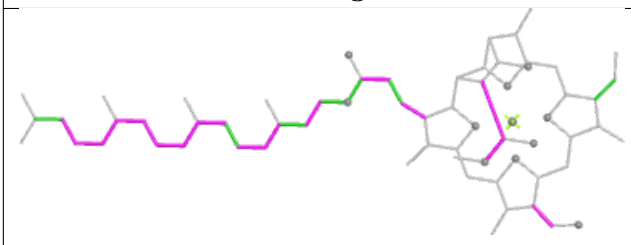
Ligand CL7 4C 510



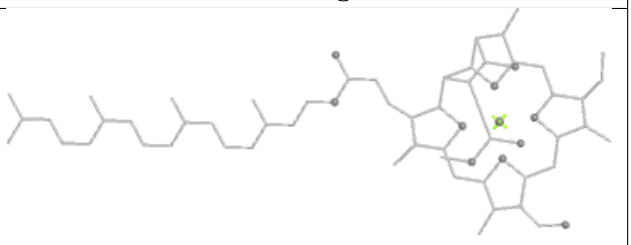
Bond lengths



Bond angles

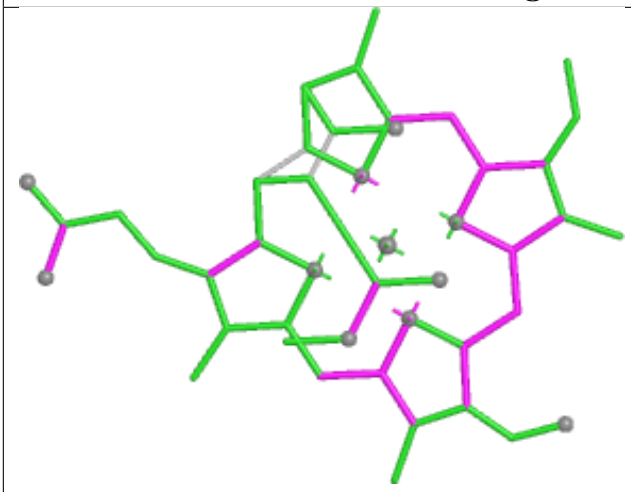


Torsions



Rings

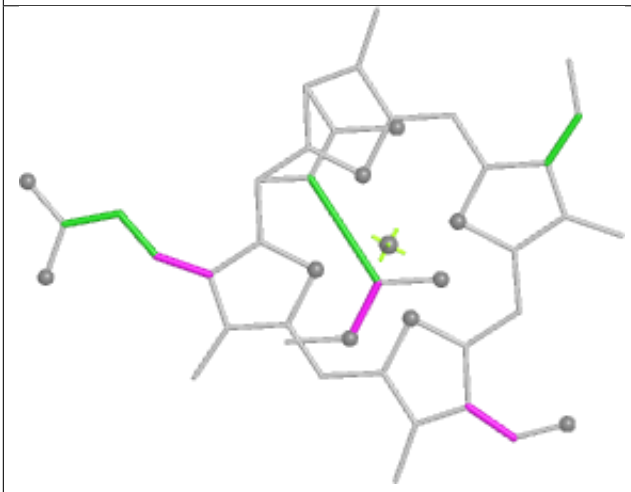
Ligand CL7 42 504



Bond lengths



Bond angles

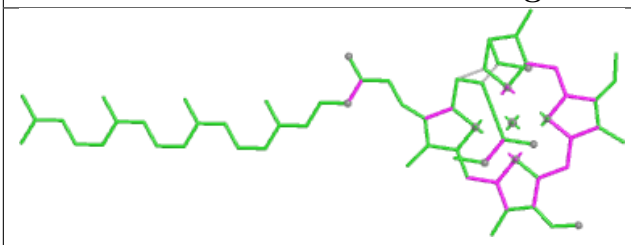


Torsions

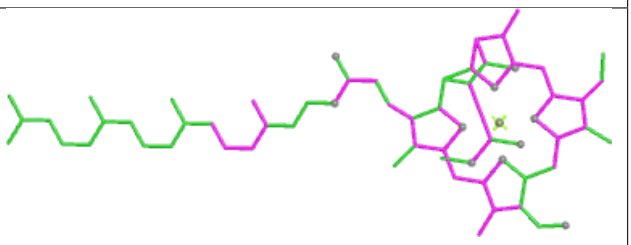


Rings

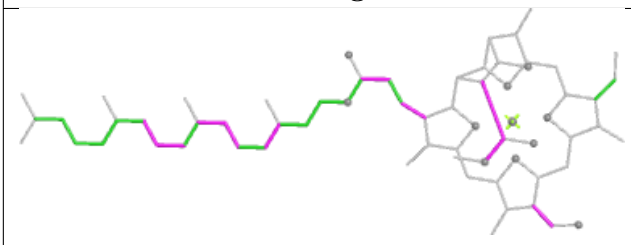
Ligand CL7 13 510



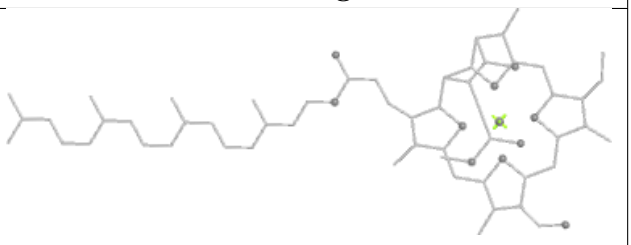
Bond lengths



Bond angles

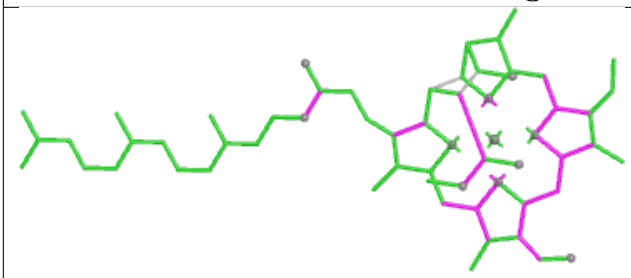


Torsions

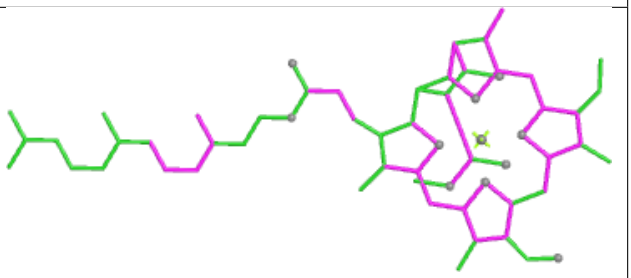


Rings

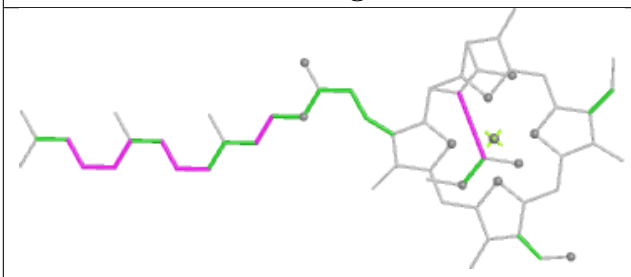
Ligand CL7 44 413



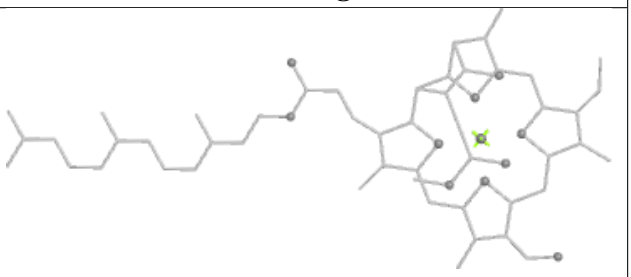
Bond lengths



Bond angles

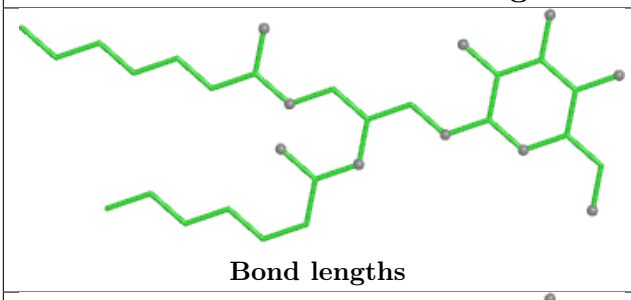


Torsions

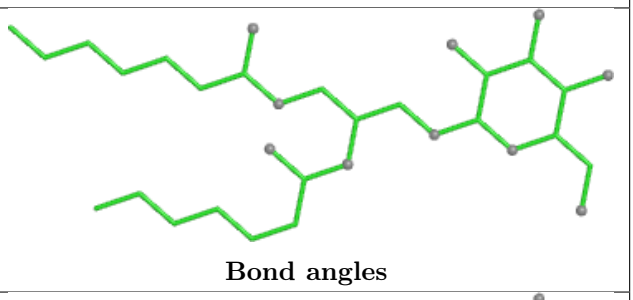


Rings

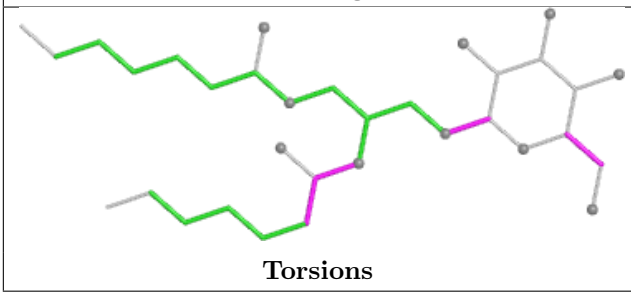
Ligand LMG 1D 410



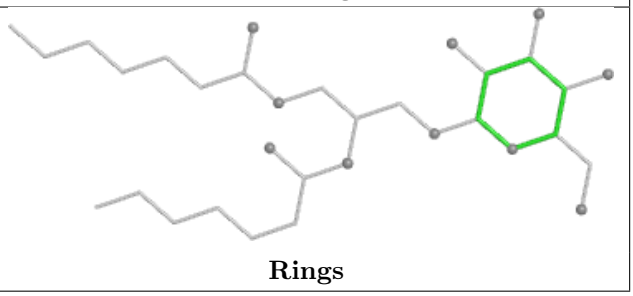
Bond lengths



Bond angles

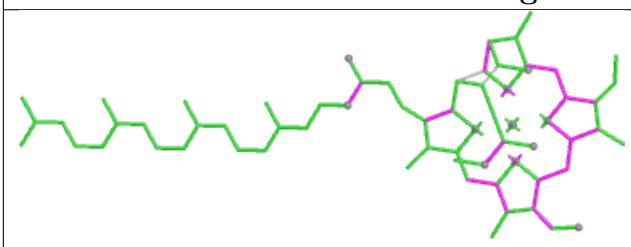


Torsions

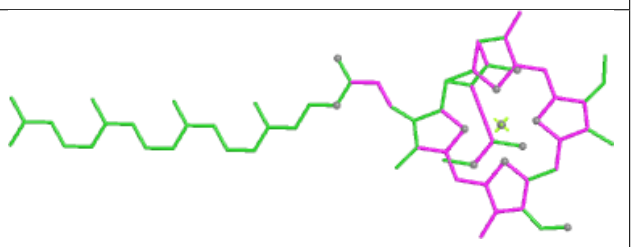


Rings

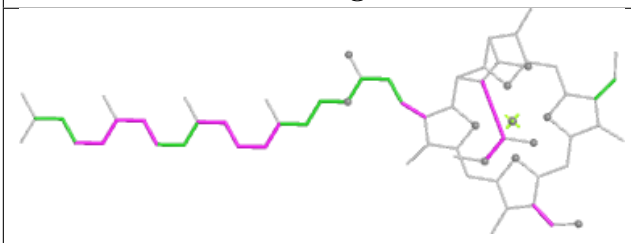
Ligand CL7 4B 606



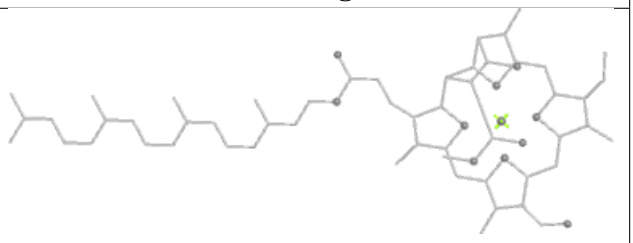
Bond lengths



Bond angles

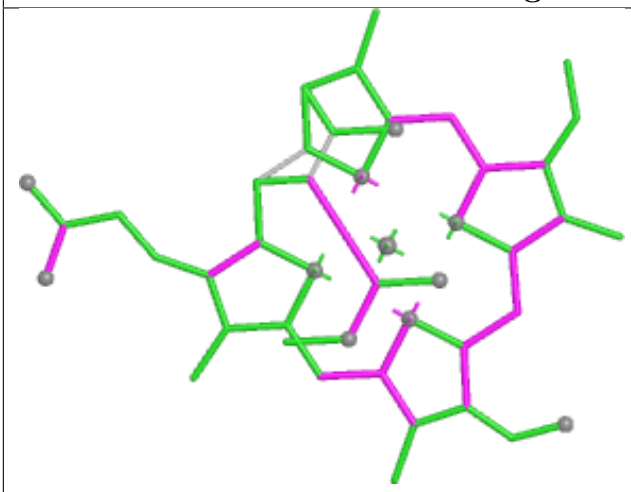


Torsions

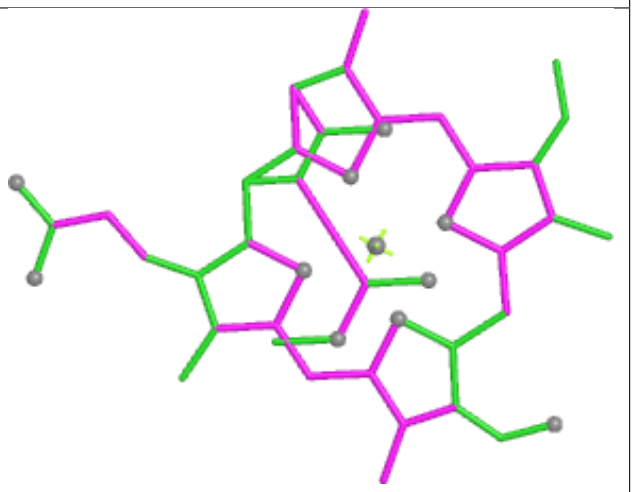


Rings

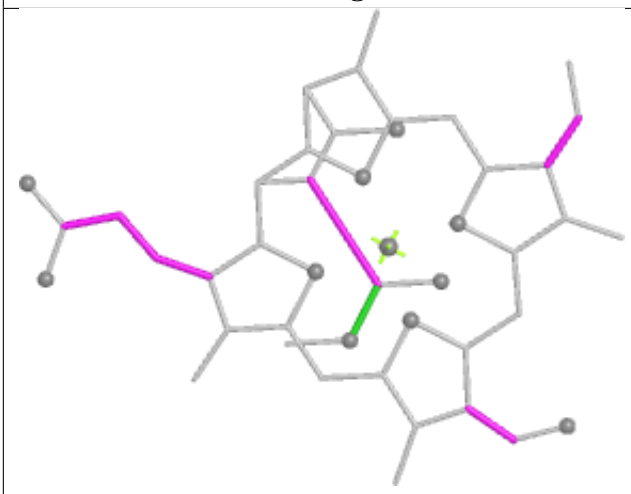
Ligand CL7 13 513



Bond lengths



Bond angles

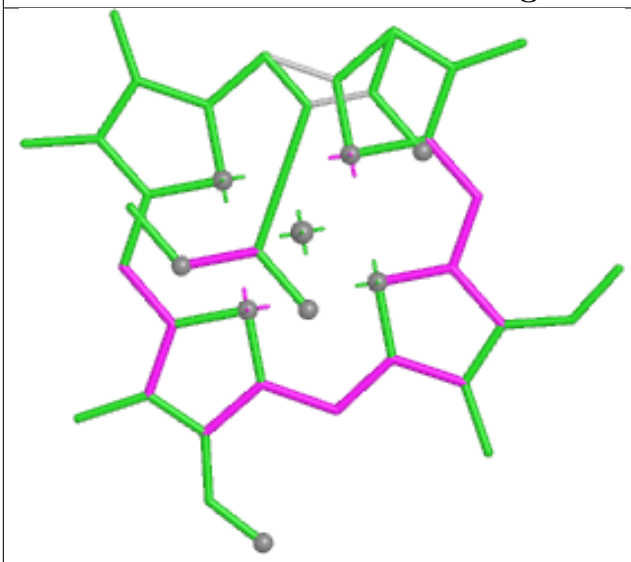


Torsions

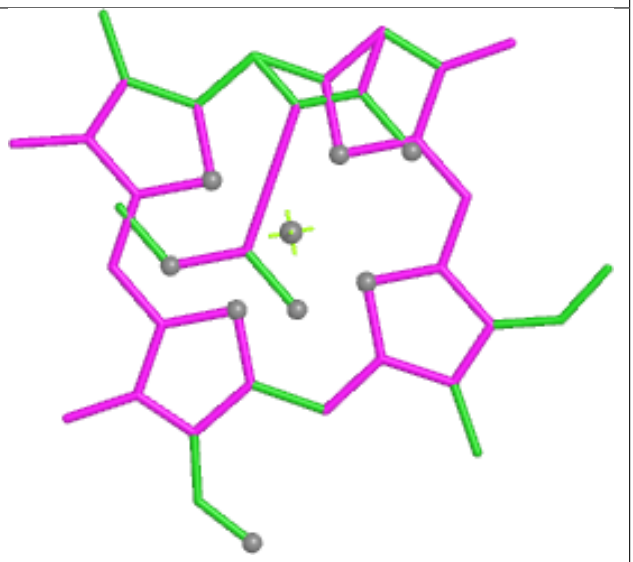


Rings

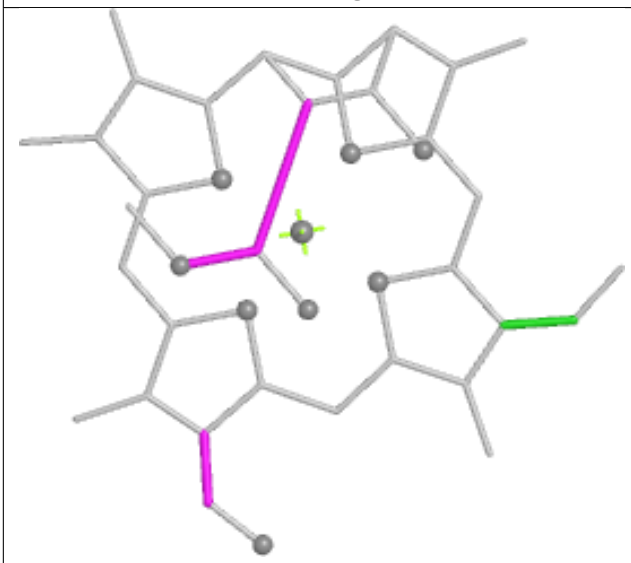
Ligand CL7 2C 517



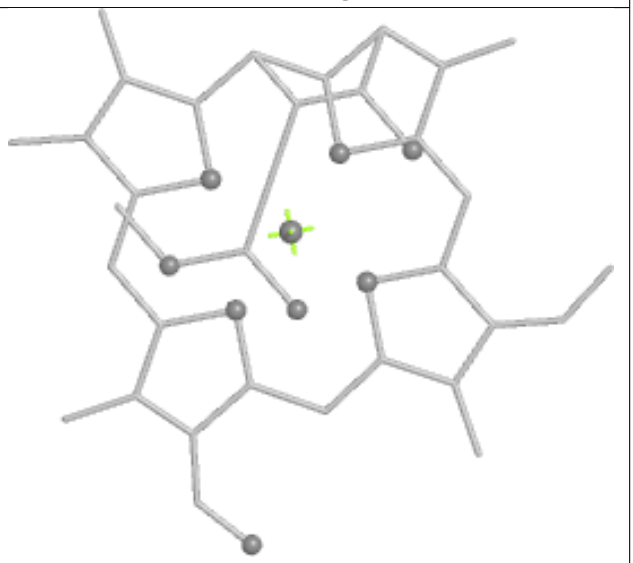
Bond lengths



Bond angles

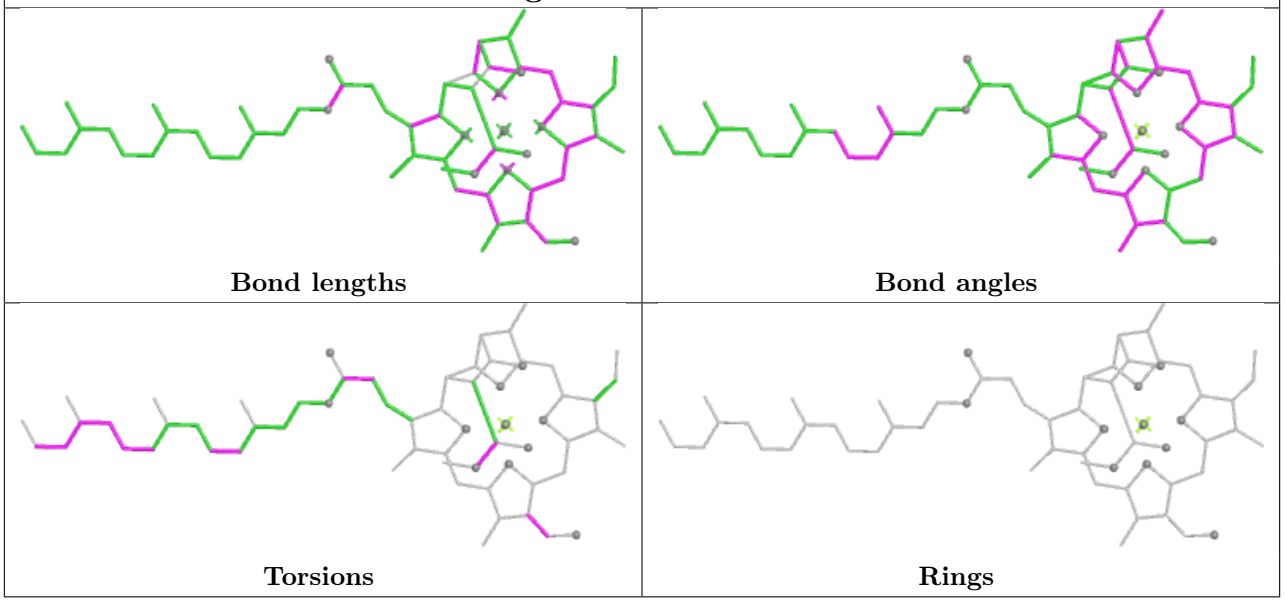


Torsions

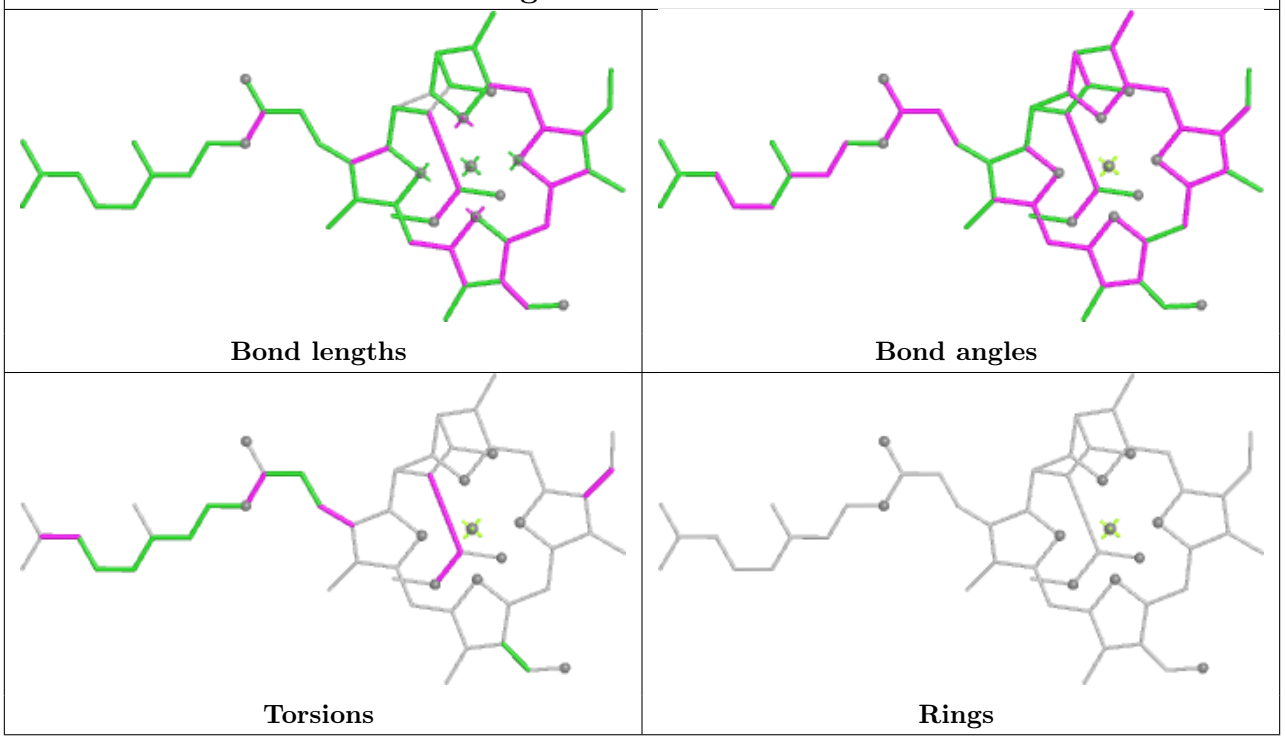


Rings

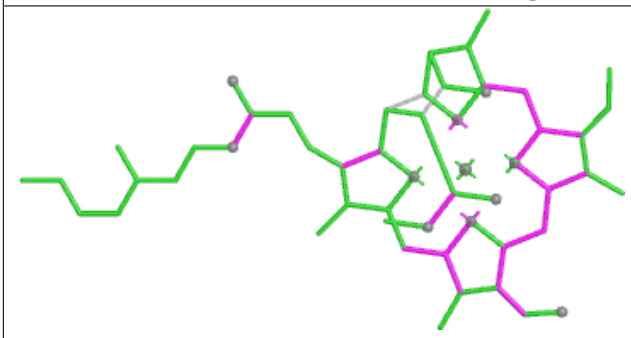
Ligand CL7 41 406



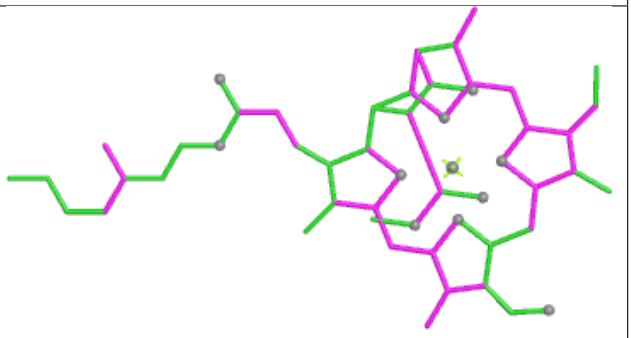
Ligand CL7 2A 403



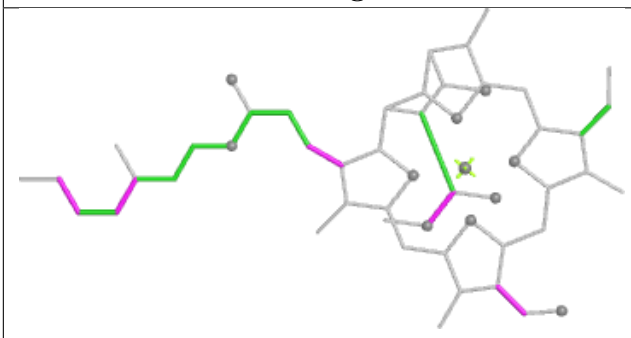
Ligand CL7 24 414



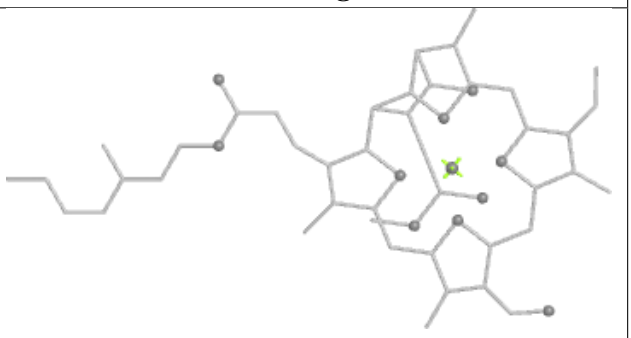
Bond lengths



Bond angles

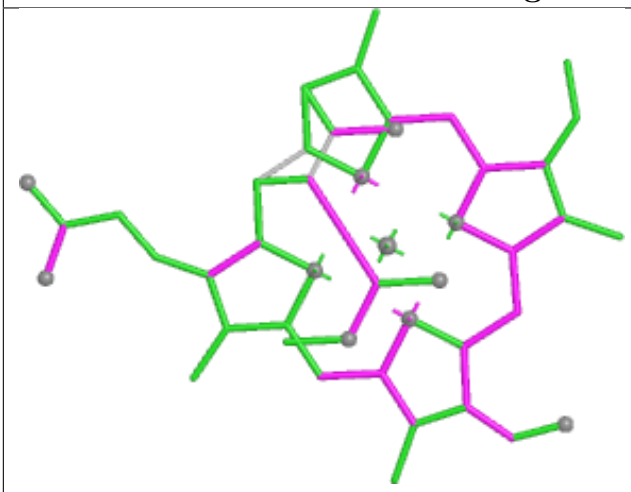


Torsions

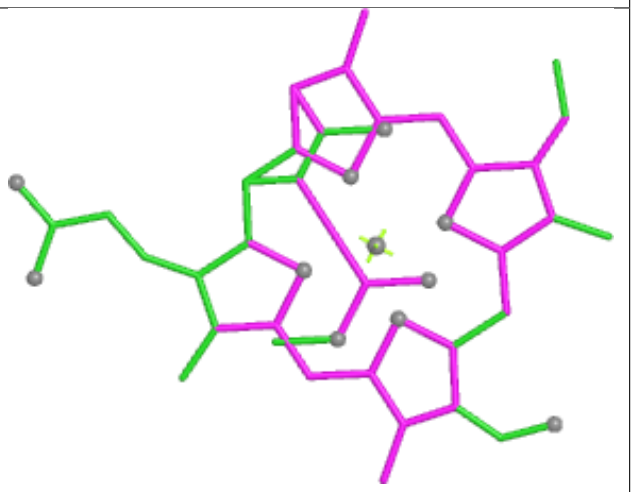


Rings

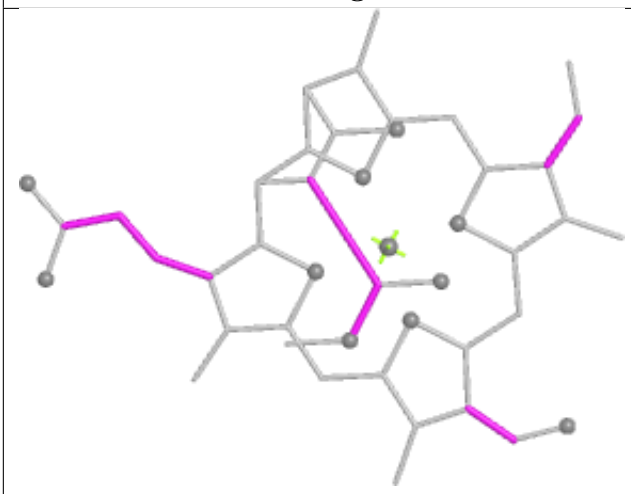
Ligand CL7 14 415



Bond lengths



Bond angles

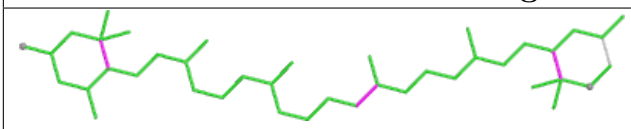


Torsions

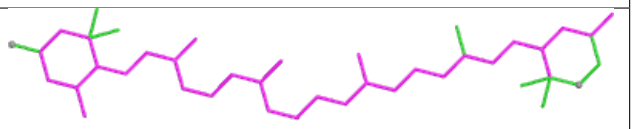


Rings

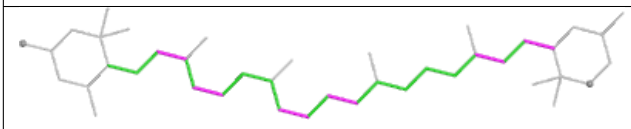
Ligand ZEX 34 419



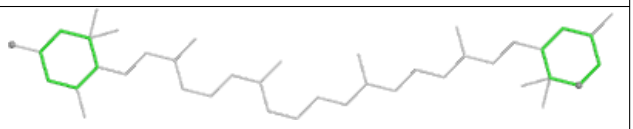
Bond lengths



Bond angles

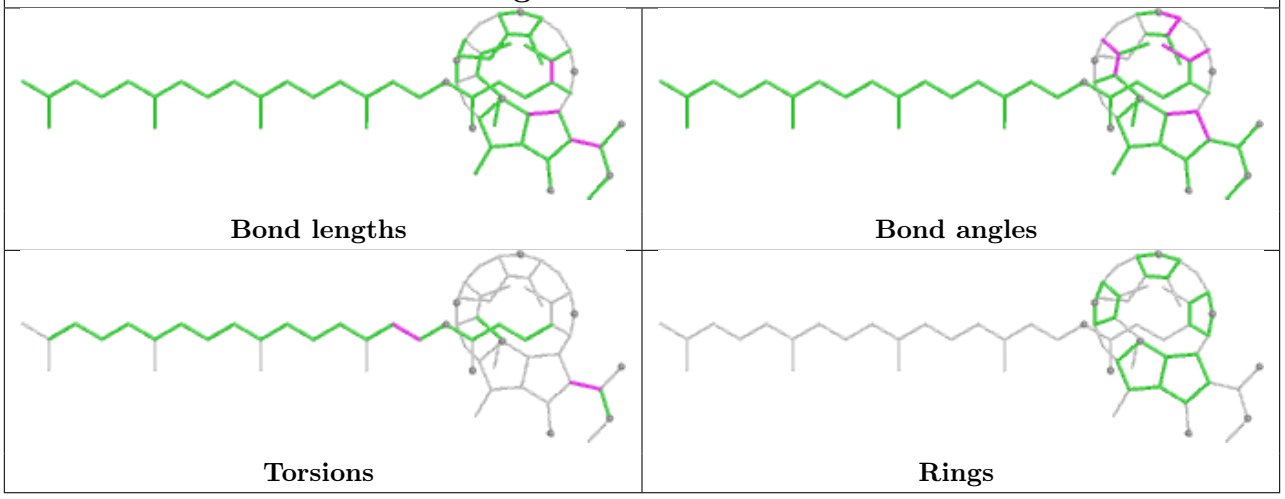


Torsions

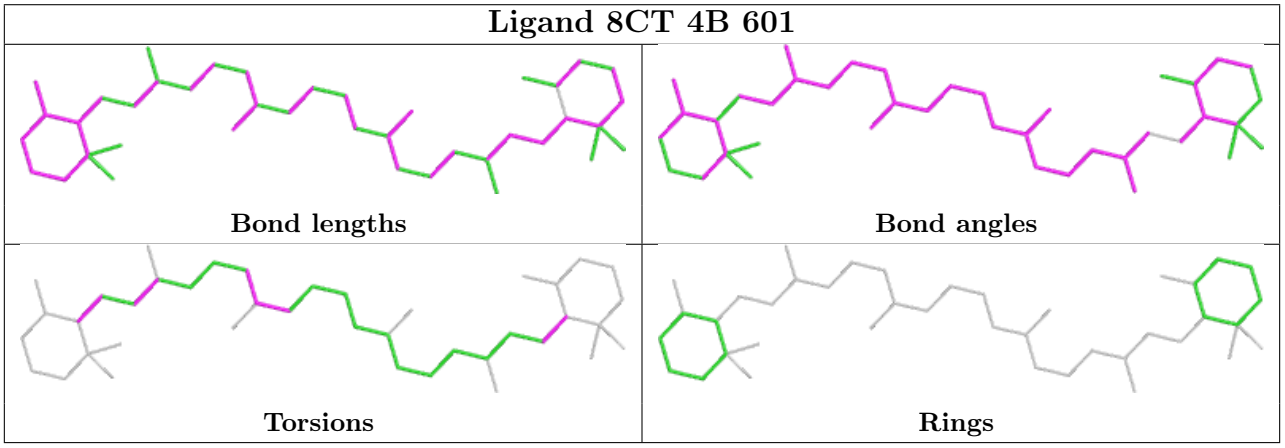


Rings

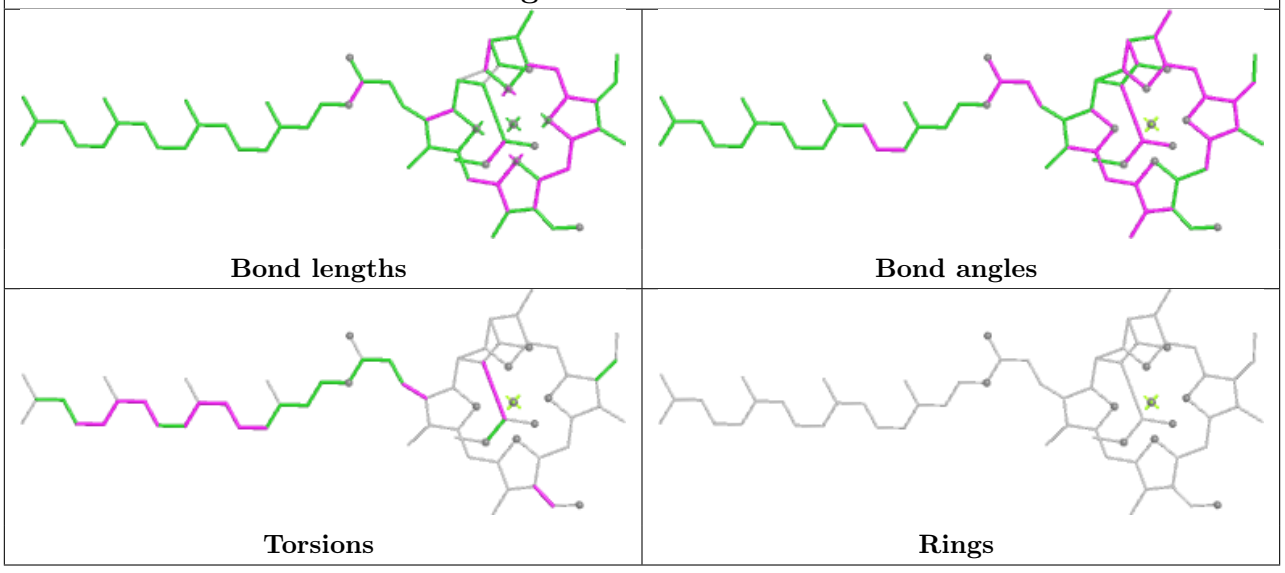
Ligand PHO 1A 402



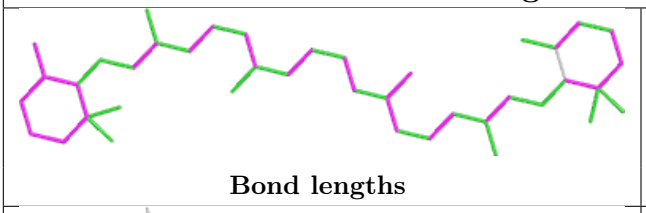
Ligand 8CT 4B 601

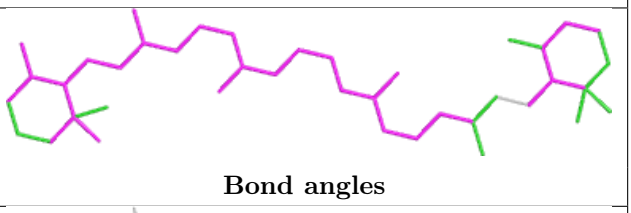


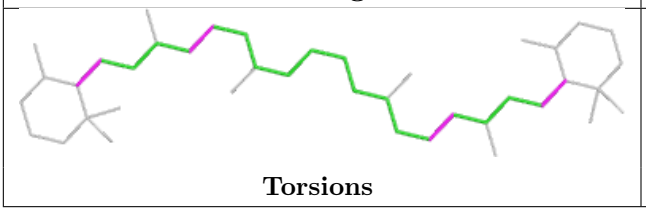
Ligand CL7 3B 612

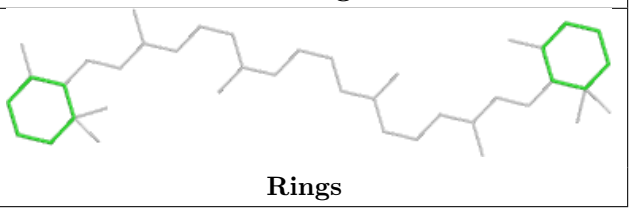


Ligand 8CT 14 402

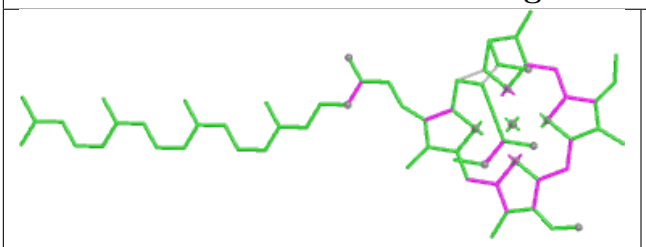

Bond lengths

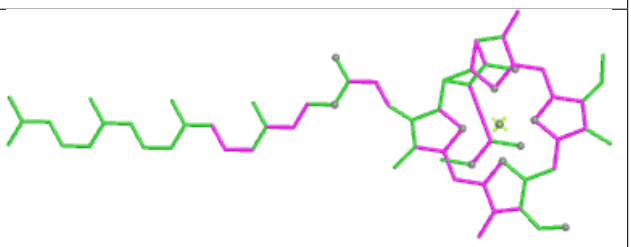

Bond angles

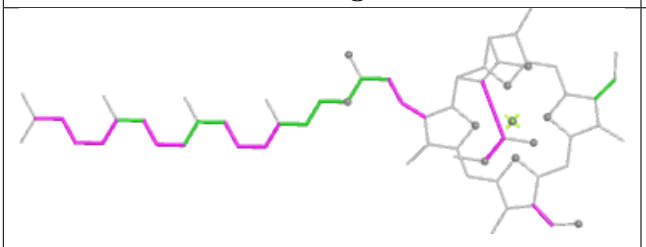

Torsions

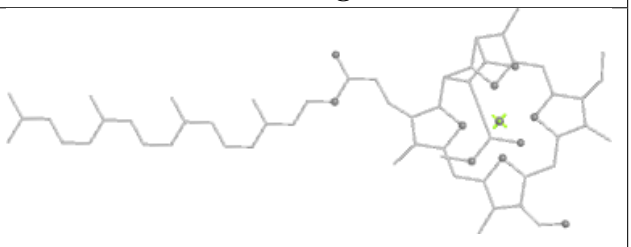

Rings

Ligand CL7 12 517

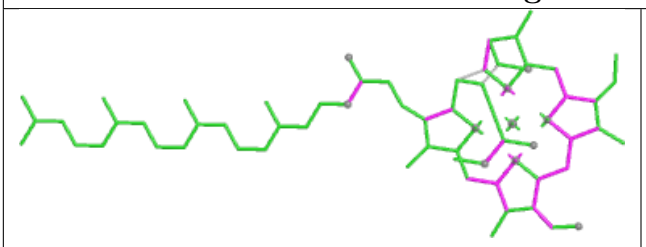

Bond lengths

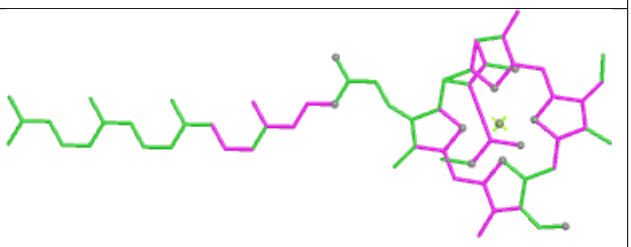

Bond angles

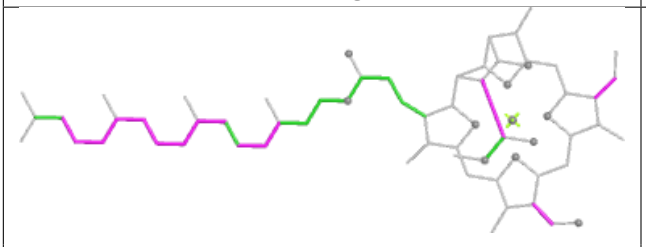

Torsions

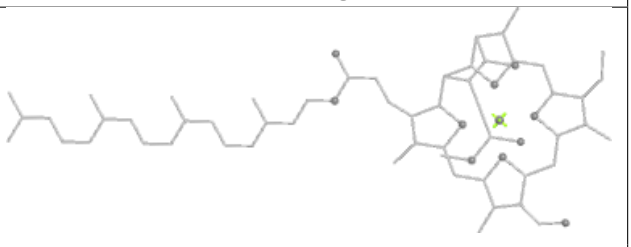

Rings

Ligand CL7 22 505

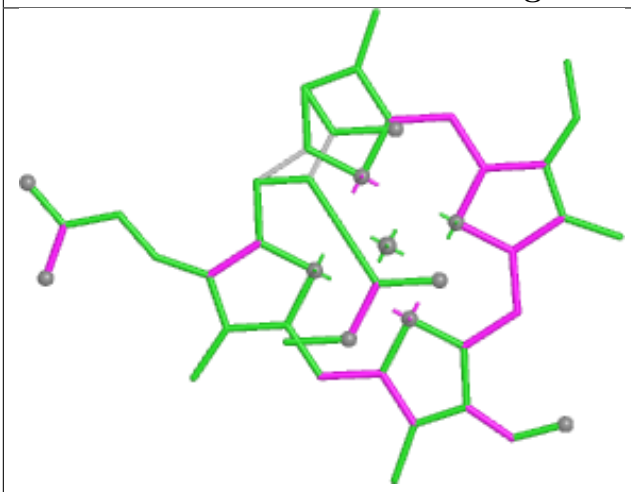

Bond lengths


Bond angles

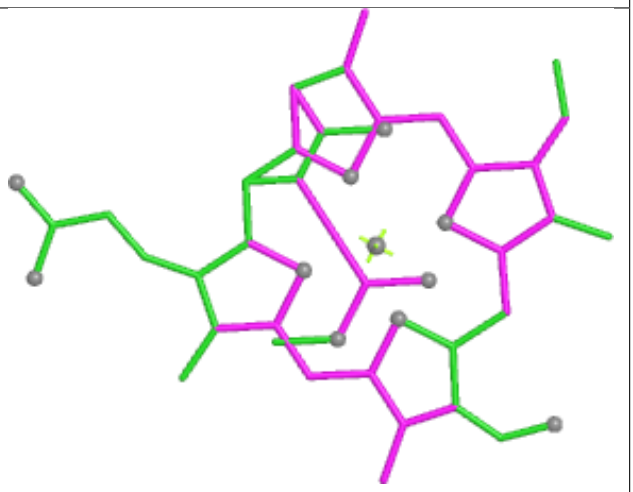

Torsions


Rings

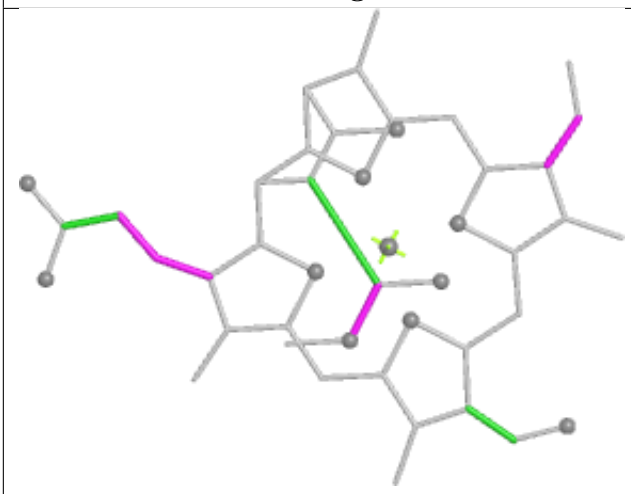
Ligand CL7 33 514



Bond lengths



Bond angles

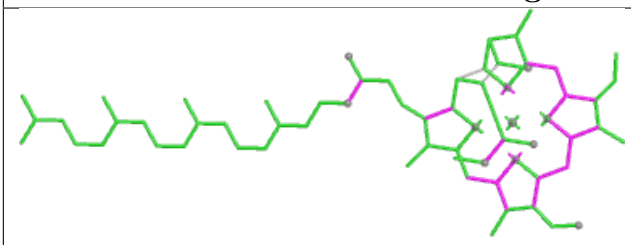


Torsions

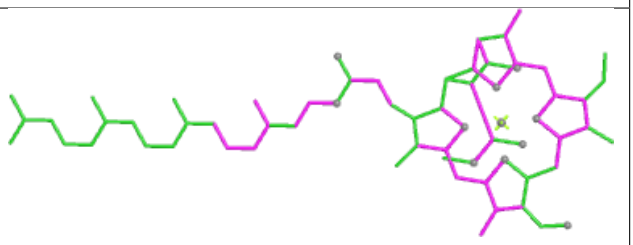


Rings

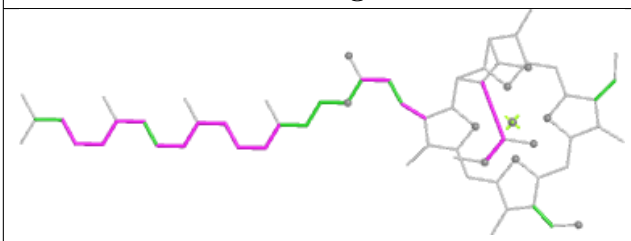
Ligand CL7 22 510



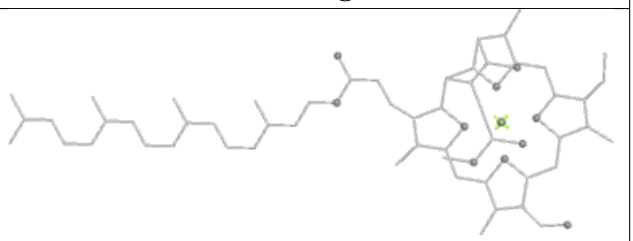
Bond lengths



Bond angles

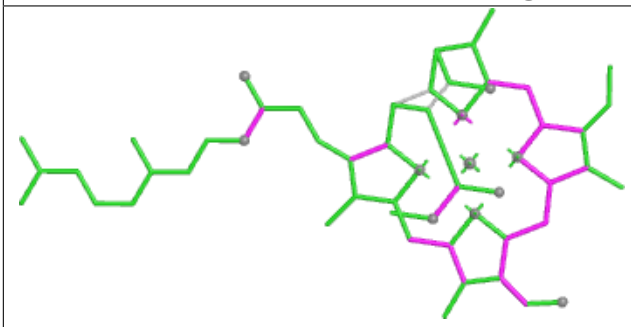


Torsions

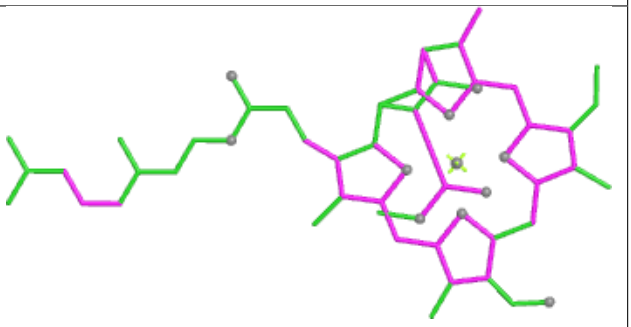


Rings

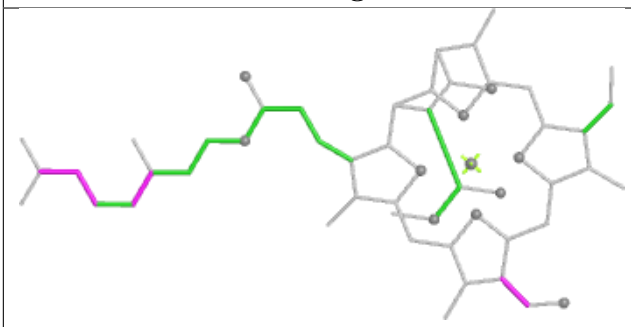
Ligand CL7 1B 606



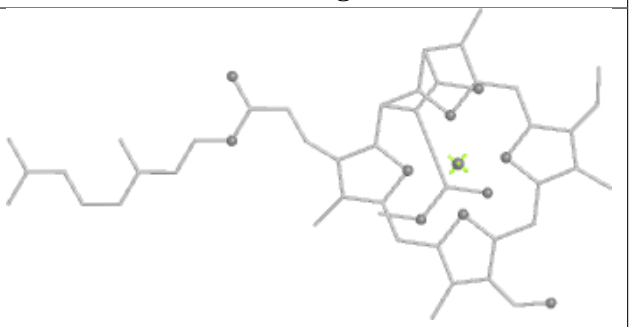
Bond lengths



Bond angles

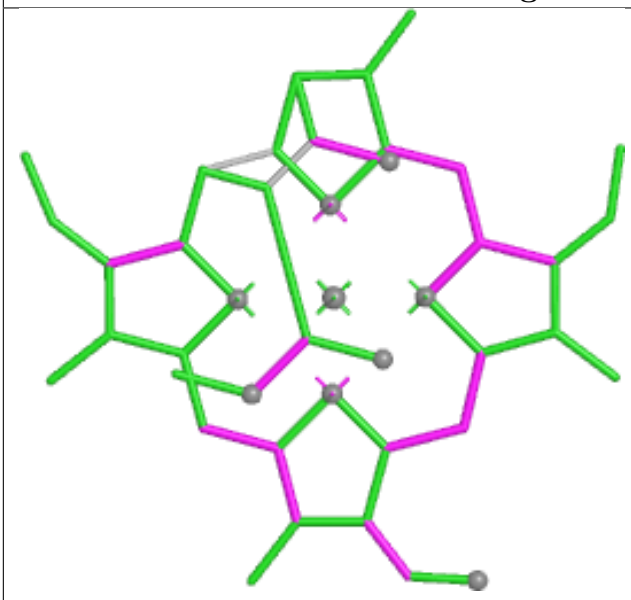


Torsions

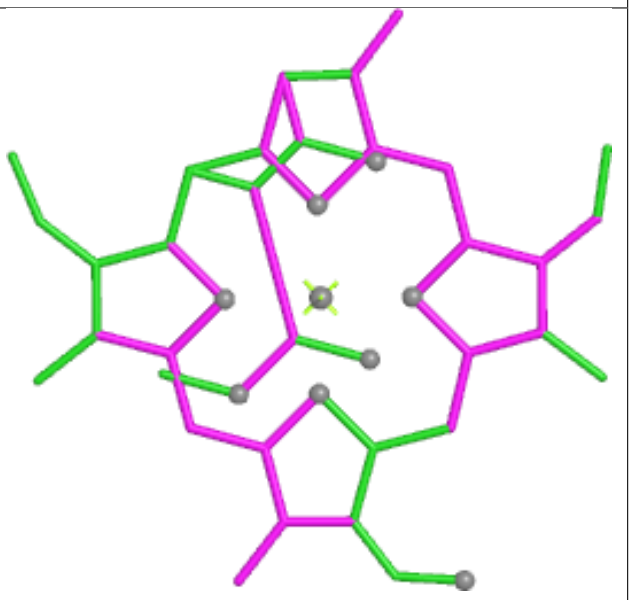


Rings

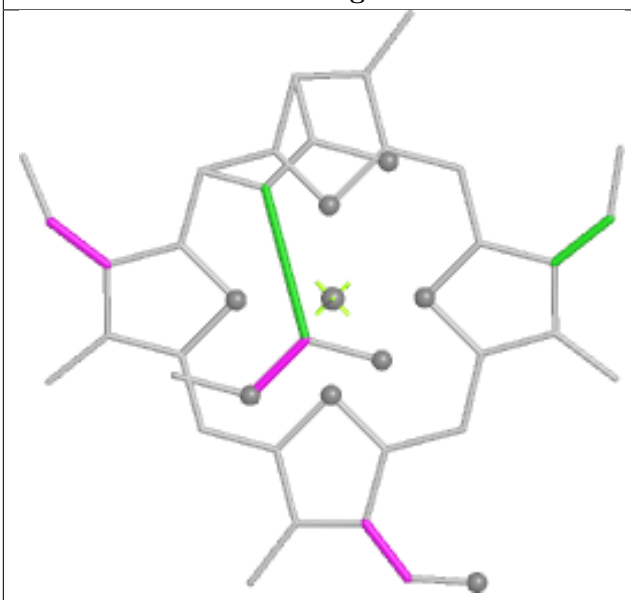
Ligand CL7 4C 511



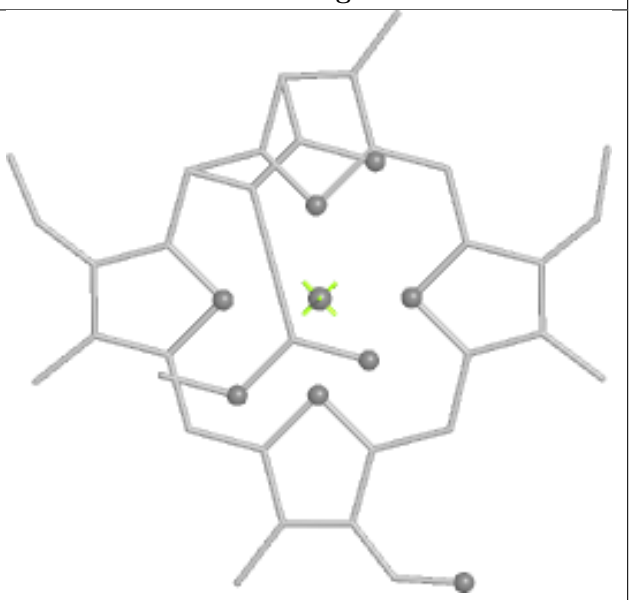
Bond lengths



Bond angles

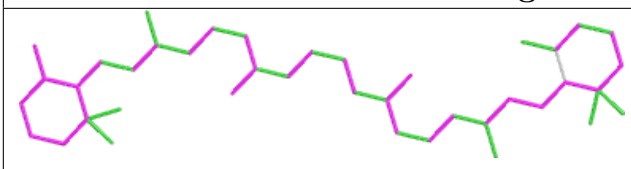


Torsions

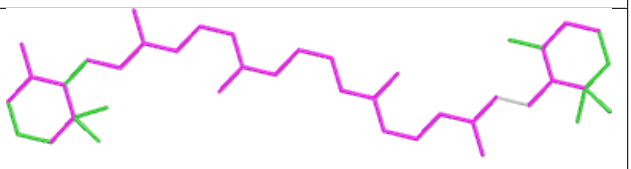


Rings

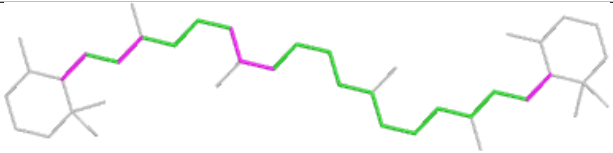
Ligand 8CT 2B 601



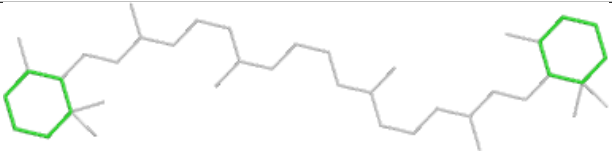
Bond lengths



Bond angles

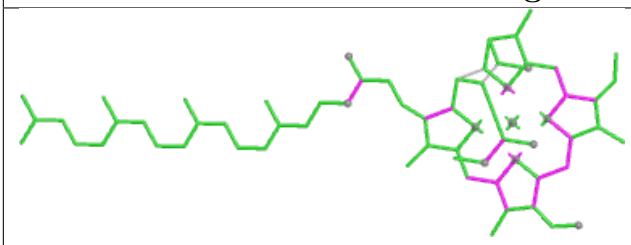


Torsions

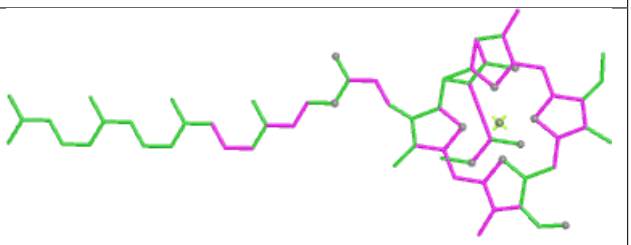


Rings

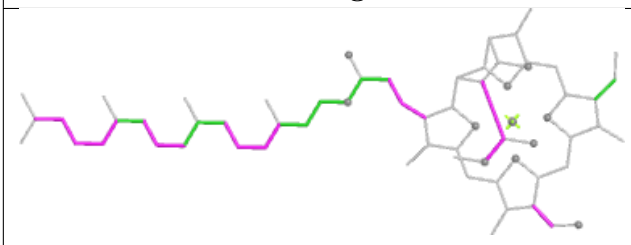
Ligand CL7 42 517



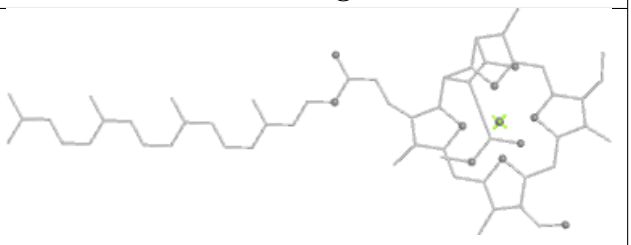
Bond lengths



Bond angles

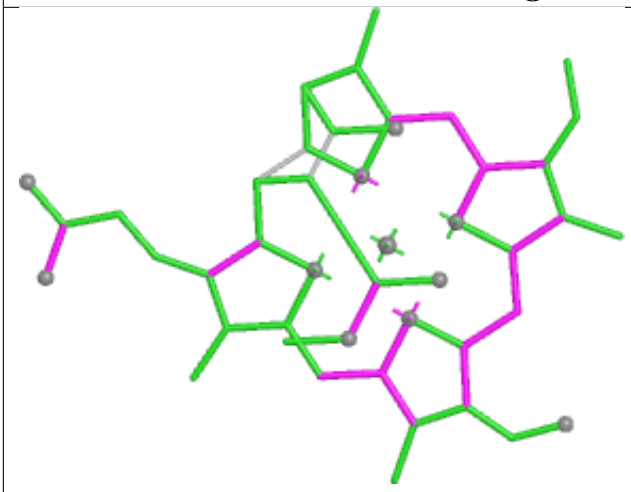


Torsions

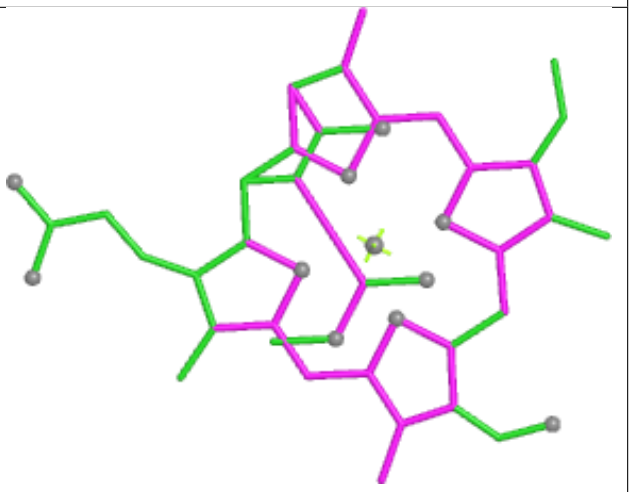


Rings

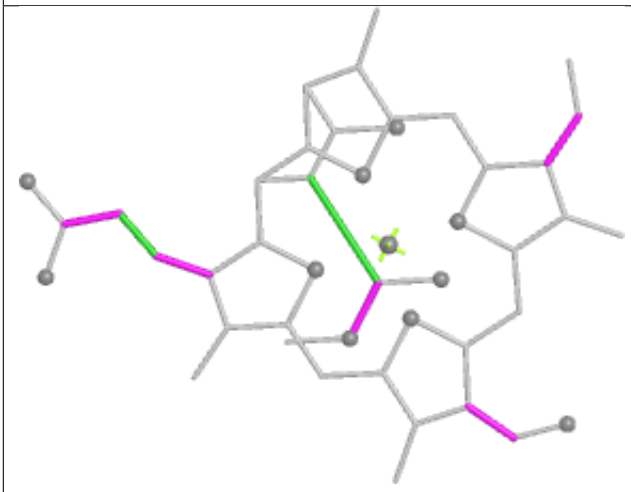
Ligand CL7 12 514



Bond lengths



Bond angles

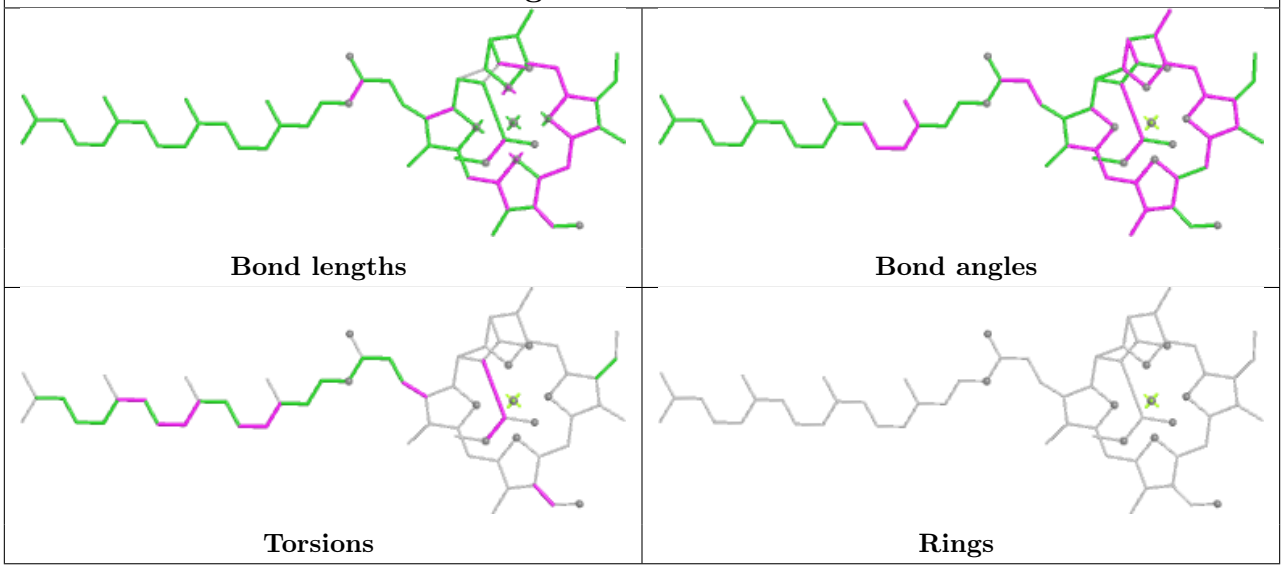


Torsions

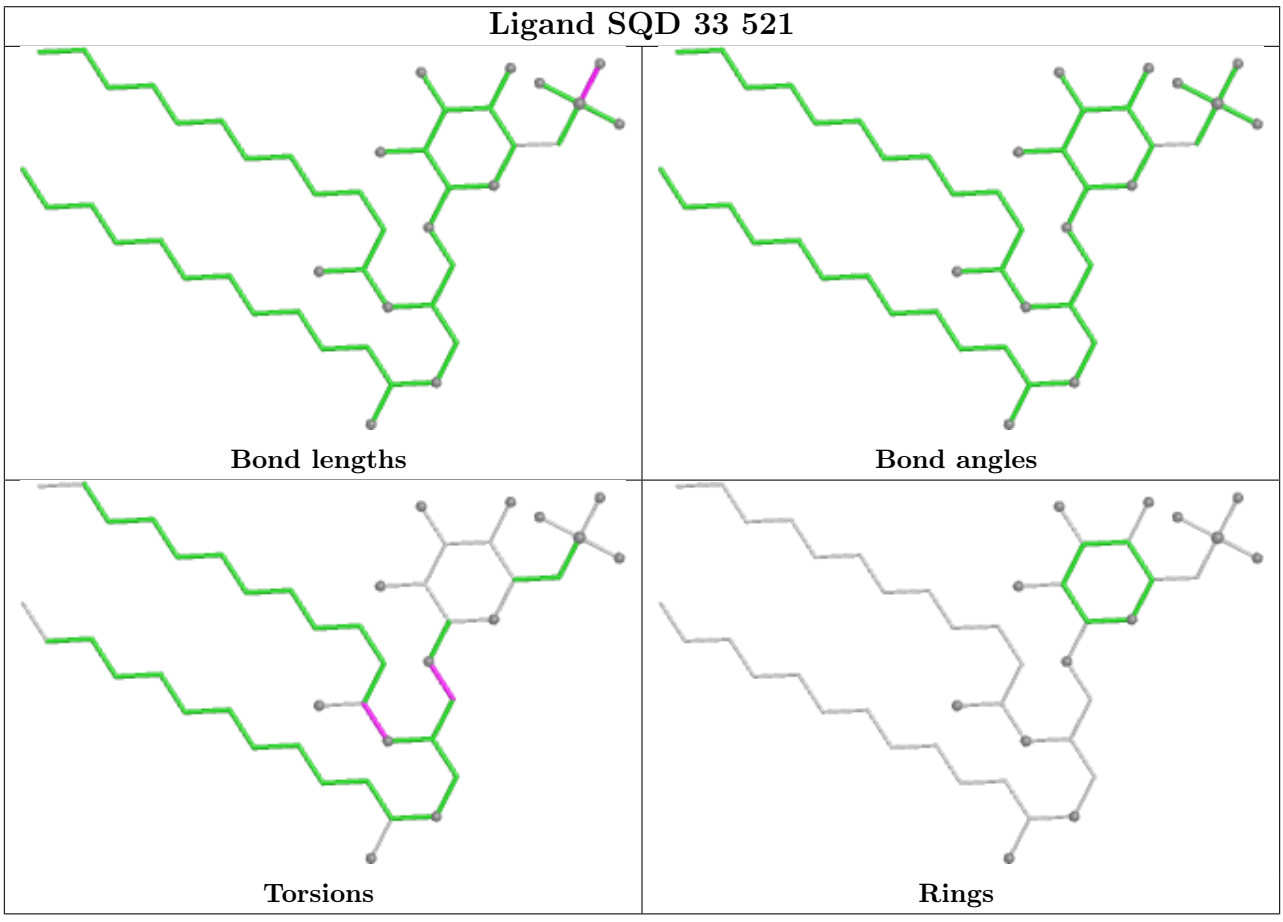


Rings

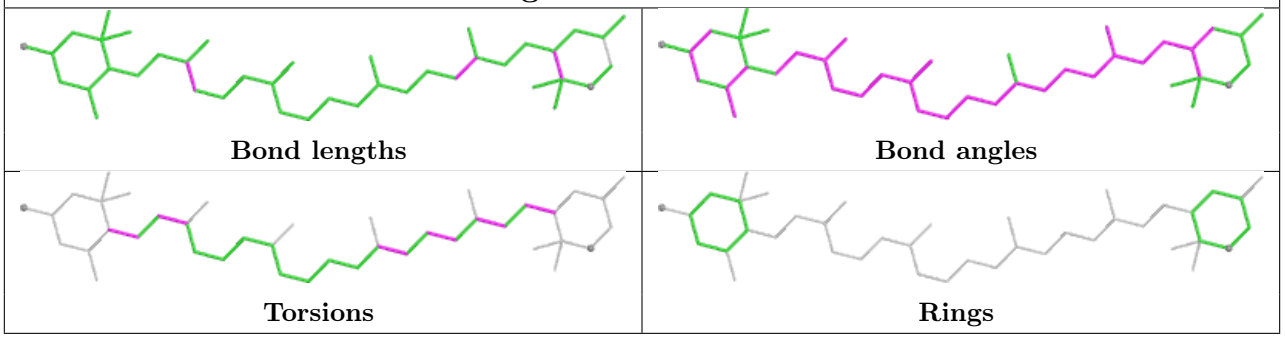
Ligand CL7 32 506



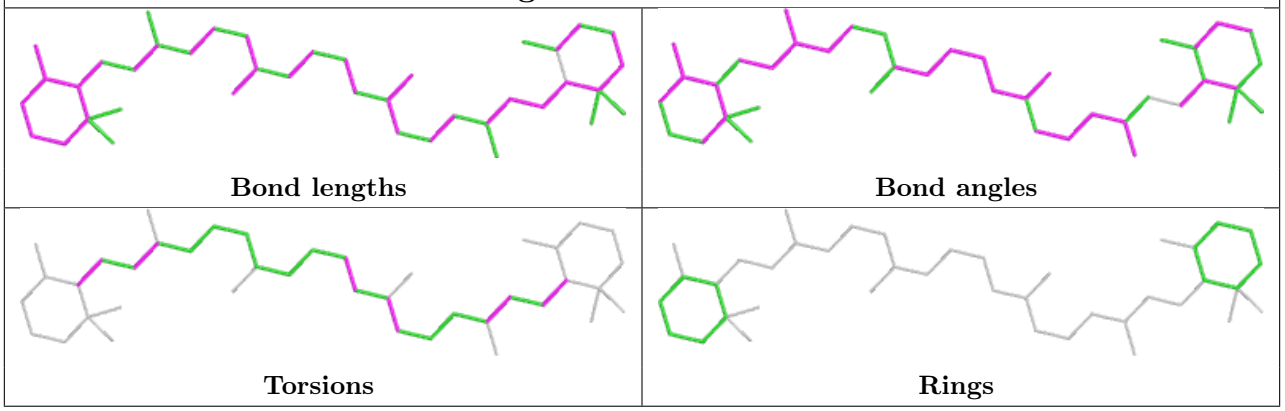
Ligand SQD 33 521



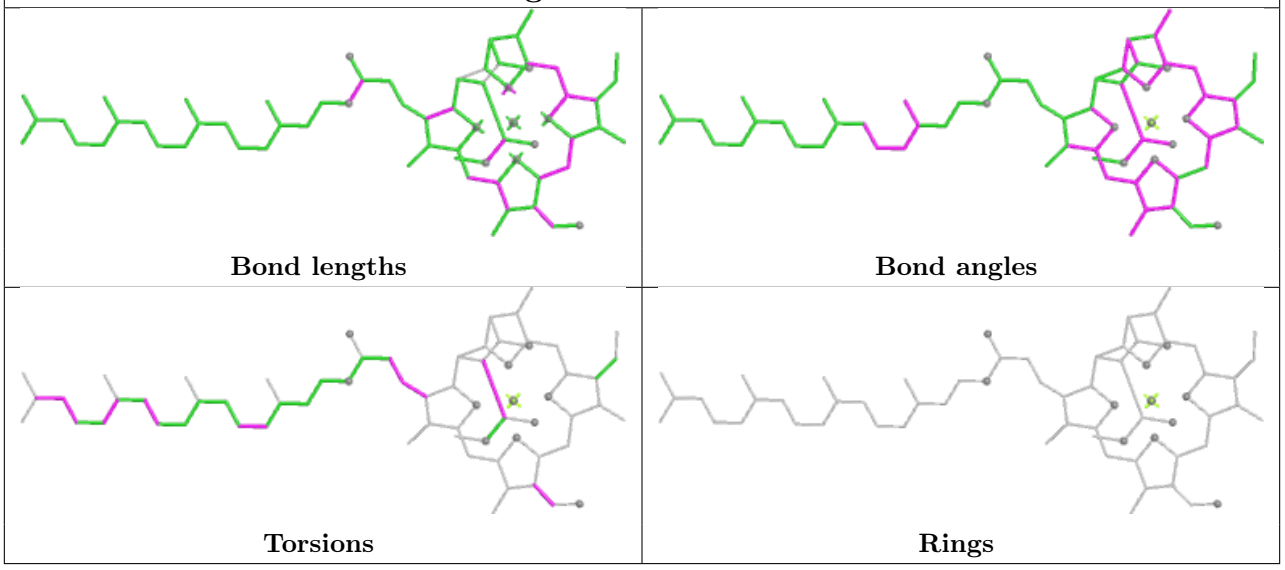
Ligand ZEX 33 519



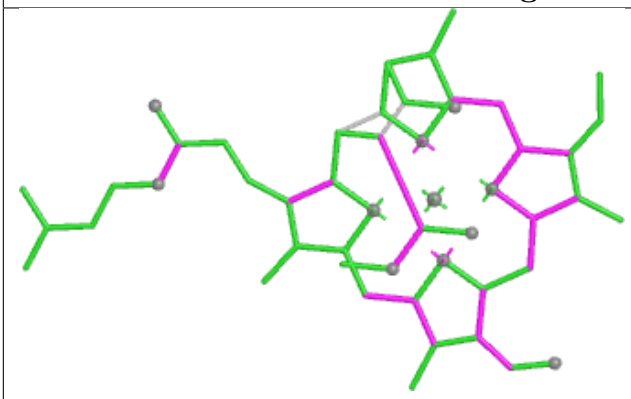
Ligand 8CT 1K 101



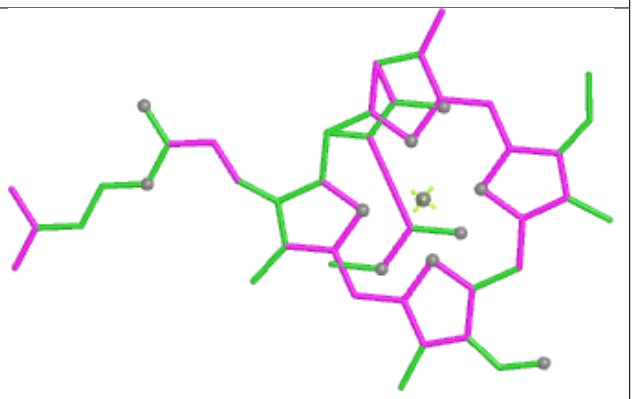
Ligand CL7 32 518



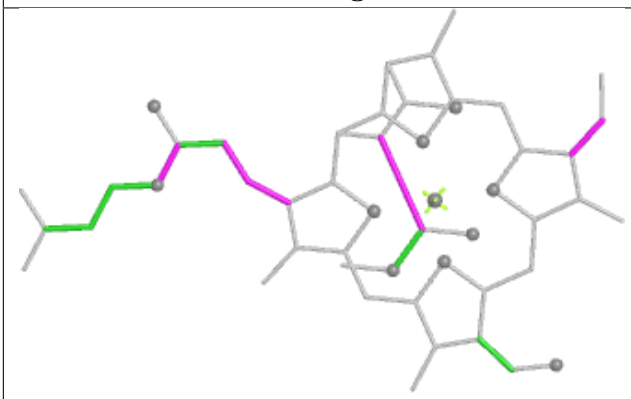
Ligand CL7 4B 616



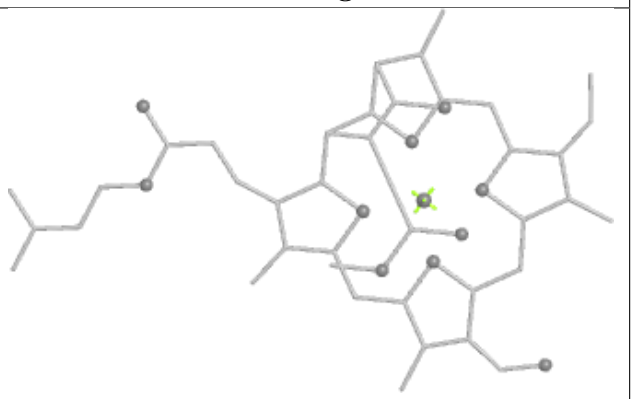
Bond lengths



Bond angles

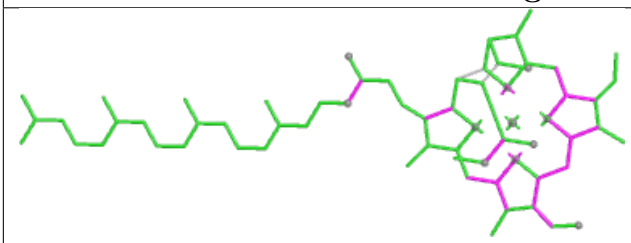


Torsions

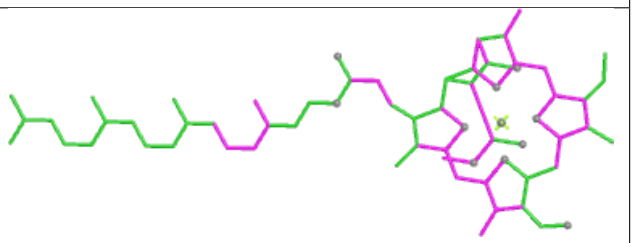


Rings

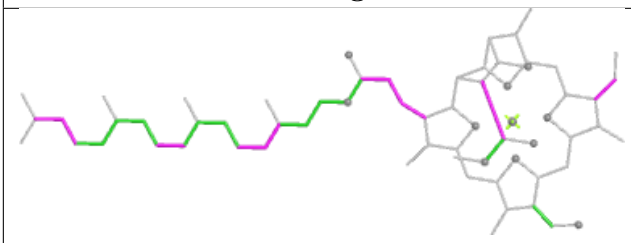
Ligand CL7 13 505



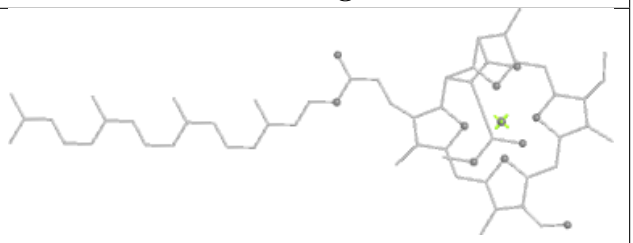
Bond lengths



Bond angles

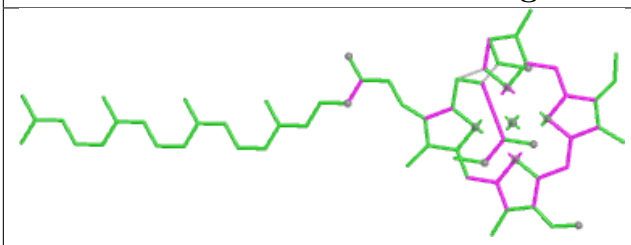


Torsions

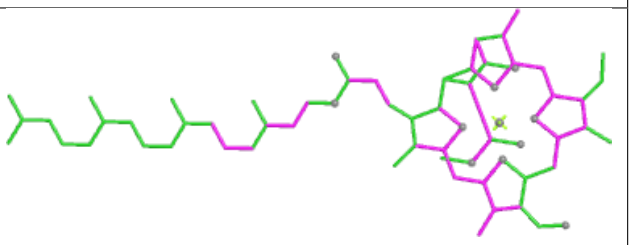


Rings

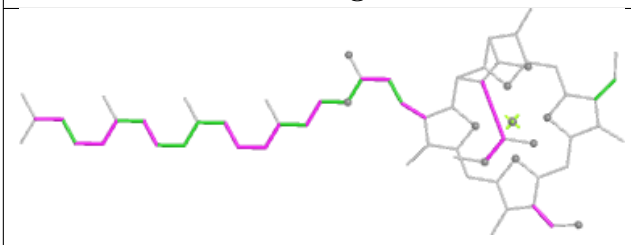
Ligand CL7 4C 509



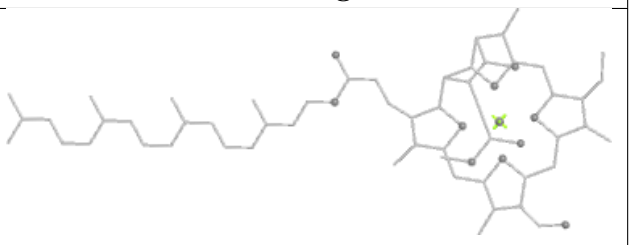
Bond lengths



Bond angles

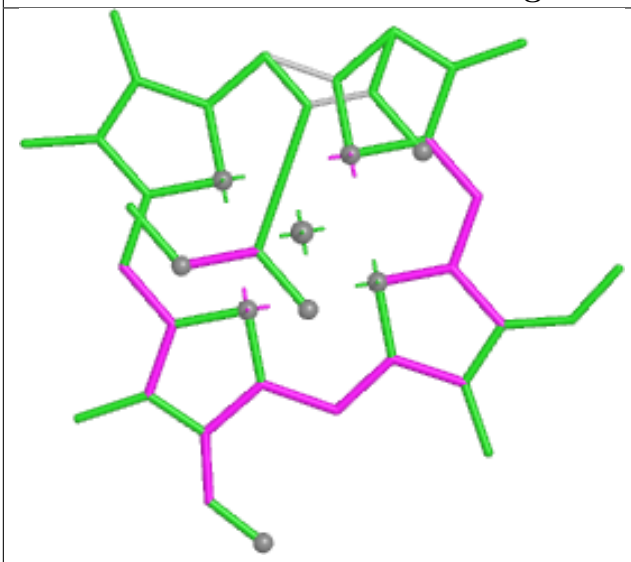


Torsions

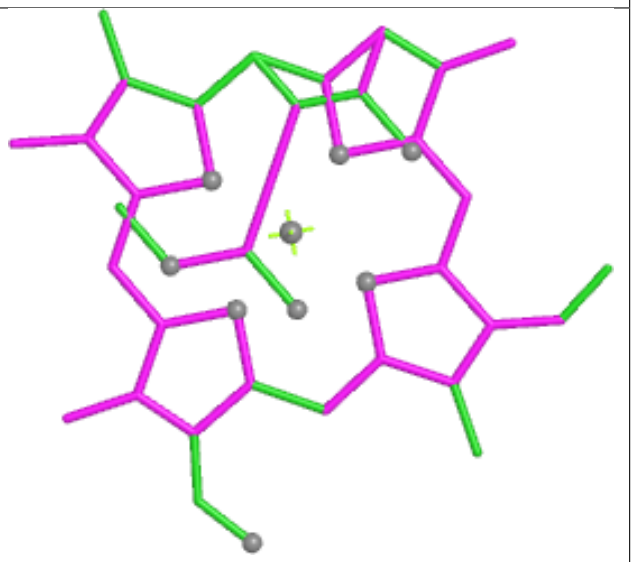


Rings

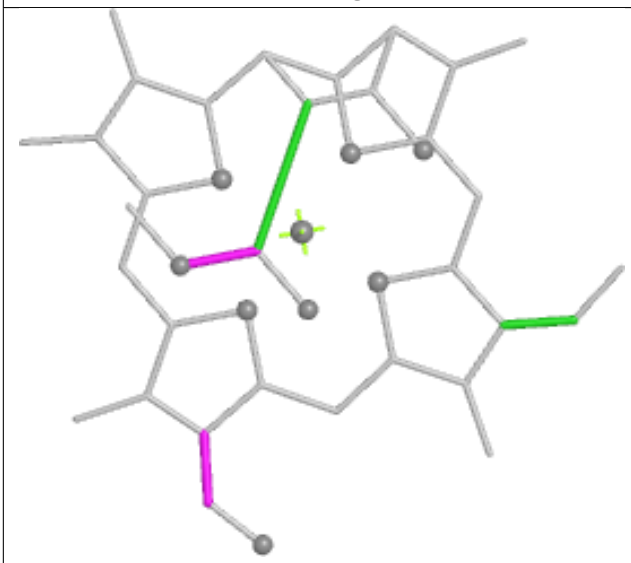
Ligand CL7 41 407



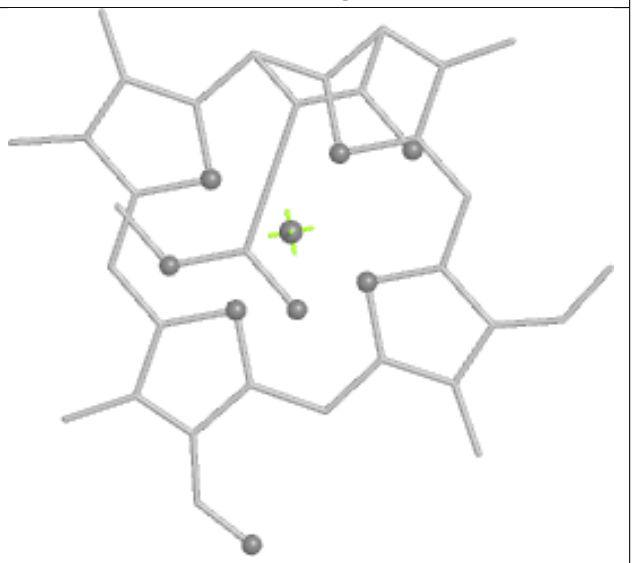
Bond lengths



Bond angles

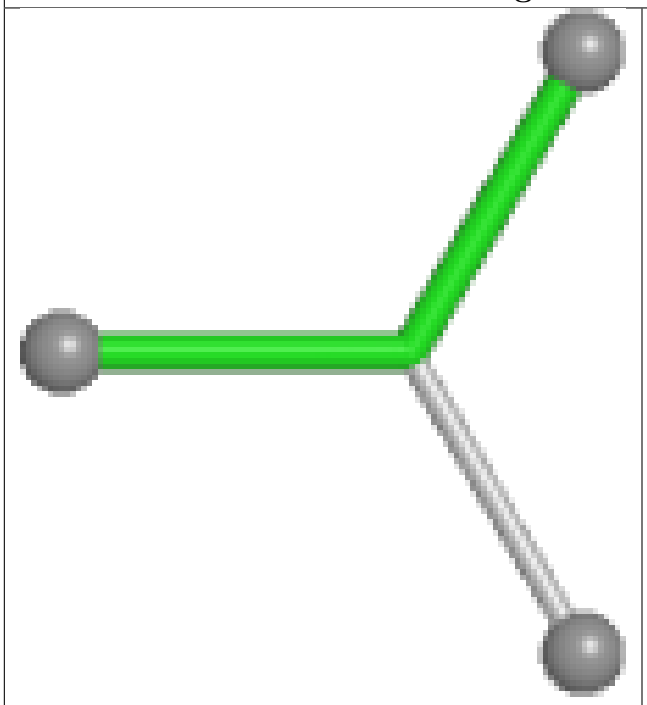


Torsions

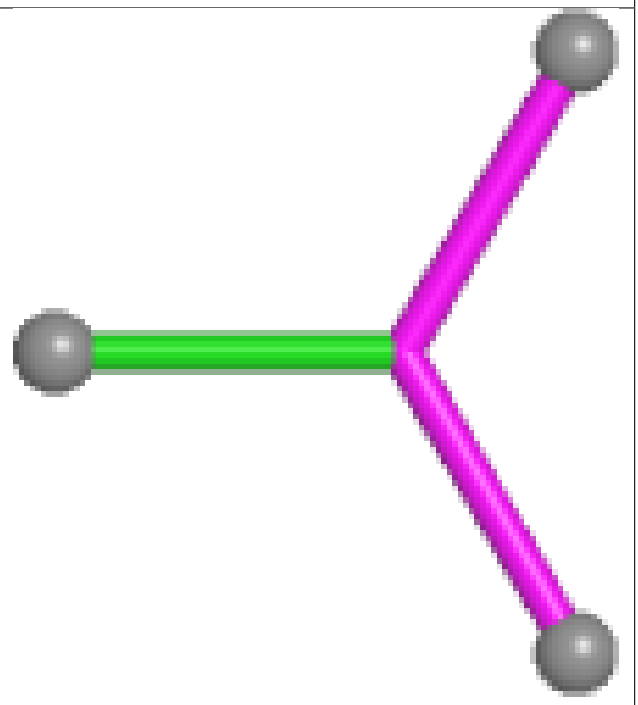


Rings

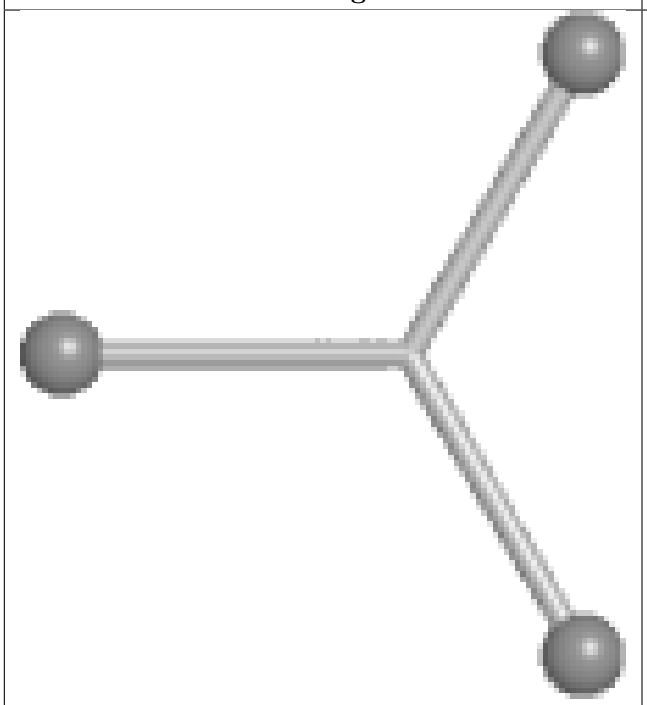
Ligand BCT 3D 403



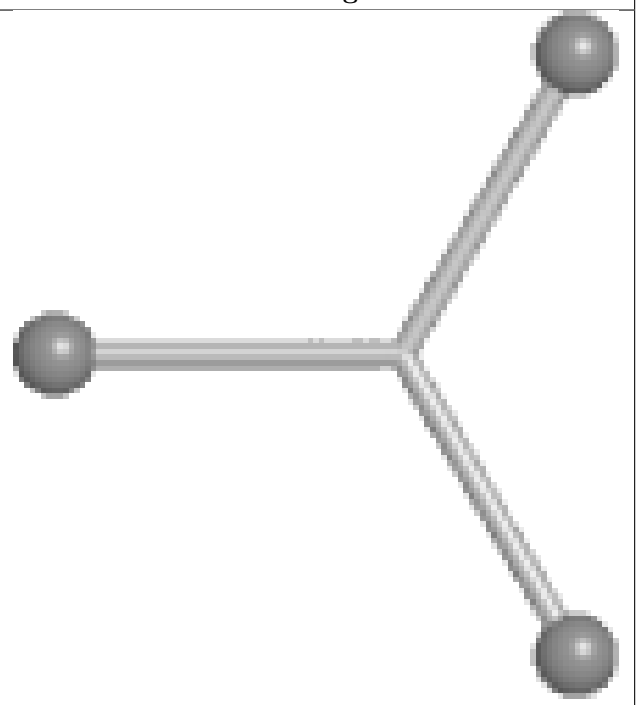
Bond lengths



Bond angles

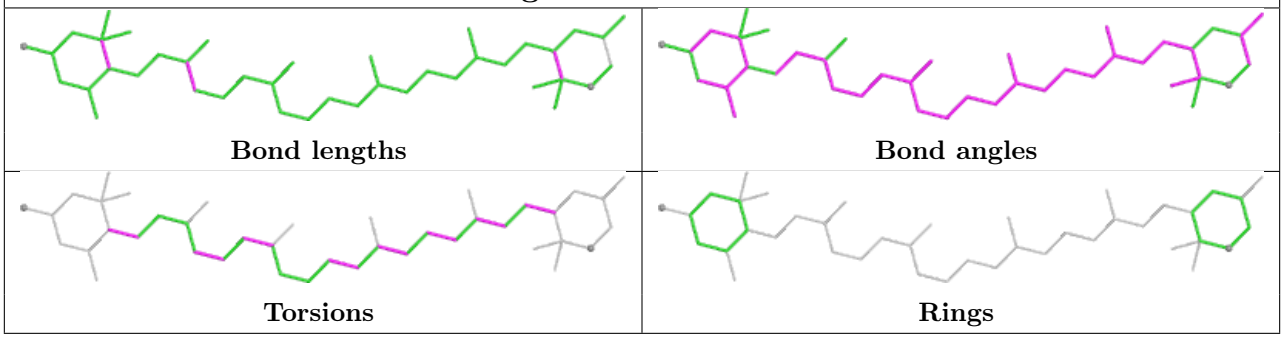


Torsions

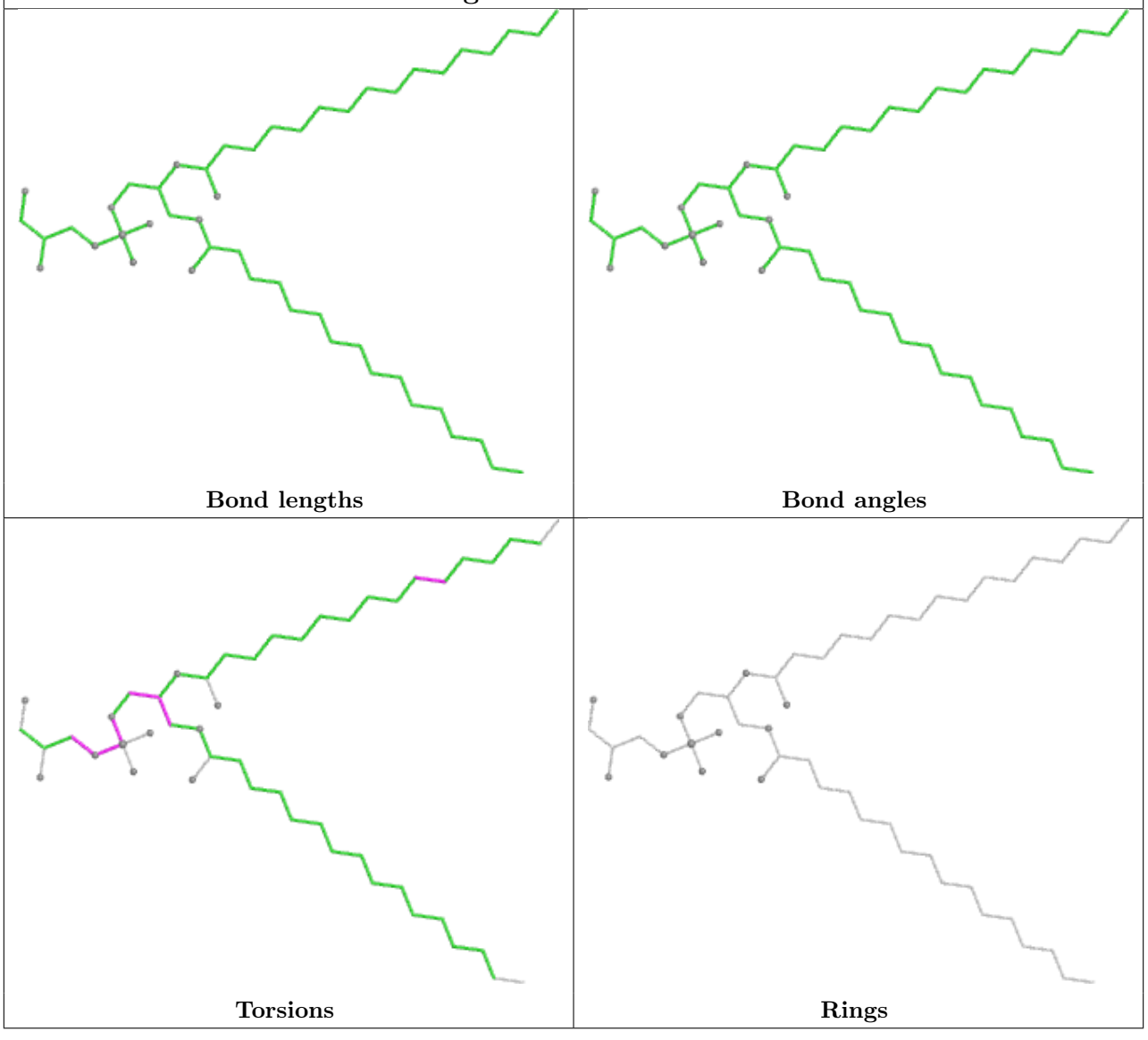


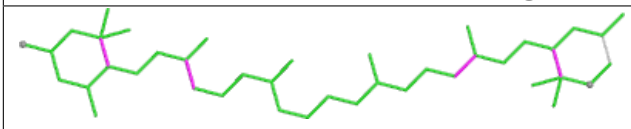
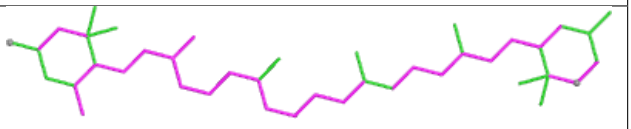
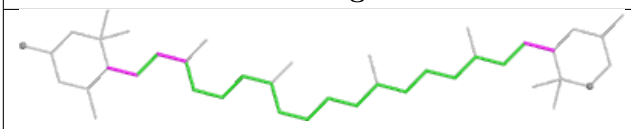
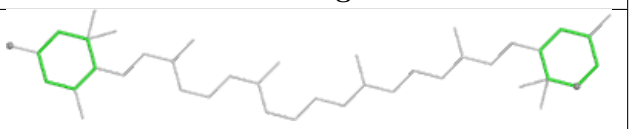
Rings

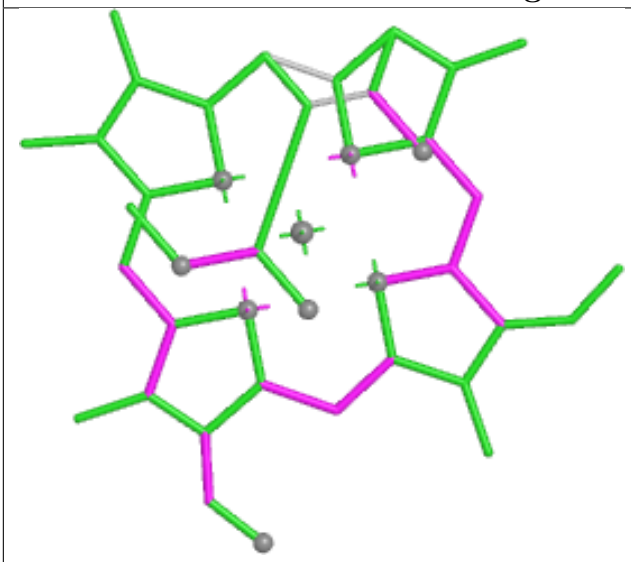
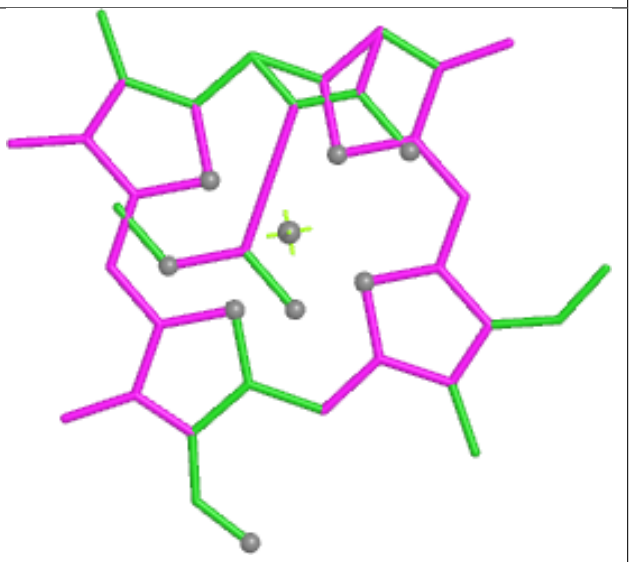
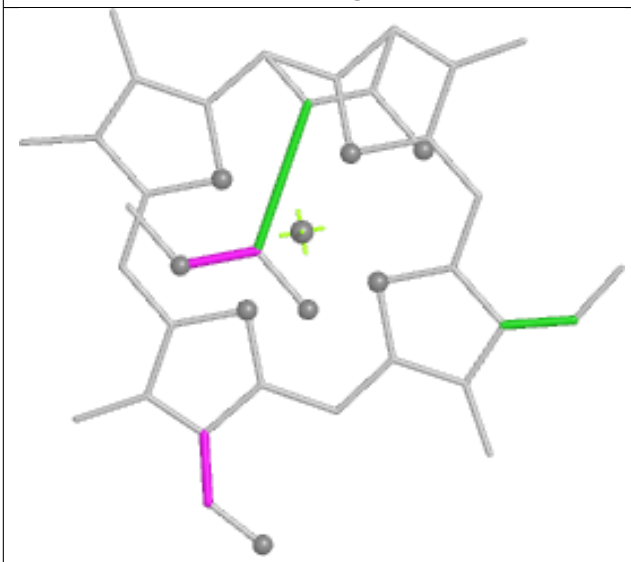
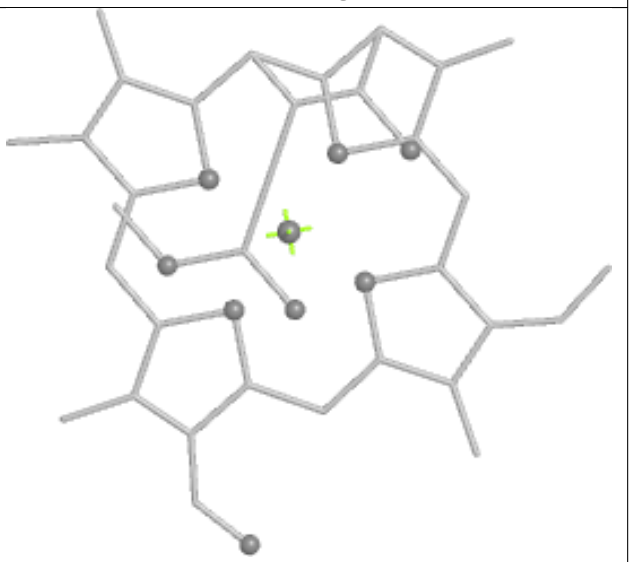
Ligand ZEX 24 420



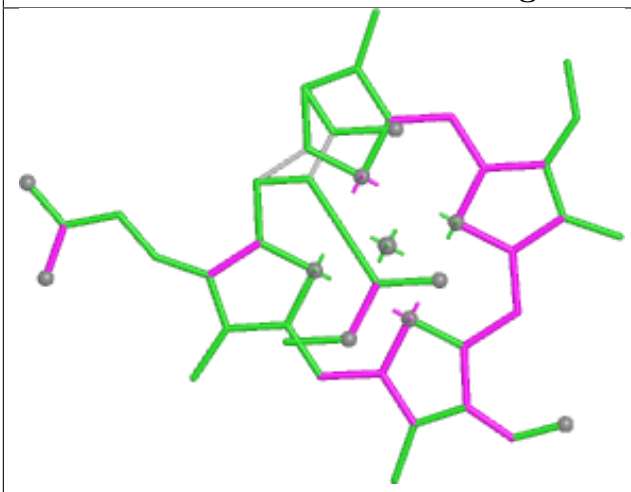
Ligand LHG 34 401



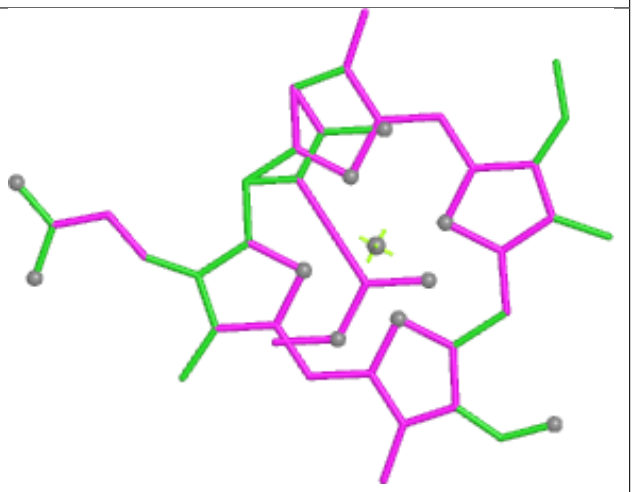
Ligand ZEX 13 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CL7 31 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

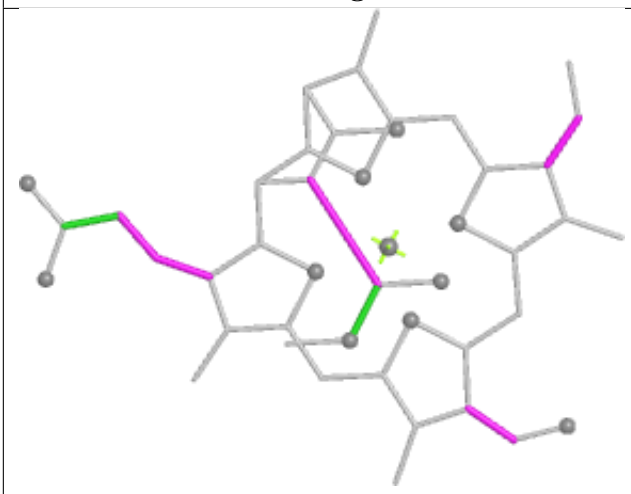
Ligand CL7 3D 405



Bond lengths



Bond angles

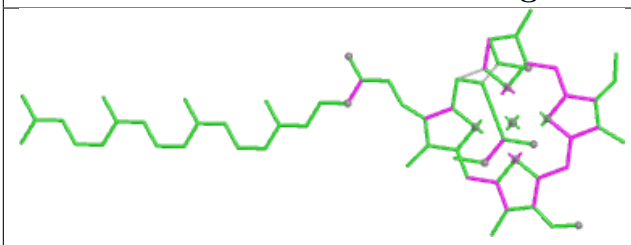


Torsions

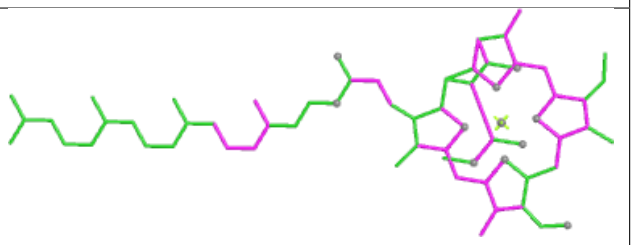


Rings

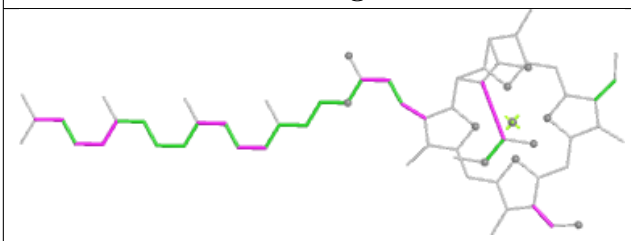
Ligand CL7 3B 609



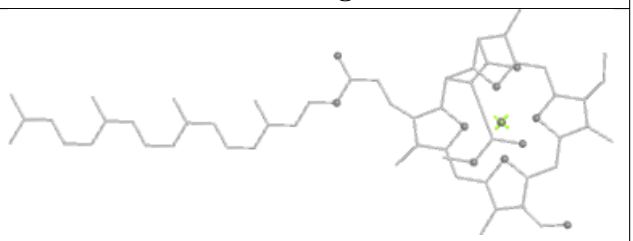
Bond lengths



Bond angles

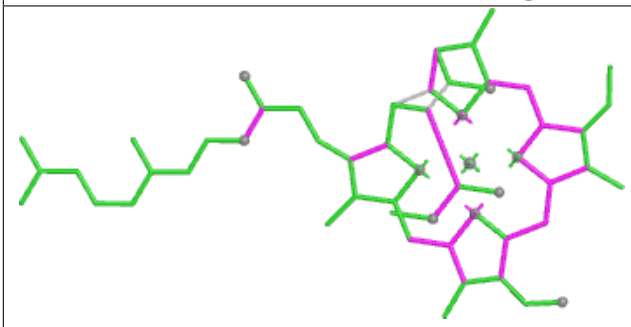


Torsions

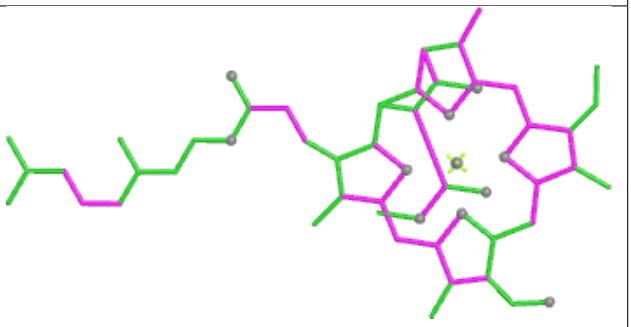


Rings

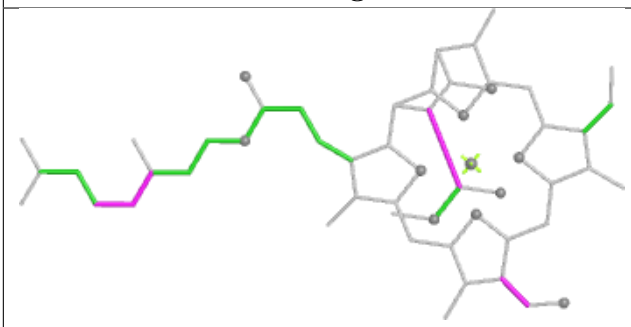
Ligand CL7 3B 613



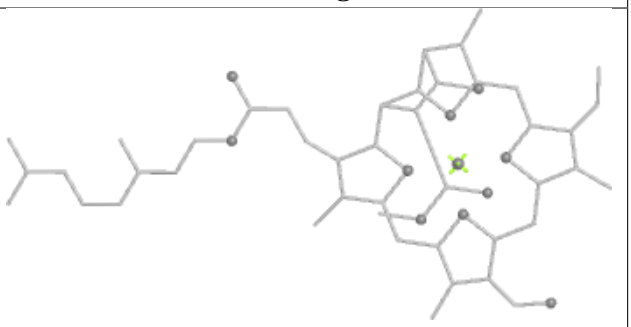
Bond lengths



Bond angles

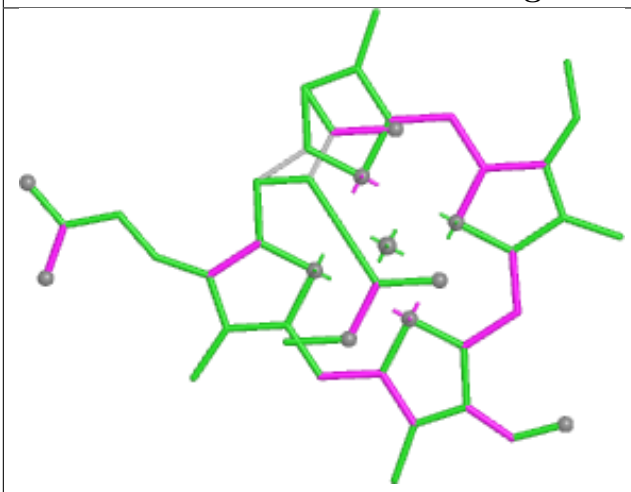


Torsions

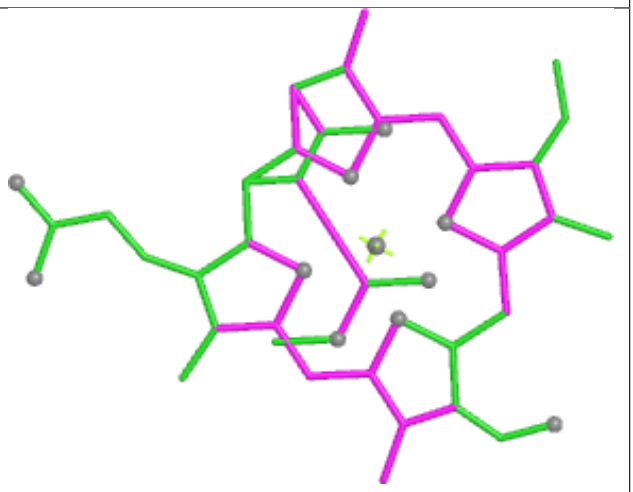


Rings

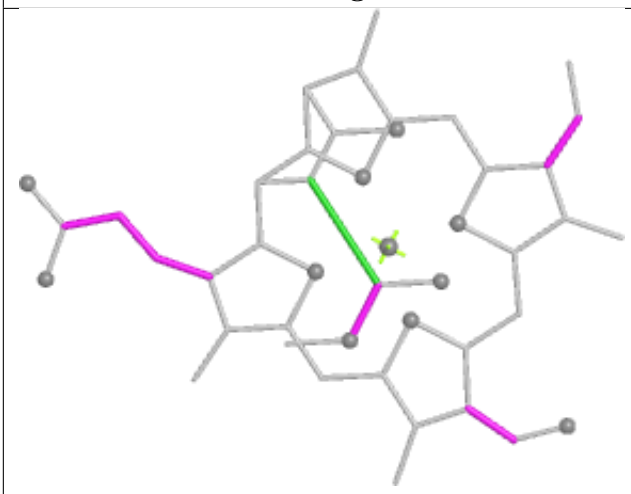
Ligand CL7 41 419



Bond lengths



Bond angles

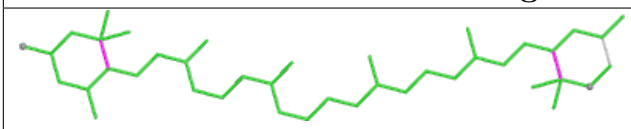


Torsions

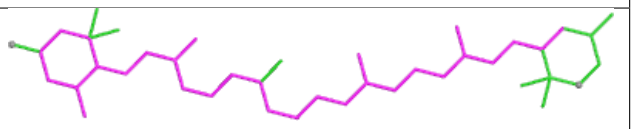


Rings

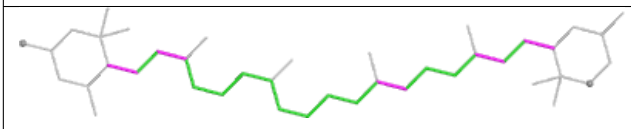
Ligand ZEX 43 421



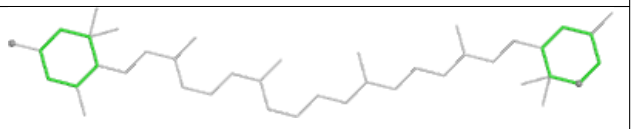
Bond lengths



Bond angles

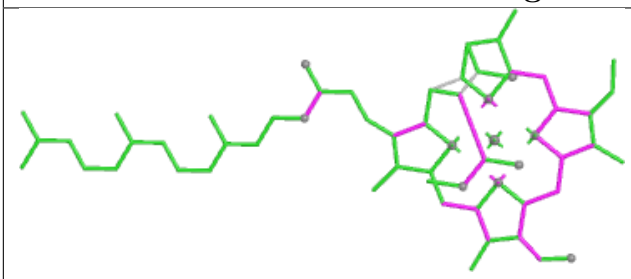


Torsions

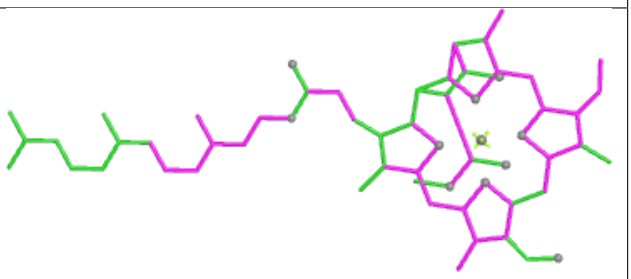


Rings

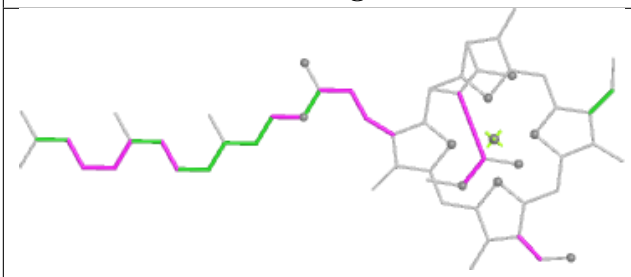
Ligand CL7 34 409



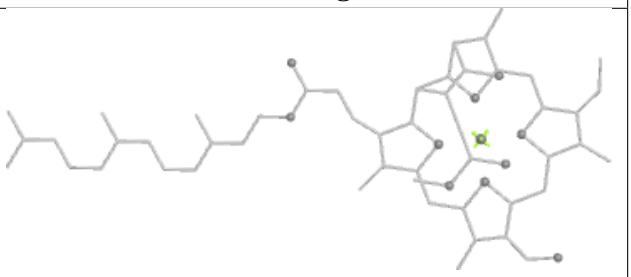
Bond lengths



Bond angles

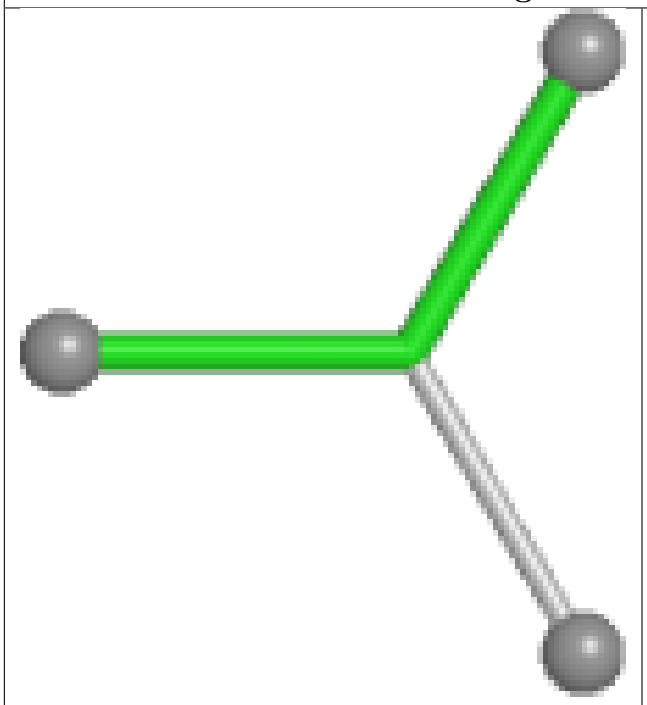


Torsions

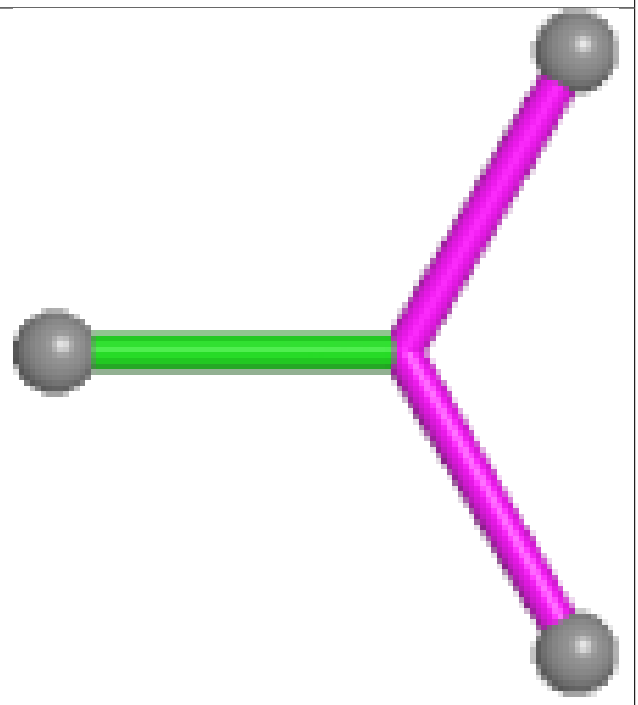


Rings

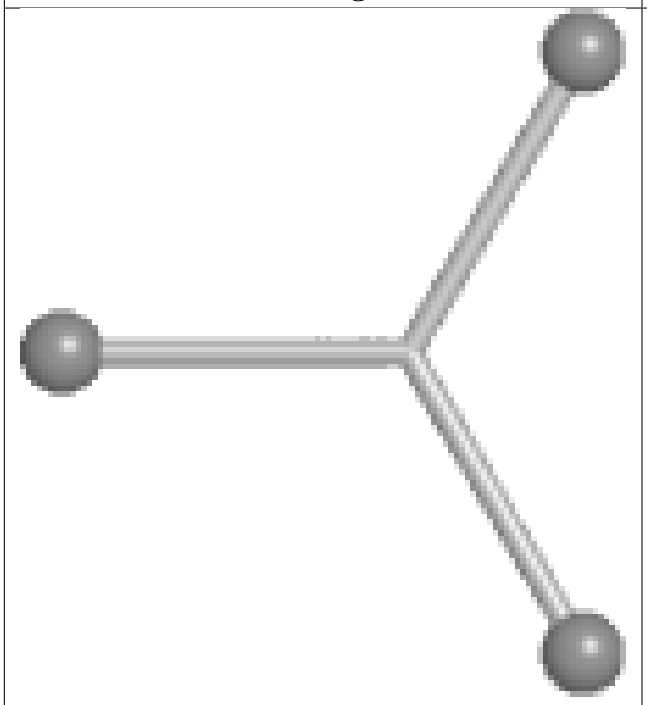
Ligand BCT 2D 403



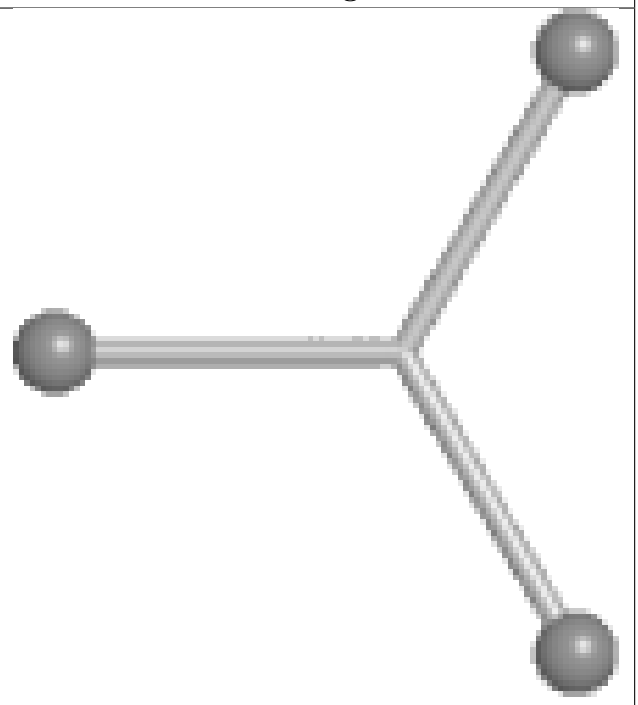
Bond lengths



Bond angles

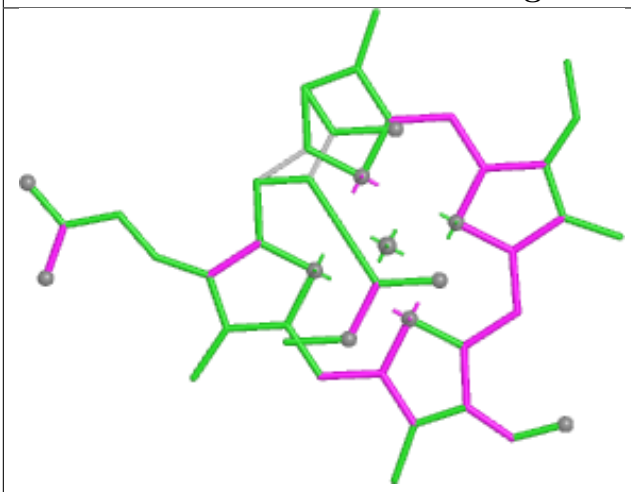


Torsions

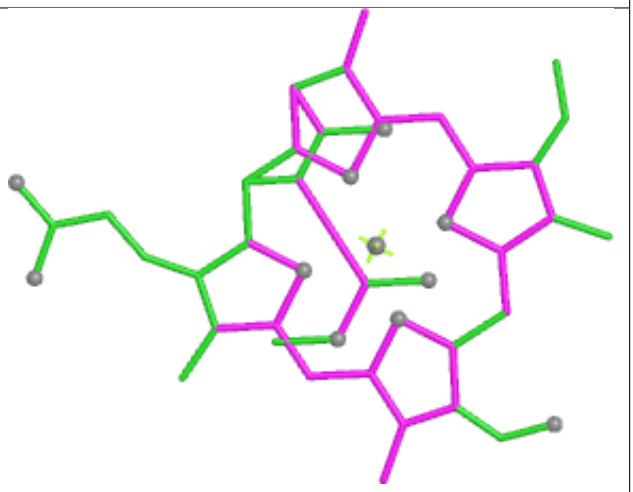


Rings

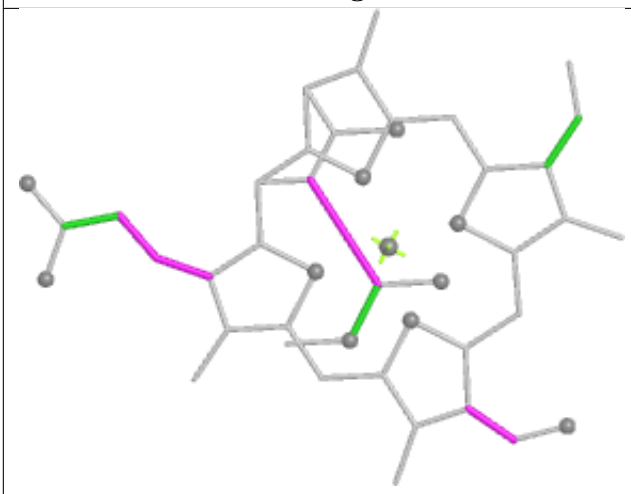
Ligand CL7 32 508



Bond lengths



Bond angles

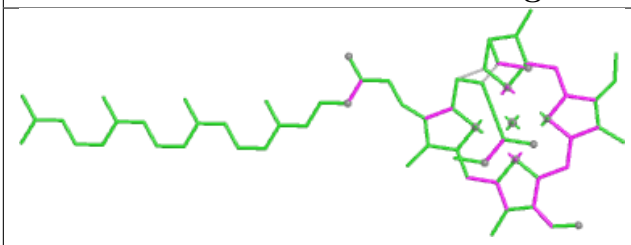


Torsions

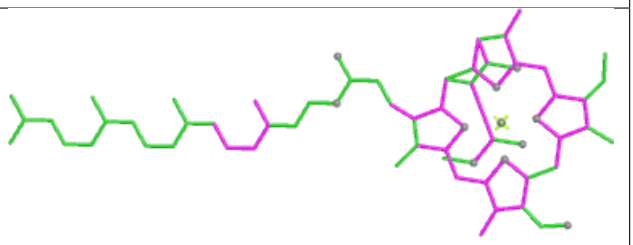


Rings

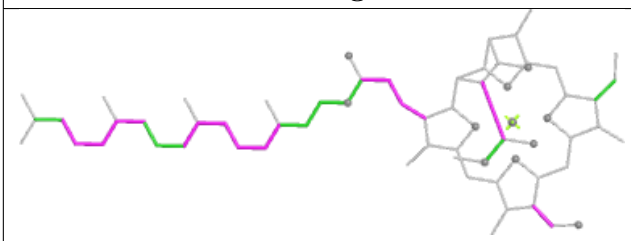
Ligand CL7 33 501



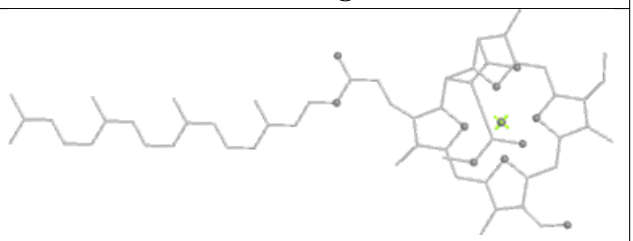
Bond lengths



Bond angles

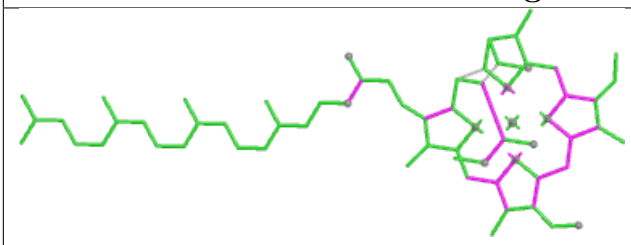


Torsions

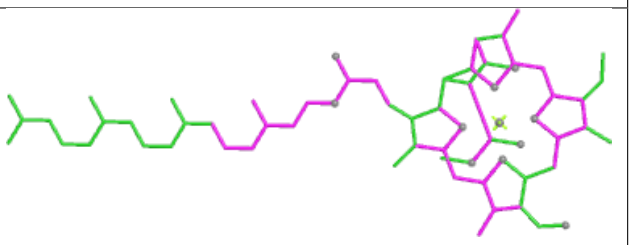


Rings

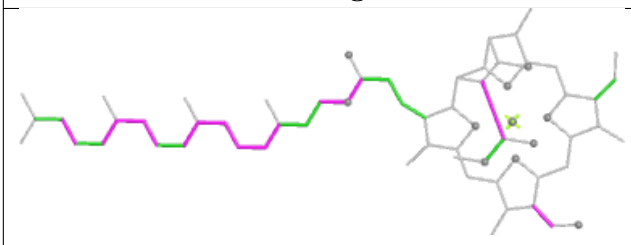
Ligand CL7 13 511



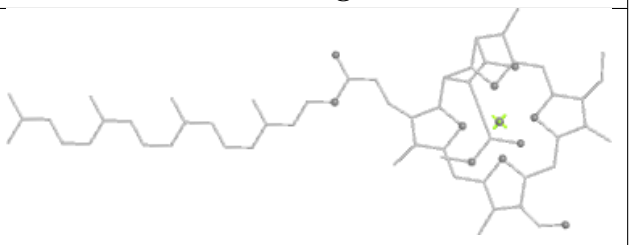
Bond lengths



Bond angles

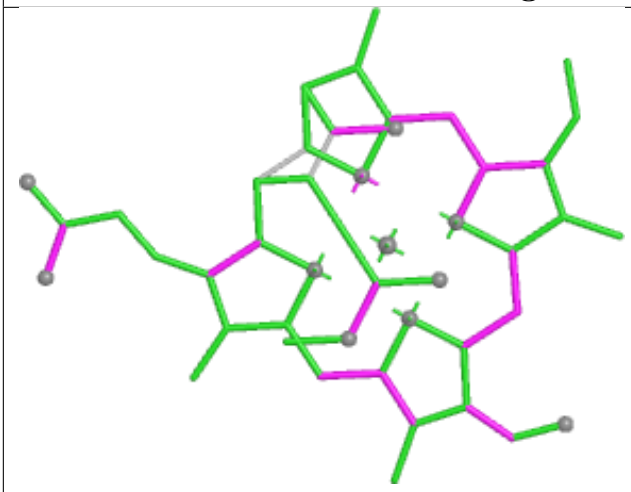


Torsions



Rings

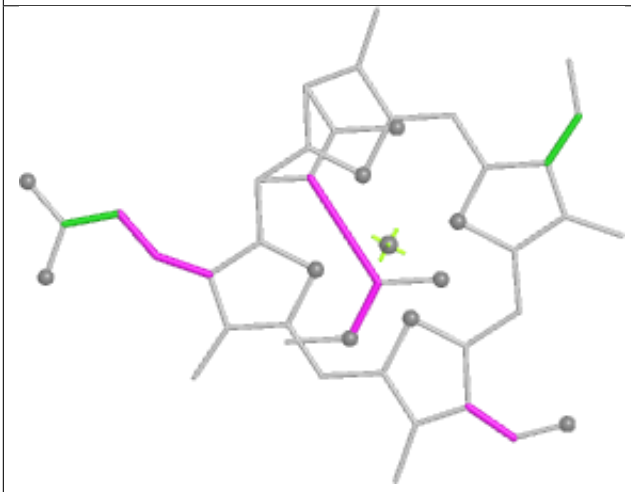
Ligand CL7 1C 513



Bond lengths



Bond angles

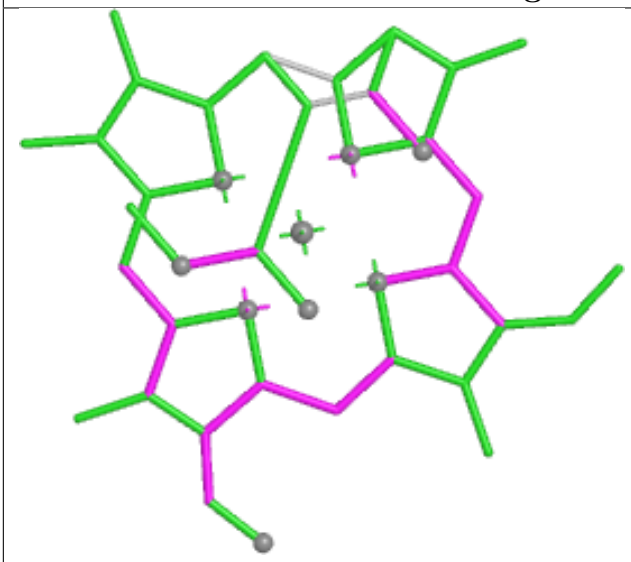


Torsions

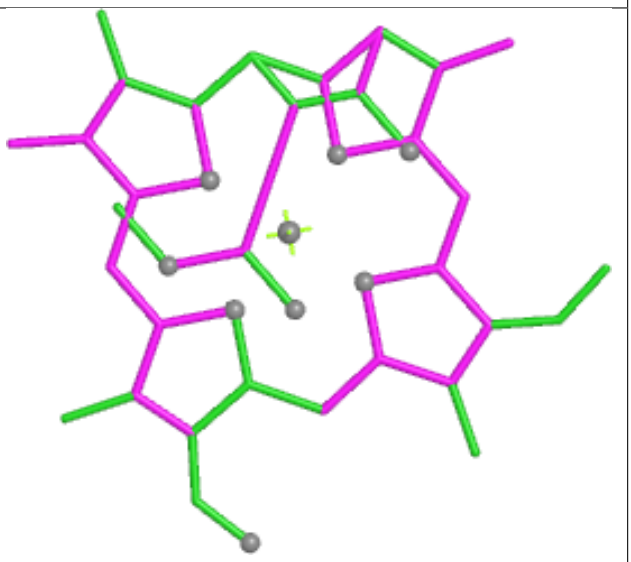


Rings

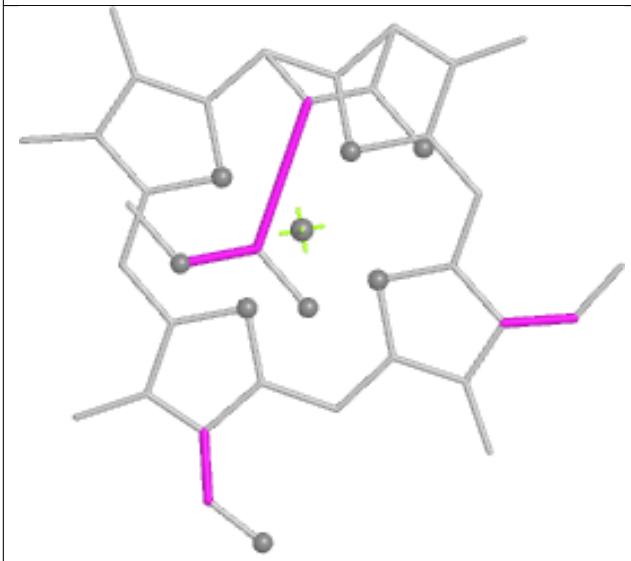
Ligand CL7 24 416



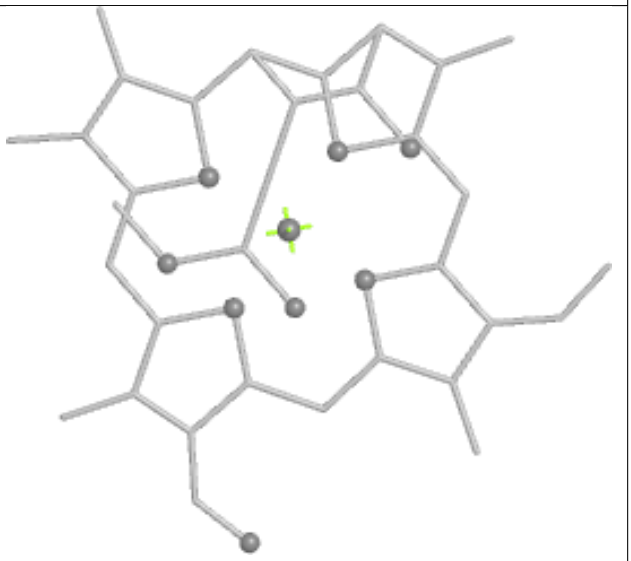
Bond lengths



Bond angles

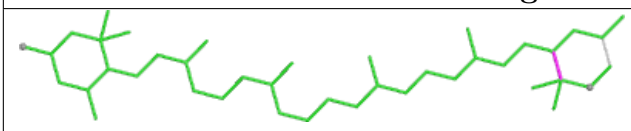


Torsions

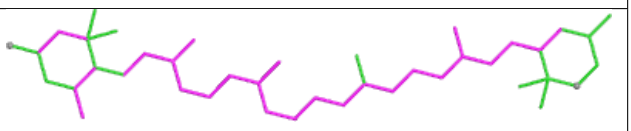


Rings

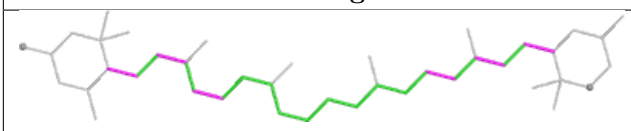
Ligand ZEX 44 418



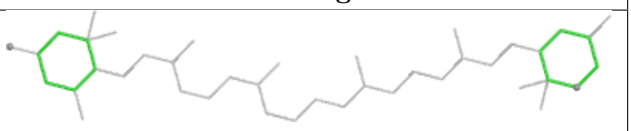
Bond lengths



Bond angles

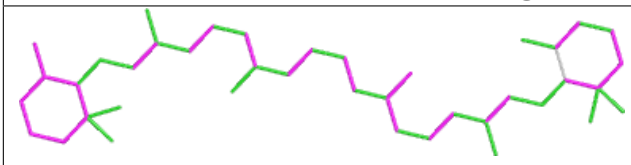


Torsions

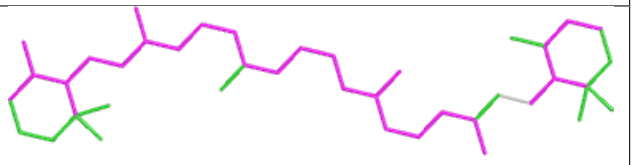


Rings

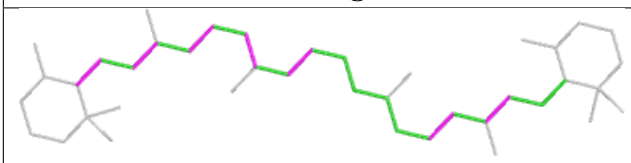
Ligand 8CT 2C 515



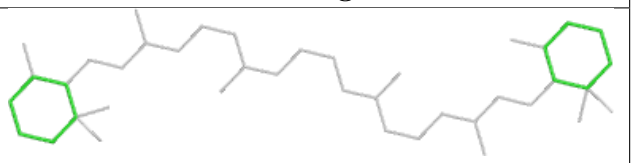
Bond lengths



Bond angles

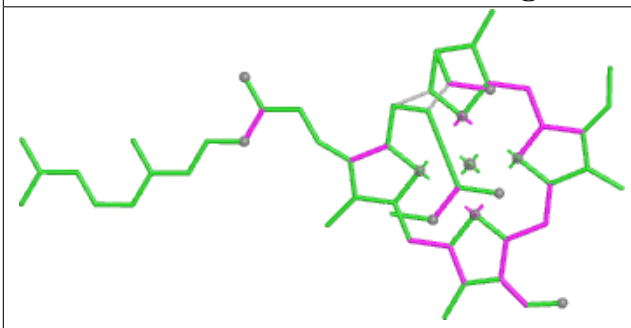


Torsions

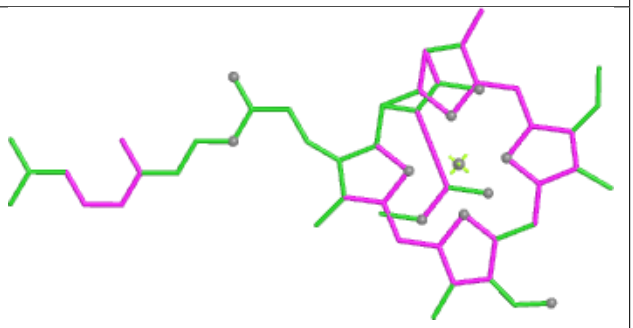


Rings

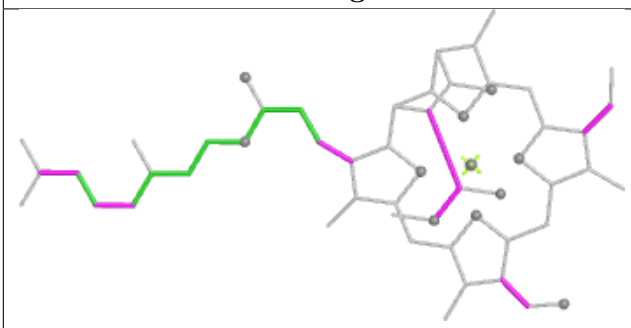
Ligand CL7 4C 504



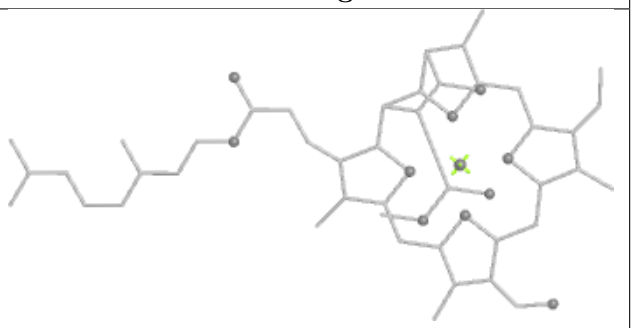
Bond lengths



Bond angles

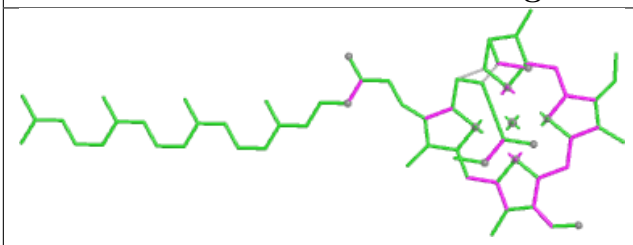


Torsions

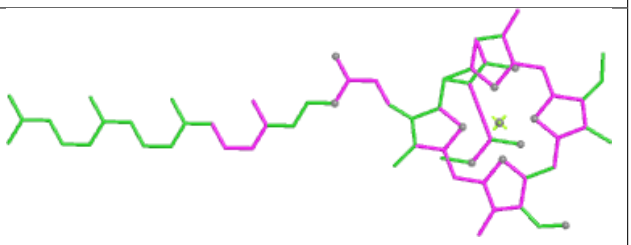


Rings

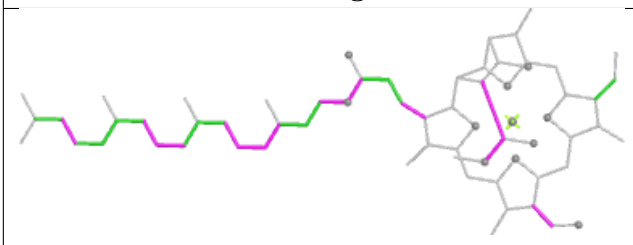
Ligand CL7 31 410



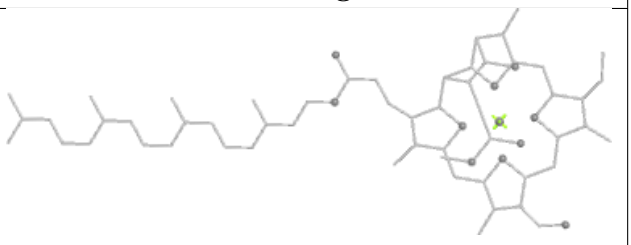
Bond lengths



Bond angles

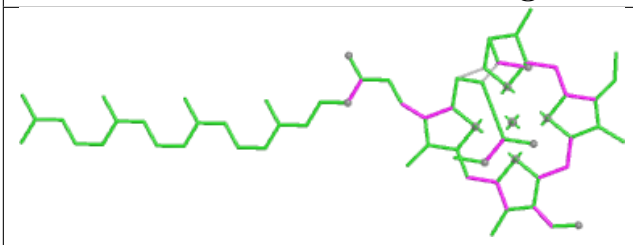


Torsions

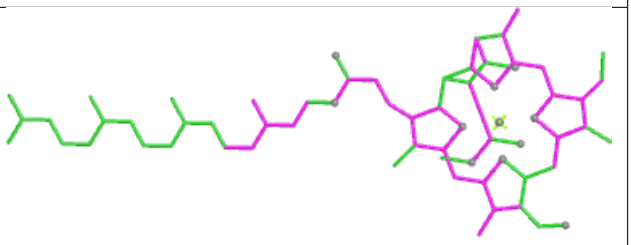


Rings

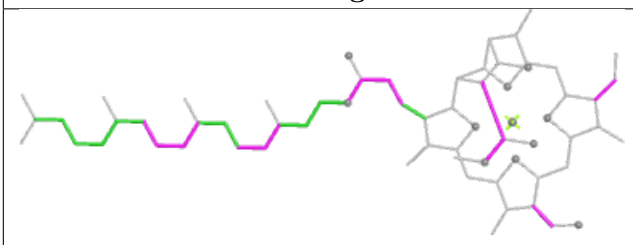
Ligand CL7 4A 401



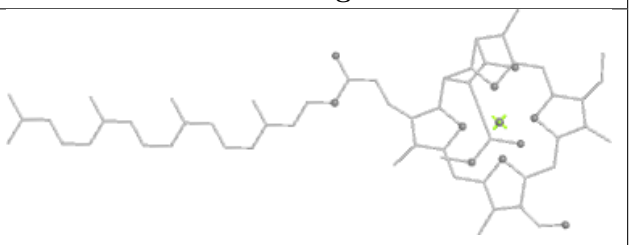
Bond lengths



Bond angles

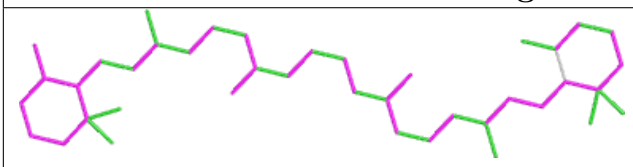


Torsions

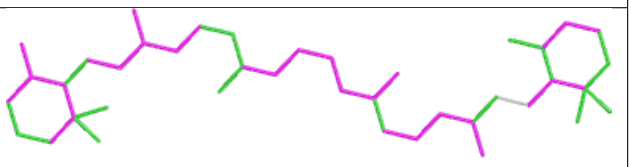


Rings

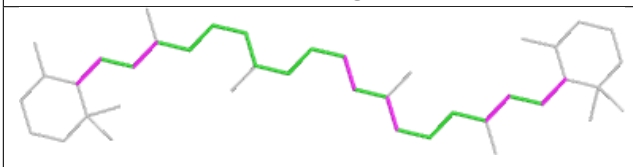
Ligand 8CT 3K 101



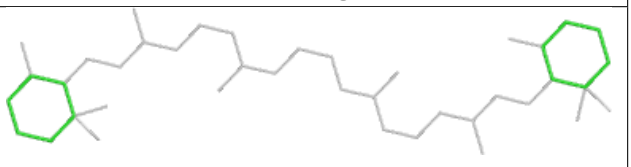
Bond lengths



Bond angles

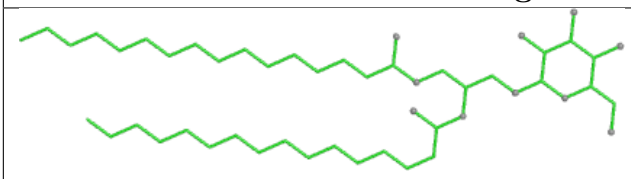


Torsions

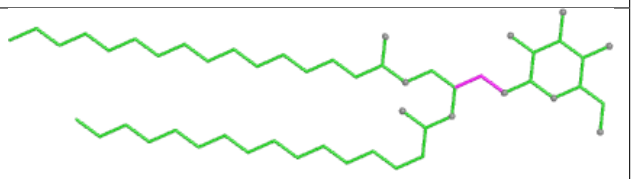


Rings

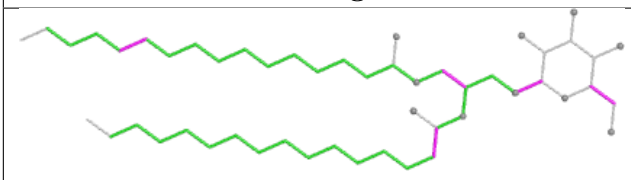
Ligand LMG 11 401



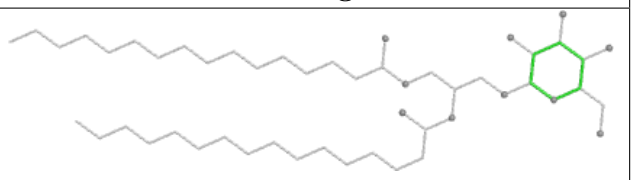
Bond lengths



Bond angles

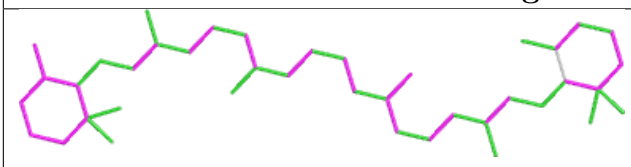


Torsions

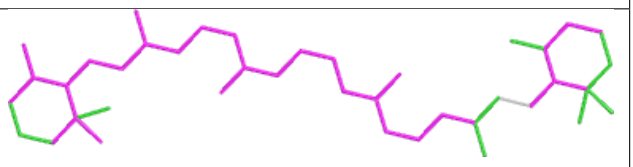


Rings

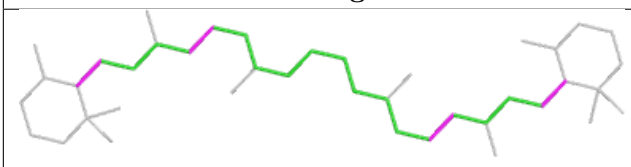
Ligand 8CT 24 402



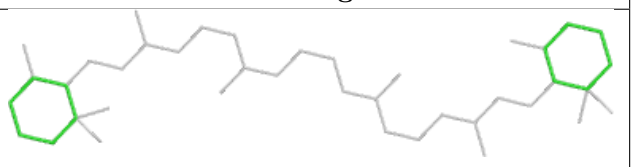
Bond lengths



Bond angles

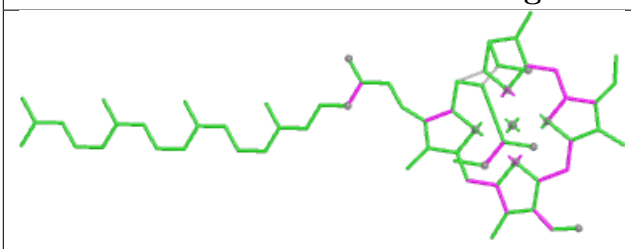


Torsions

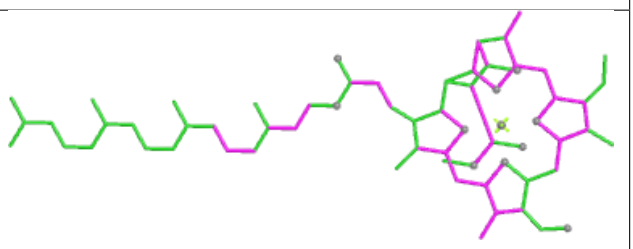


Rings

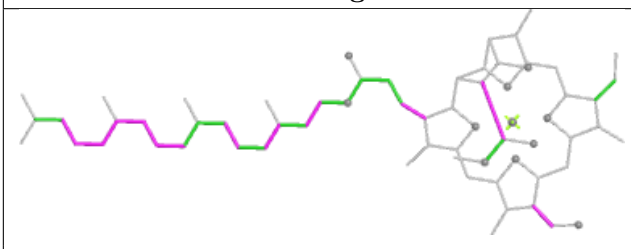
Ligand CL7 41 404



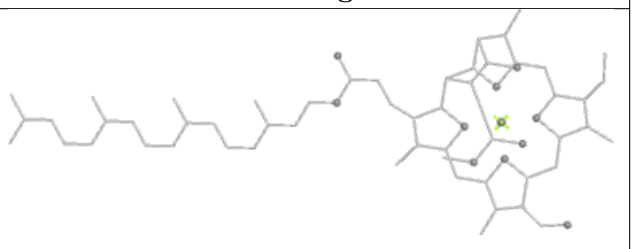
Bond lengths



Bond angles

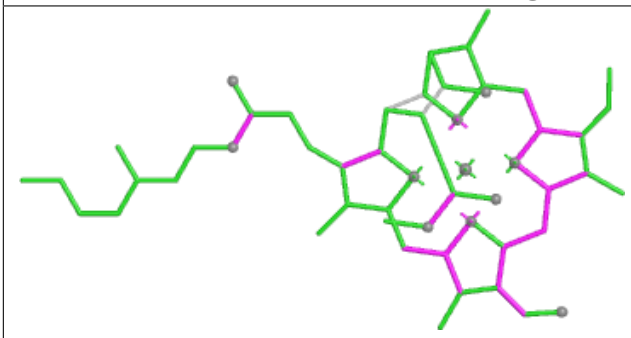


Torsions

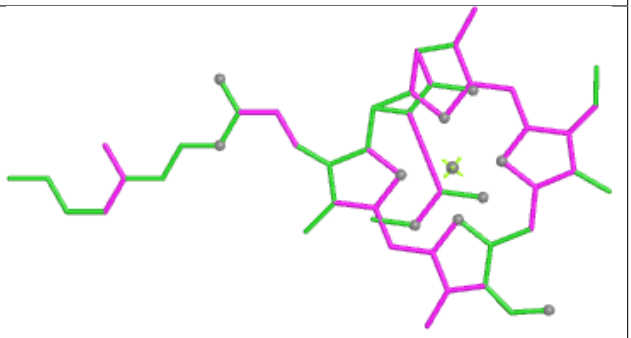


Rings

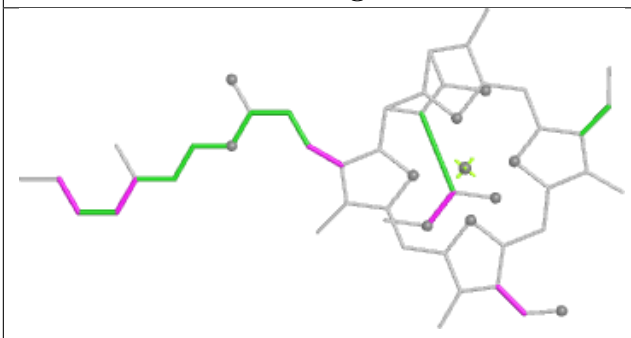
Ligand CL7 14 414



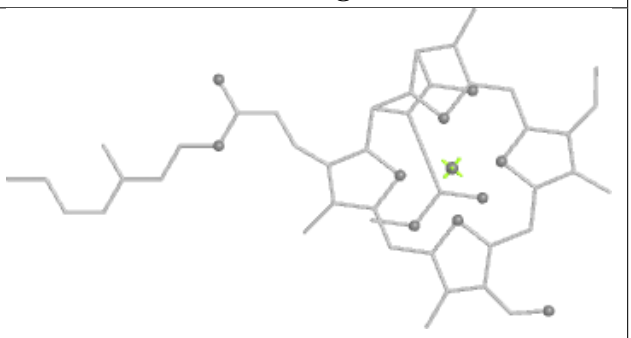
Bond lengths



Bond angles

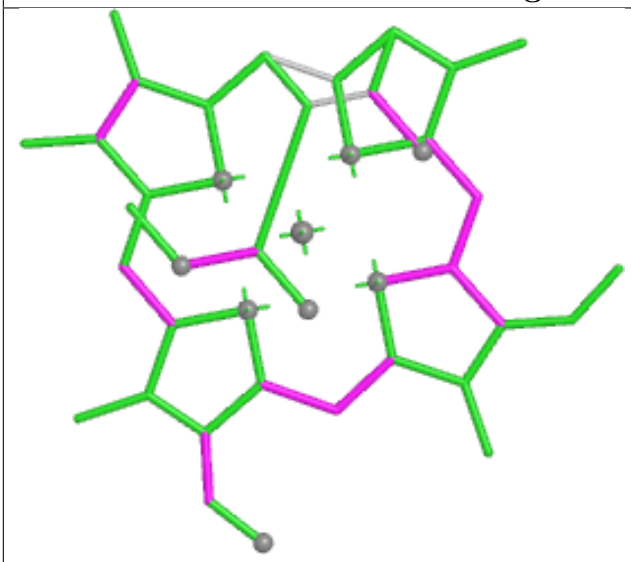


Torsions

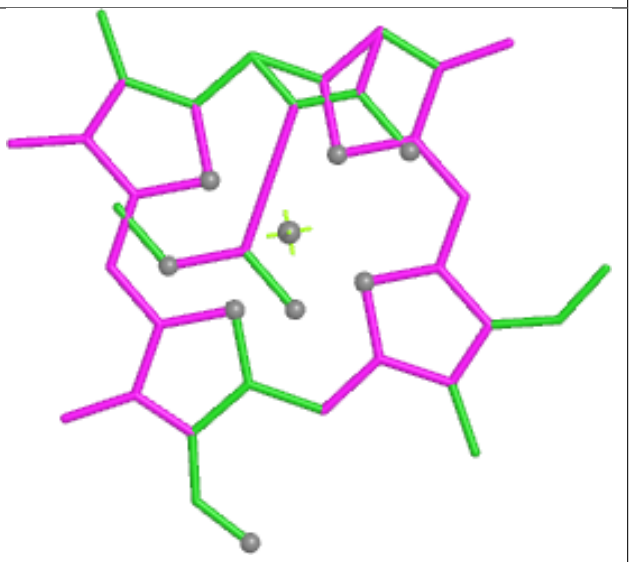


Rings

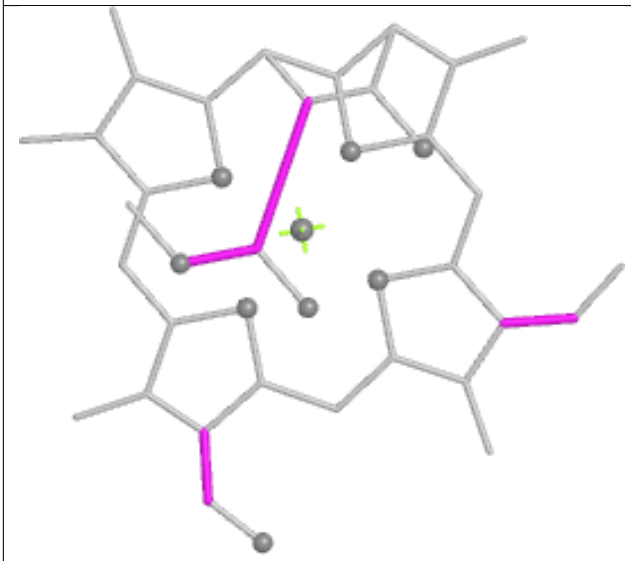
Ligand CL7 41 415



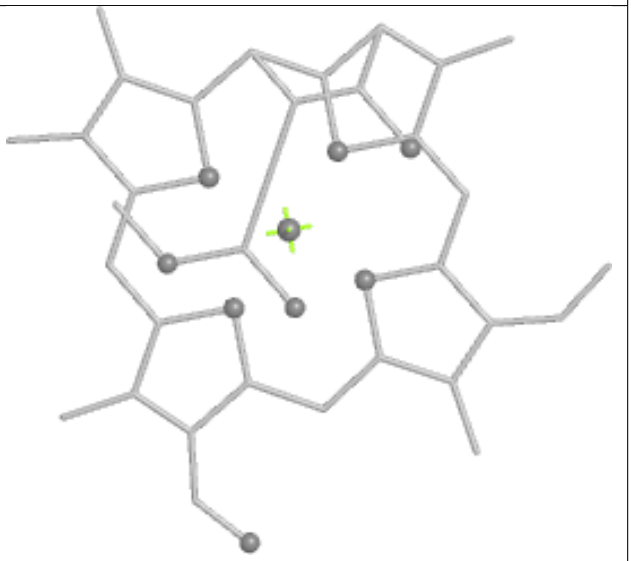
Bond lengths



Bond angles

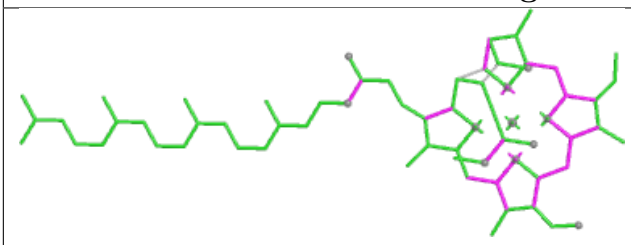


Torsions

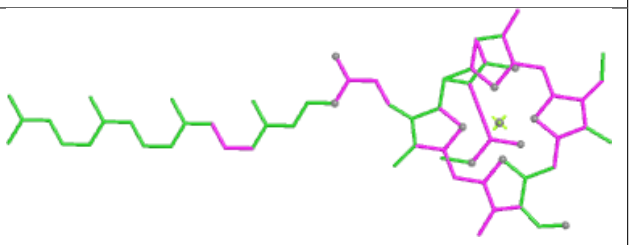


Rings

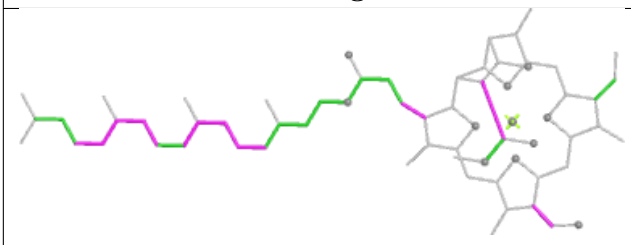
Ligand CL7 2B 613



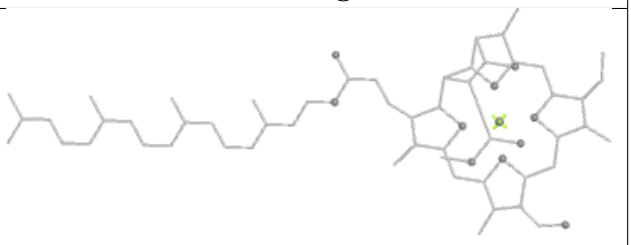
Bond lengths



Bond angles

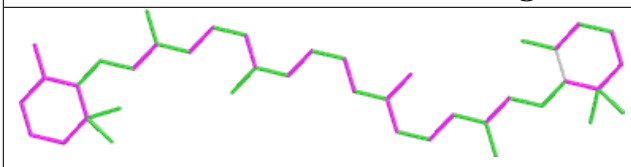


Torsions

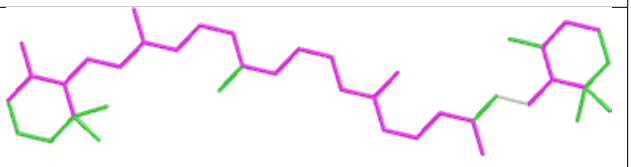


Rings

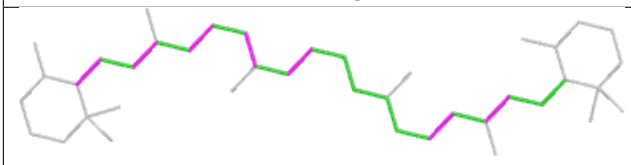
Ligand 8CT 4C 515



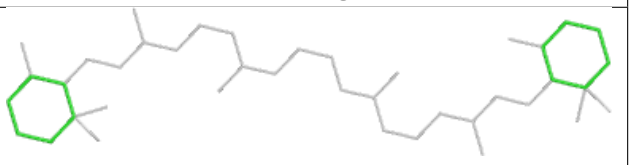
Bond lengths



Bond angles

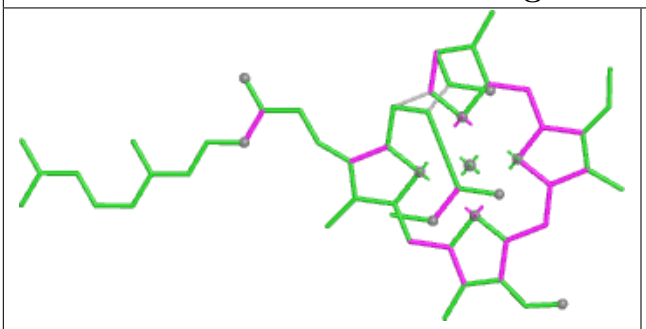


Torsions

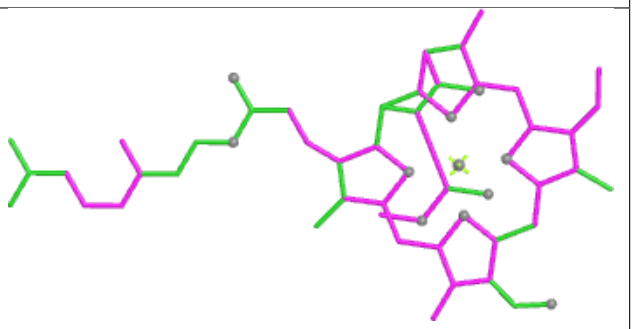


Rings

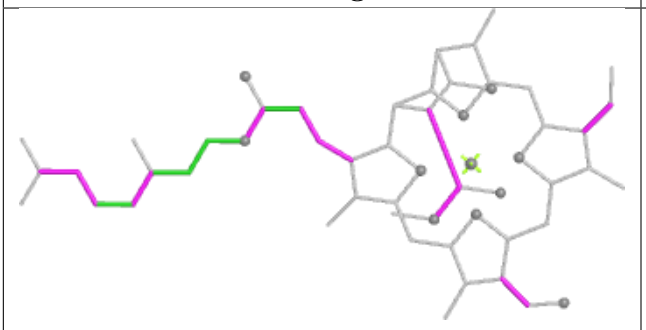
Ligand CL7 13 516



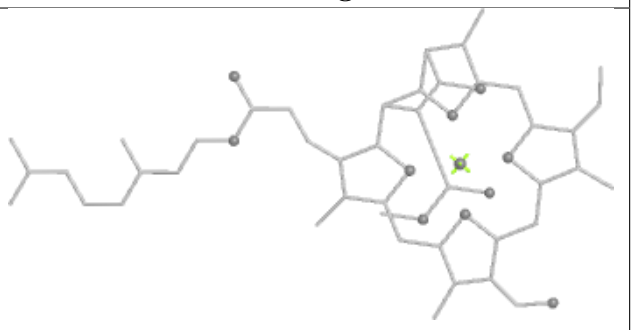
Bond lengths



Bond angles

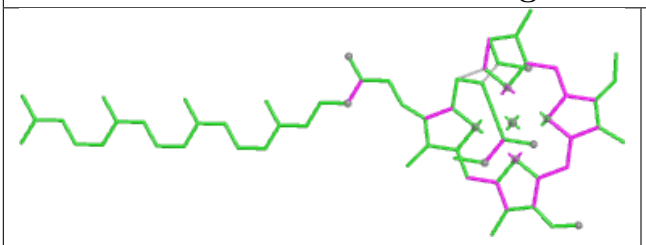


Torsions

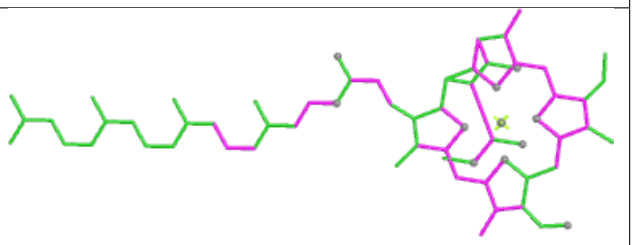


Rings

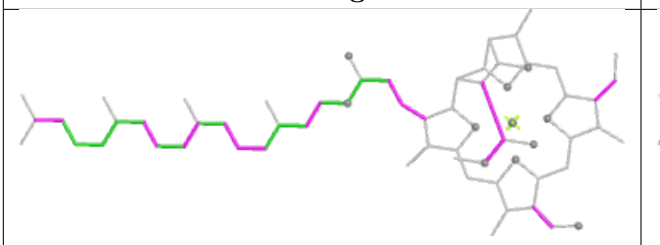
Ligand CL7 1A 407



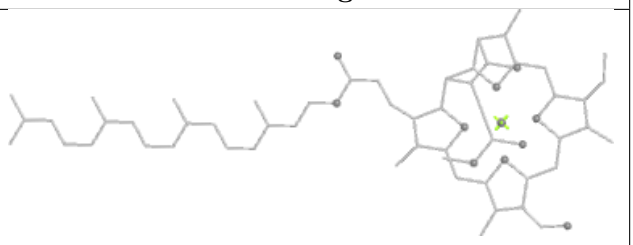
Bond lengths



Bond angles

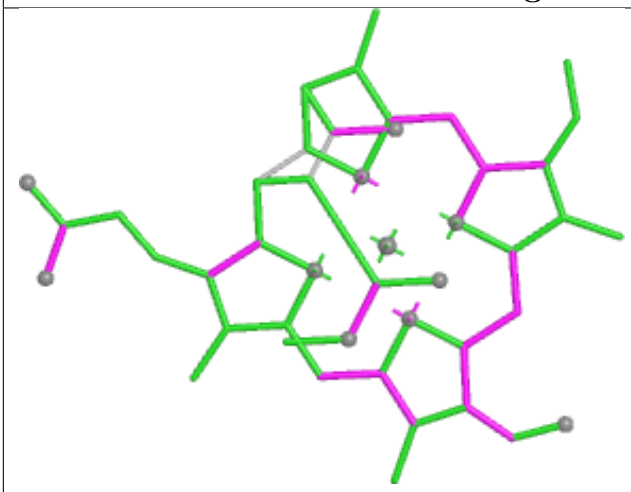


Torsions

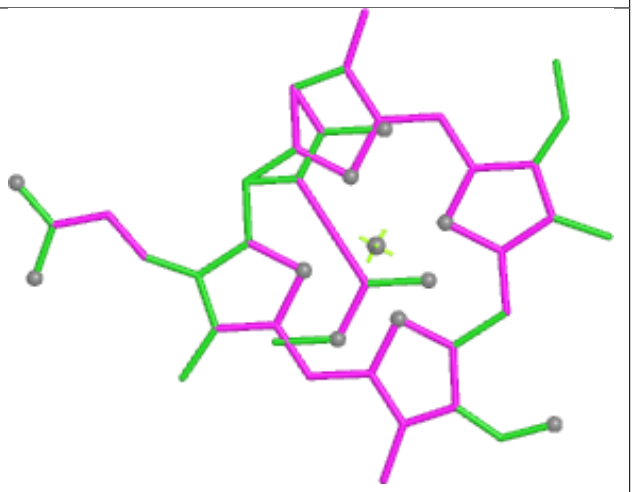


Rings

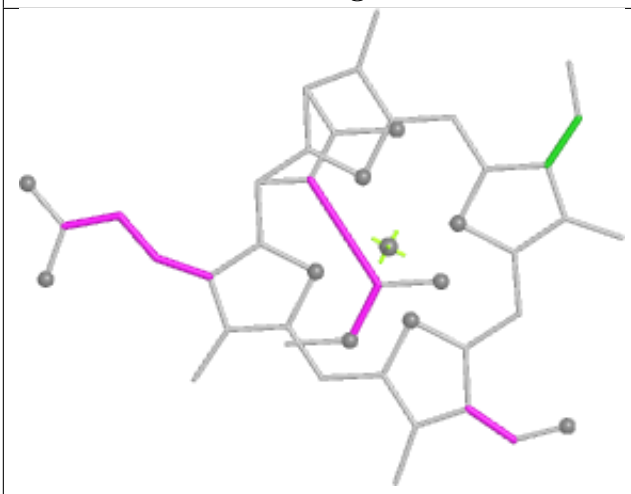
Ligand CL7 31 412



Bond lengths



Bond angles

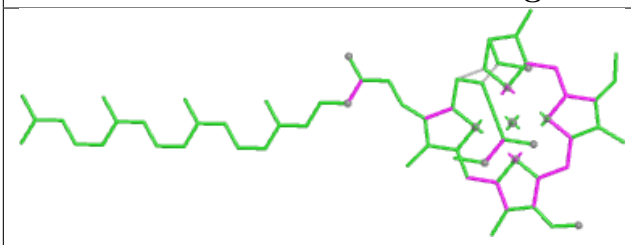


Torsions

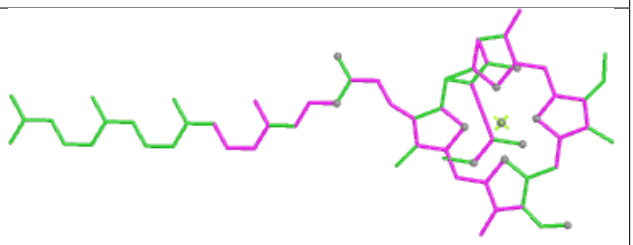


Rings

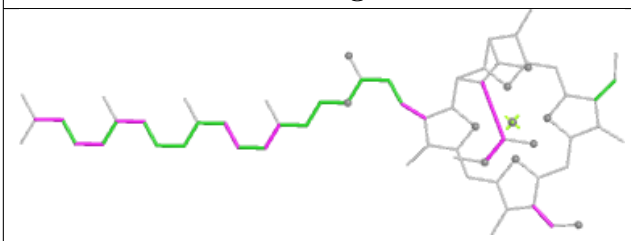
Ligand CL7 44 411



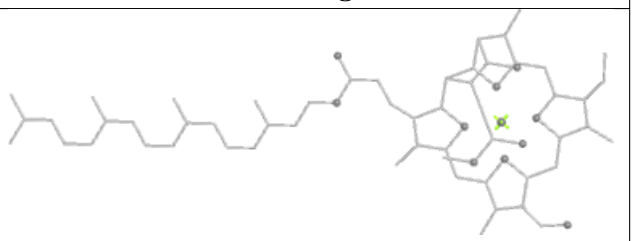
Bond lengths



Bond angles

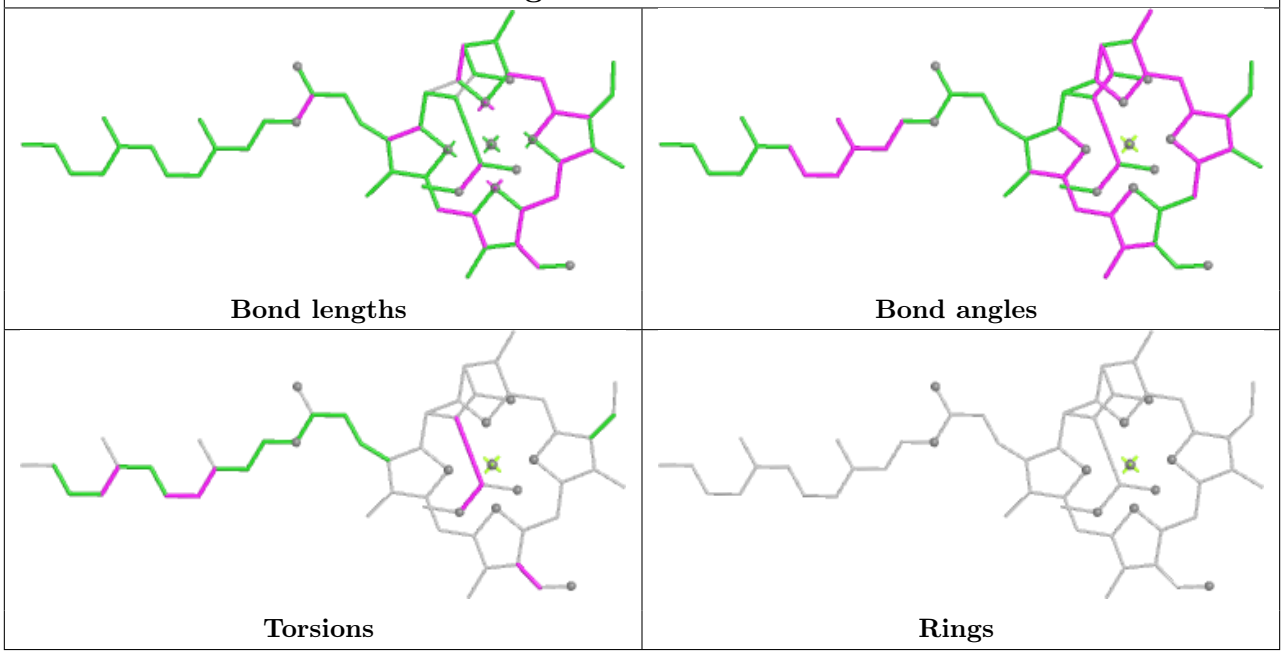


Torsions

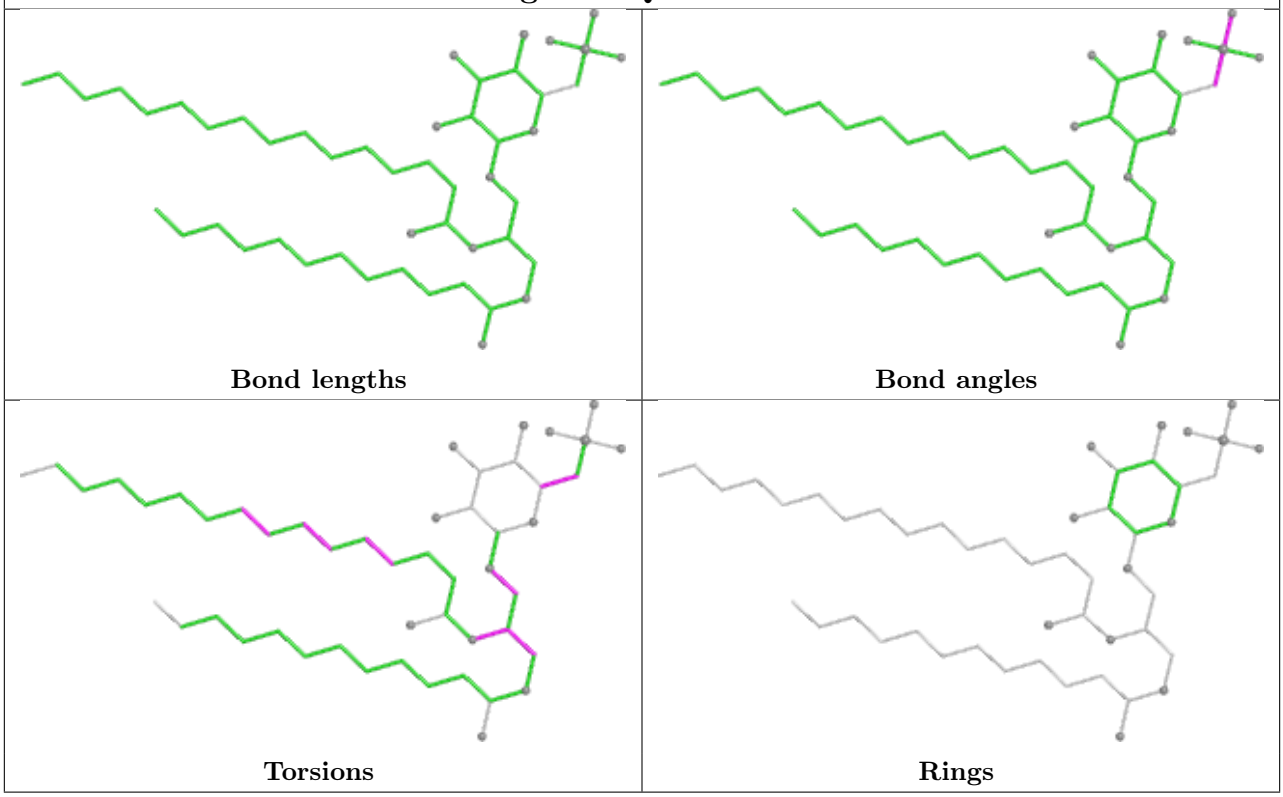


Rings

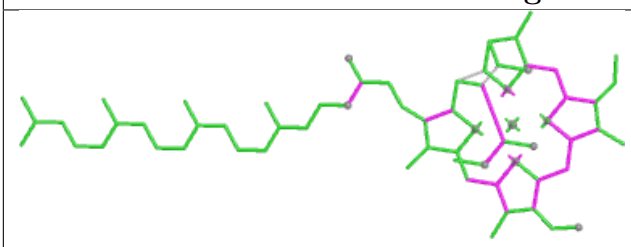
Ligand CL7 43 403



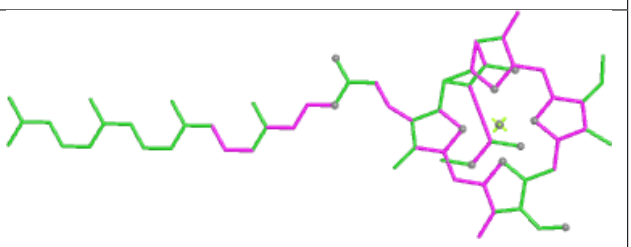
Ligand SQD 43 424



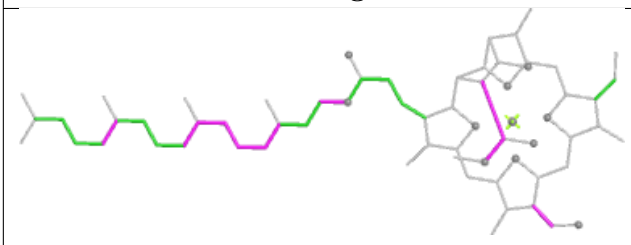
Ligand CL7 13 508



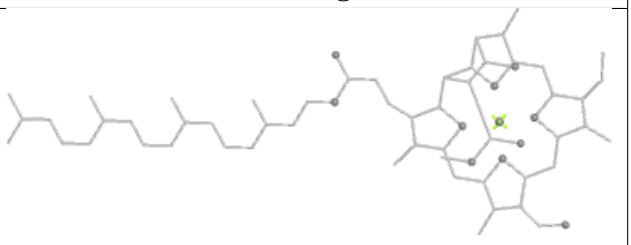
Bond lengths



Bond angles

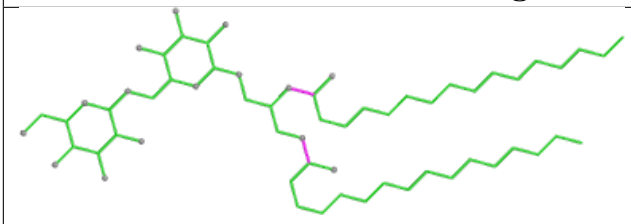


Torsions

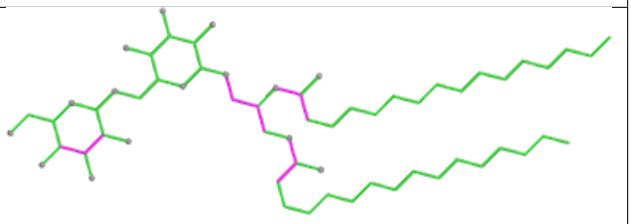


Rings

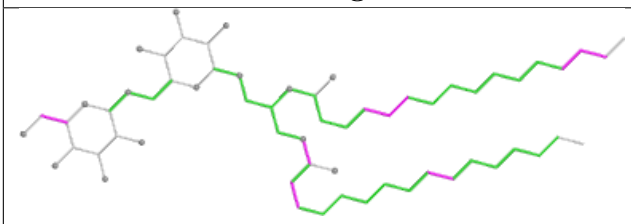
Ligand DGD 4C 516



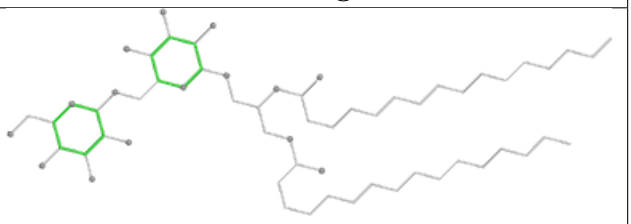
Bond lengths



Bond angles

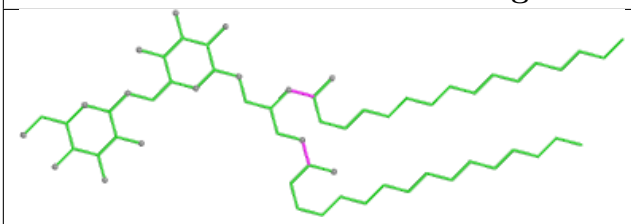


Torsions

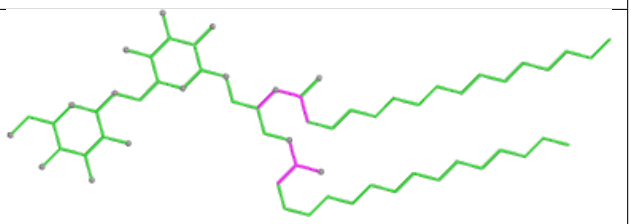


Rings

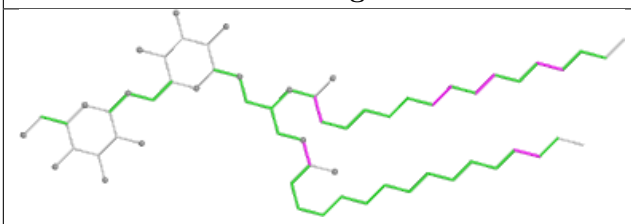
Ligand DGD 3B 624



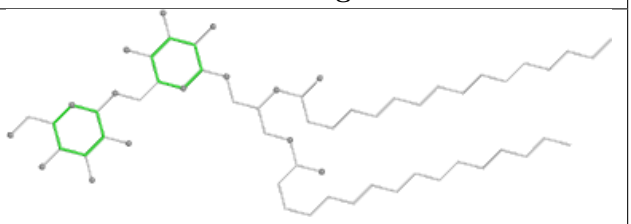
Bond lengths



Bond angles

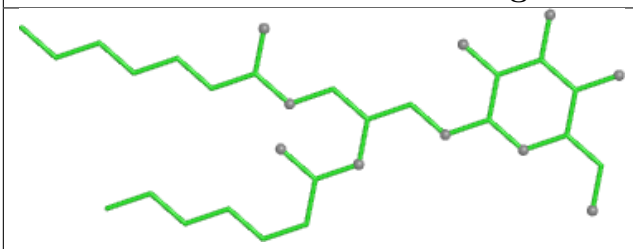


Torsions

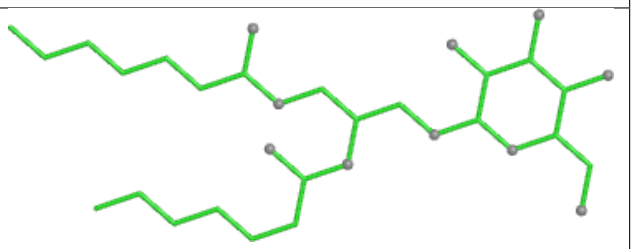


Rings

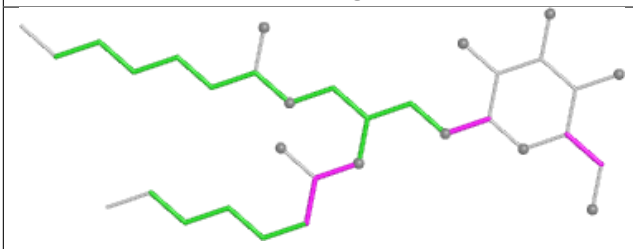
Ligand LMG 2D 410



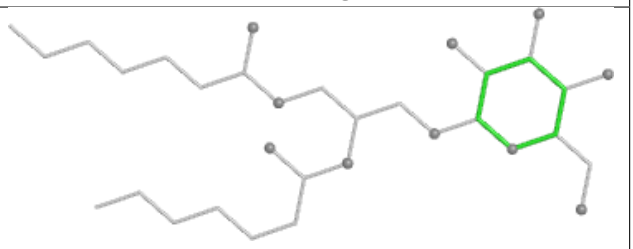
Bond lengths



Bond angles

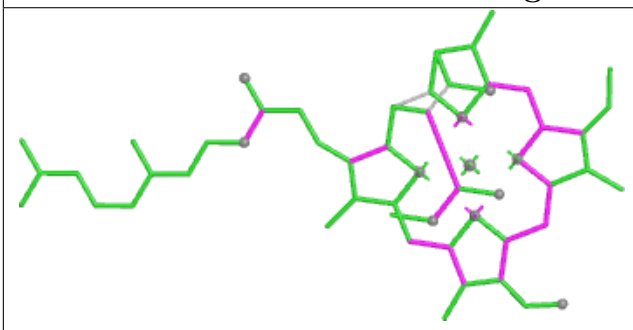


Torsions

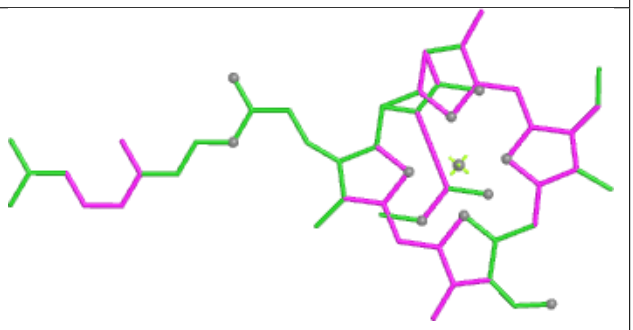


Rings

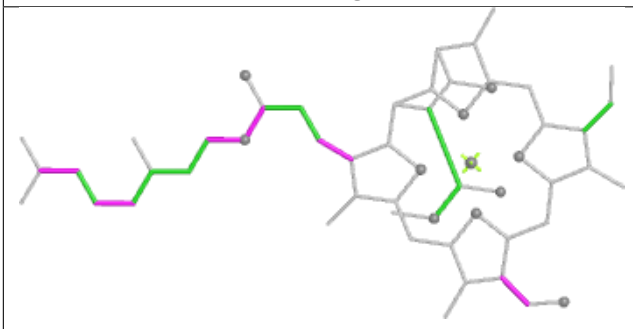
Ligand CL7 11 417



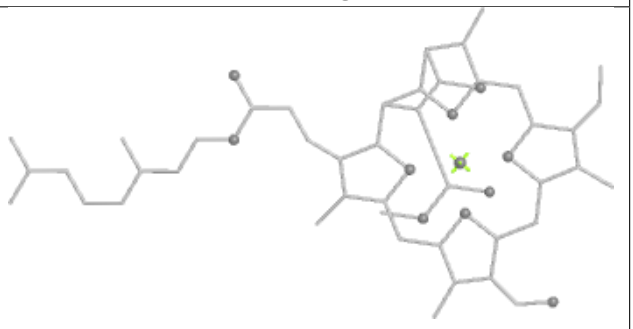
Bond lengths



Bond angles

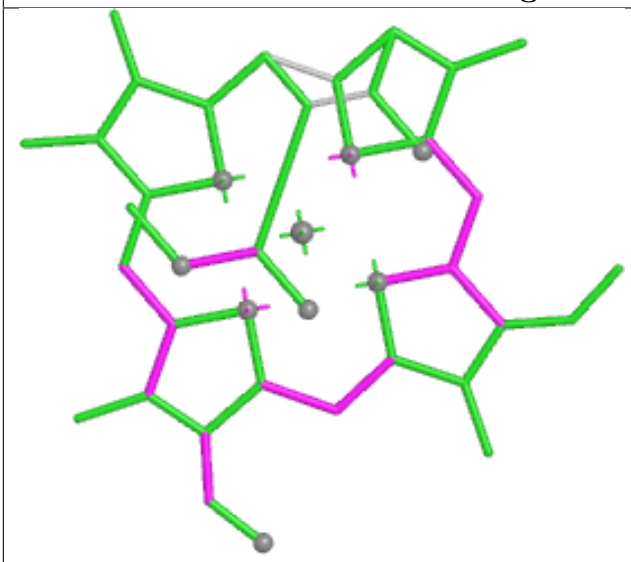


Torsions

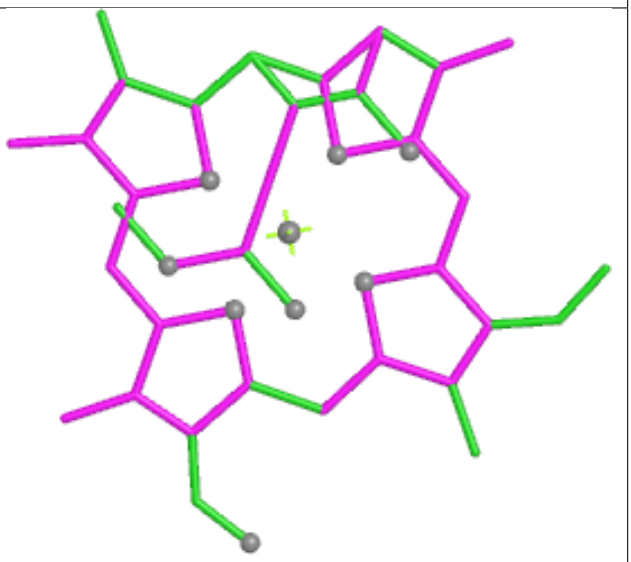


Rings

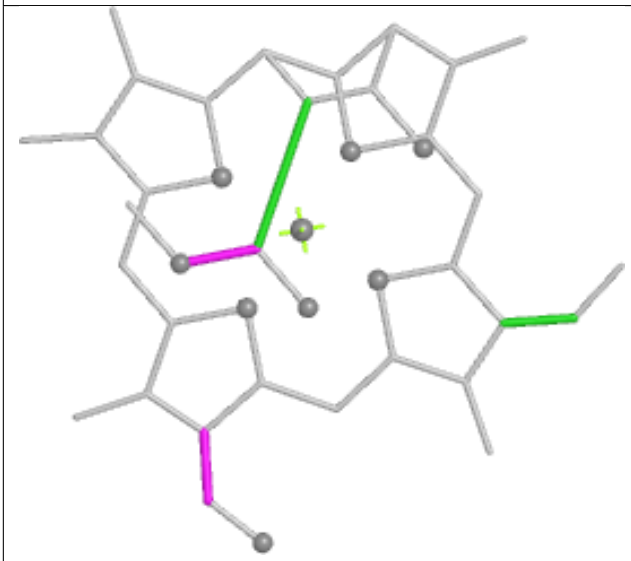
Ligand CL7 3C 512



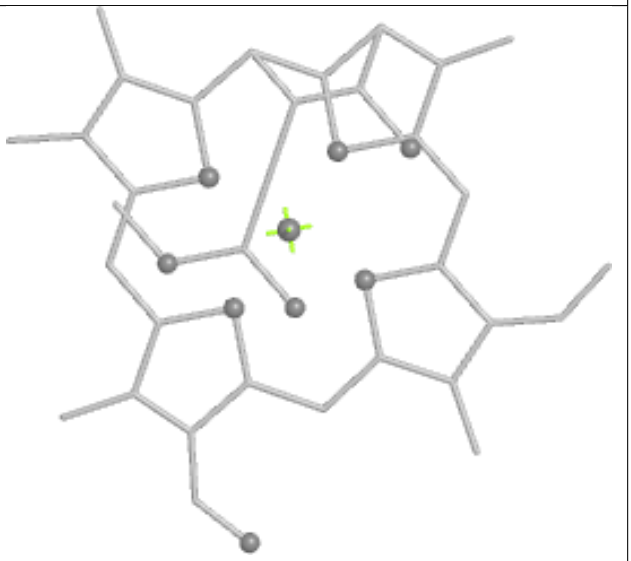
Bond lengths



Bond angles

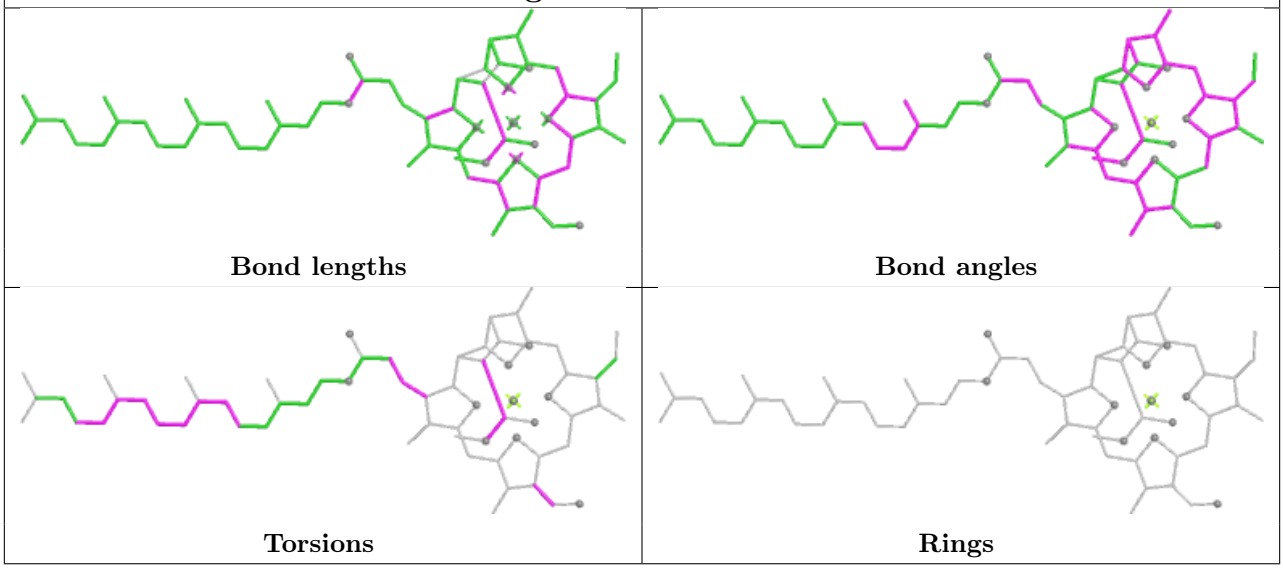


Torsions

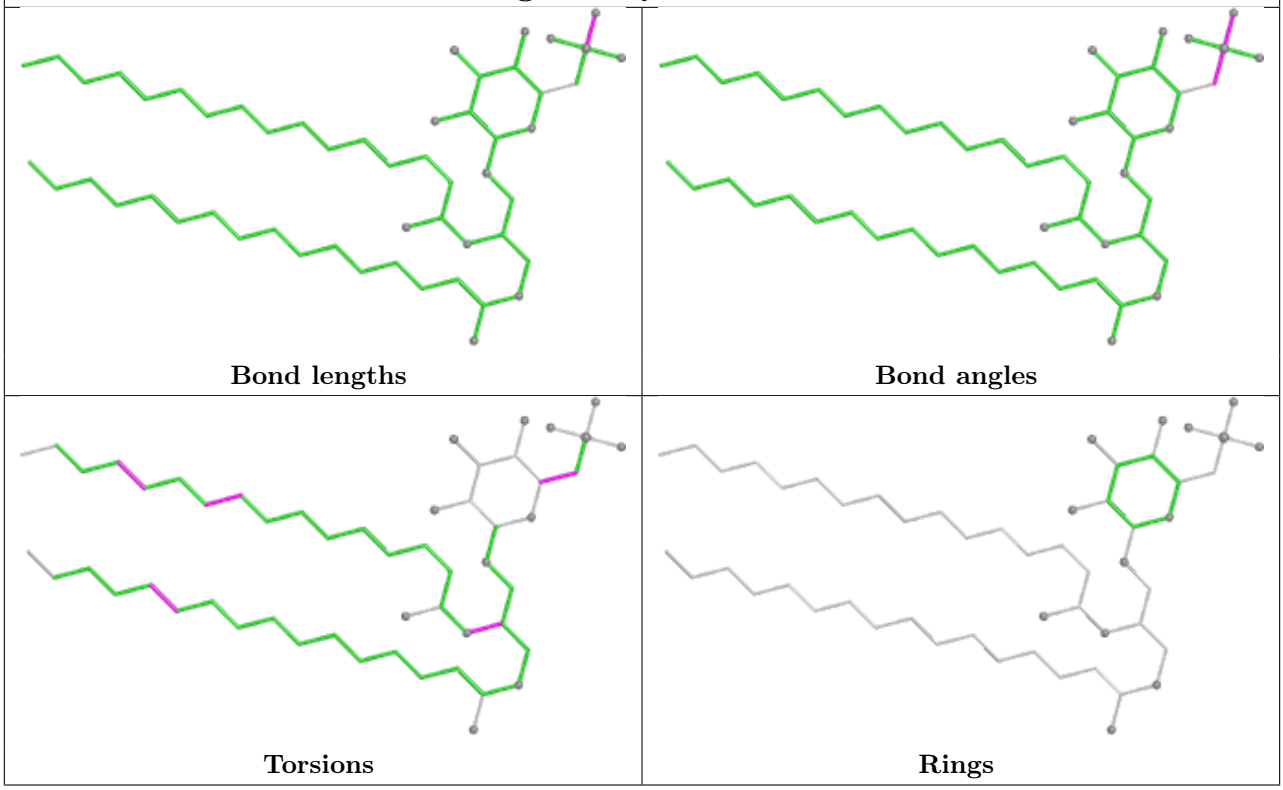


Rings

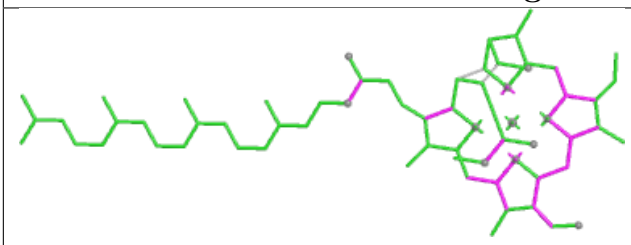
Ligand CL7 13 503



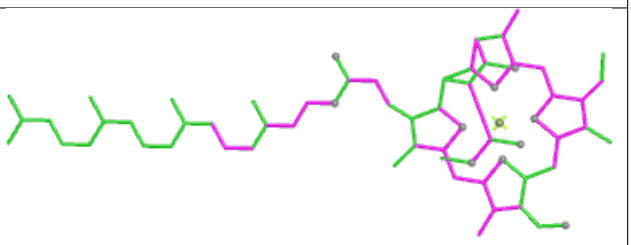
Ligand SQD 2B 621



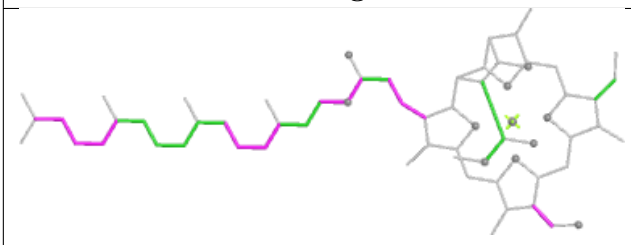
Ligand CL7 22 516



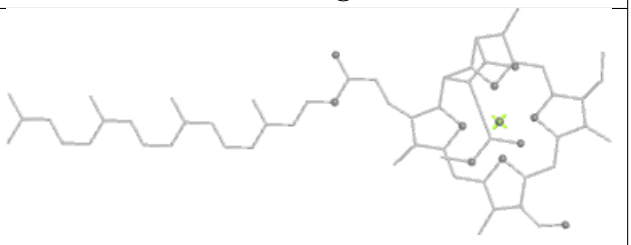
Bond lengths



Bond angles

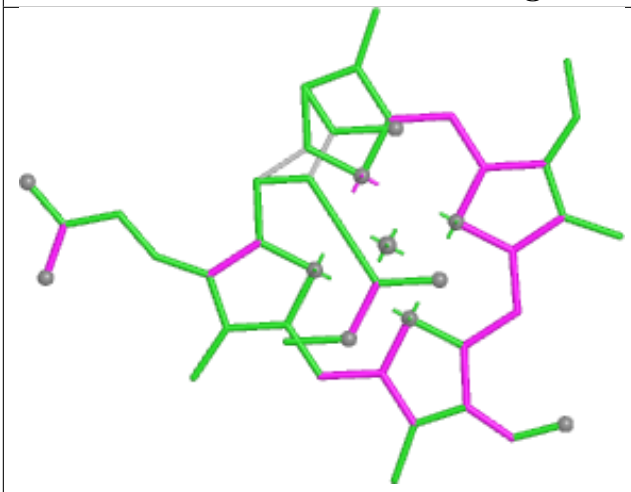


Torsions

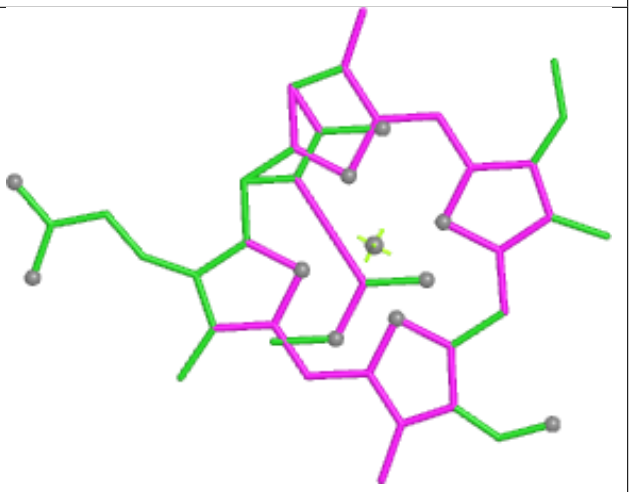


Rings

Ligand CL7 33 506



Bond lengths



Bond angles

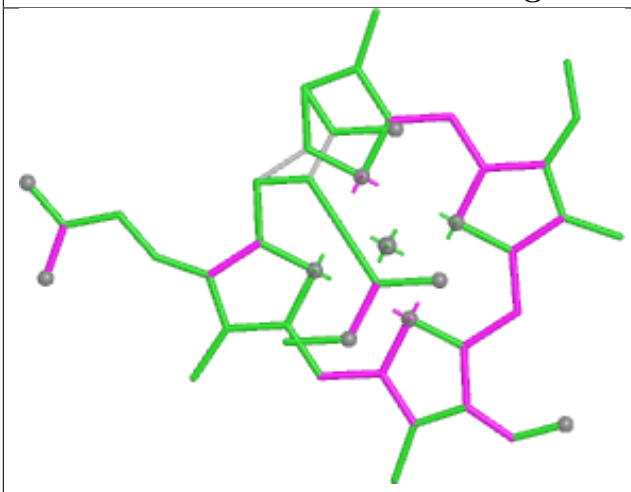


Torsions

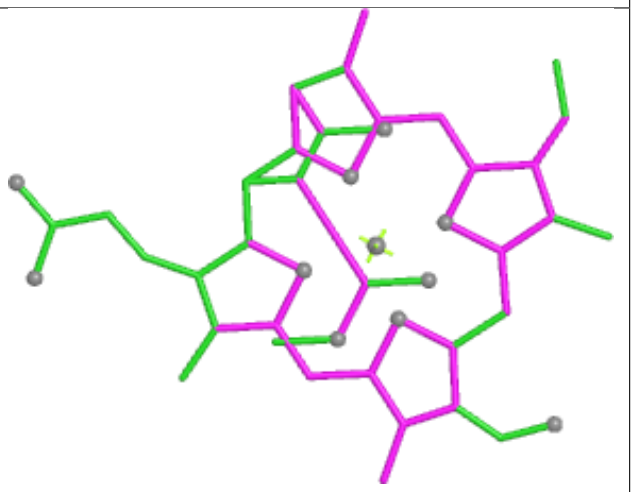


Rings

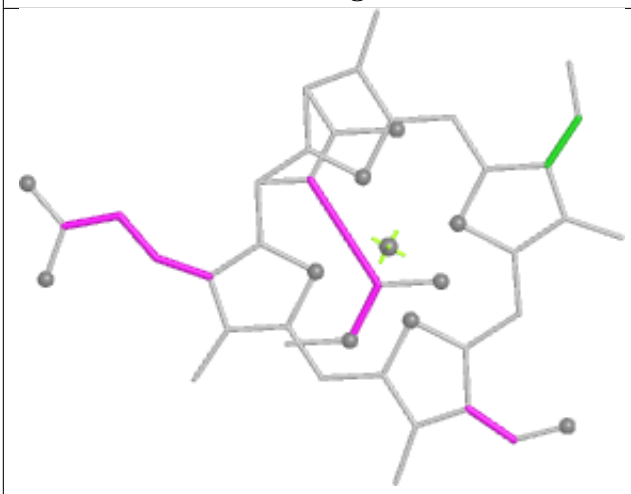
Ligand CL7 24 410



Bond lengths



Bond angles

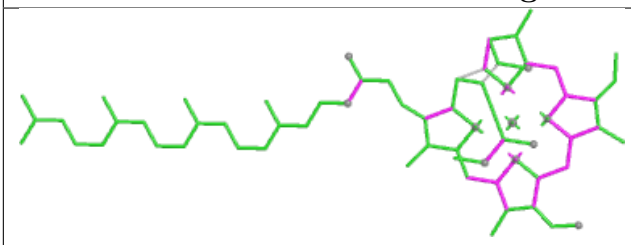


Torsions

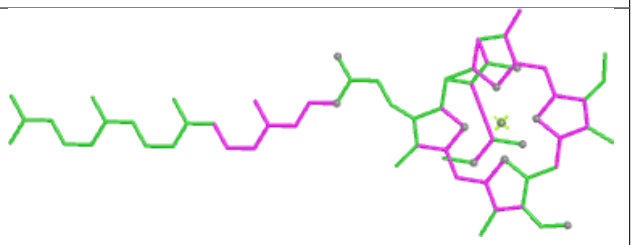


Rings

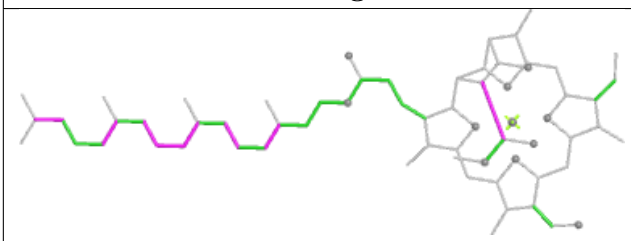
Ligand CL7 1B 603



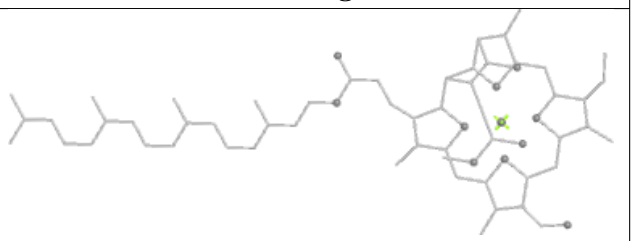
Bond lengths



Bond angles

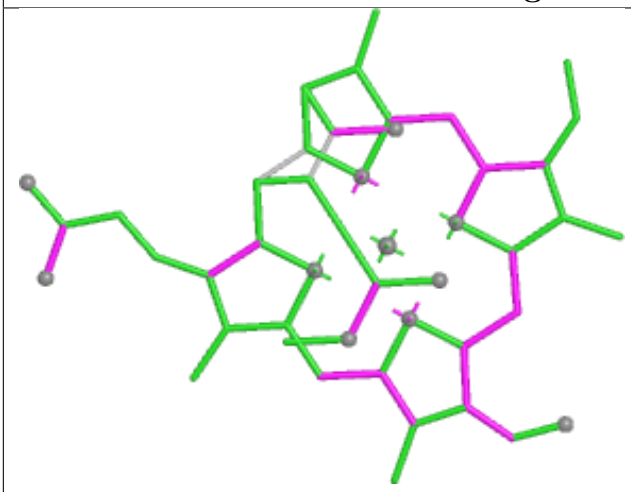


Torsions

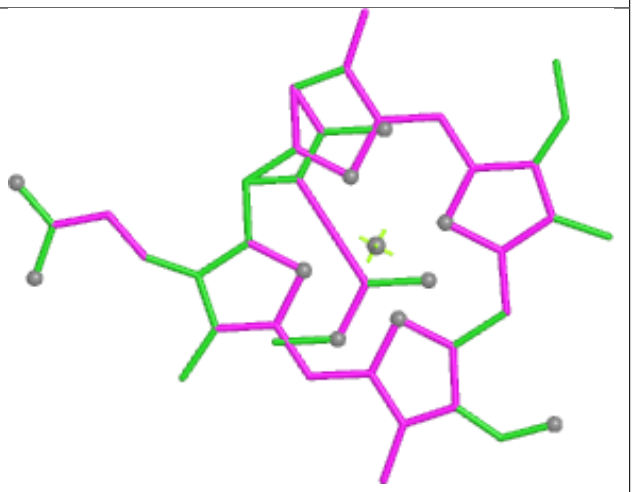


Rings

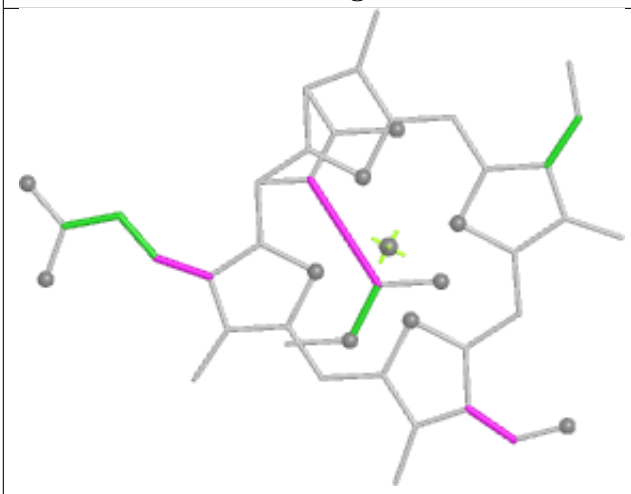
Ligand CL7 12 515



Bond lengths



Bond angles

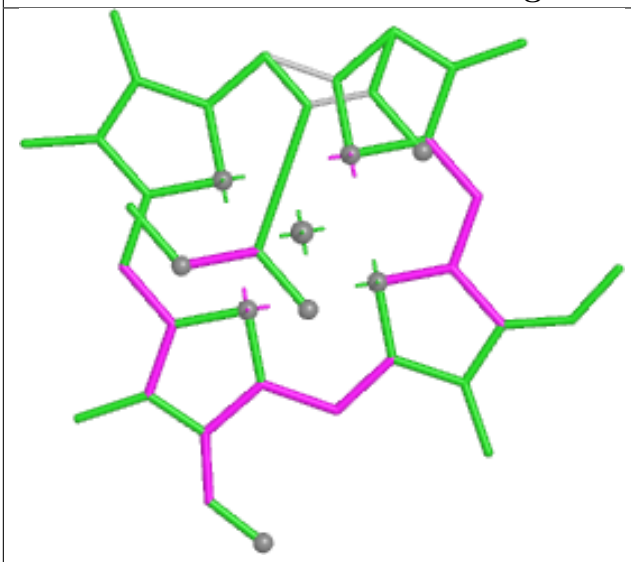


Torsions

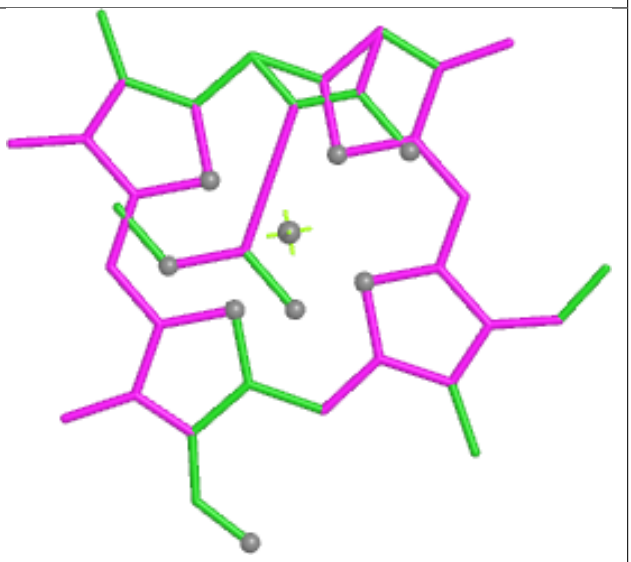


Rings

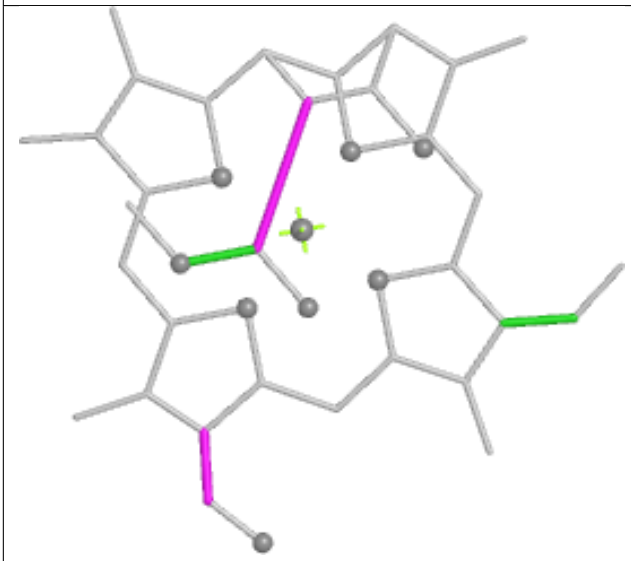
Ligand CL7 44 407



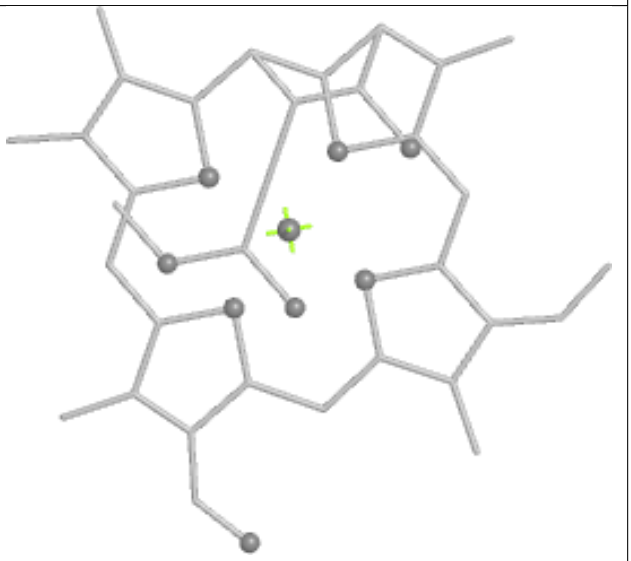
Bond lengths



Bond angles

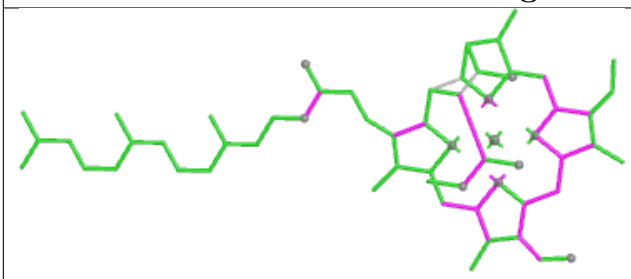


Torsions

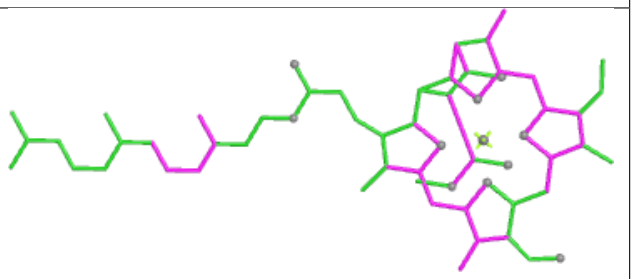


Rings

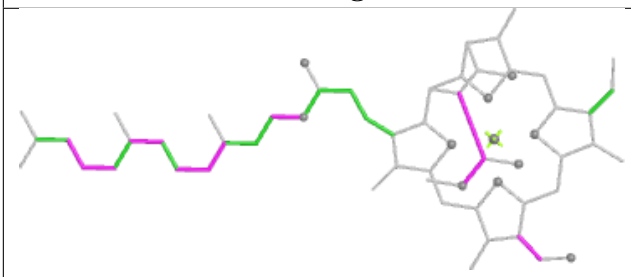
Ligand CL7 1C 502



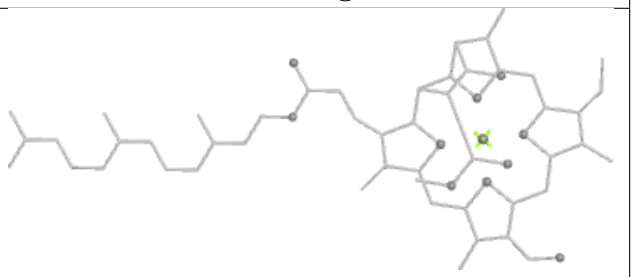
Bond lengths



Bond angles



Torsions

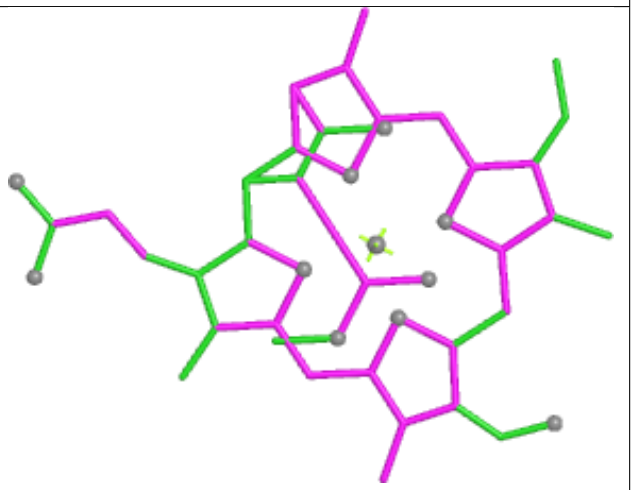


Rings

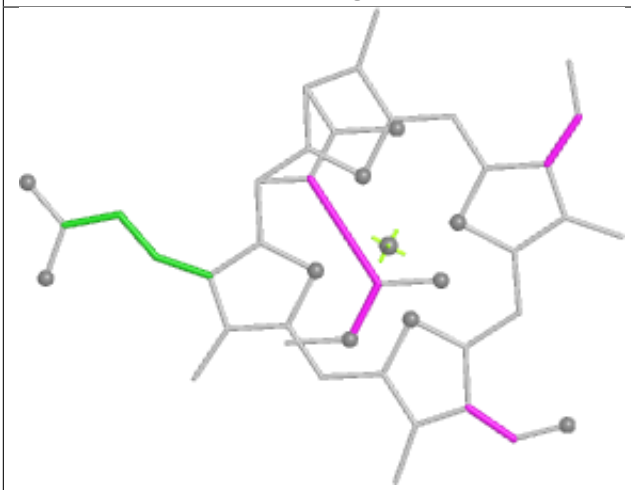
Ligand CL7 41 420



Bond lengths



Bond angles

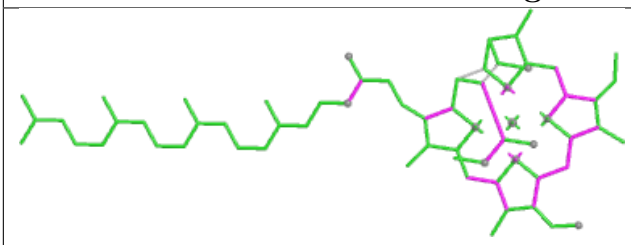


Torsions

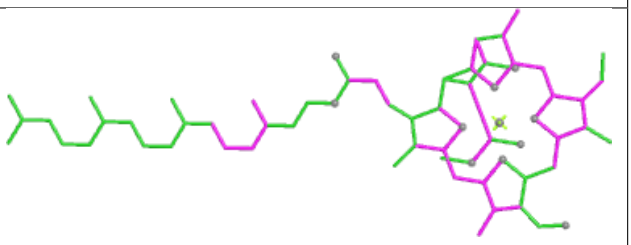


Rings

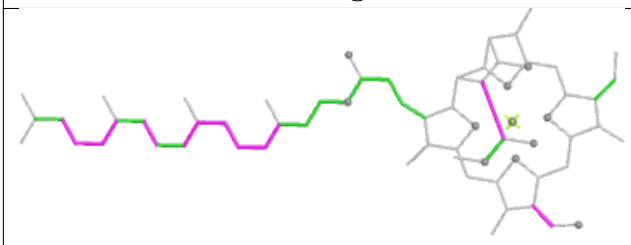
Ligand CL7 43 408



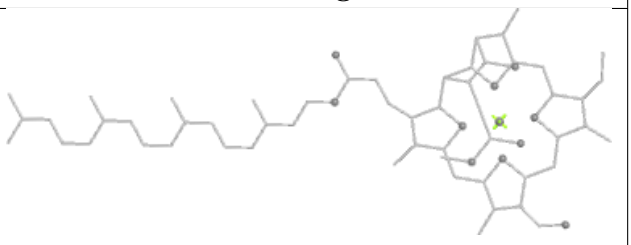
Bond lengths



Bond angles

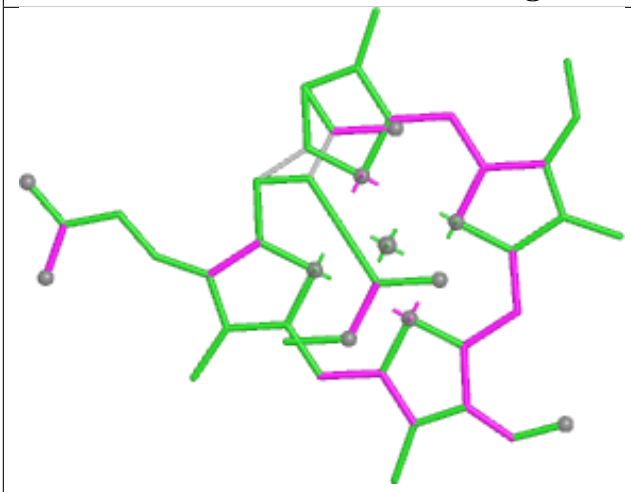


Torsions

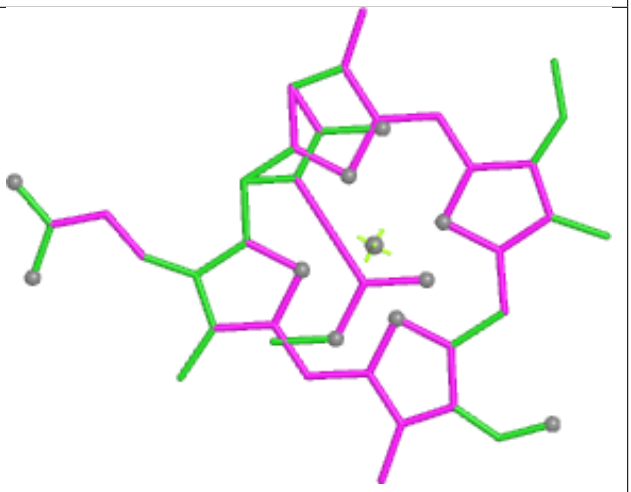


Rings

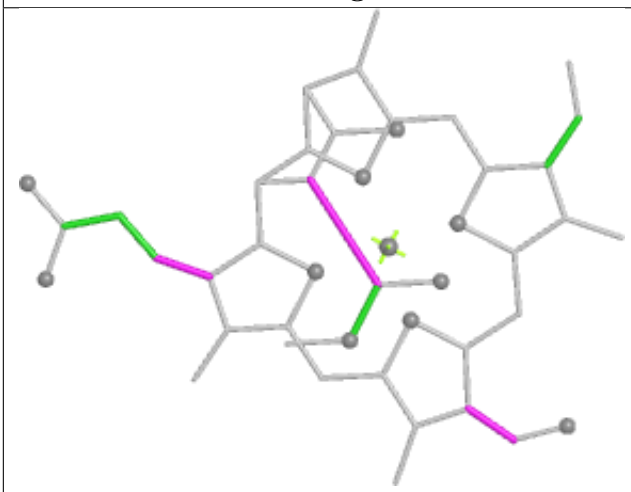
Ligand CL7 22 515



Bond lengths



Bond angles

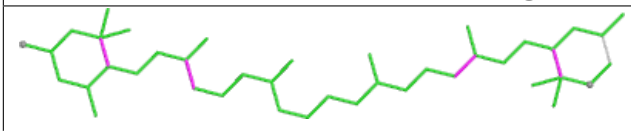


Torsions

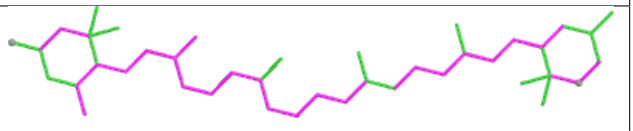


Rings

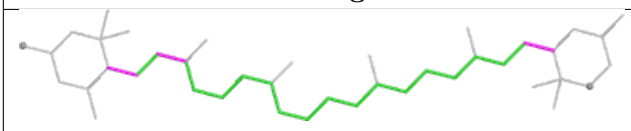
Ligand ZEX 33 522



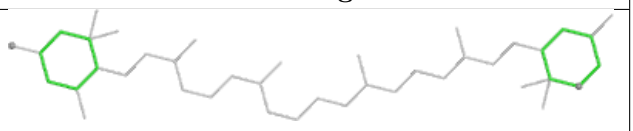
Bond lengths



Bond angles



Torsions

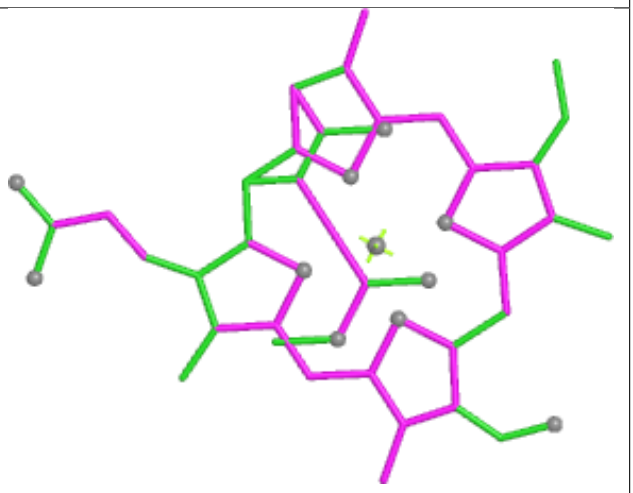


Rings

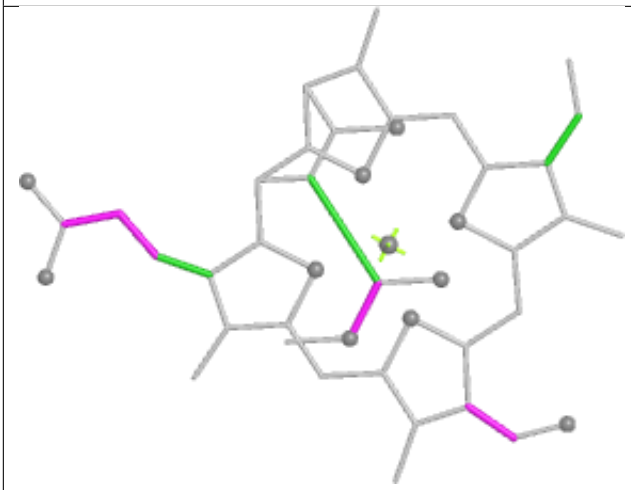
Ligand CL7 23 419



Bond lengths



Bond angles

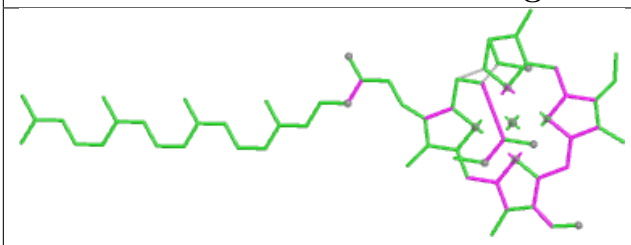


Torsions

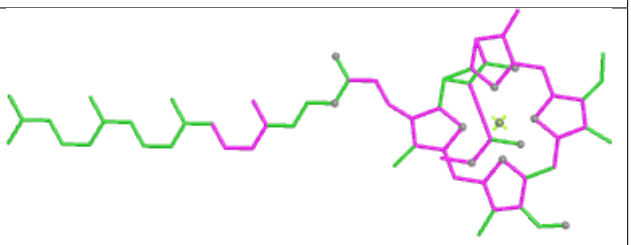


Rings

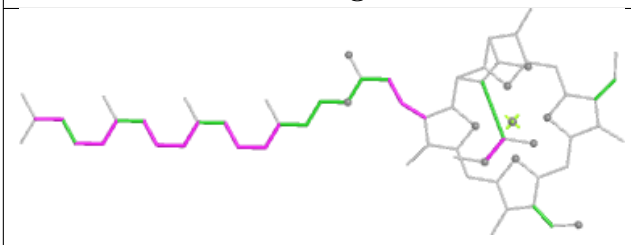
Ligand CL7 22 503



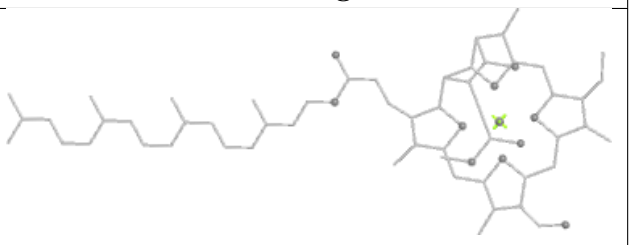
Bond lengths



Bond angles

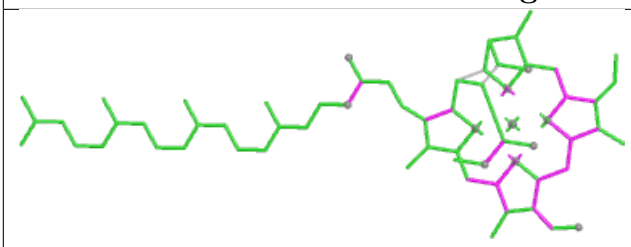


Torsions

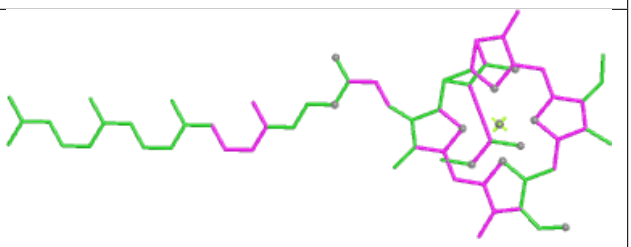


Rings

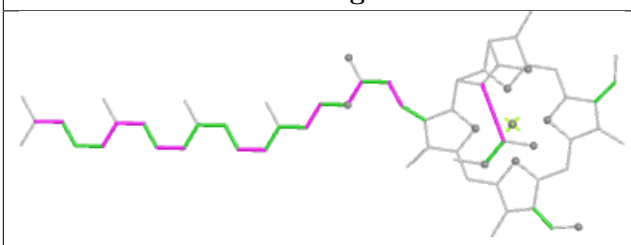
Ligand CL7 1B 610



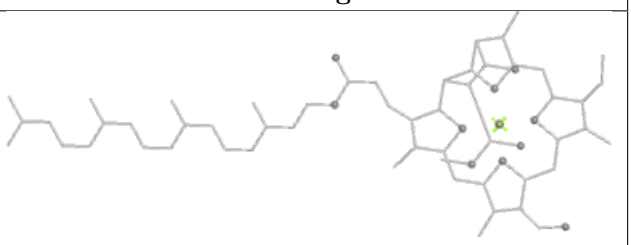
Bond lengths



Bond angles

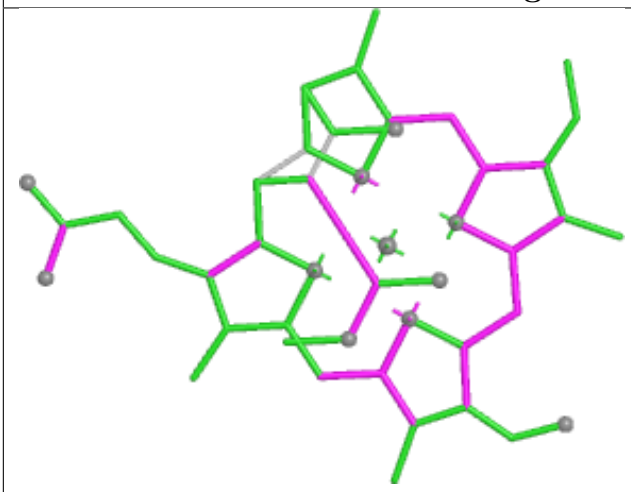


Torsions

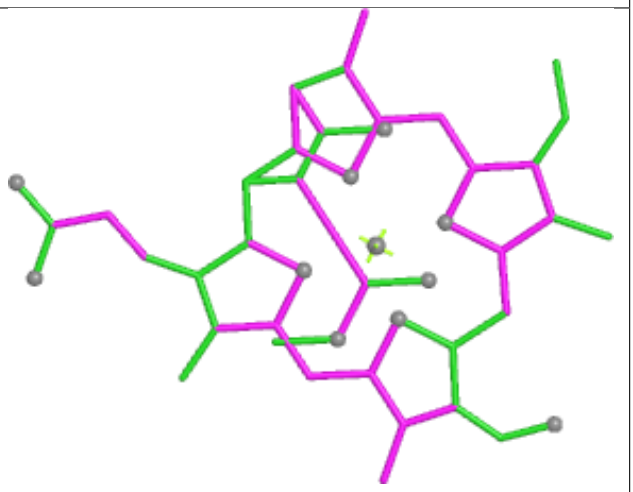


Rings

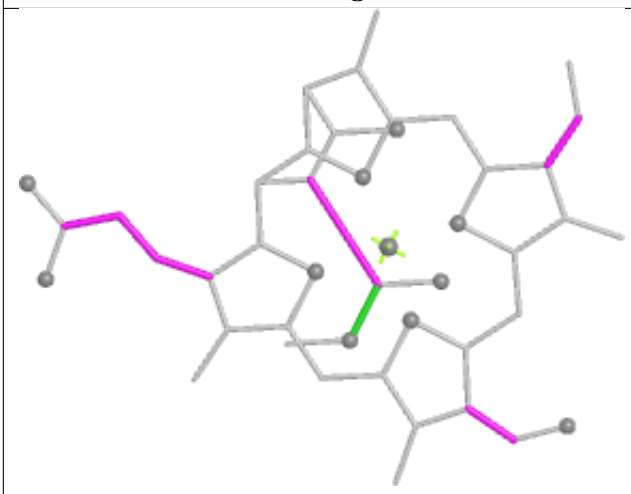
Ligand CL7 43 414



Bond lengths



Bond angles

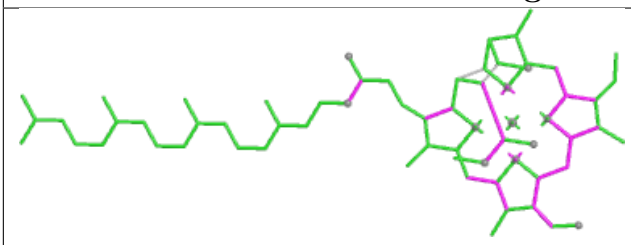


Torsions

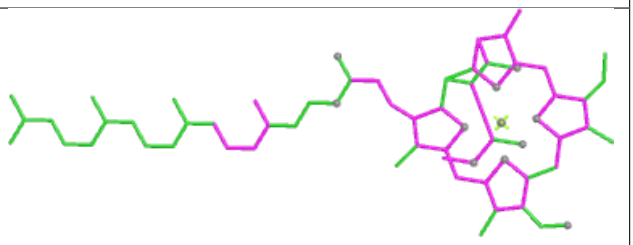


Rings

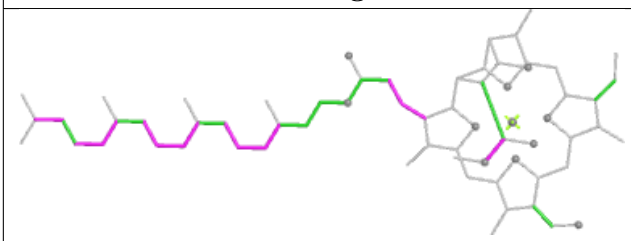
Ligand CL7 32 503



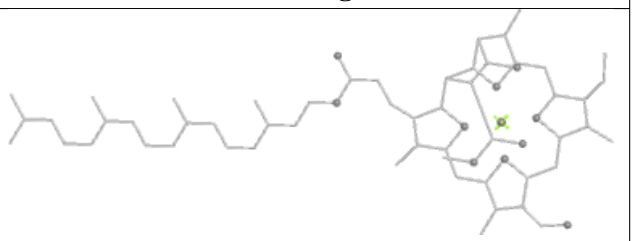
Bond lengths



Bond angles

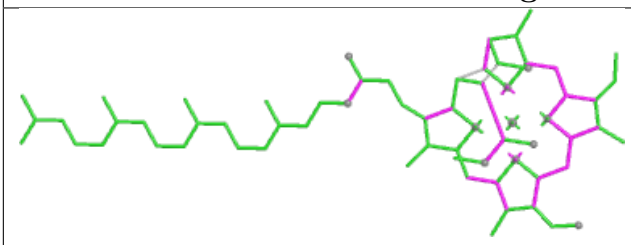


Torsions

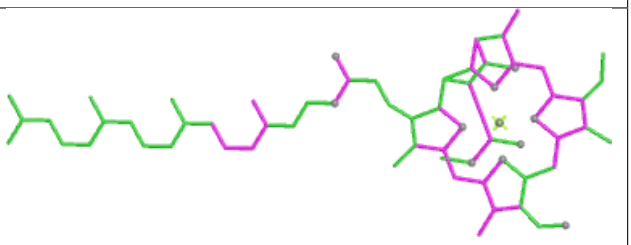


Rings

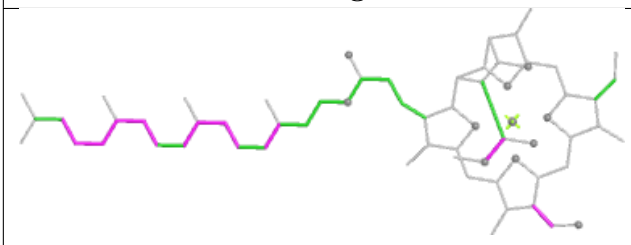
Ligand CL7 4B 612



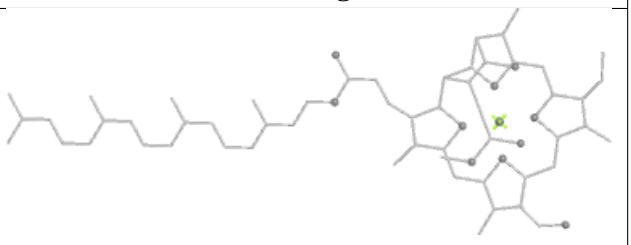
Bond lengths



Bond angles

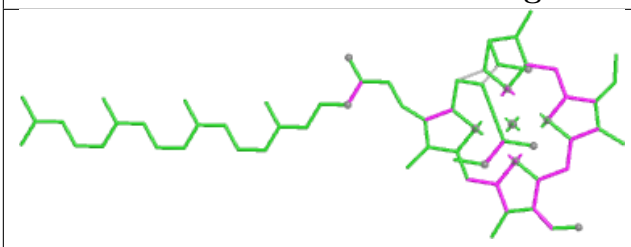


Torsions

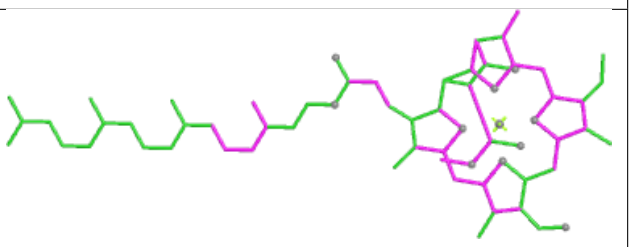


Rings

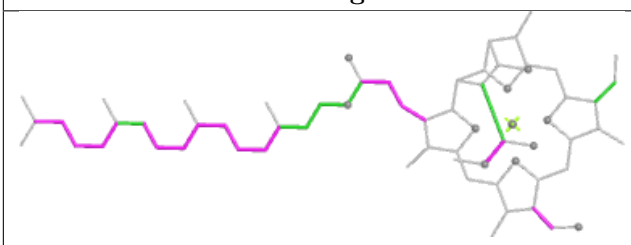
Ligand CL7 34 406



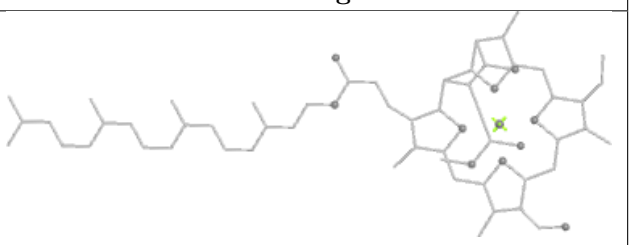
Bond lengths



Bond angles

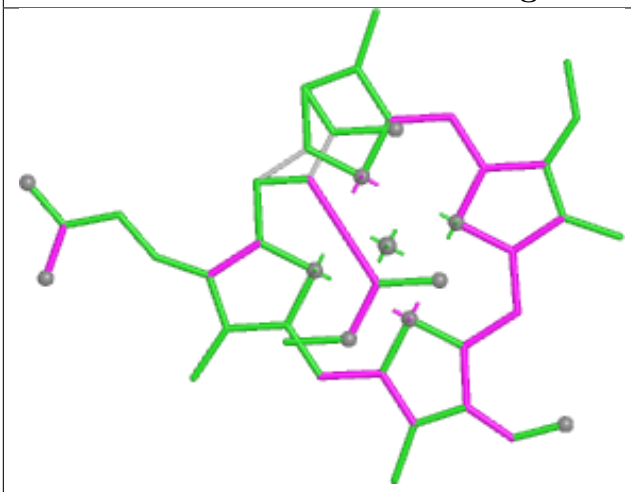


Torsions

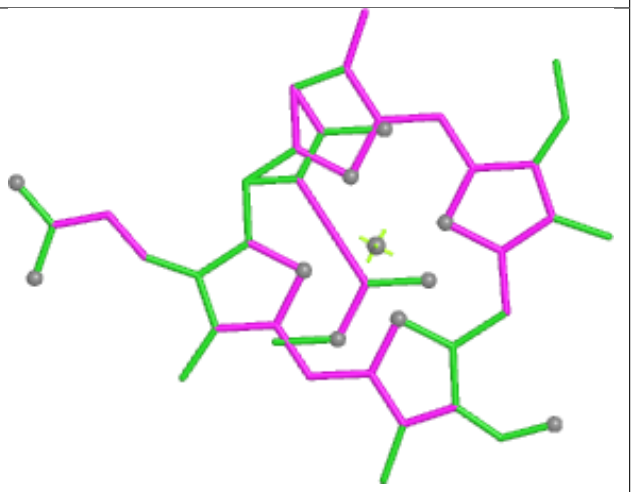


Rings

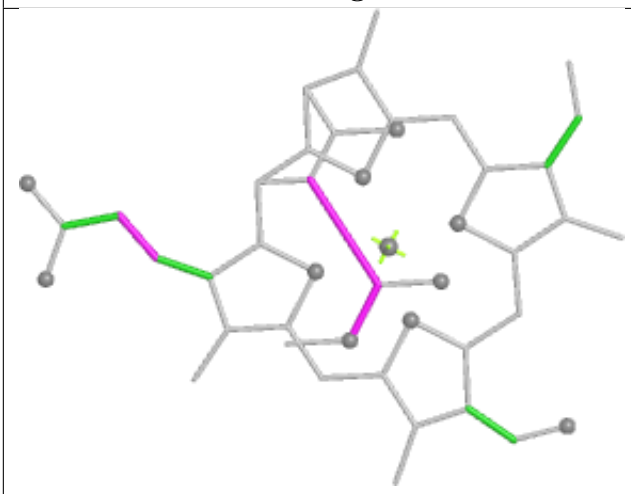
Ligand CL7 4B 617



Bond lengths



Bond angles

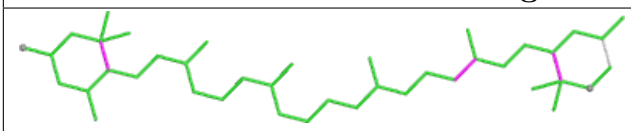


Torsions

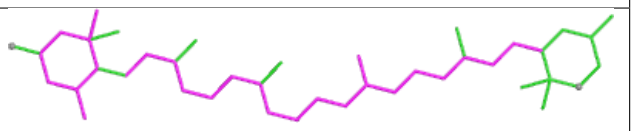


Rings

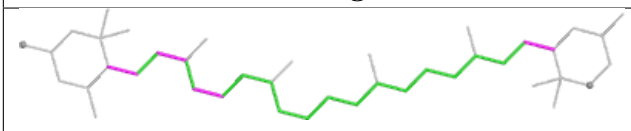
Ligand ZEX 42 520



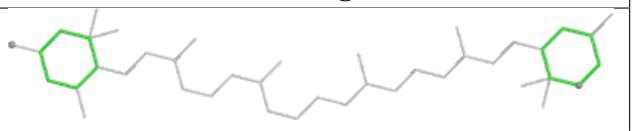
Bond lengths



Bond angles

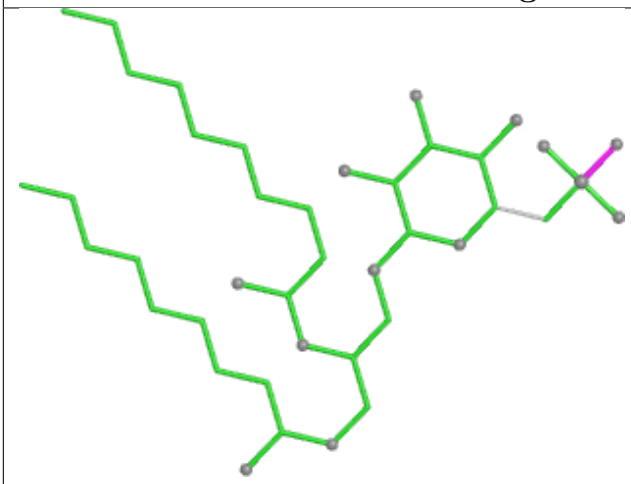


Torsions

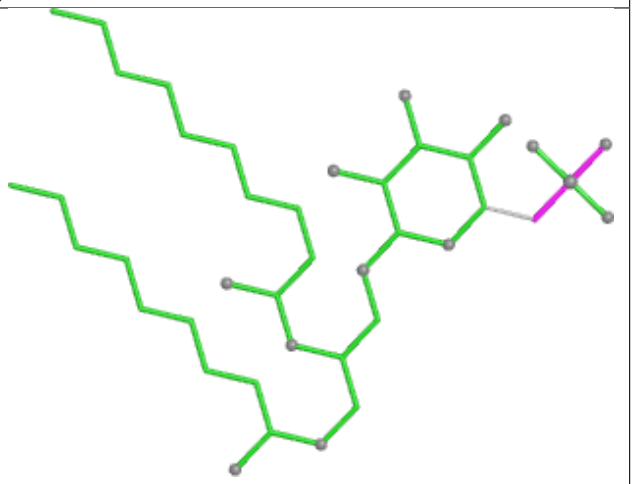


Rings

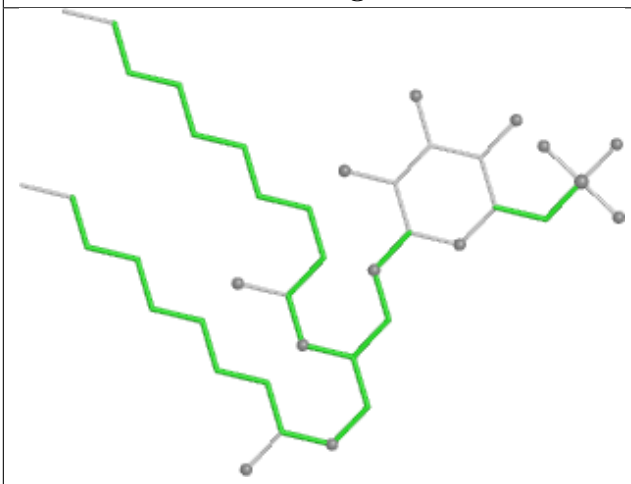
Ligand SQD 22 523



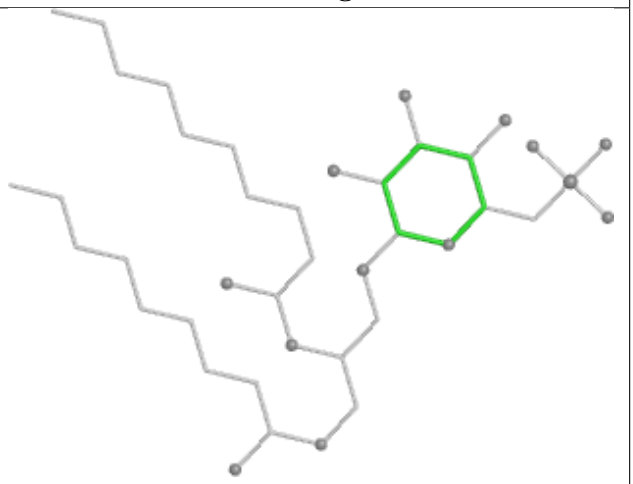
Bond lengths



Bond angles

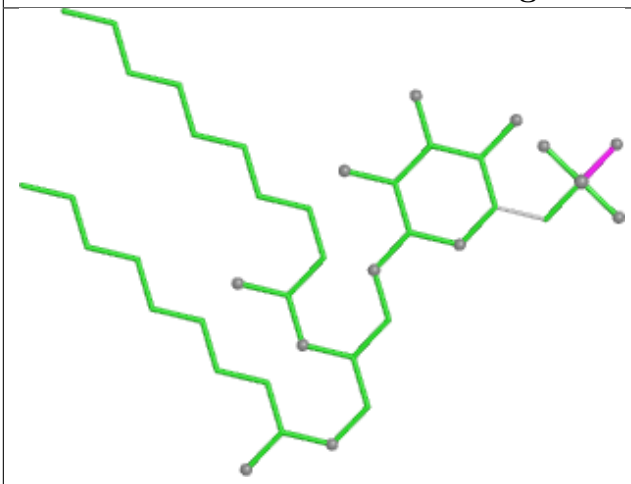


Torsions

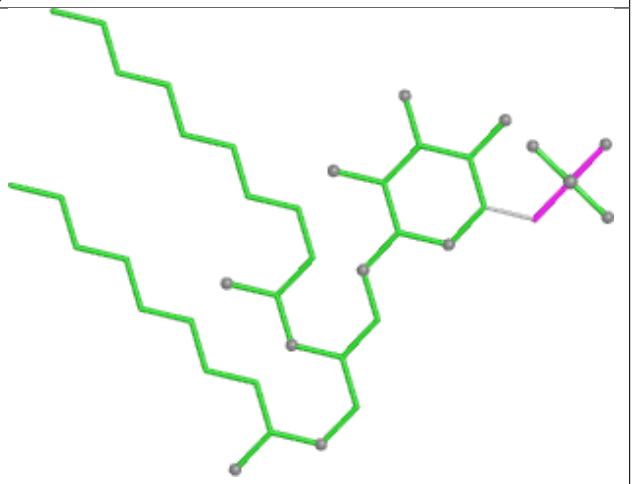


Rings

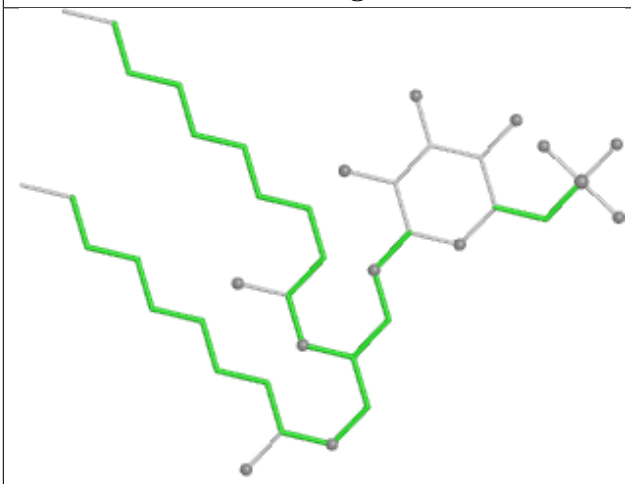
Ligand SQD 32 523



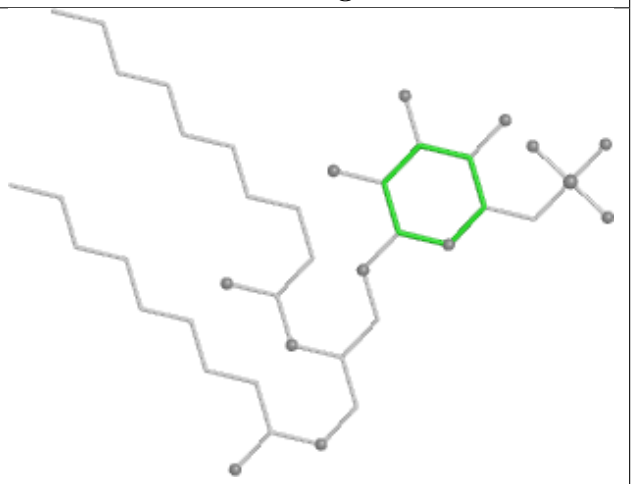
Bond lengths



Bond angles

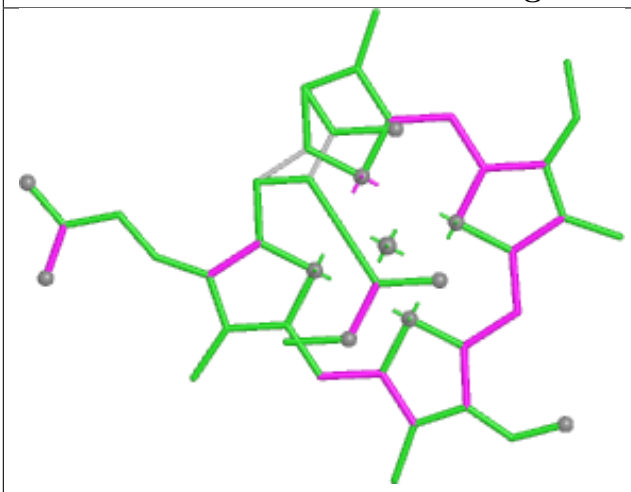


Torsions

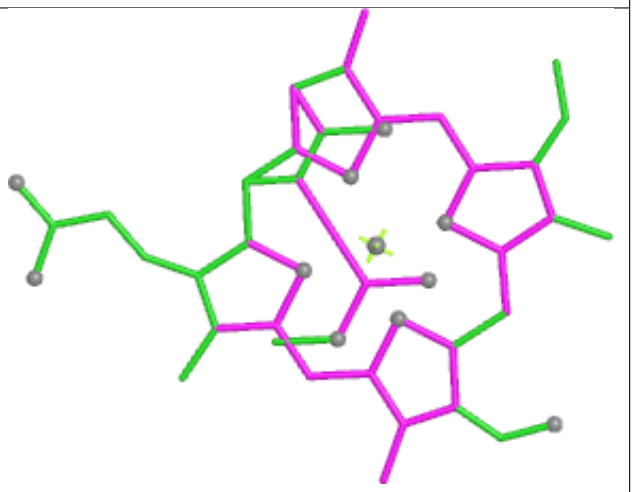


Rings

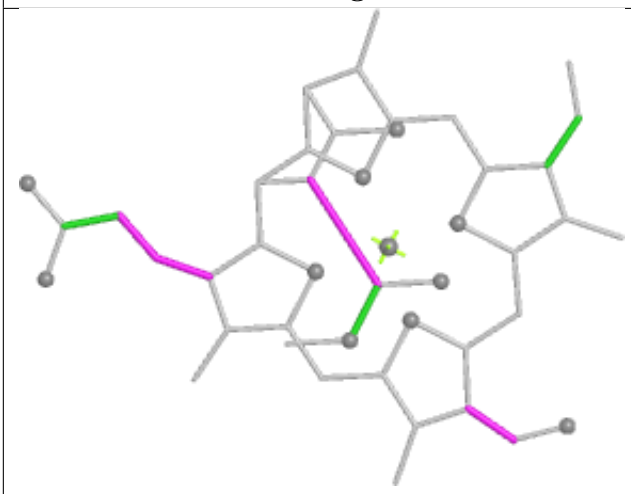
Ligand CL7 42 513



Bond lengths



Bond angles

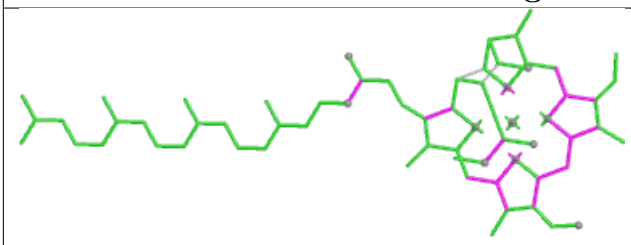


Torsions

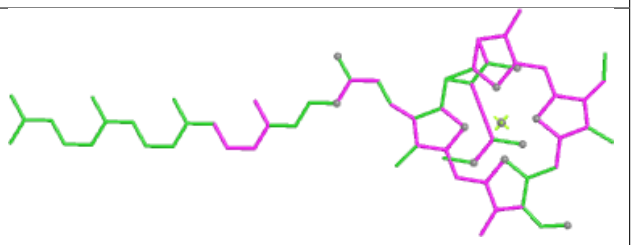


Rings

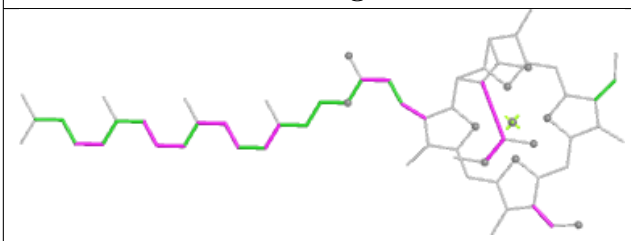
Ligand CL7 43 411



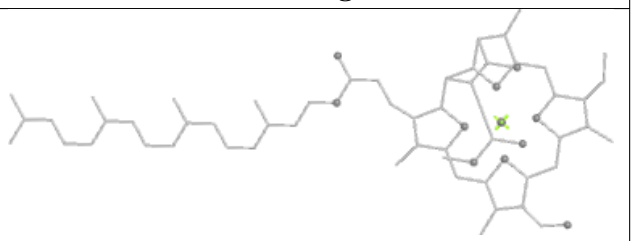
Bond lengths



Bond angles

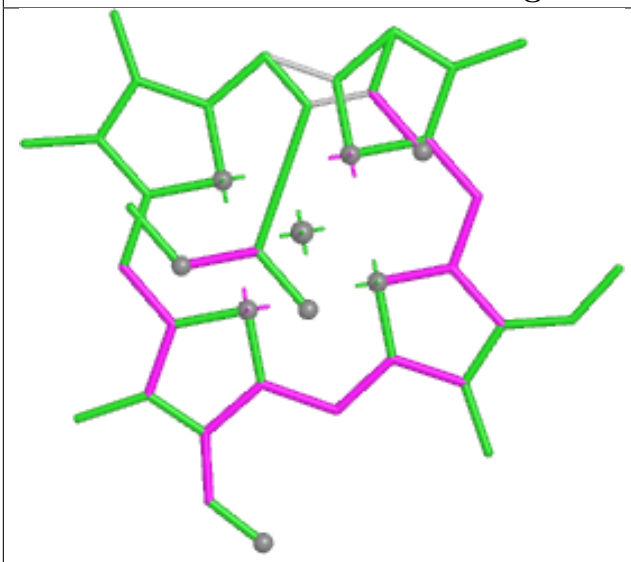


Torsions

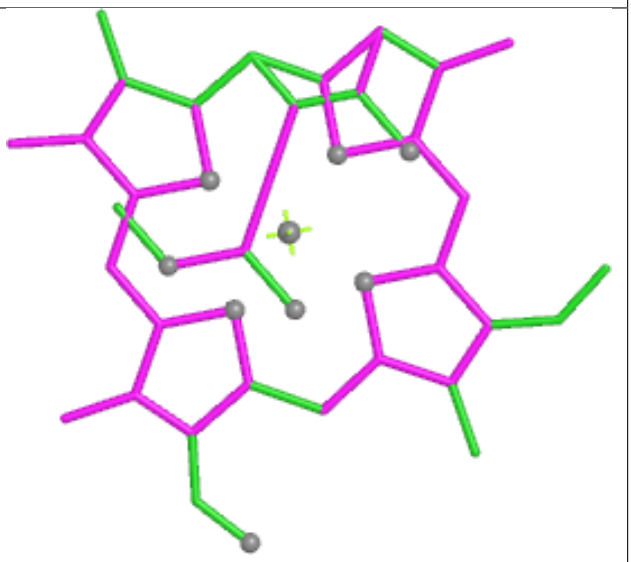


Rings

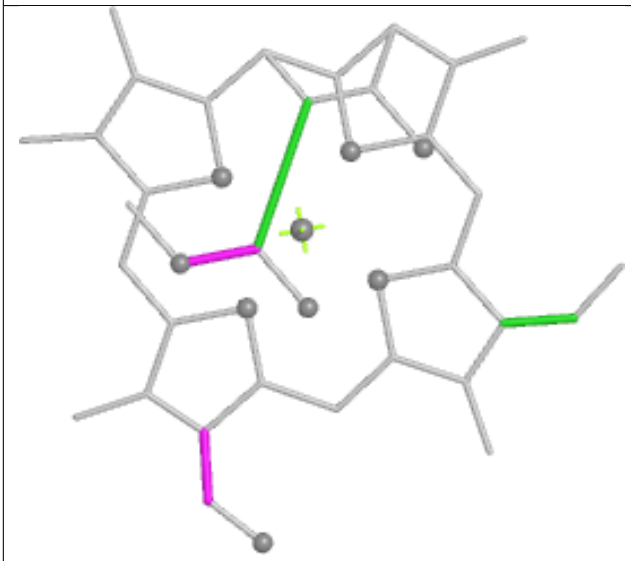
Ligand CL7 11 407



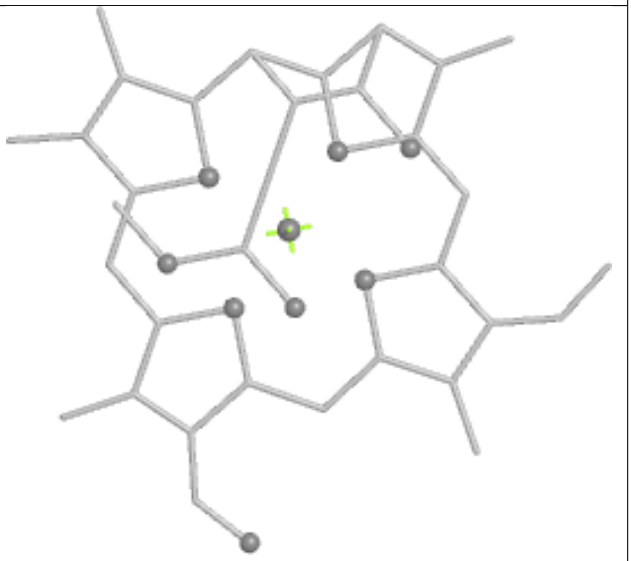
Bond lengths



Bond angles

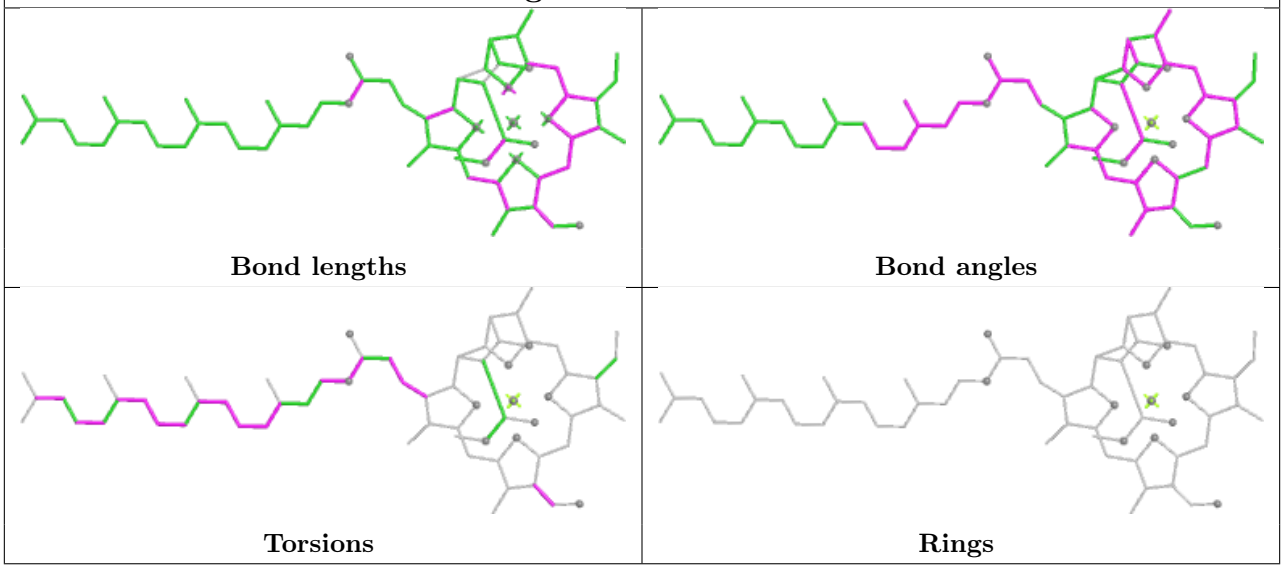


Torsions

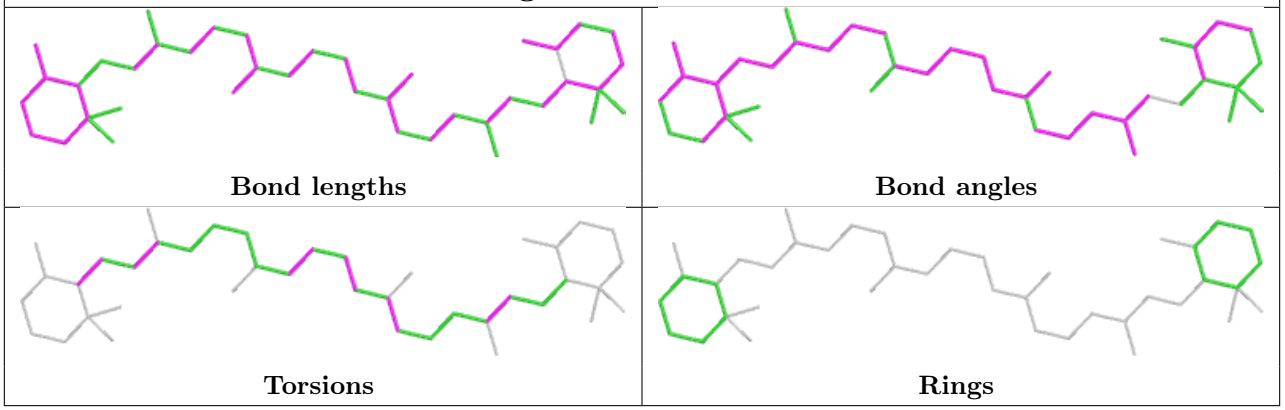


Rings

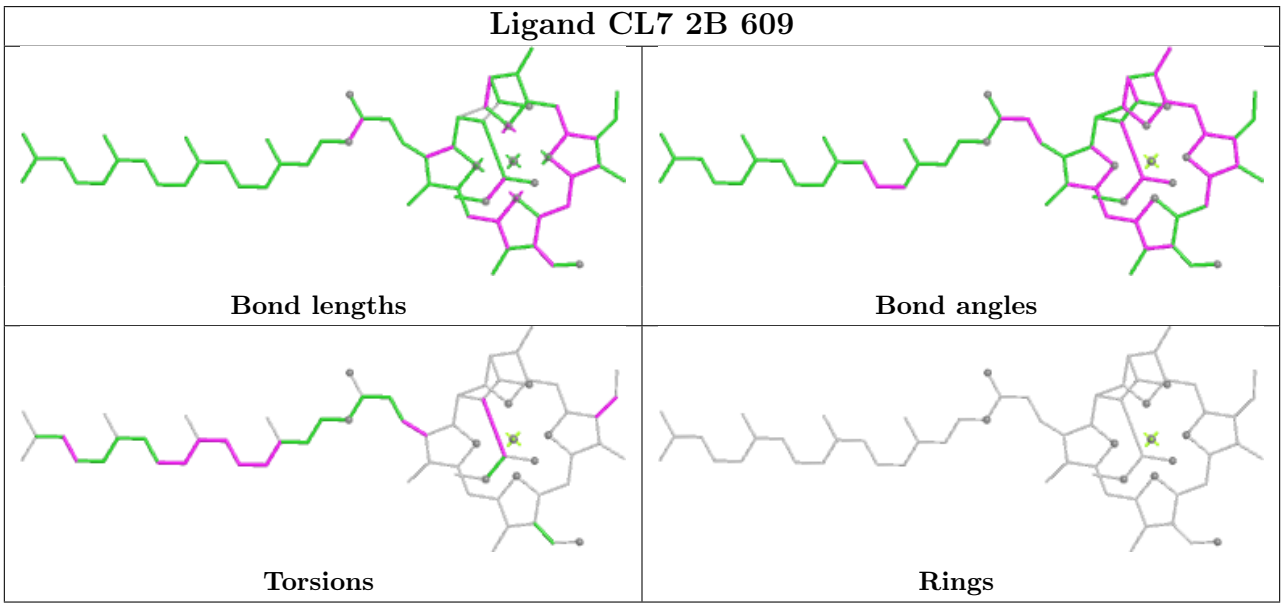
Ligand CL7 24 405



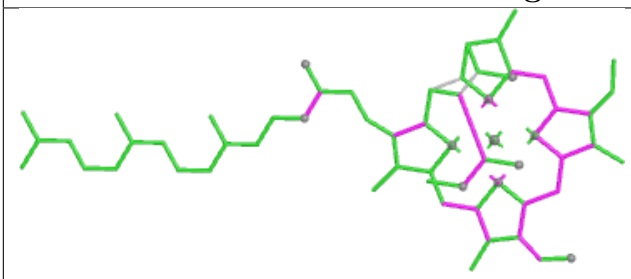
Ligand 8CT 4D 406



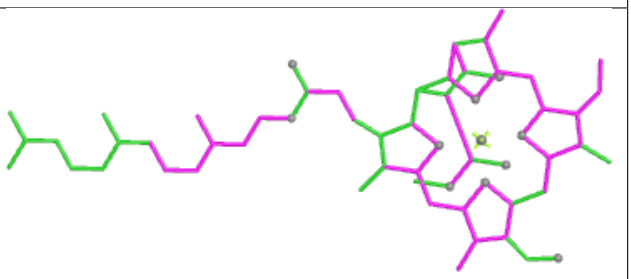
Ligand CL7 2B 609



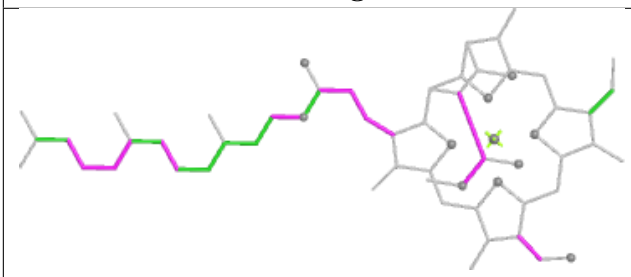
Ligand CL7 24 409



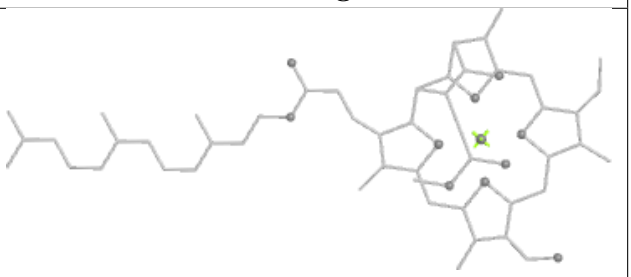
Bond lengths



Bond angles

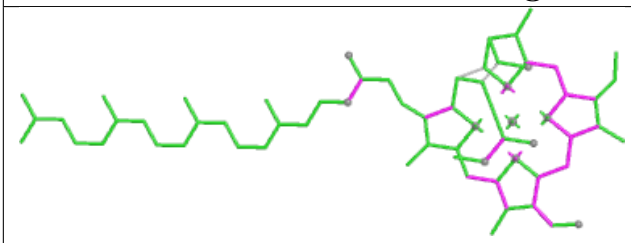


Torsions

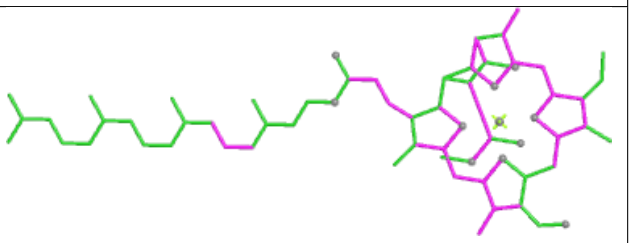


Rings

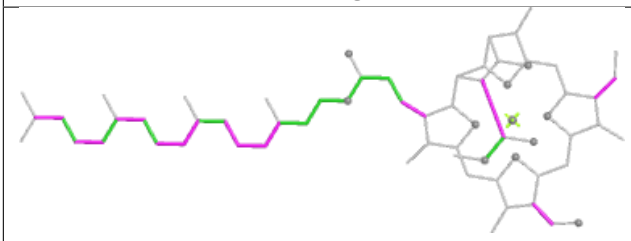
Ligand CL7 23 405



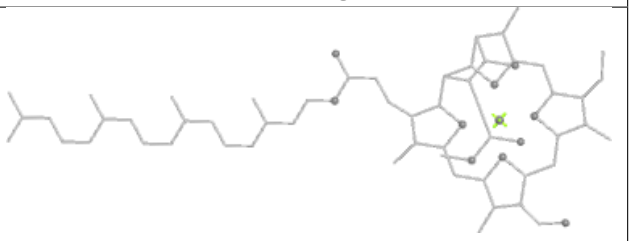
Bond lengths



Bond angles

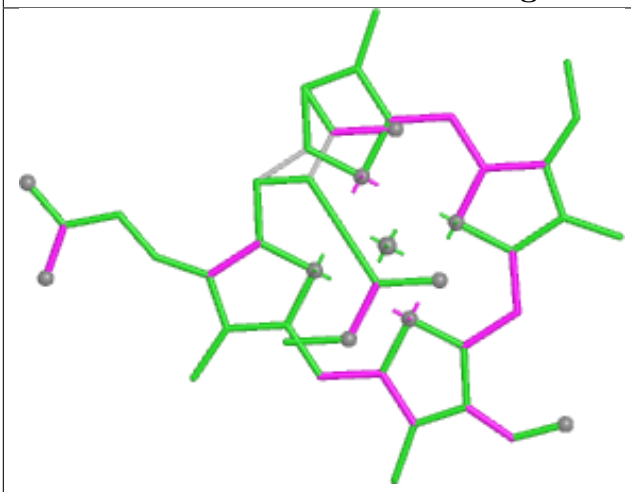


Torsions

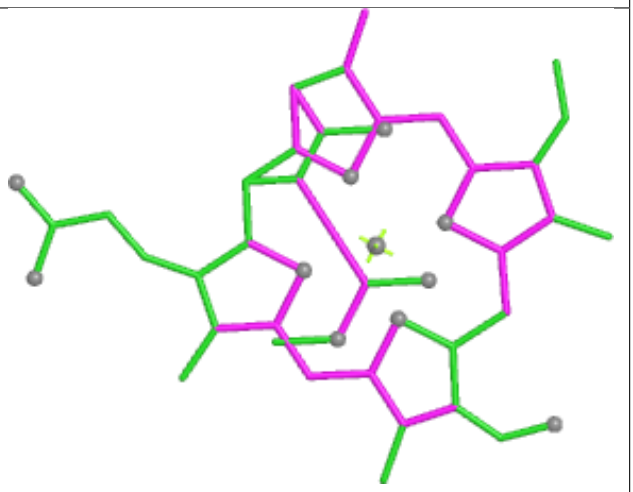


Rings

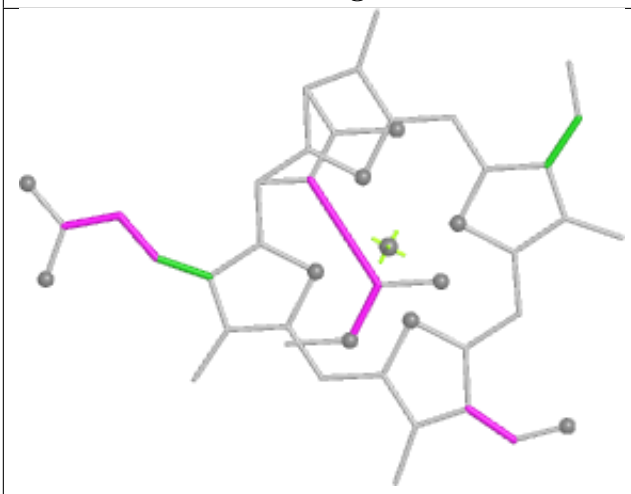
Ligand CL7 4B 623



Bond lengths



Bond angles

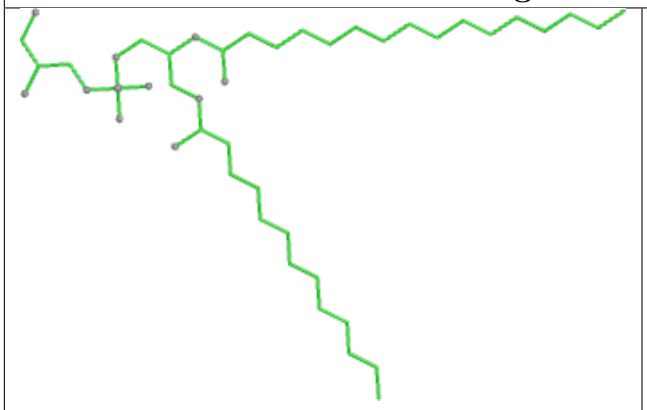


Torsions

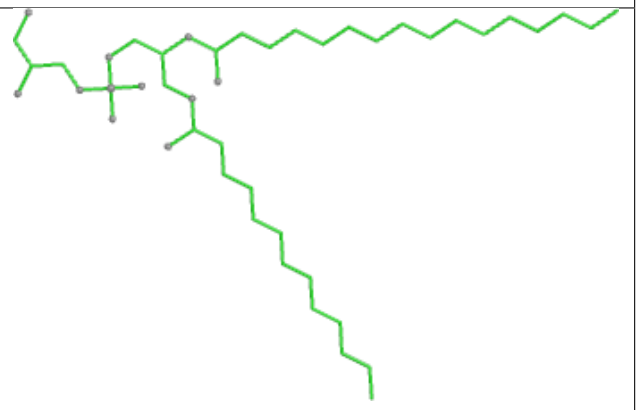


Rings

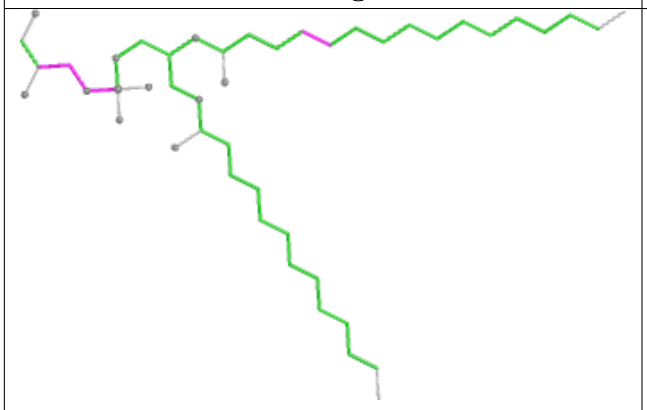
Ligand LHG 4A 408



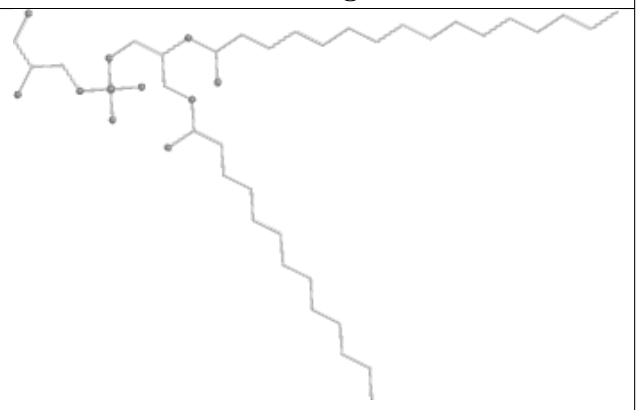
Bond lengths



Bond angles

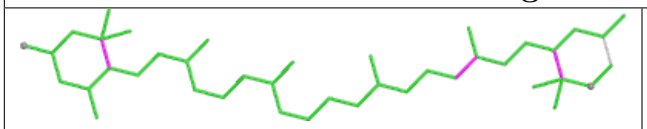


Torsions

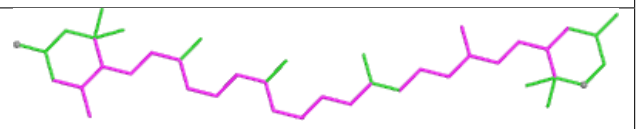


Rings

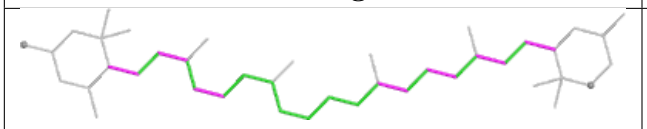
Ligand ZEX 42 524



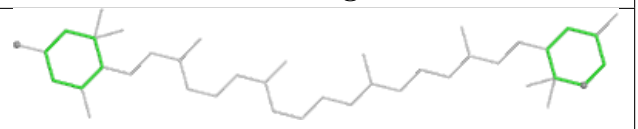
Bond lengths



Bond angles

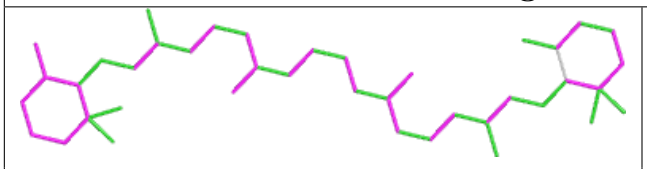


Torsions

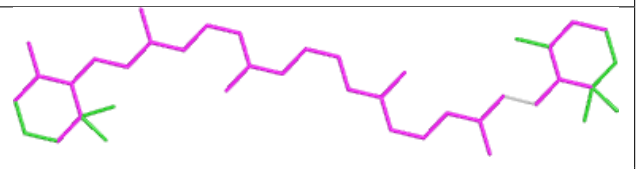


Rings

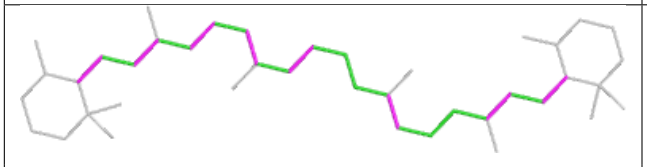
Ligand 8CT 4C 514



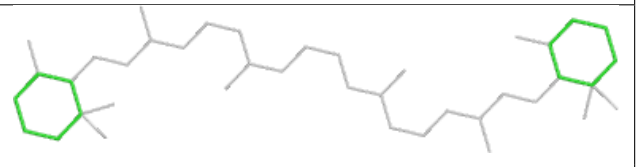
Bond lengths



Bond angles

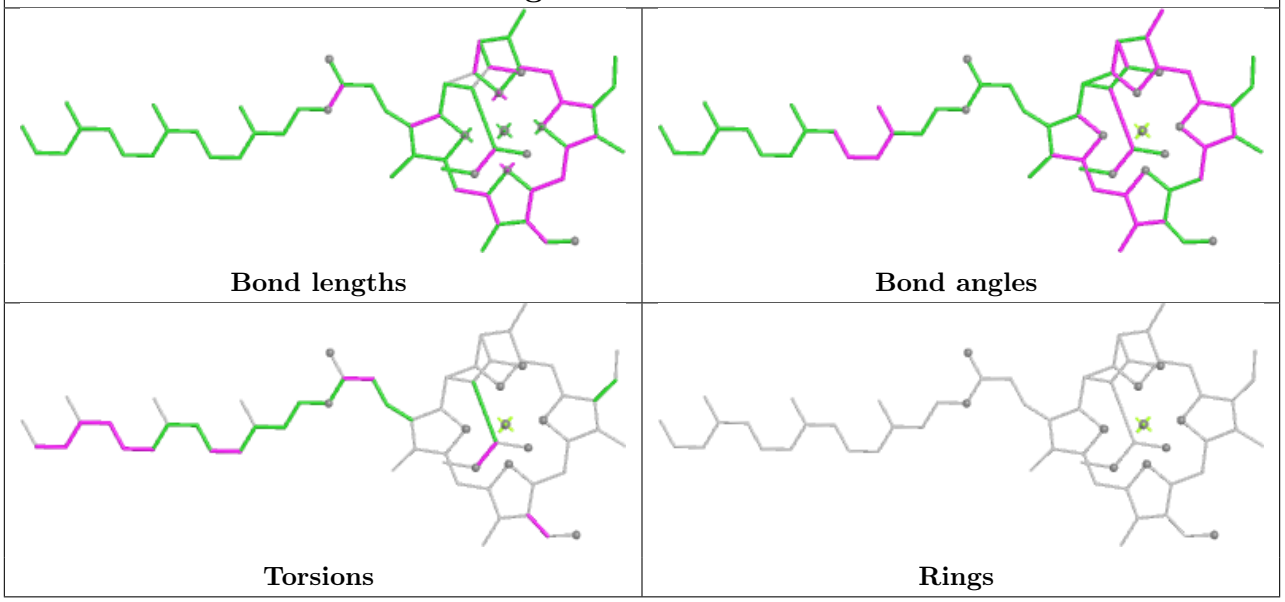


Torsions

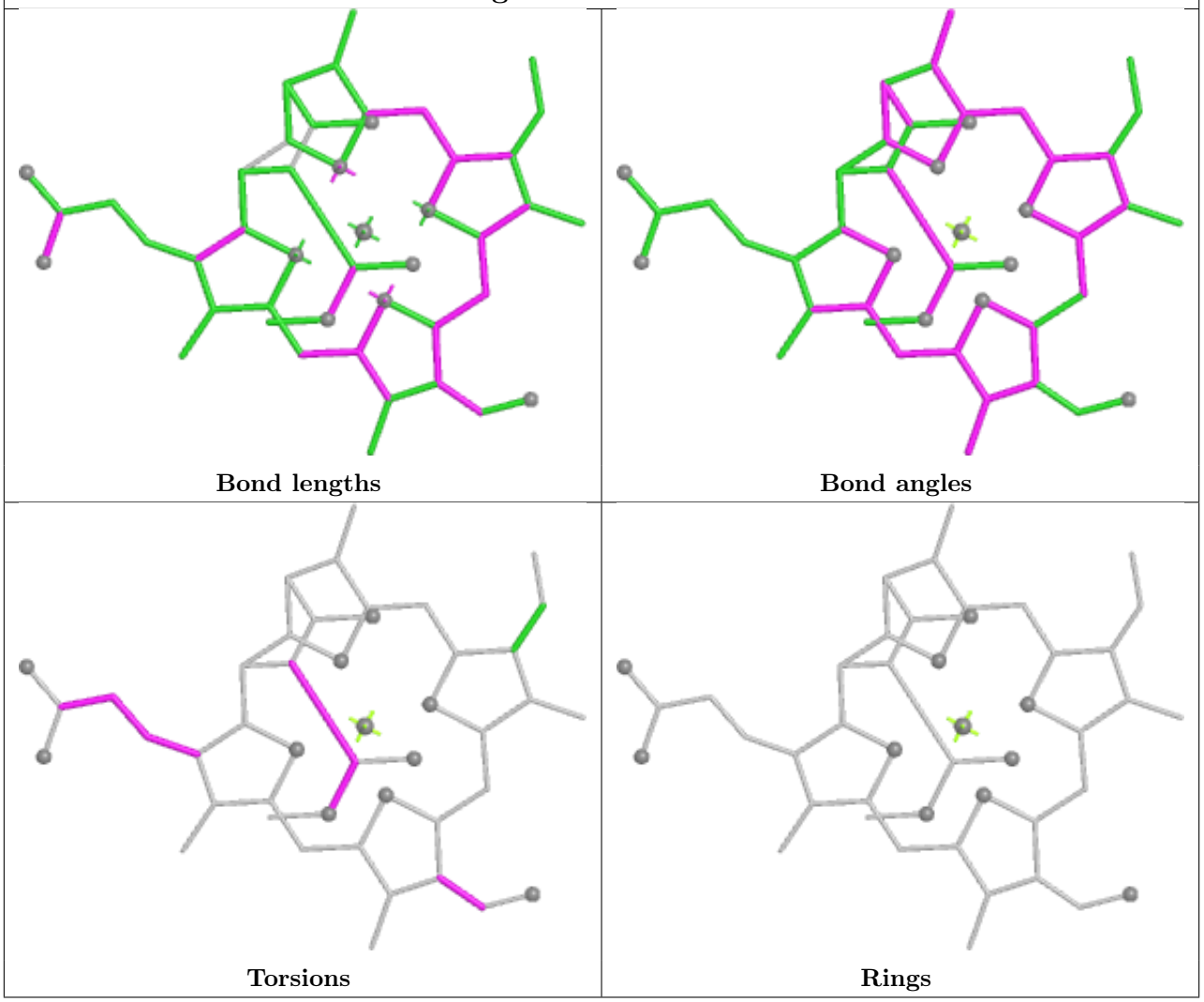


Rings

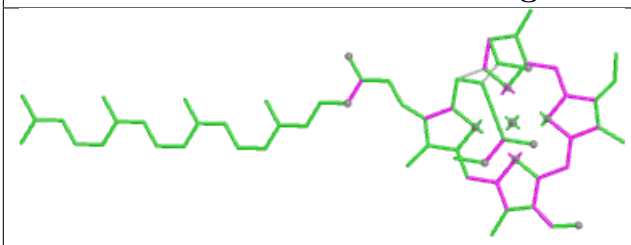
Ligand CL7 31 406



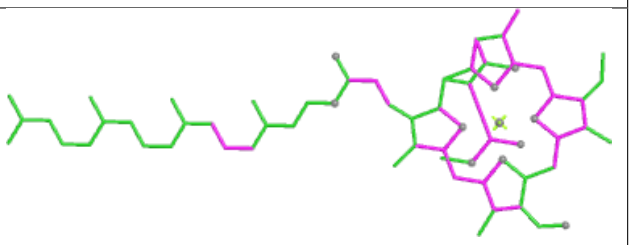
Ligand CL7 34 410



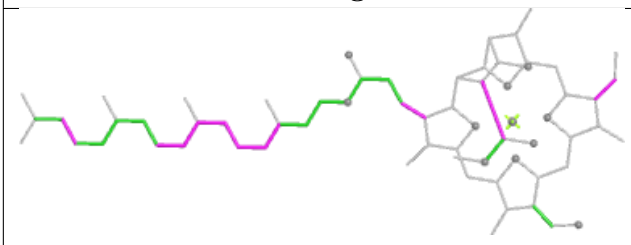
Ligand CL7 3B 608



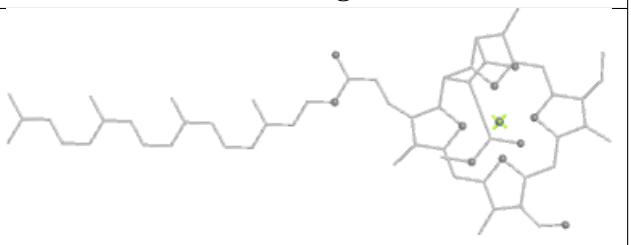
Bond lengths



Bond angles

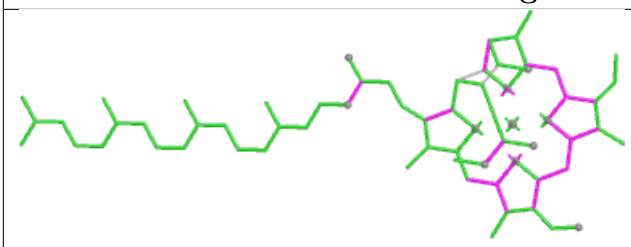


Torsions

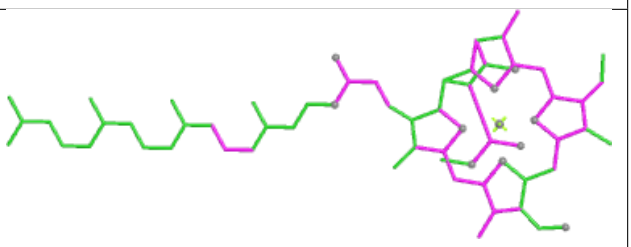


Rings

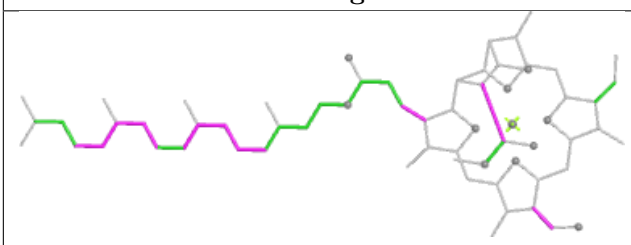
Ligand CL7 1B 612



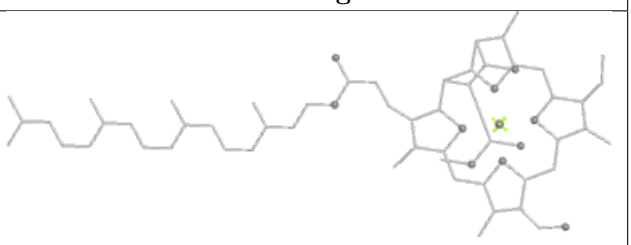
Bond lengths



Bond angles

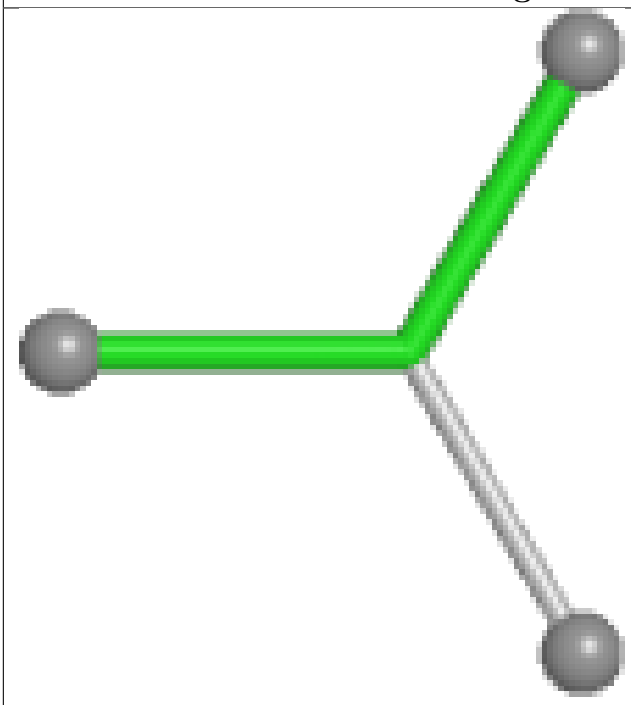


Torsions

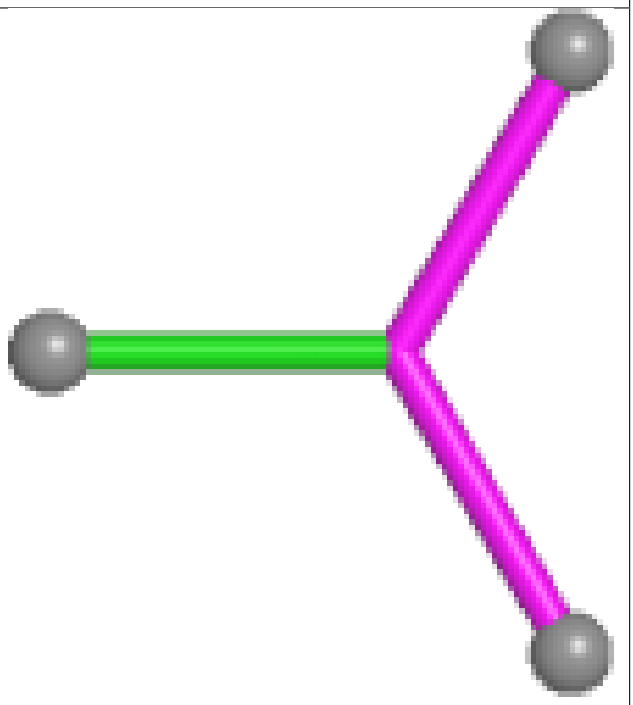


Rings

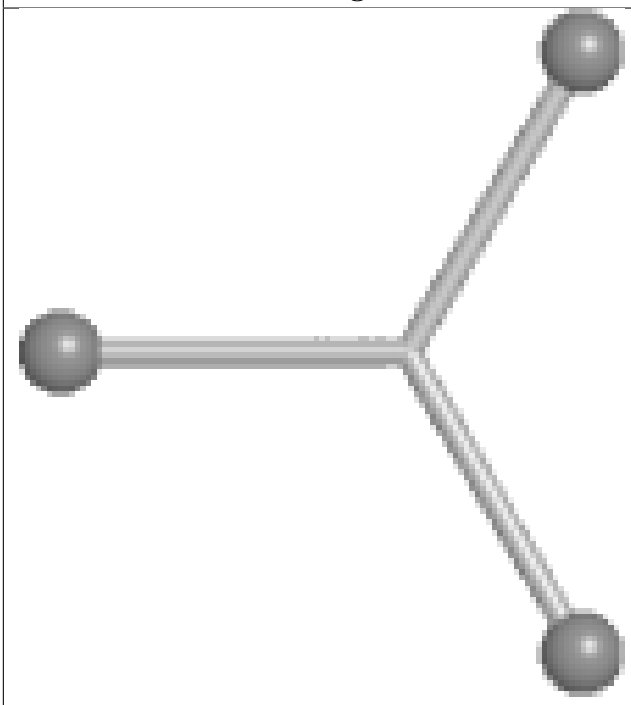
Ligand BCT 4D 403



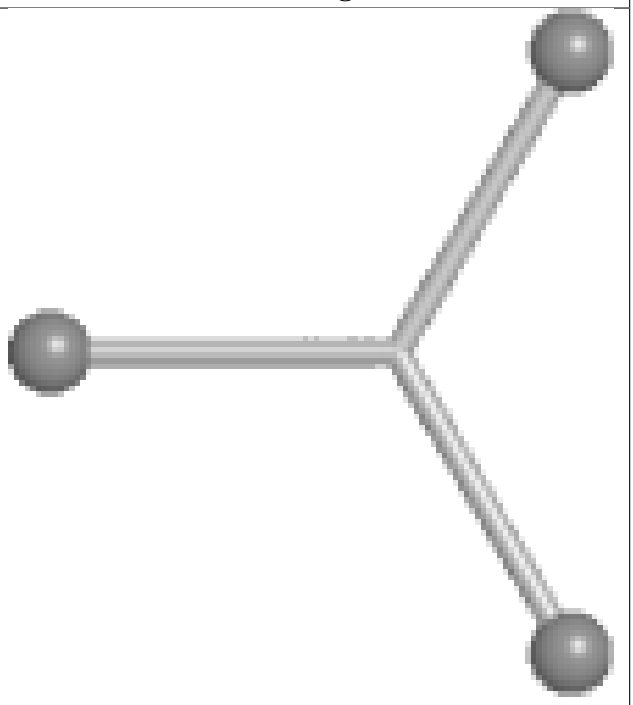
Bond lengths



Bond angles

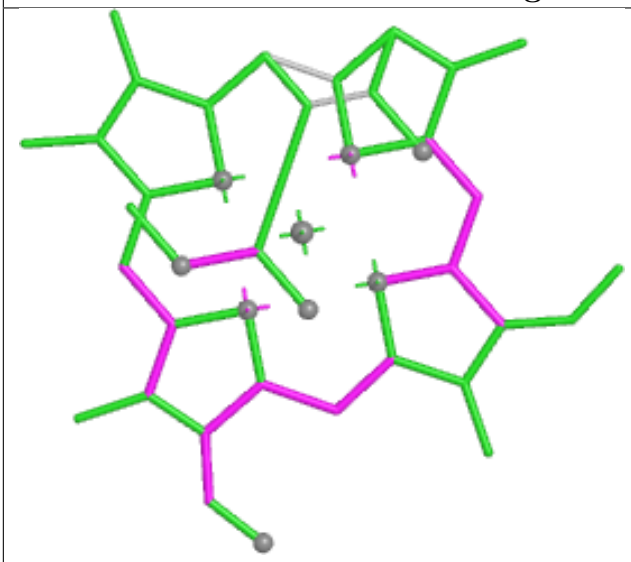


Torsions

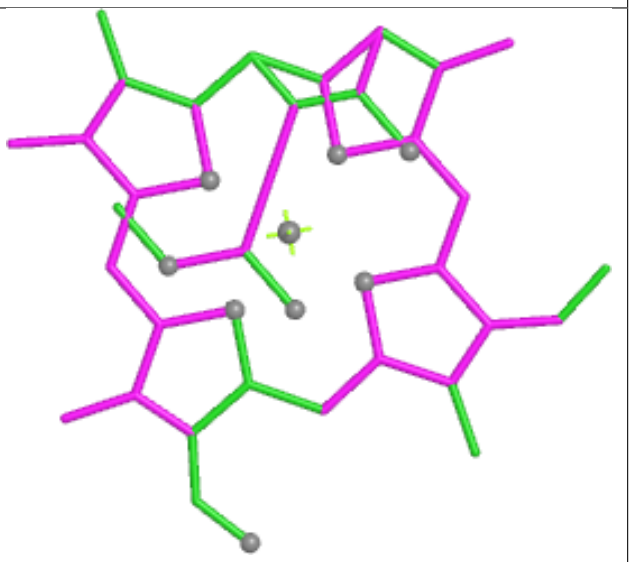


Rings

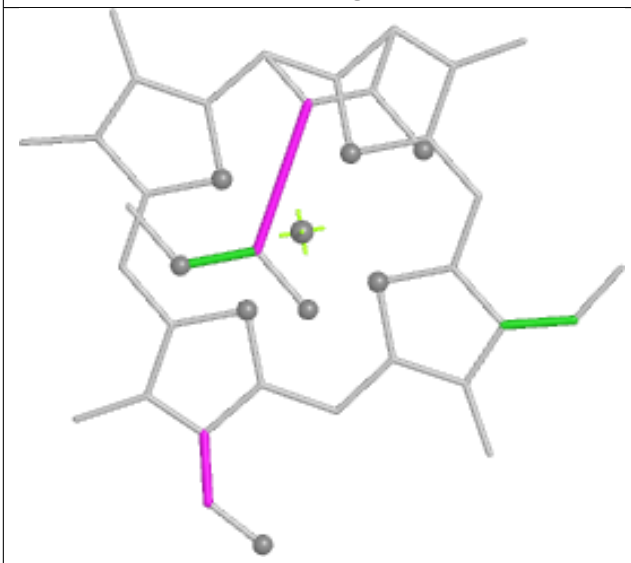
Ligand CL7 24 407



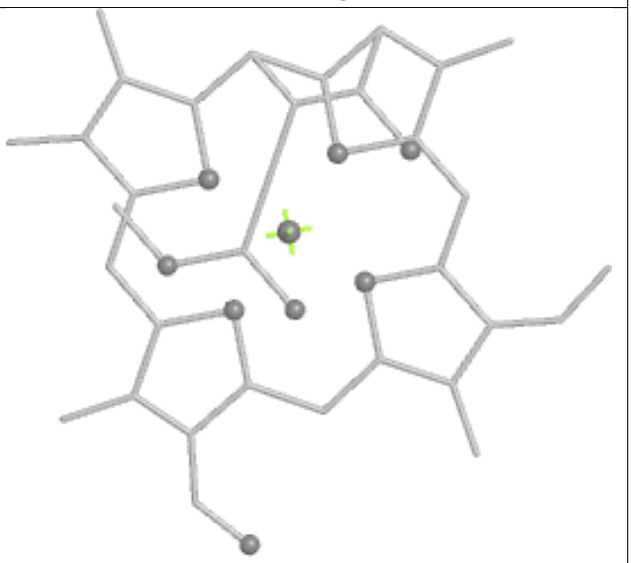
Bond lengths



Bond angles

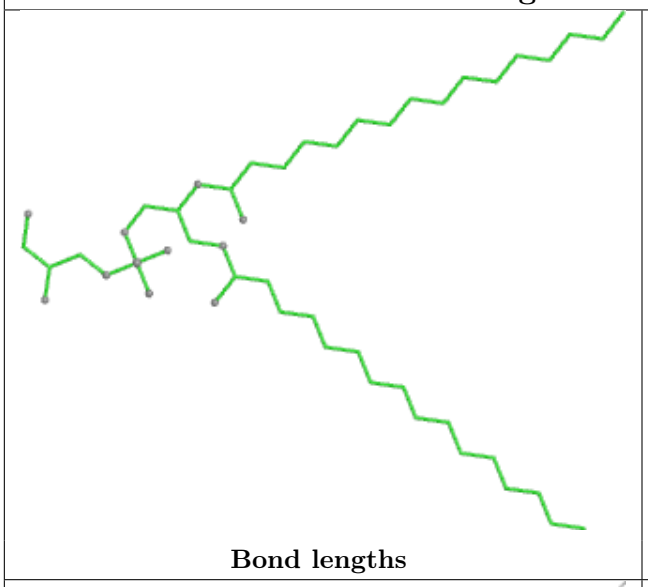


Torsions

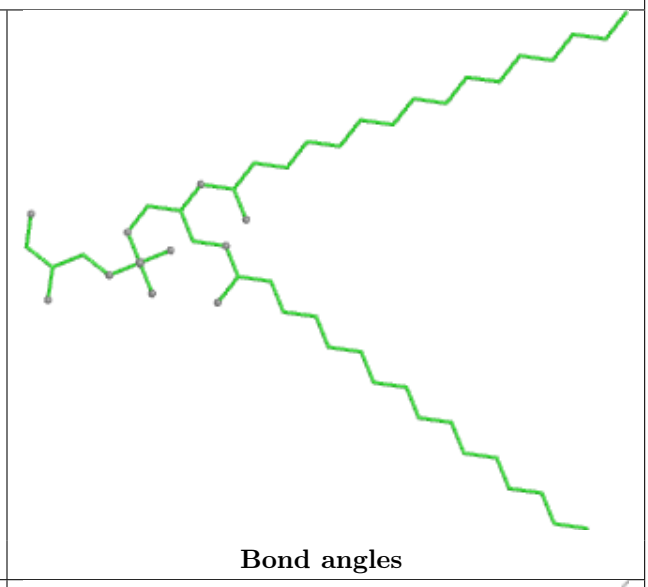


Rings

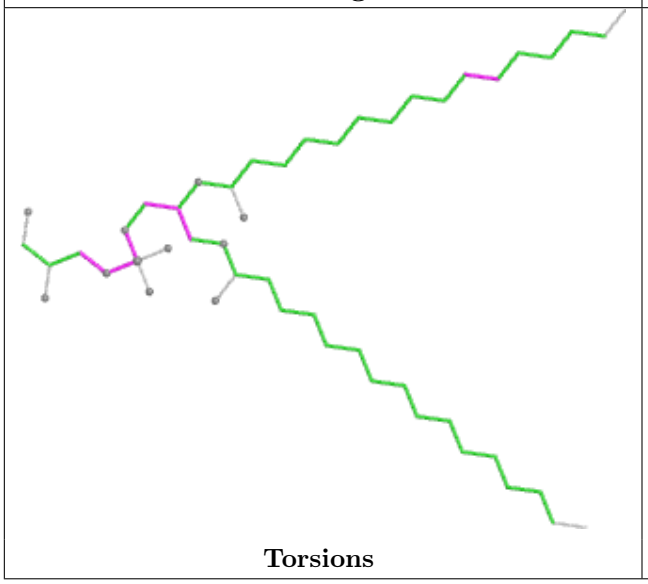
Ligand LHG 24 401



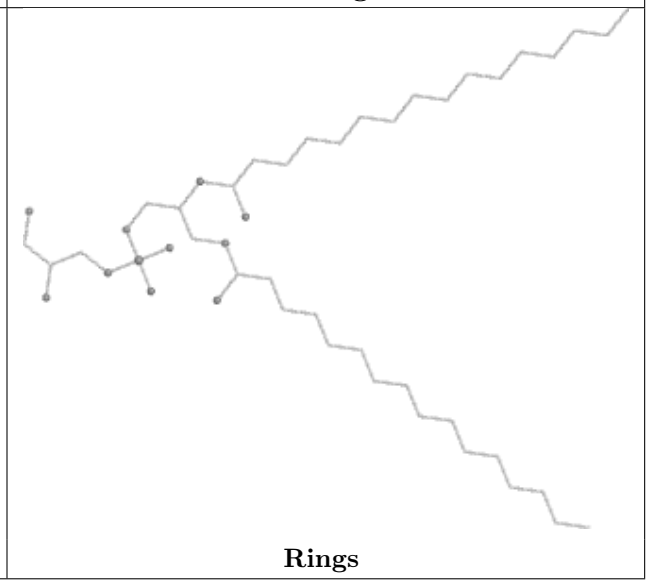
Bond lengths



Bond angles

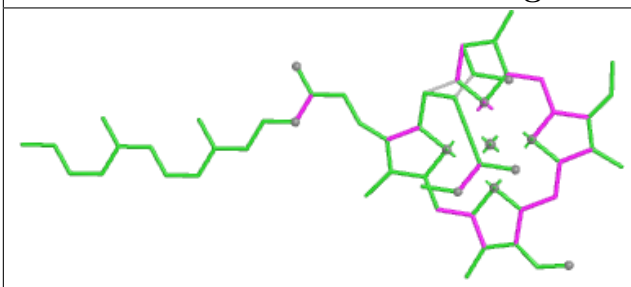


Torsions

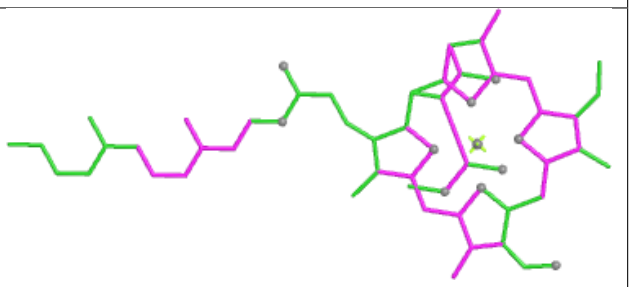


Rings

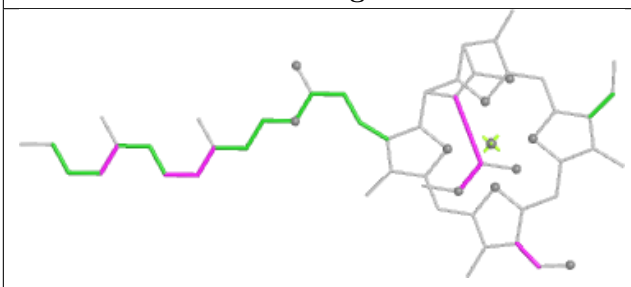
Ligand CL7 13 502



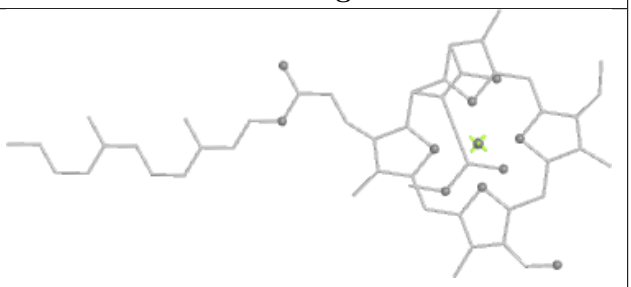
Bond lengths



Bond angles

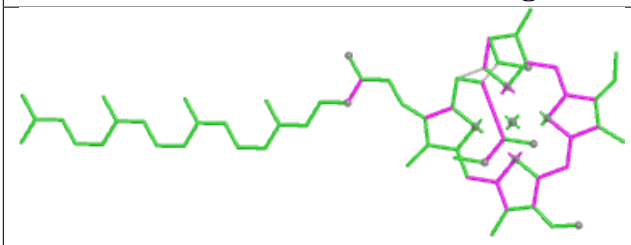


Torsions

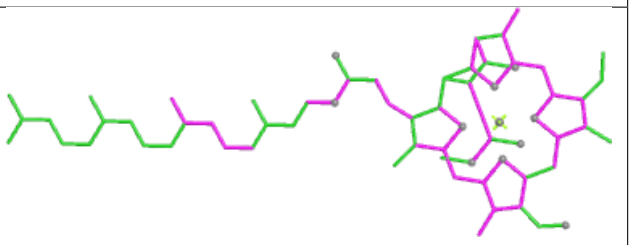


Rings

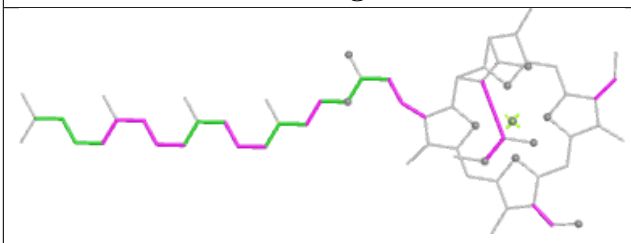
Ligand CL7 4C 505



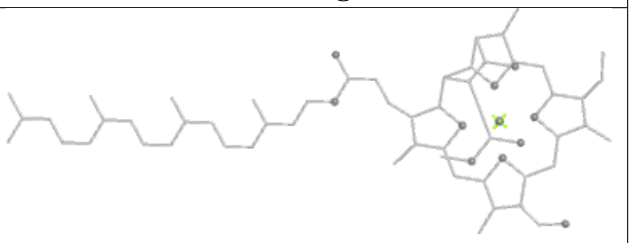
Bond lengths



Bond angles

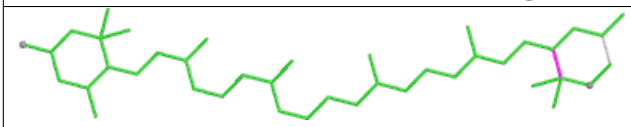


Torsions

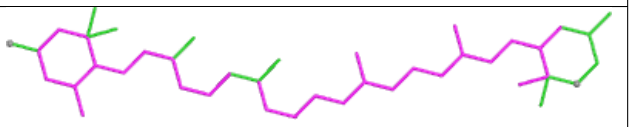


Rings

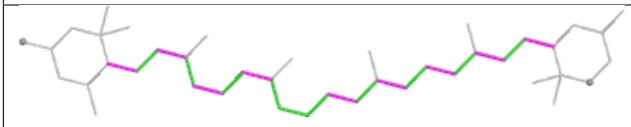
Ligand ZEX 11 421



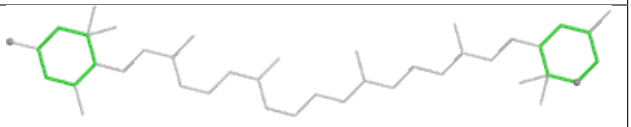
Bond lengths



Bond angles

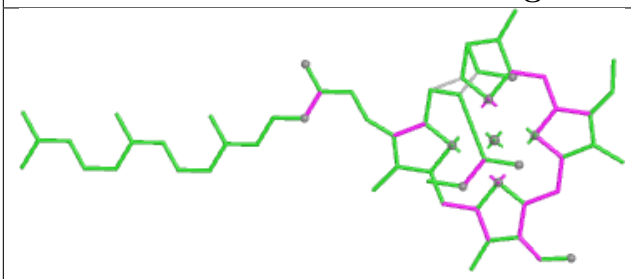


Torsions

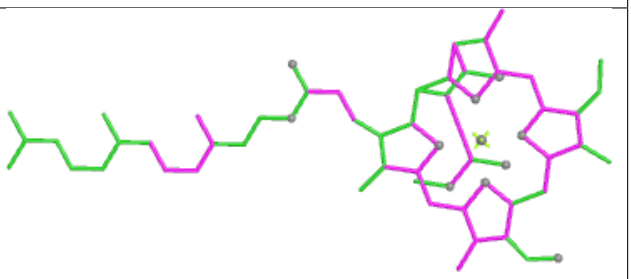


Rings

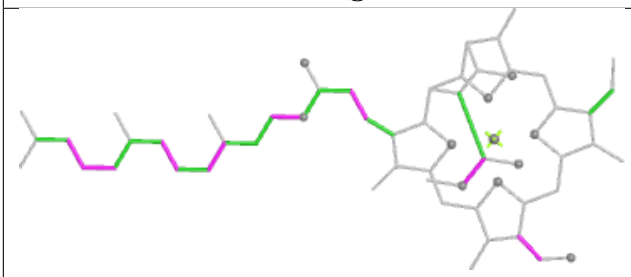
Ligand CL7 11 403



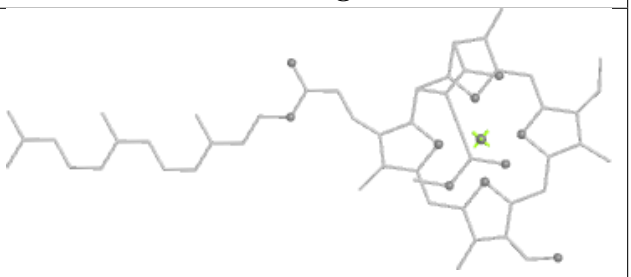
Bond lengths



Bond angles

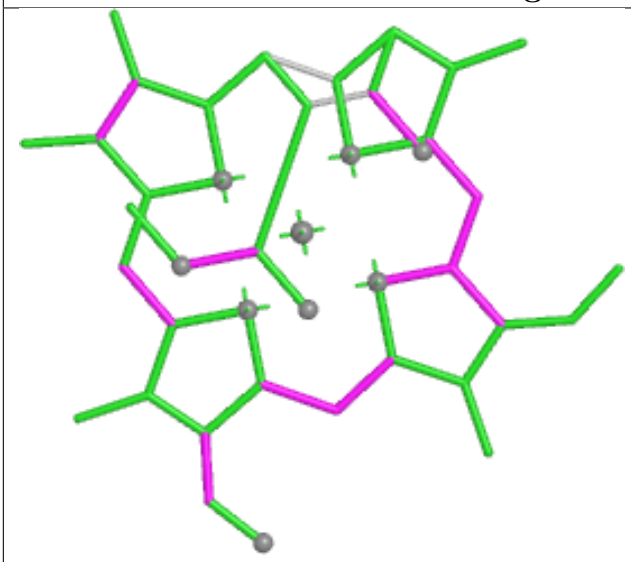


Torsions

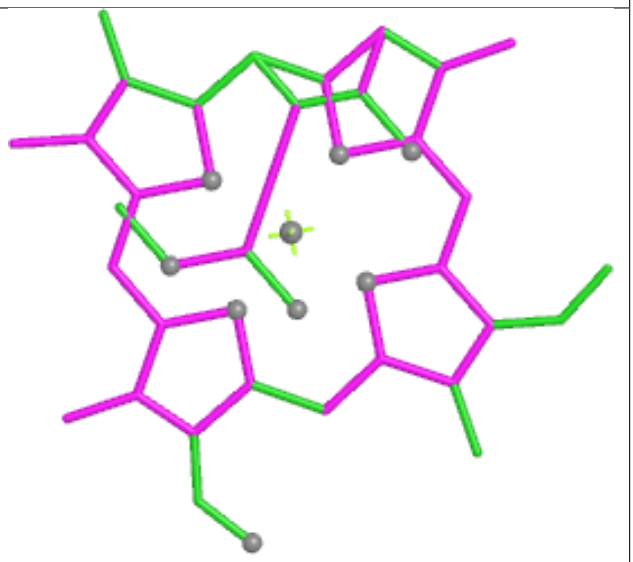


Rings

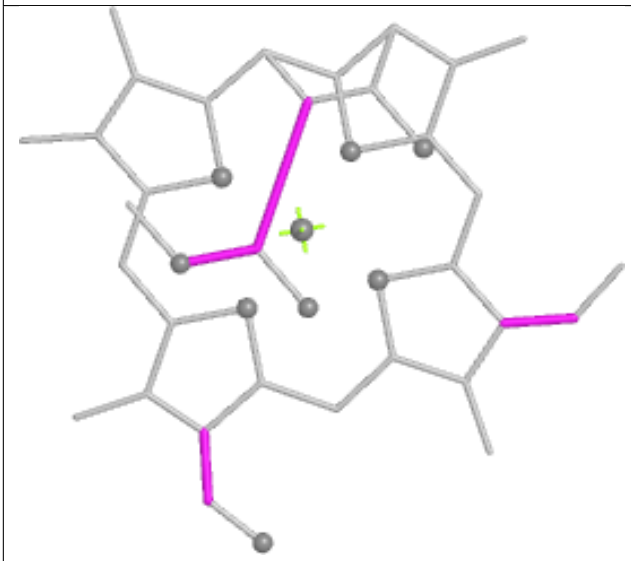
Ligand CL7 11 415



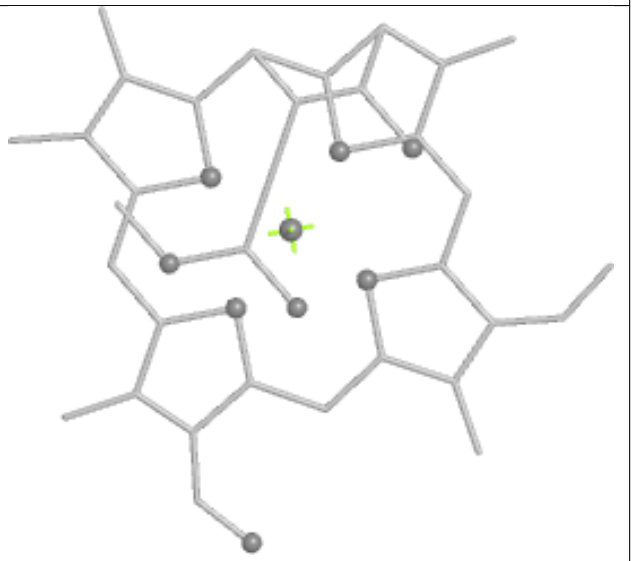
Bond lengths



Bond angles

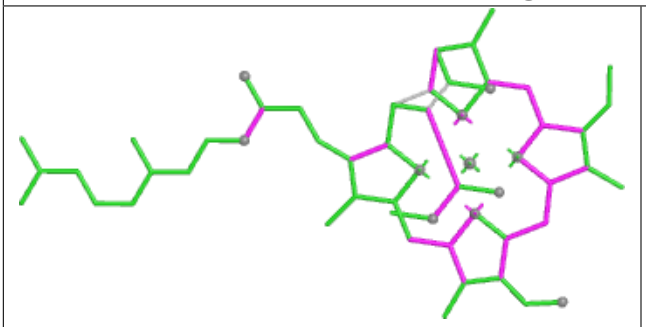


Torsions

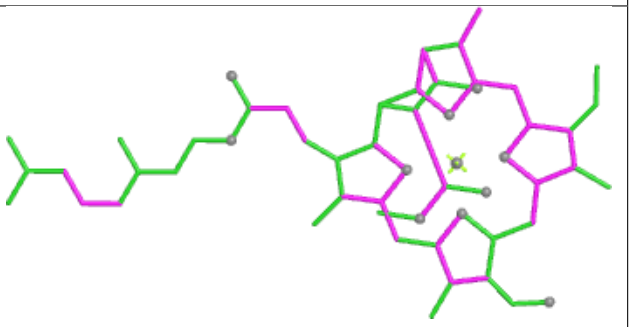


Rings

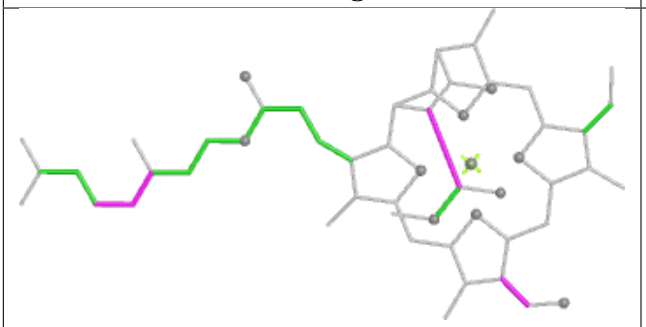
Ligand CL7 2B 614



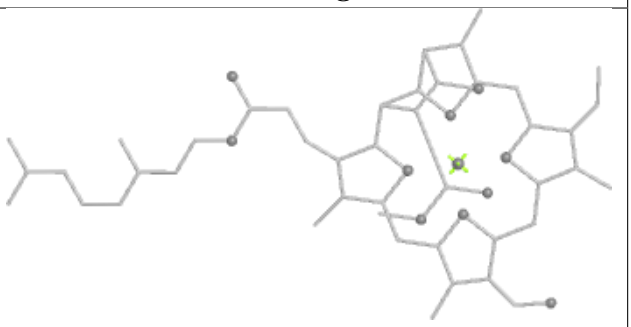
Bond lengths



Bond angles

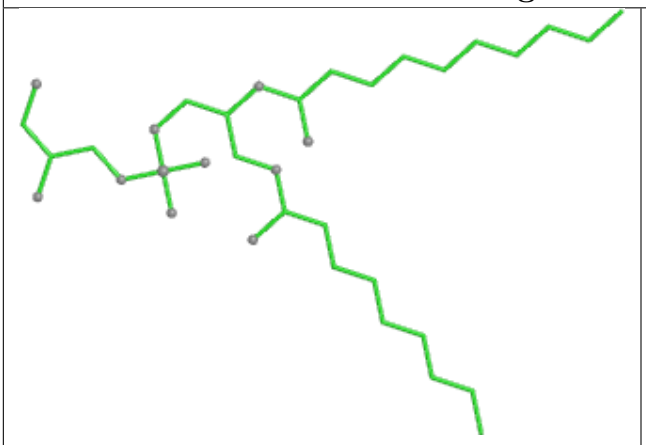


Torsions

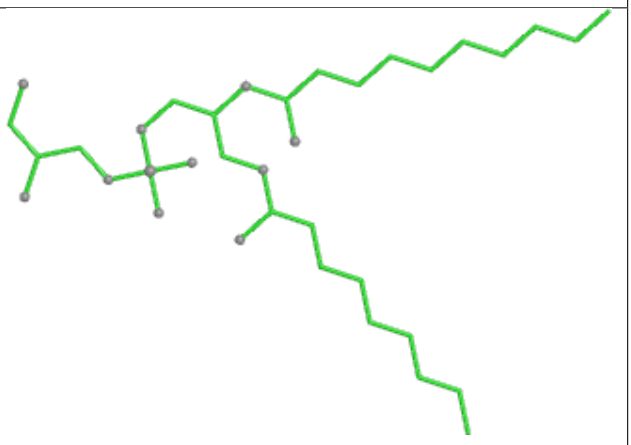


Rings

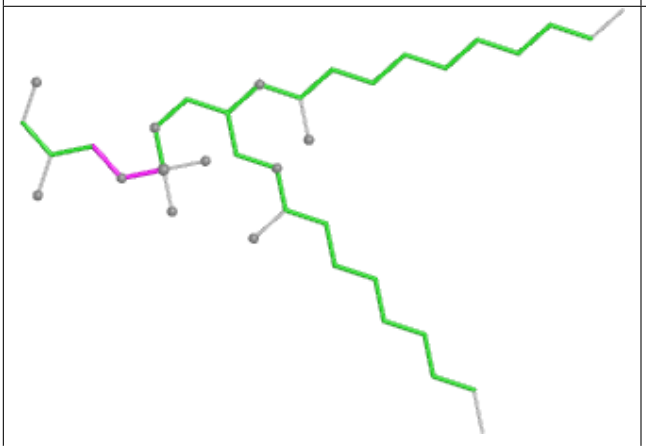
Ligand LHG 13 524



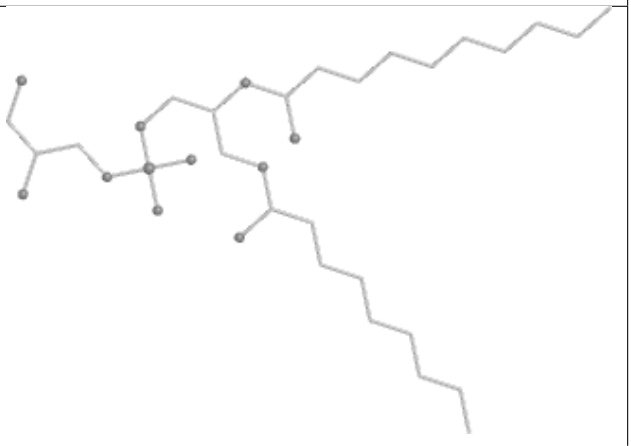
Bond lengths



Bond angles

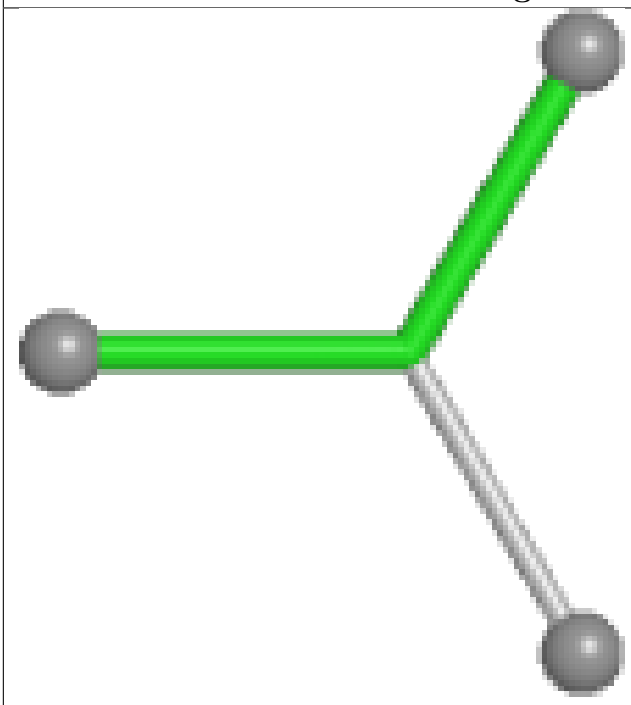


Torsions

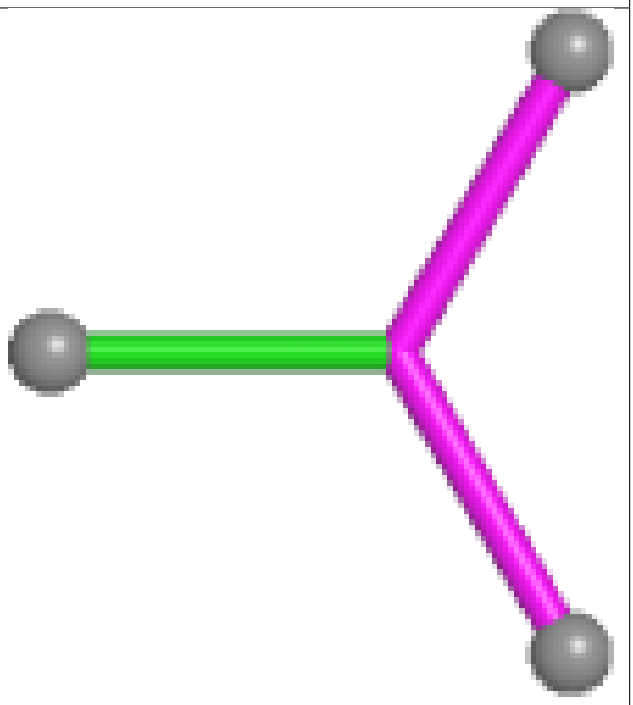


Rings

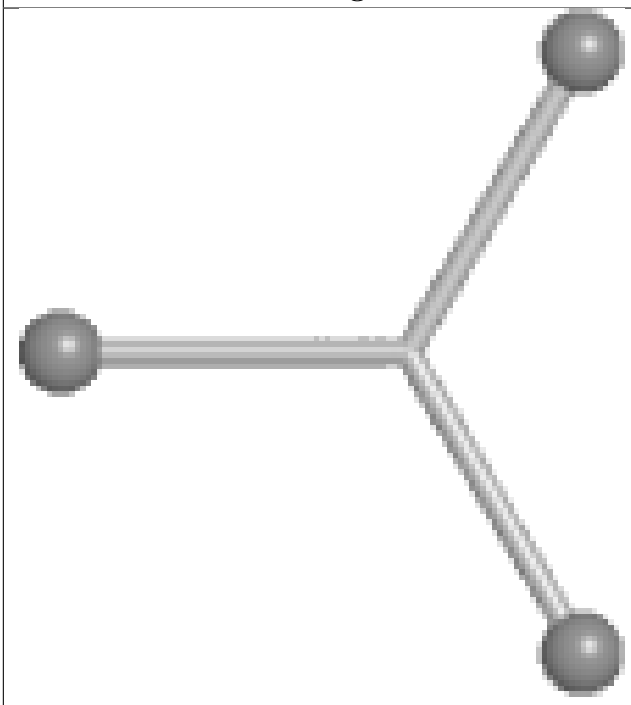
Ligand BCT 1D 403



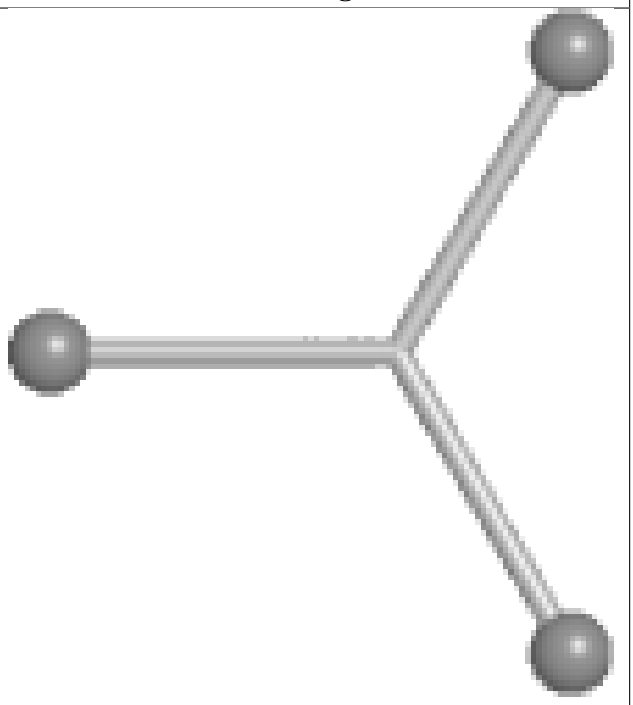
Bond lengths



Bond angles

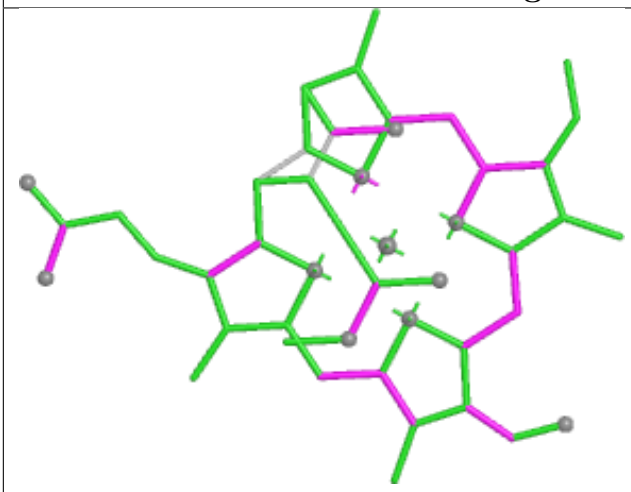


Torsions

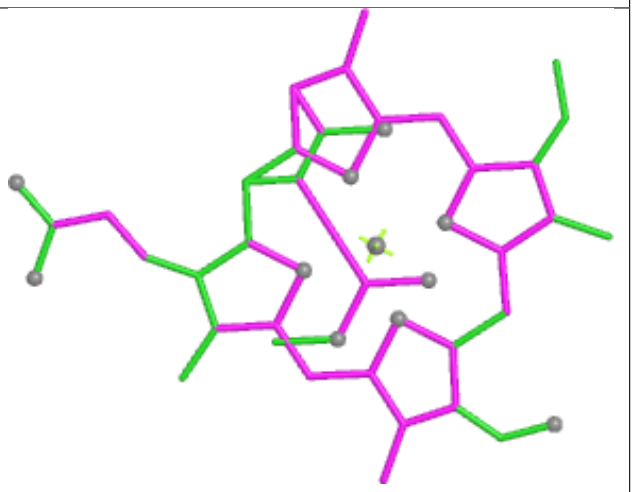


Rings

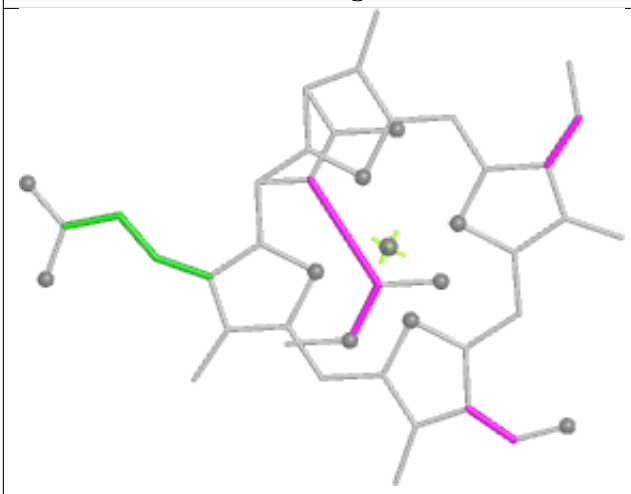
Ligand CL7 21 420



Bond lengths



Bond angles

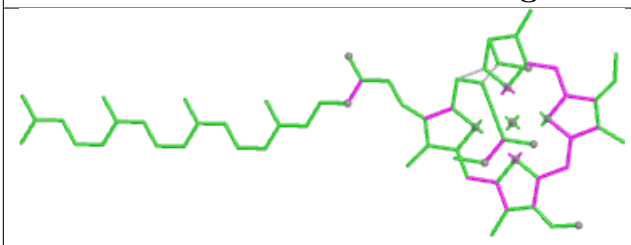


Torsions

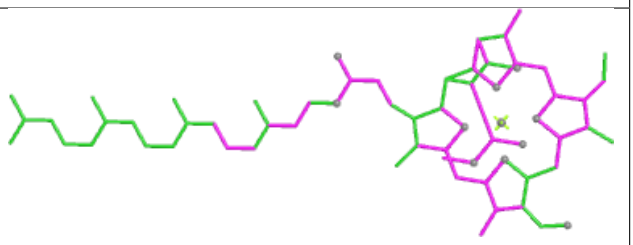


Rings

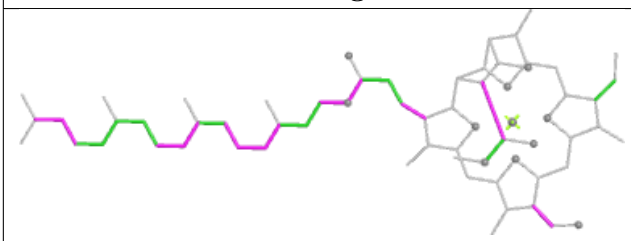
Ligand CL7 4C 508



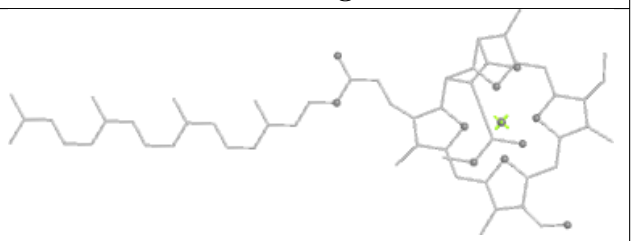
Bond lengths



Bond angles

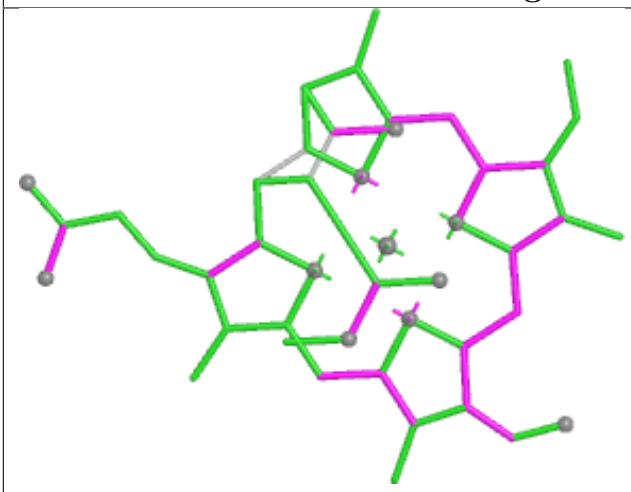


Torsions

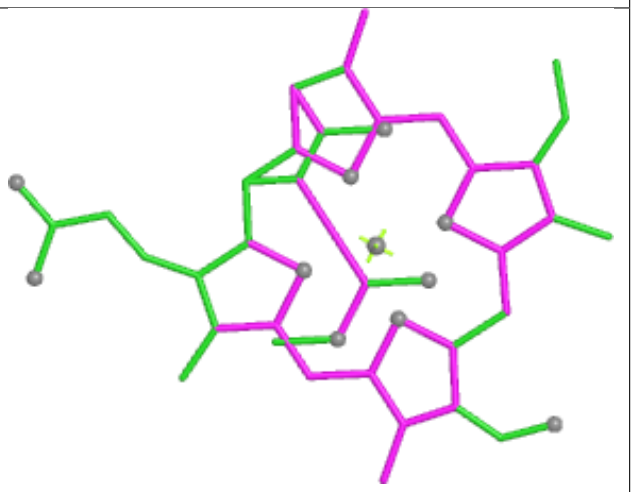


Rings

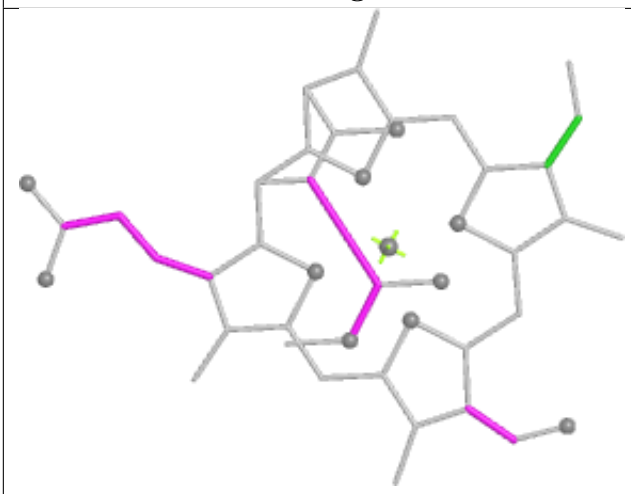
Ligand CL7 11 405



Bond lengths



Bond angles

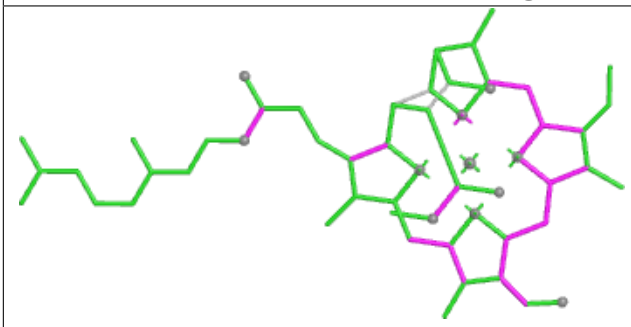


Torsions

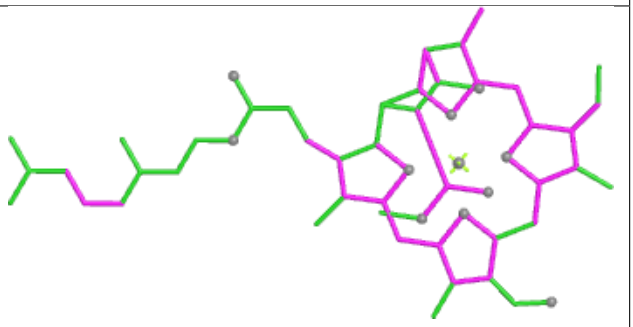


Rings

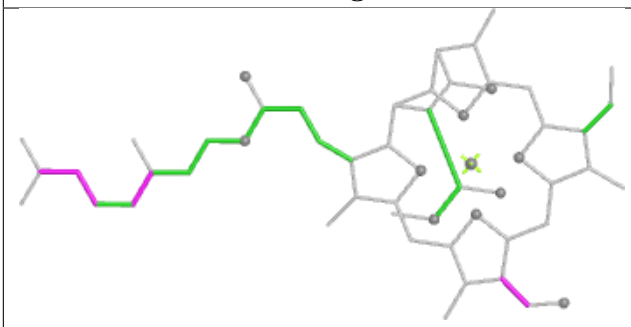
Ligand CL7 4B 607



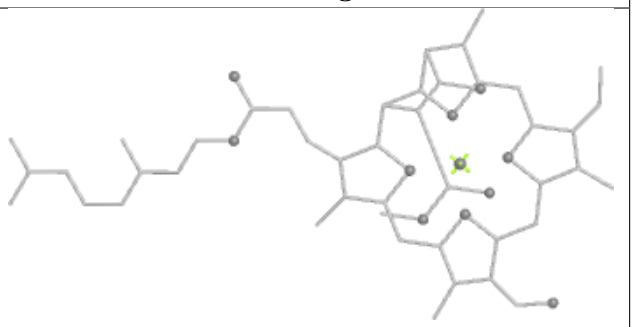
Bond lengths



Bond angles

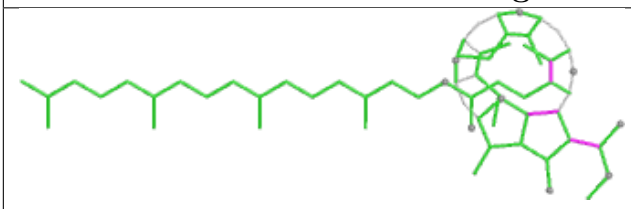


Torsions

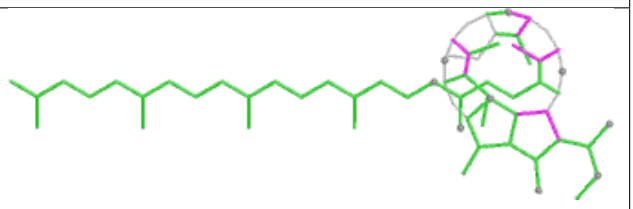


Rings

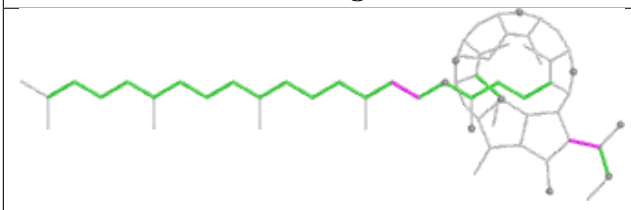
Ligand PHO 3A 402



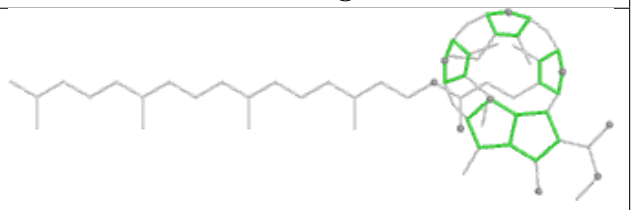
Bond lengths



Bond angles

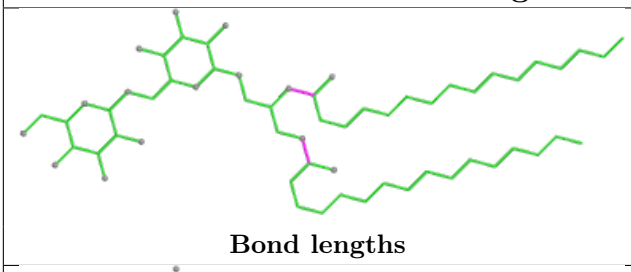


Torsions

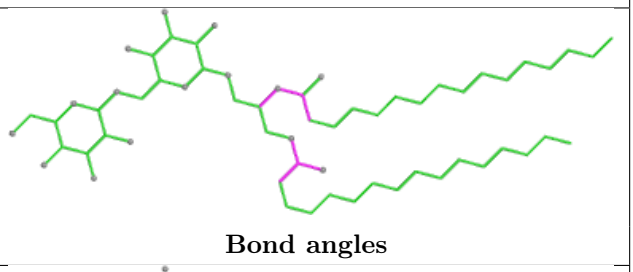


Rings

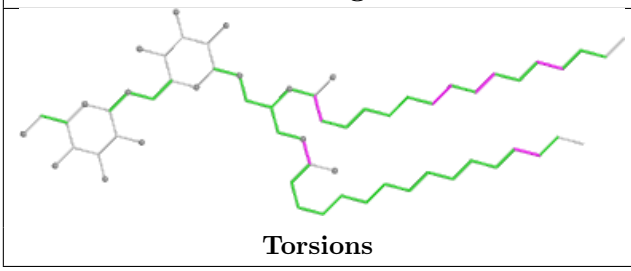
Ligand DGD 2B 625



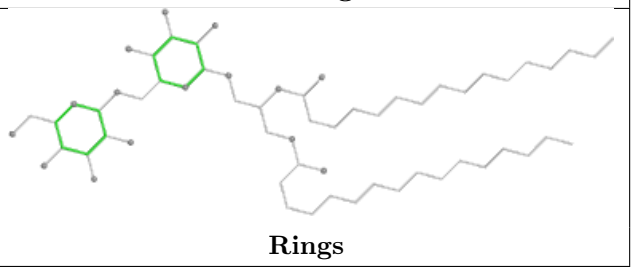
Bond lengths



Bond angles

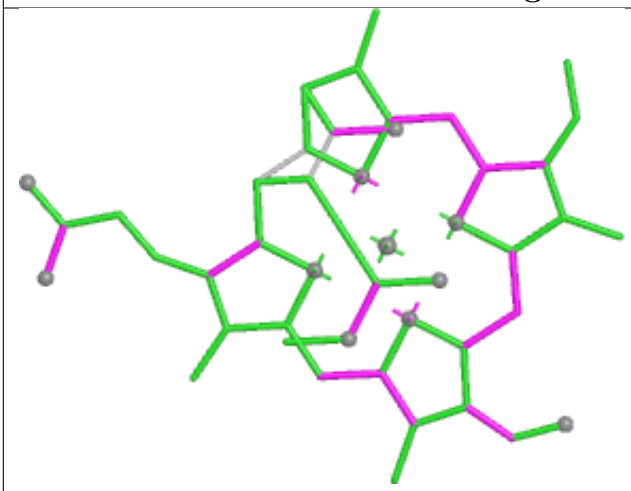


Torsions

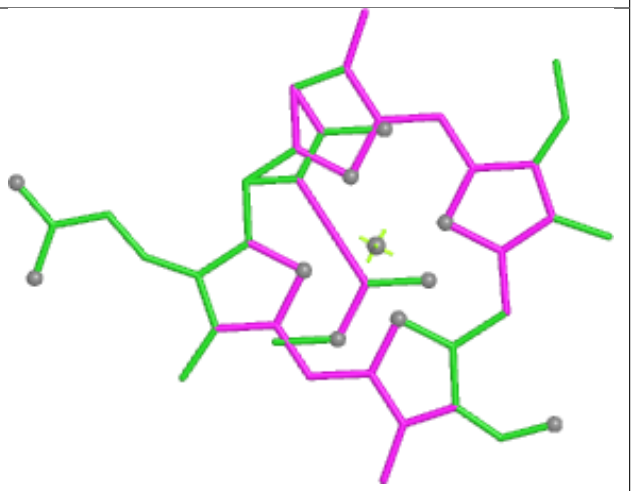


Rings

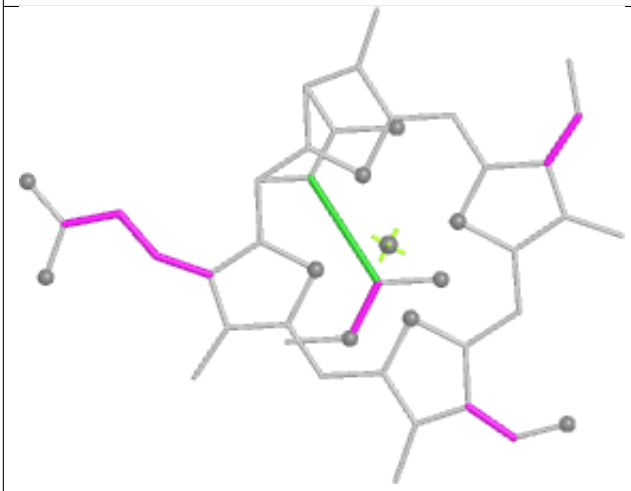
Ligand CL7 21 419



Bond lengths



Bond angles

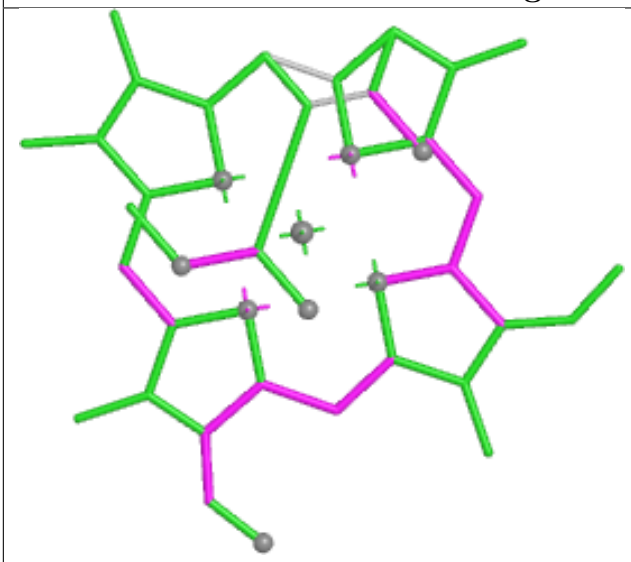


Torsions

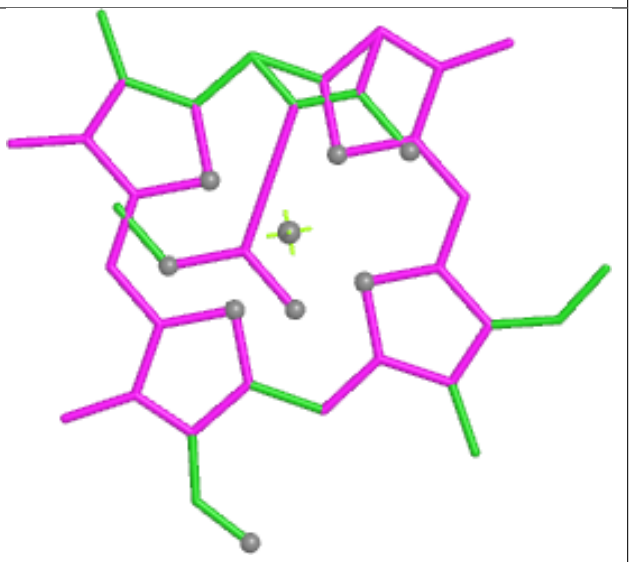


Rings

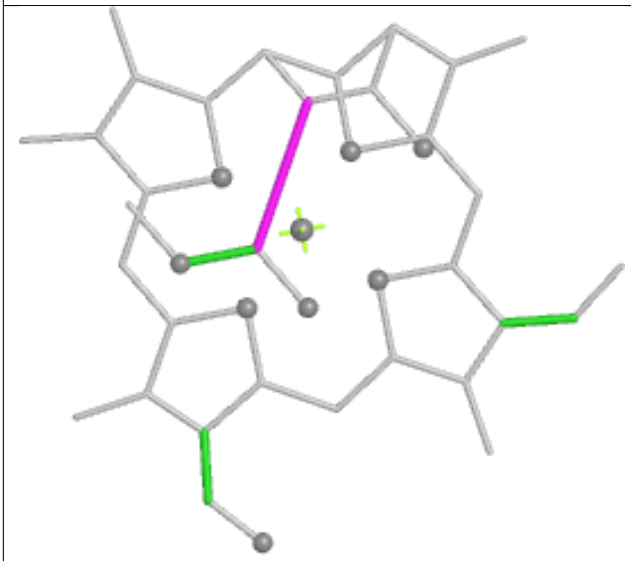
Ligand CL7 21 413



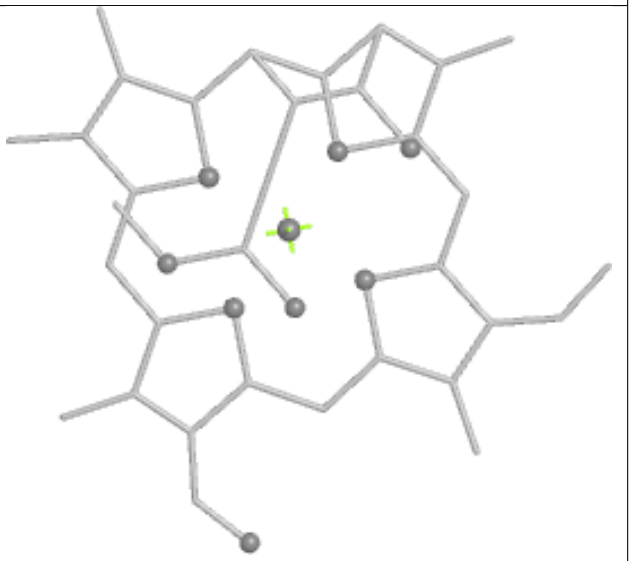
Bond lengths



Bond angles

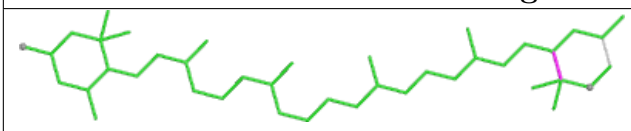


Torsions

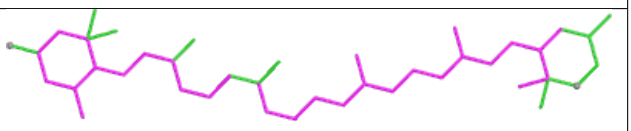


Rings

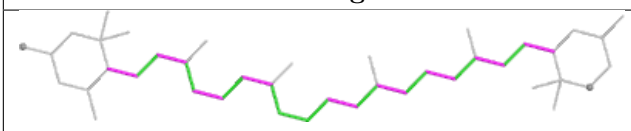
Ligand ZEX 31 421



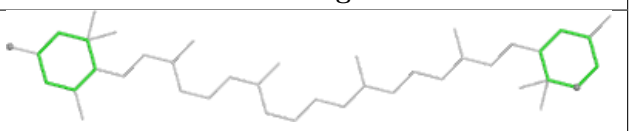
Bond lengths



Bond angles

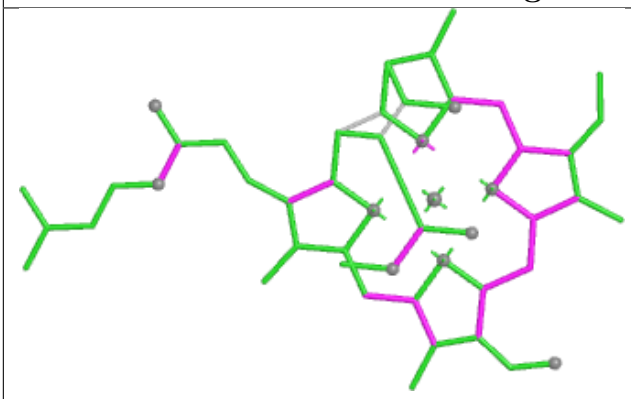


Torsions

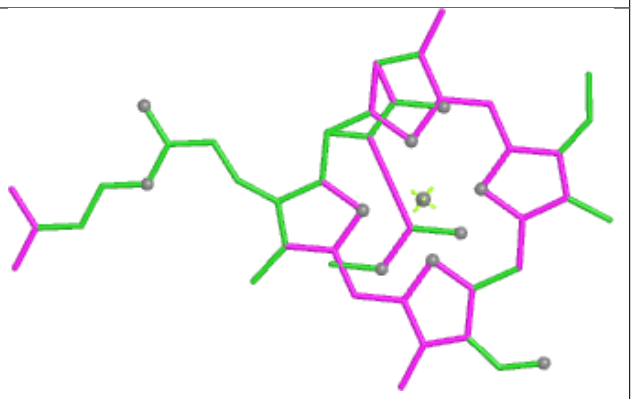


Rings

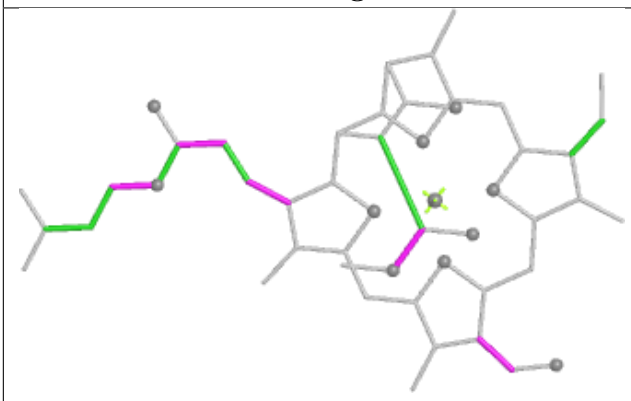
Ligand CL7 33 517



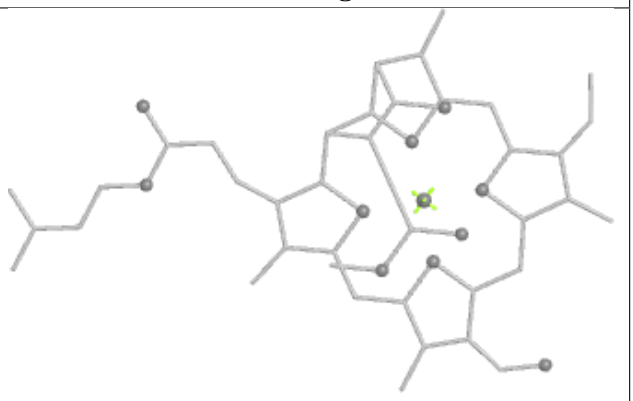
Bond lengths



Bond angles

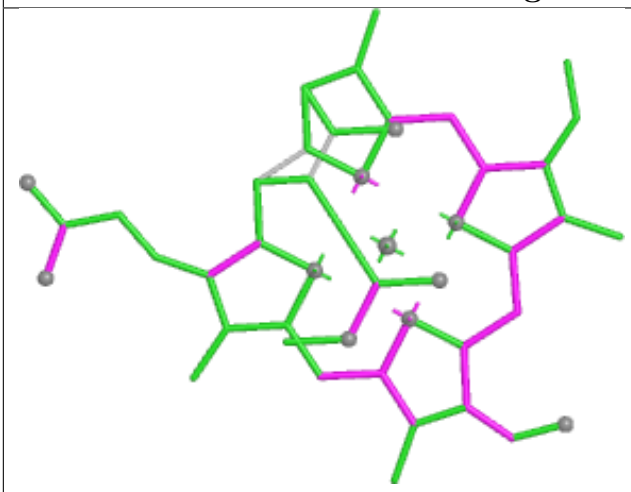


Torsions

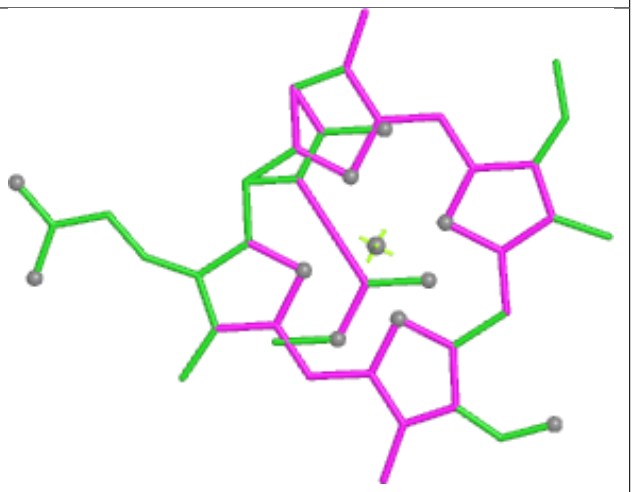


Rings

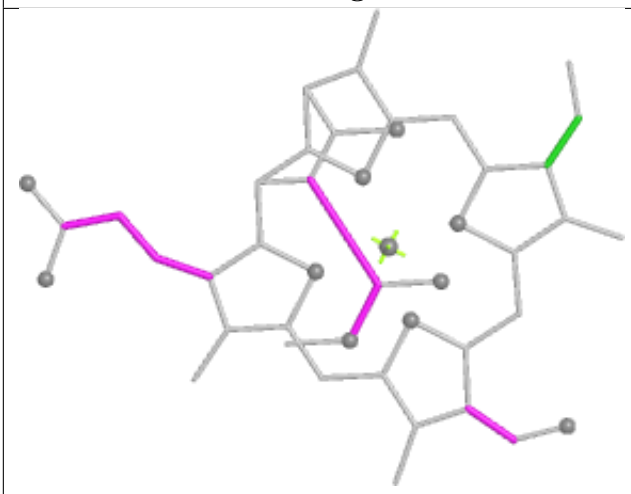
Ligand CL7 41 405



Bond lengths



Bond angles

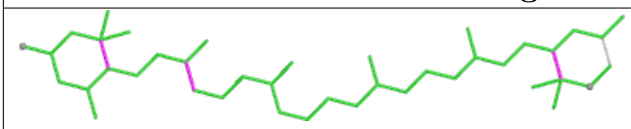


Torsions

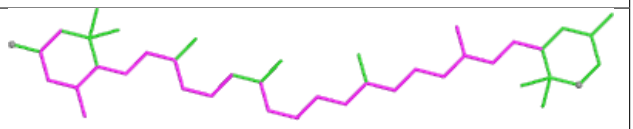


Rings

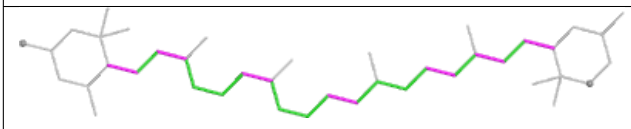
Ligand ZEX 32 519



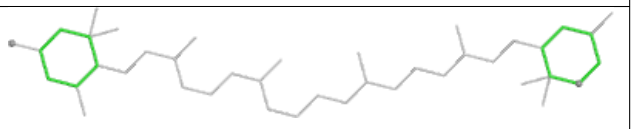
Bond lengths



Bond angles

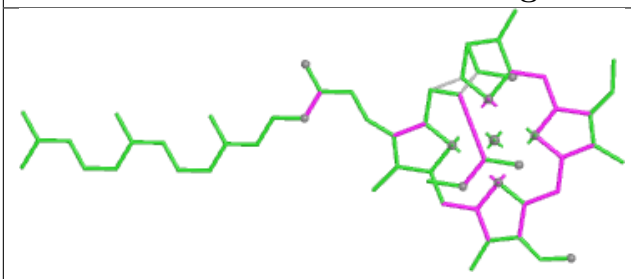


Torsions

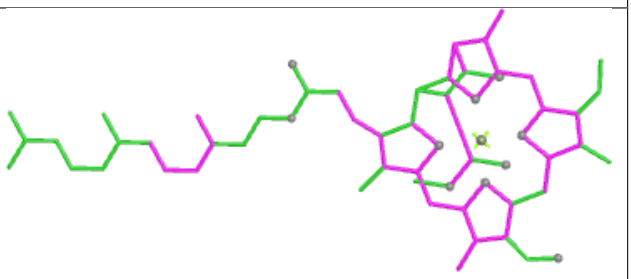


Rings

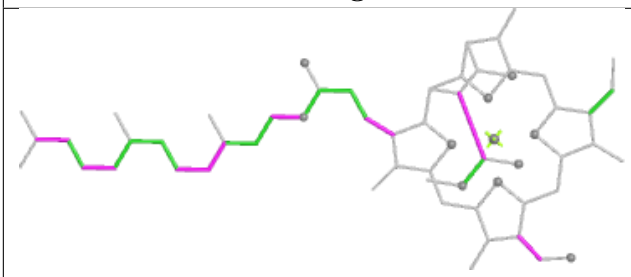
Ligand CL7 3B 614



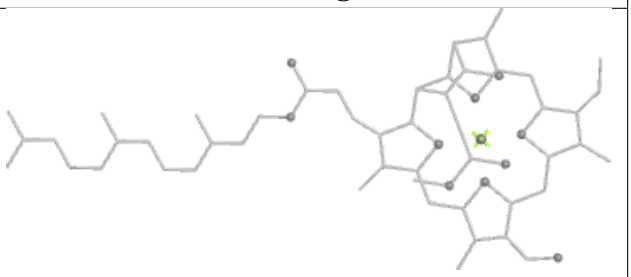
Bond lengths



Bond angles



Torsions

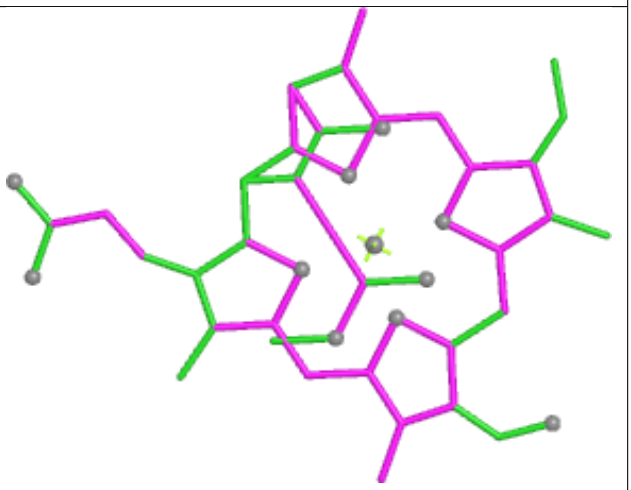


Rings

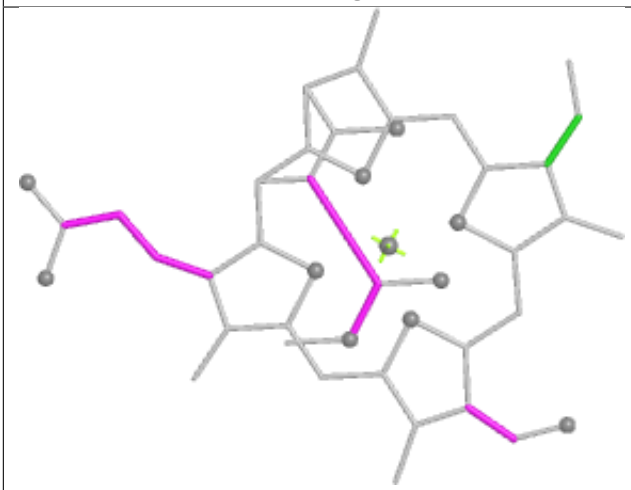
Ligand CL7 11 412



Bond lengths



Bond angles

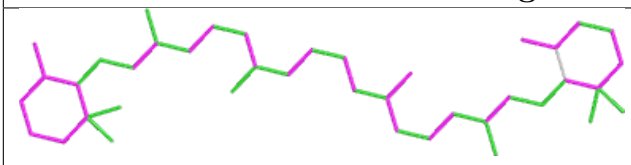


Torsions

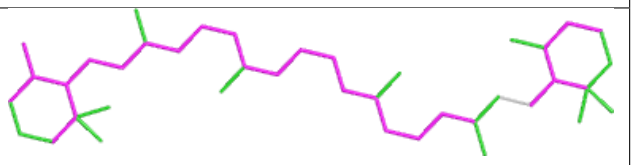


Rings

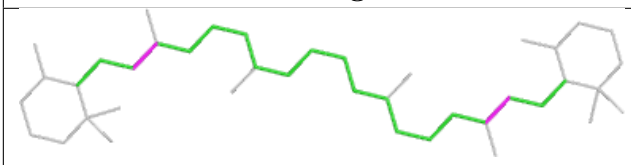
Ligand 8CT 2B 620



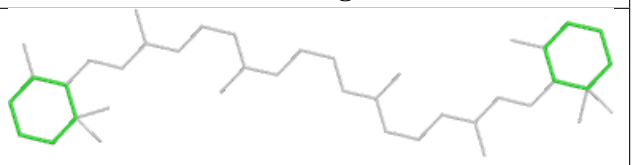
Bond lengths



Bond angles

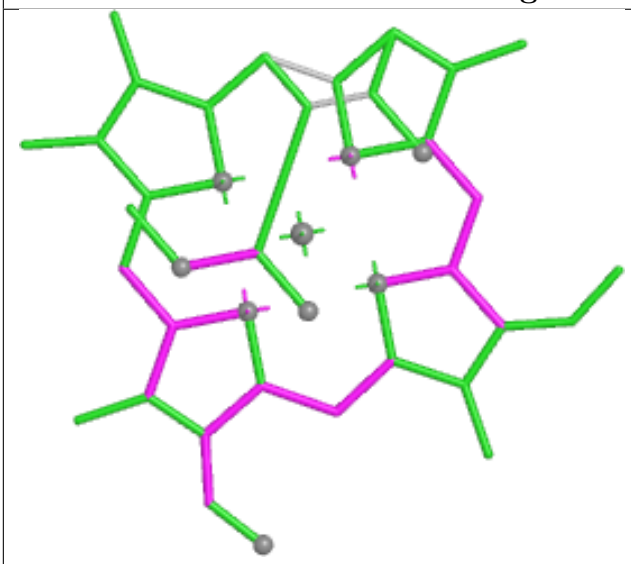


Torsions

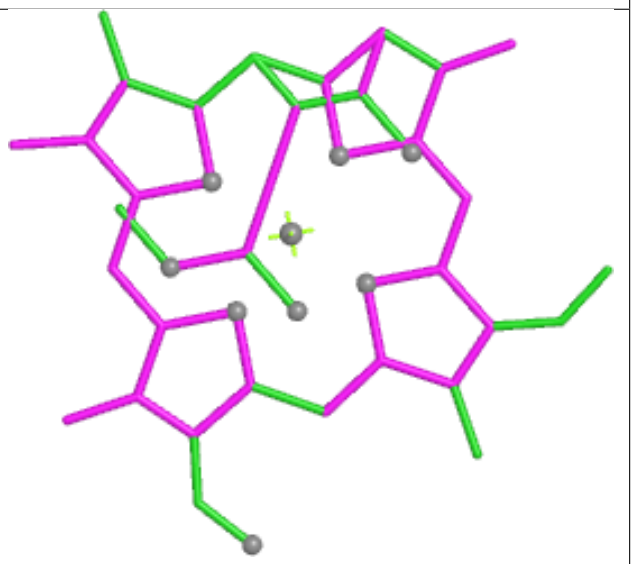


Rings

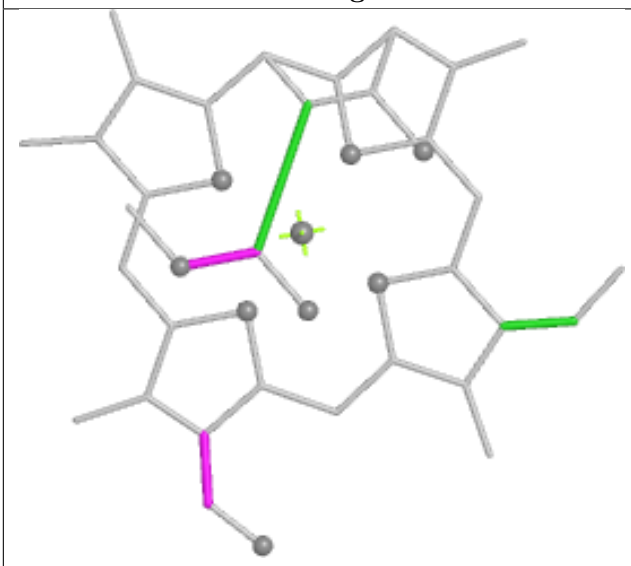
Ligand CL7 4C 512



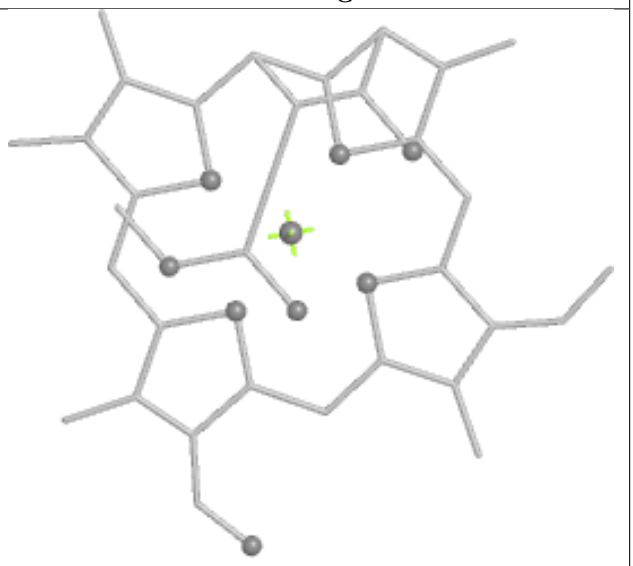
Bond lengths



Bond angles

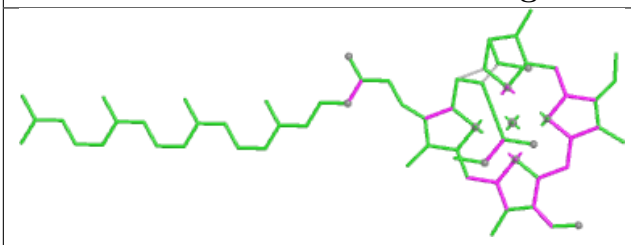


Torsions

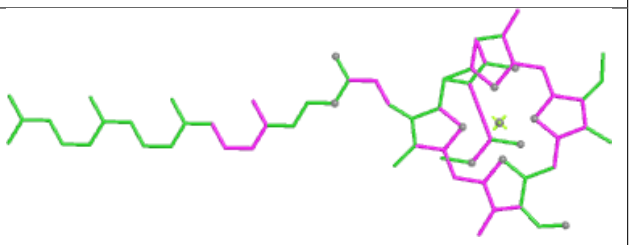


Rings

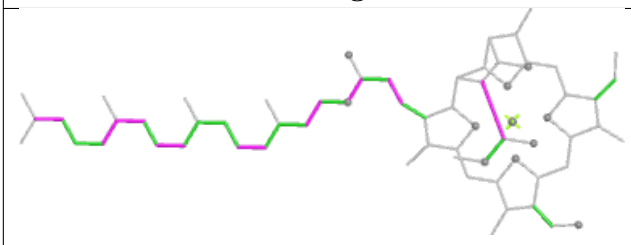
Ligand CL7 3B 610



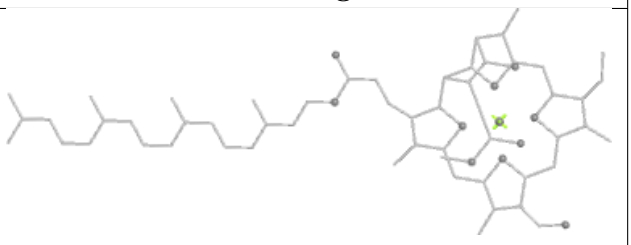
Bond lengths



Bond angles

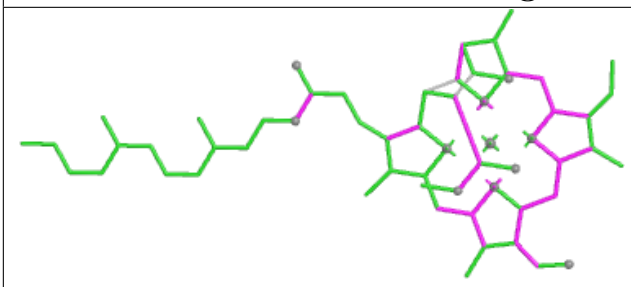


Torsions

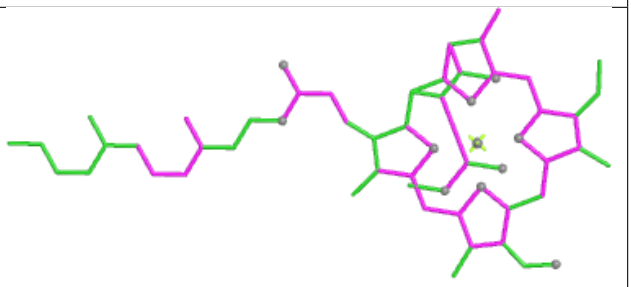


Rings

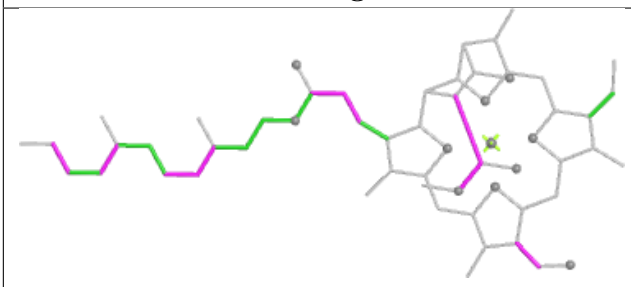
Ligand CL7 3D 404



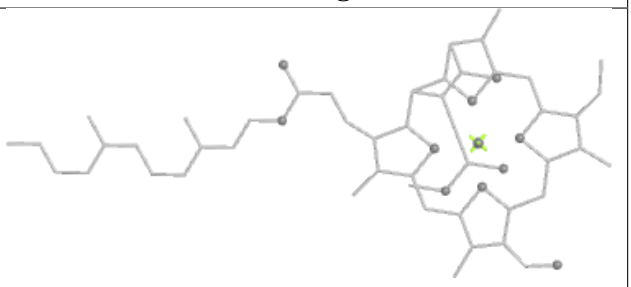
Bond lengths



Bond angles

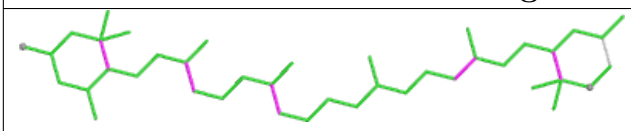


Torsions

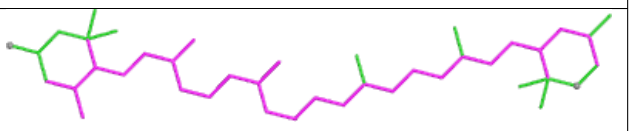


Rings

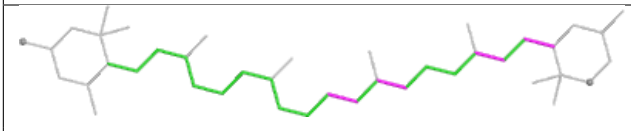
Ligand ZEX 23 401



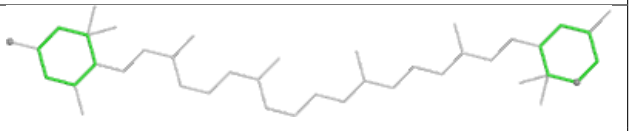
Bond lengths



Bond angles

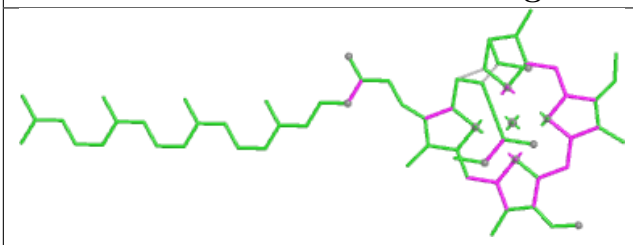


Torsions

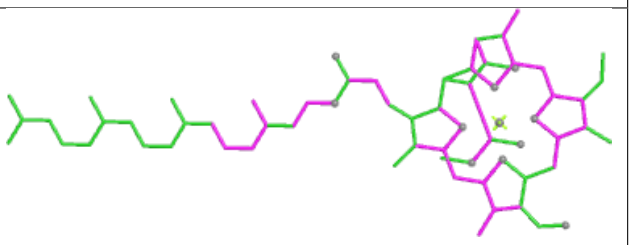


Rings

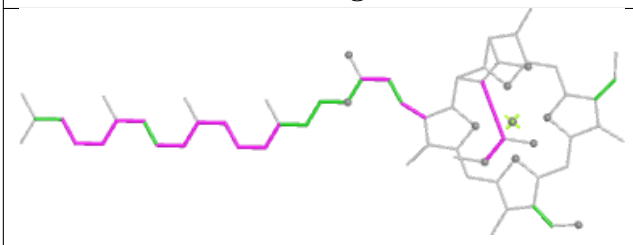
Ligand CL7 12 510



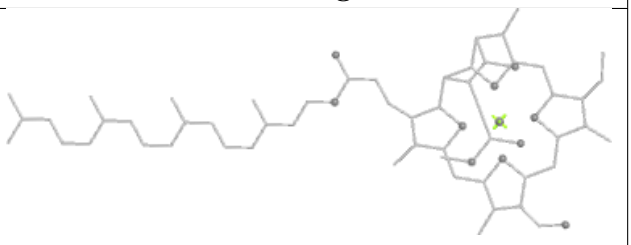
Bond lengths



Bond angles

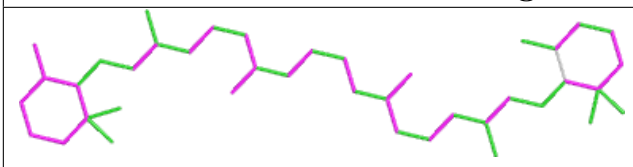


Torsions

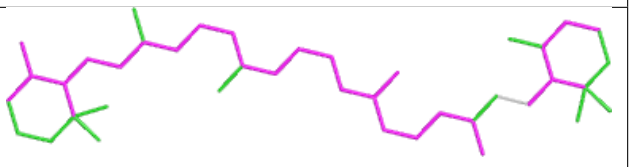


Rings

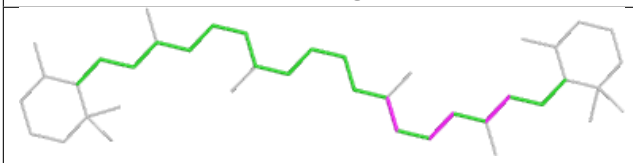
Ligand 8CT 3A 404



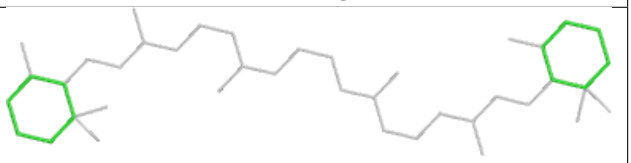
Bond lengths



Bond angles

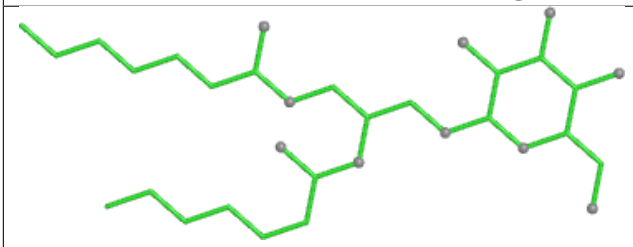


Torsions

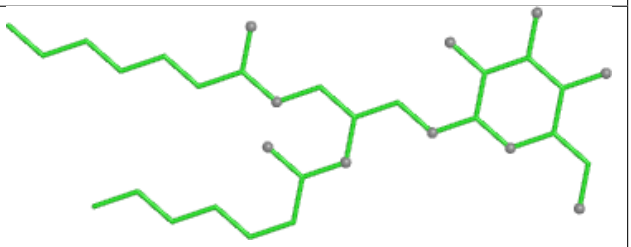


Rings

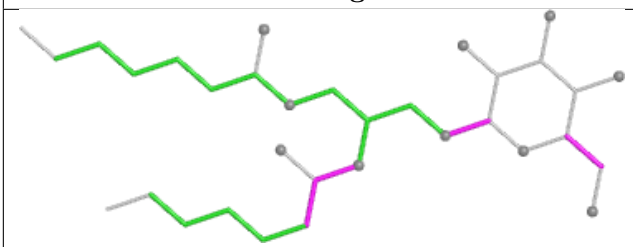
Ligand LMG 4D 410



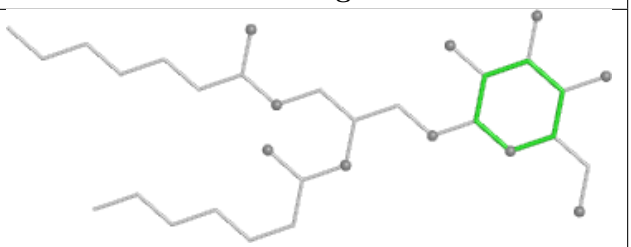
Bond lengths



Bond angles

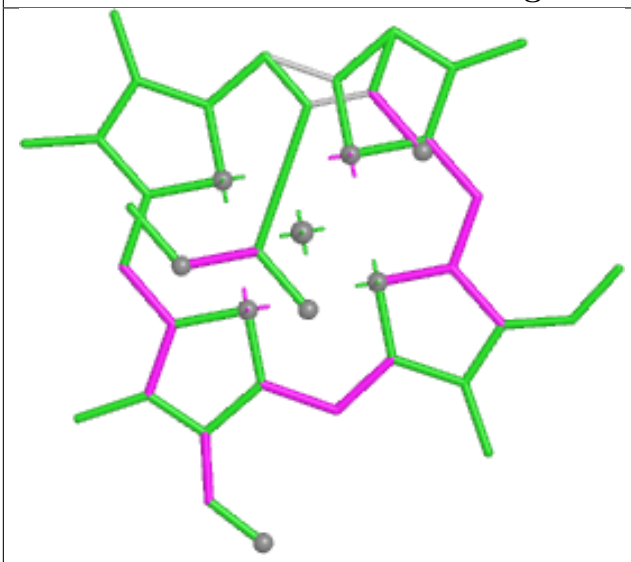


Torsions

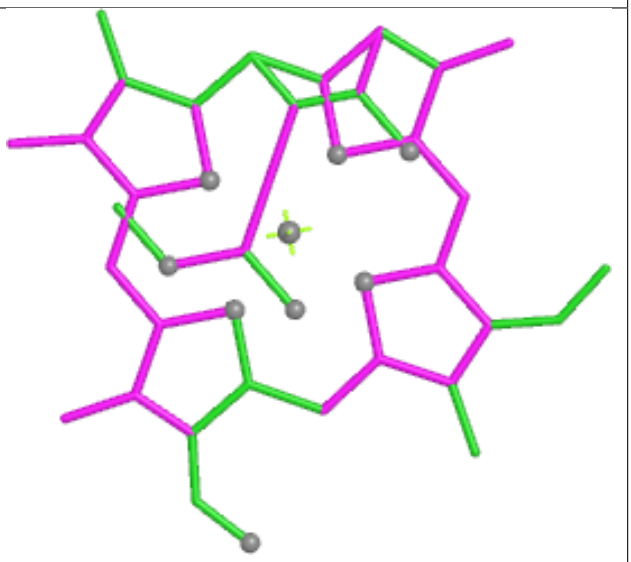


Rings

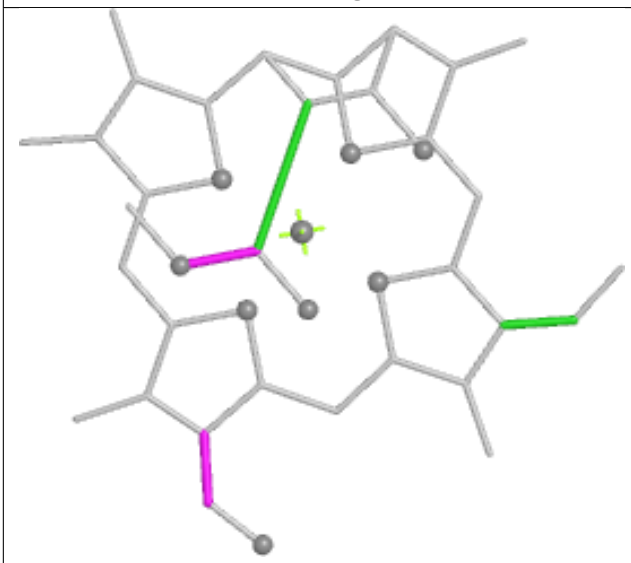
Ligand CL7 21 416



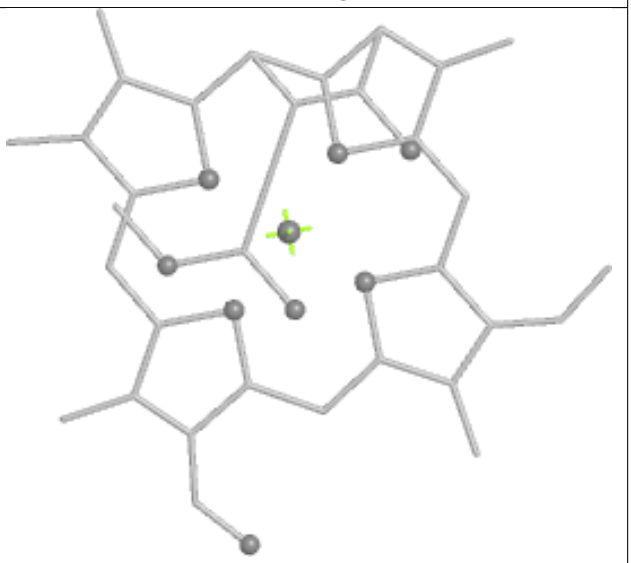
Bond lengths



Bond angles

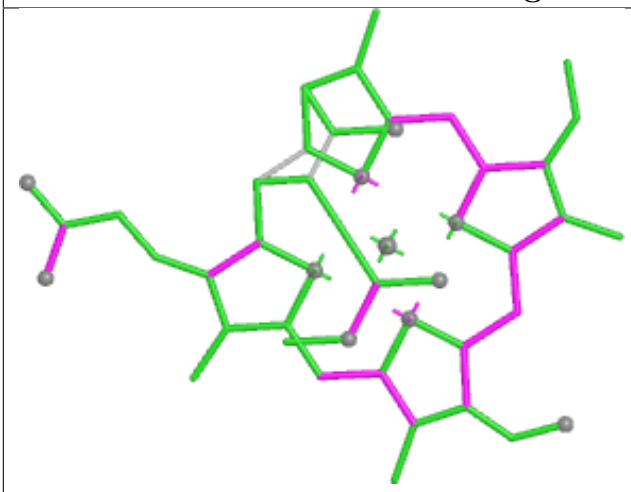


Torsions

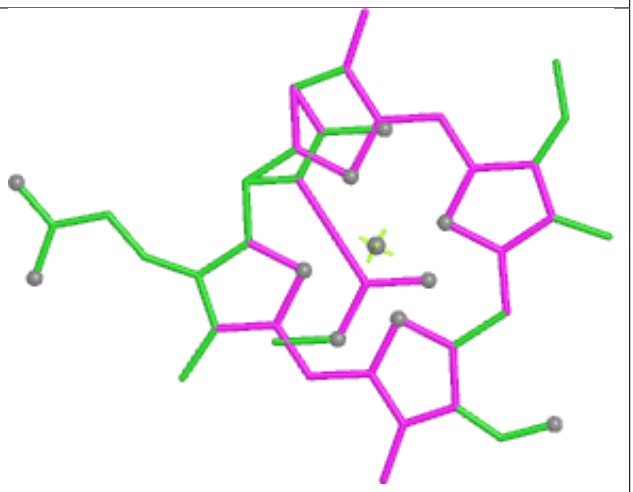


Rings

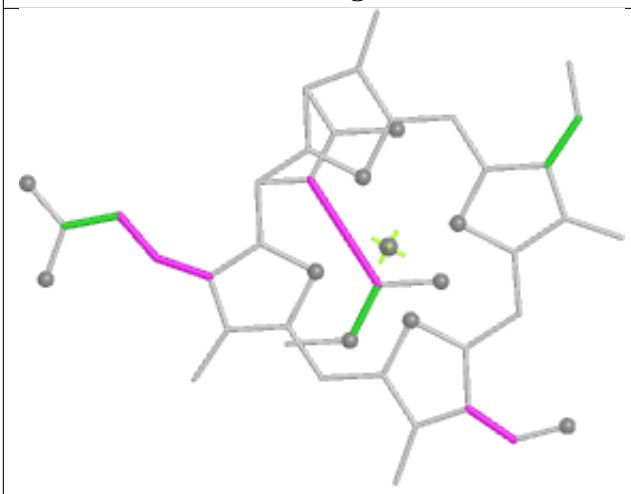
Ligand CL7 12 513



Bond lengths



Bond angles

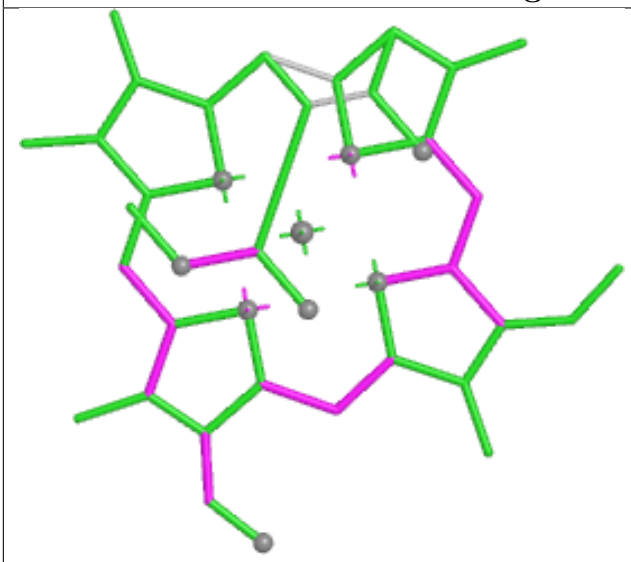


Torsions

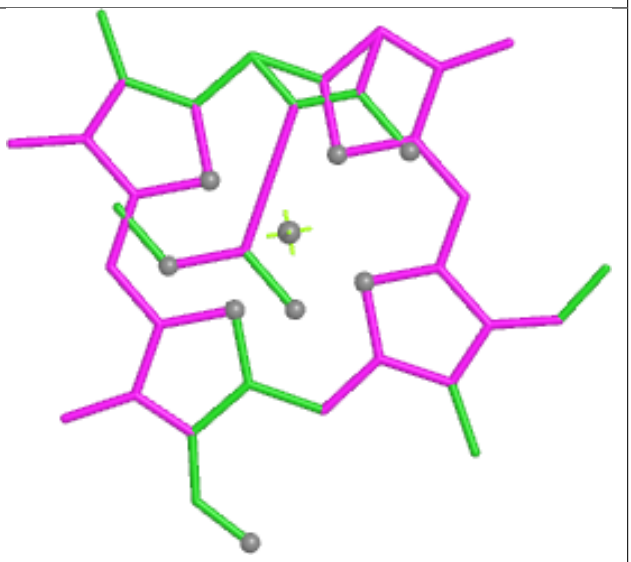


Rings

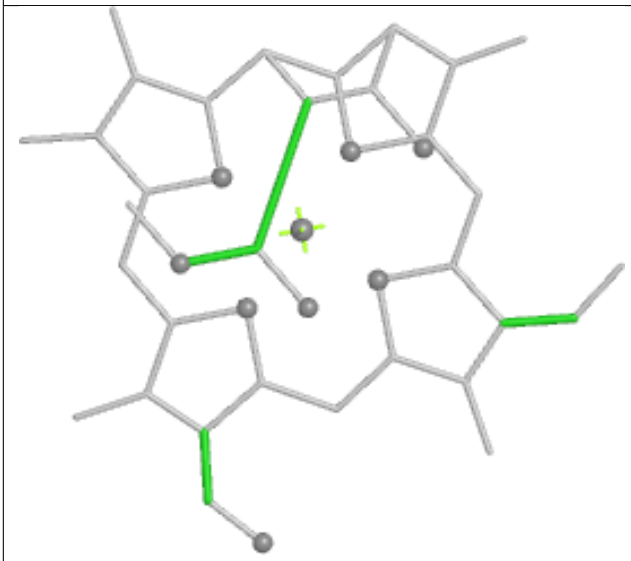
Ligand CL7 13 515



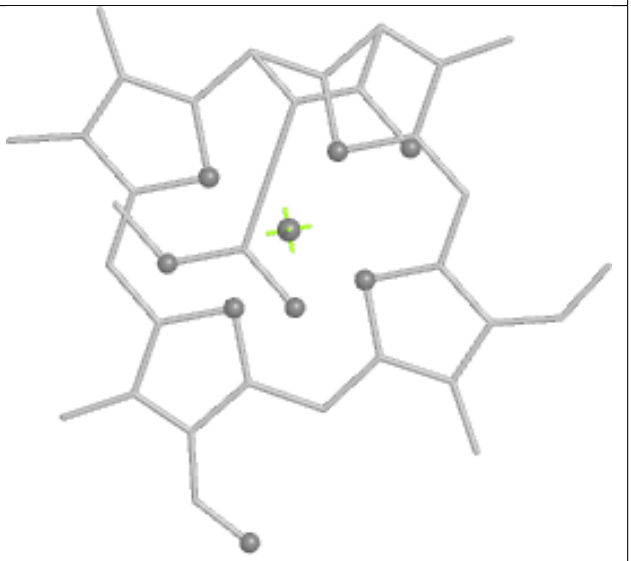
Bond lengths



Bond angles

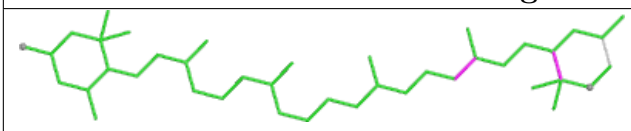


Torsions

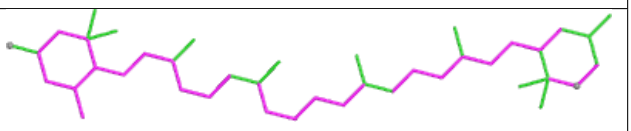


Rings

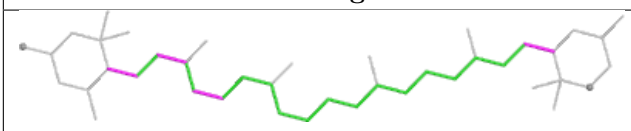
Ligand ZEX 31 422



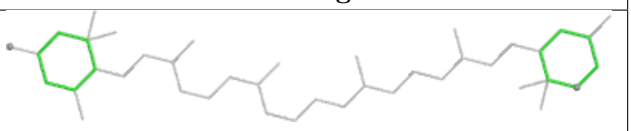
Bond lengths



Bond angles

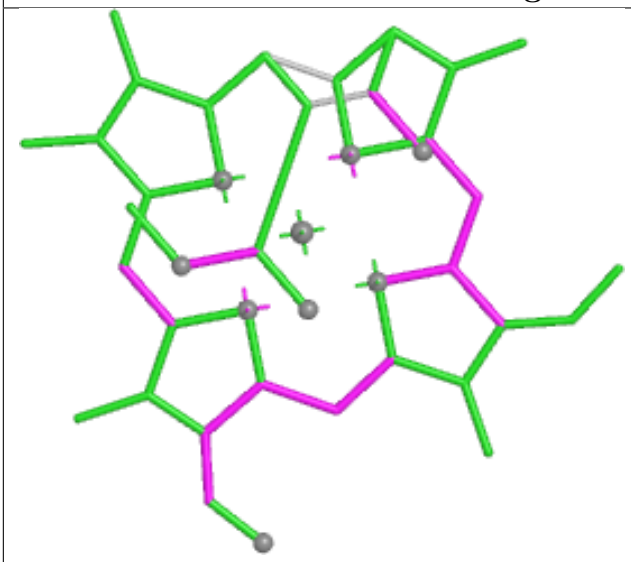


Torsions

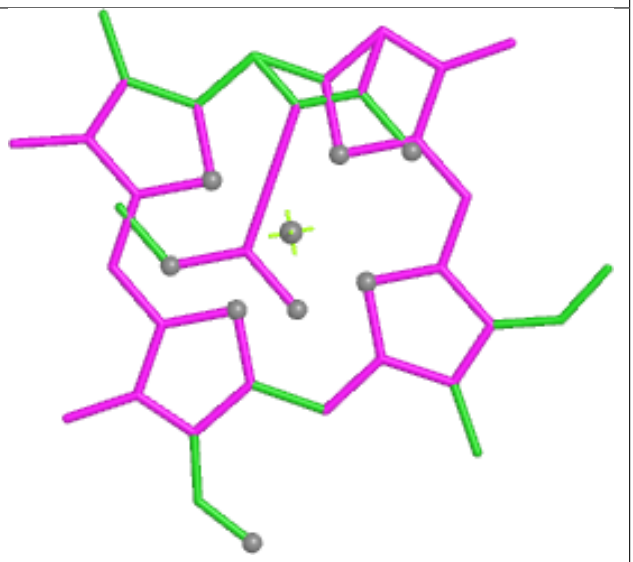


Rings

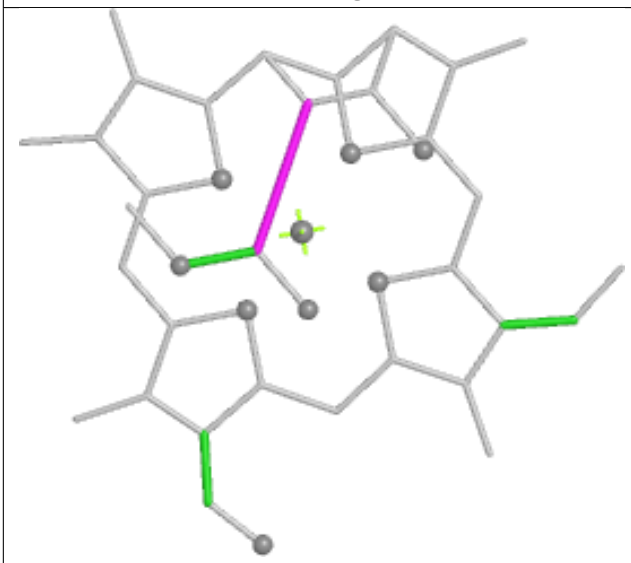
Ligand CL7 11 413



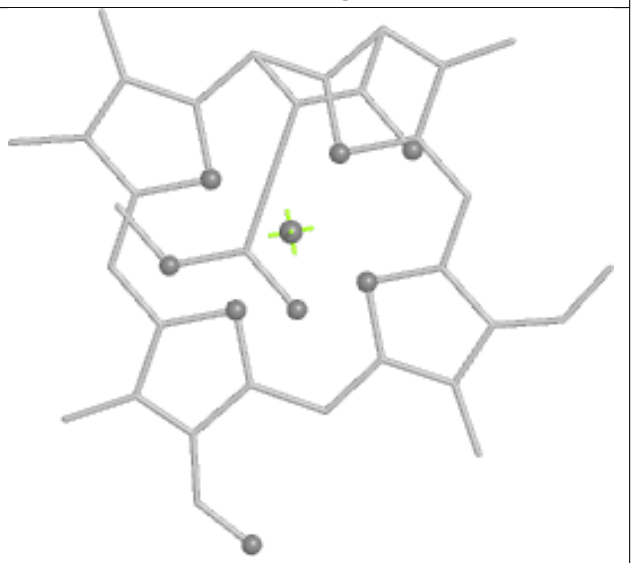
Bond lengths



Bond angles

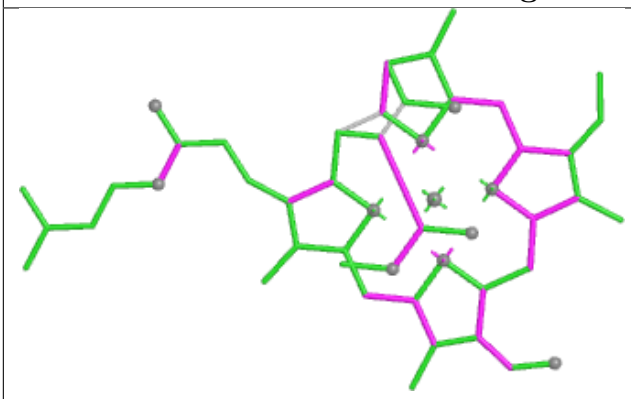


Torsions

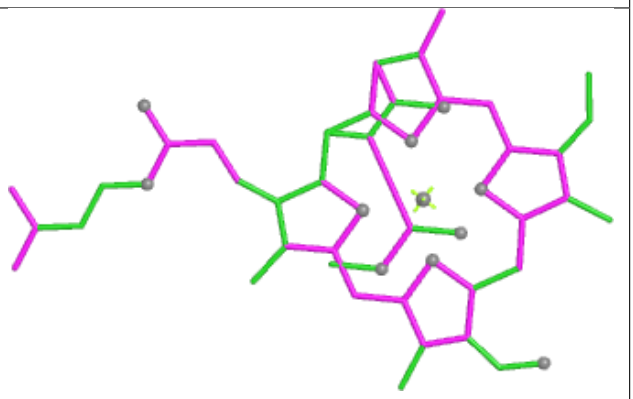


Rings

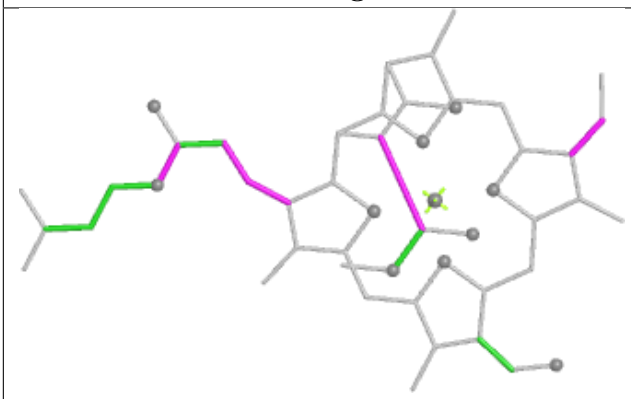
Ligand CL7 3B 615



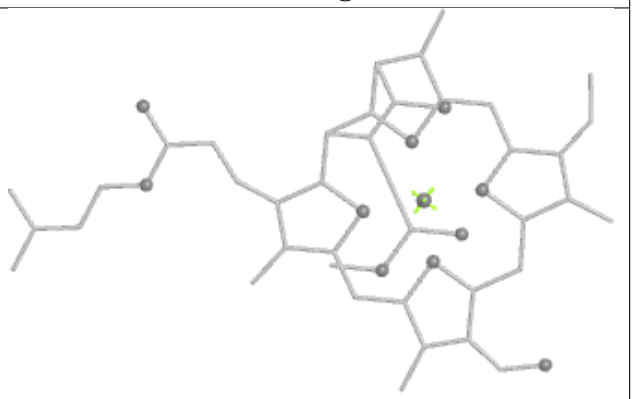
Bond lengths



Bond angles

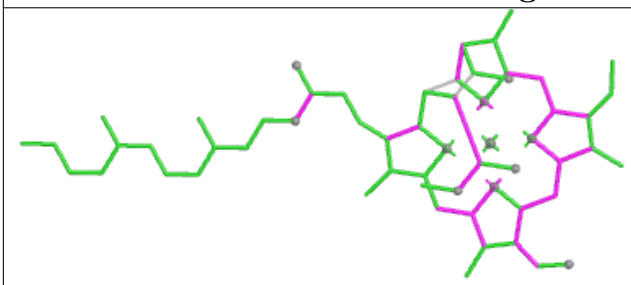


Torsions

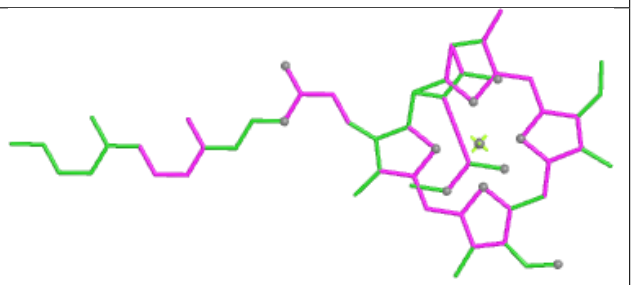


Rings

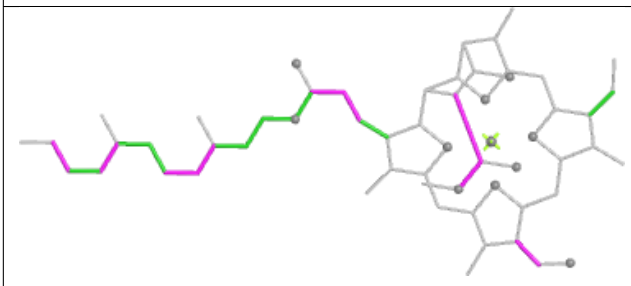
Ligand CL7 1D 404



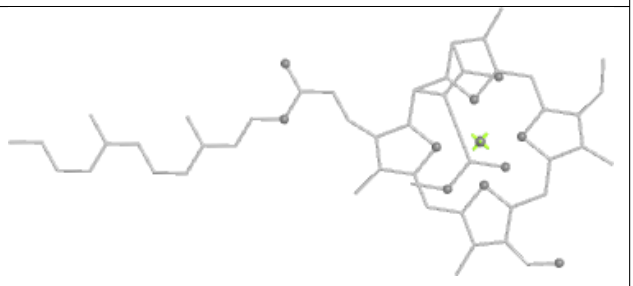
Bond lengths



Bond angles

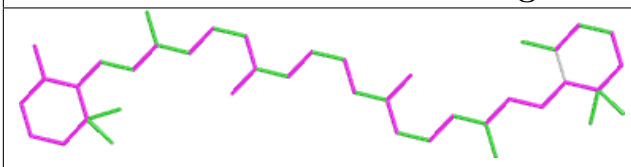


Torsions

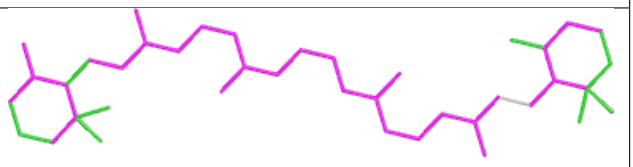


Rings

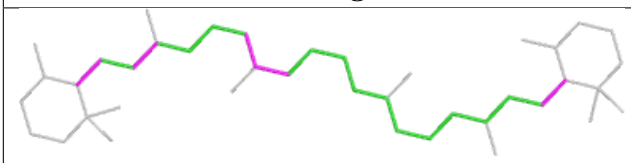
Ligand 8CT 3B 626



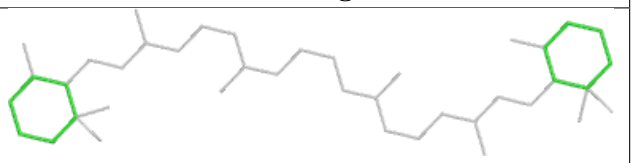
Bond lengths



Bond angles

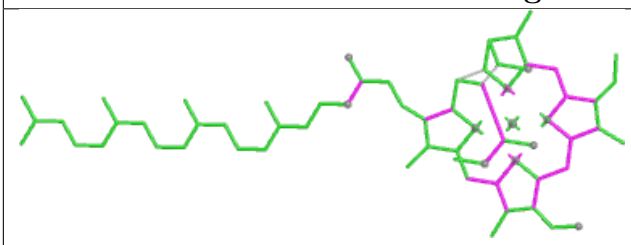


Torsions

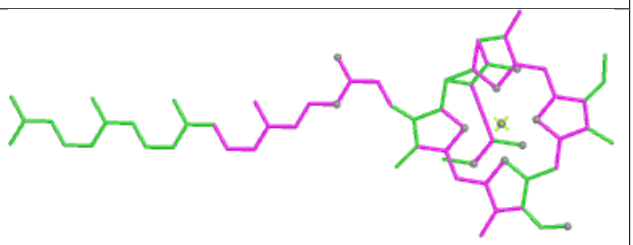


Rings

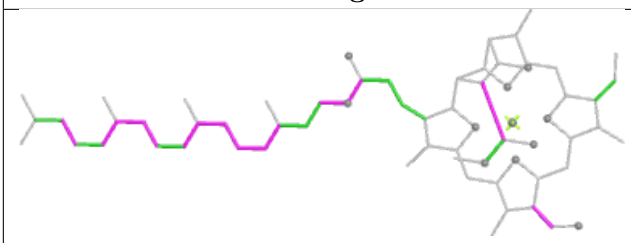
Ligand CL7 23 412



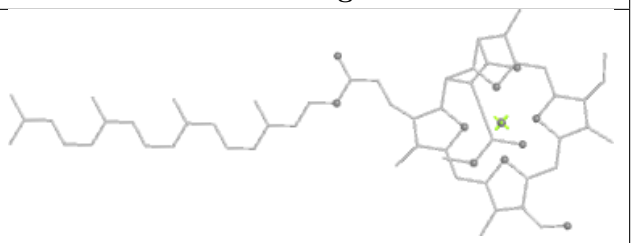
Bond lengths



Bond angles

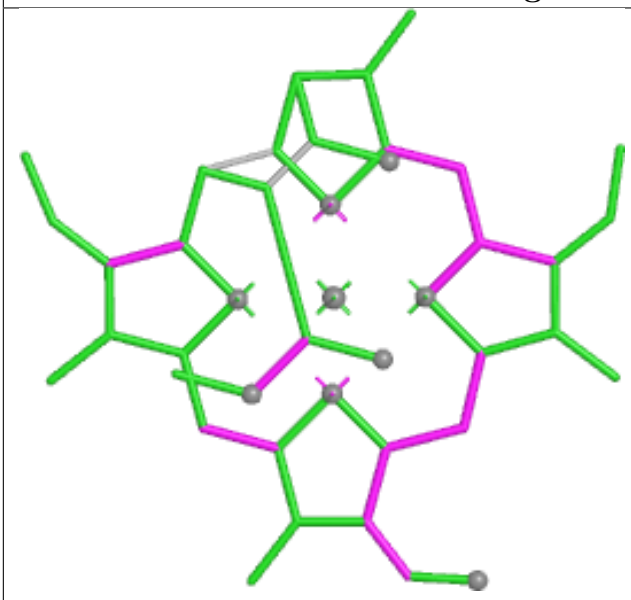


Torsions

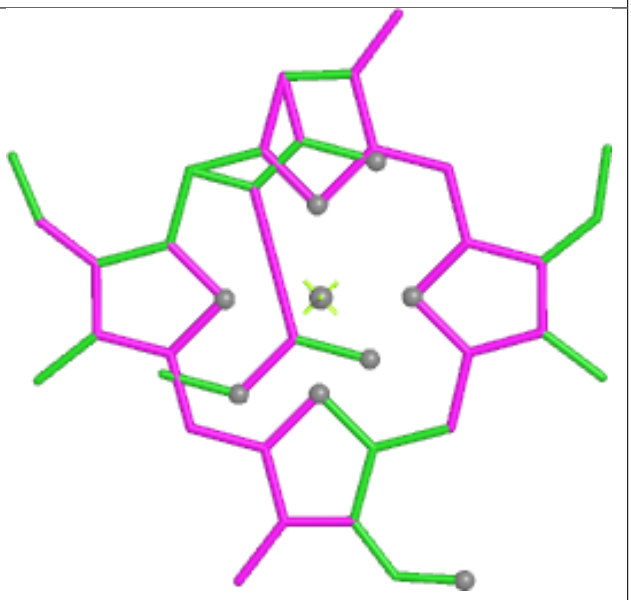


Rings

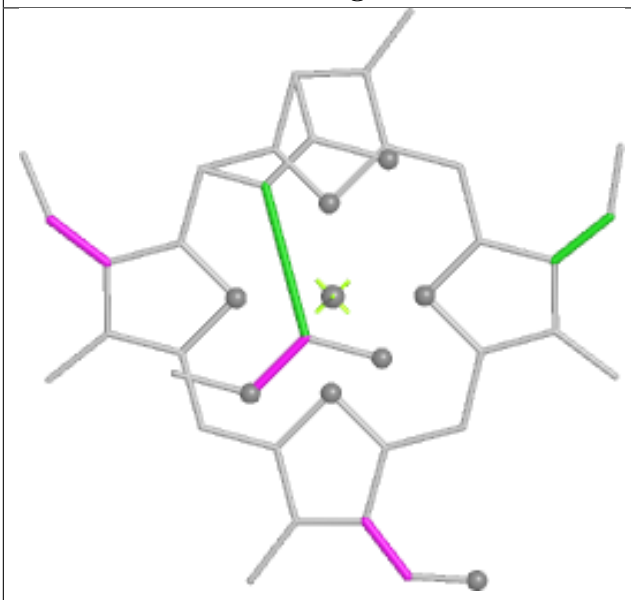
Ligand CL7 34 417



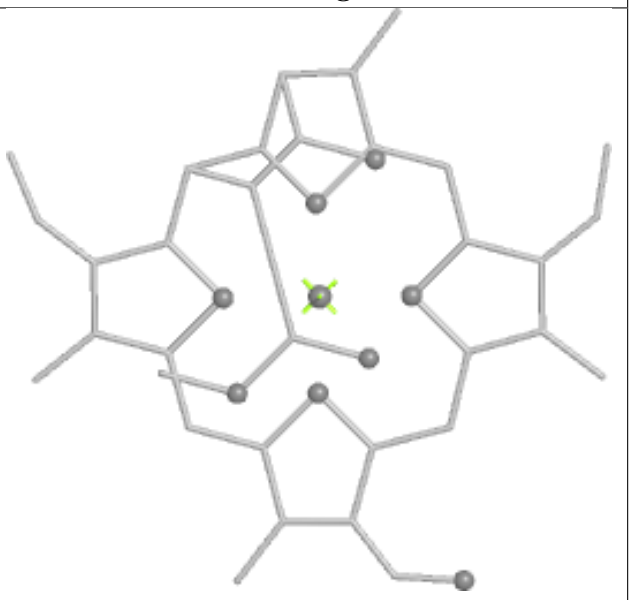
Bond lengths



Bond angles

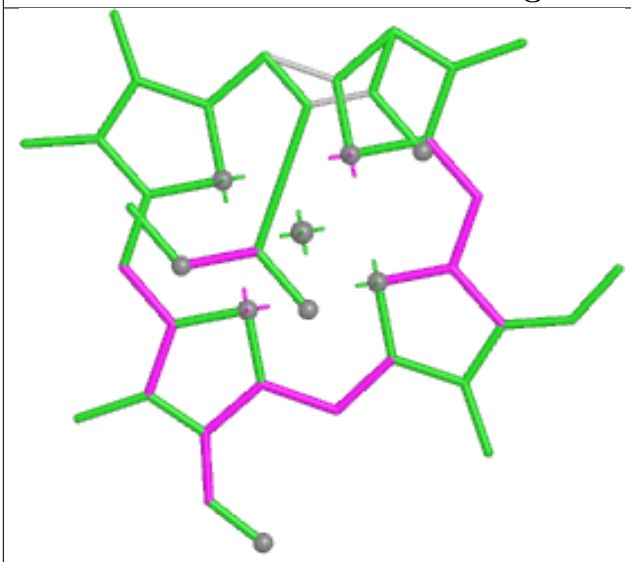


Torsions

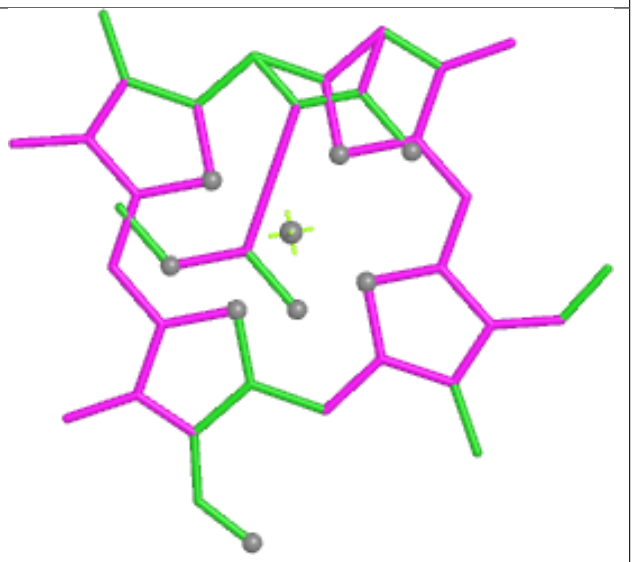


Rings

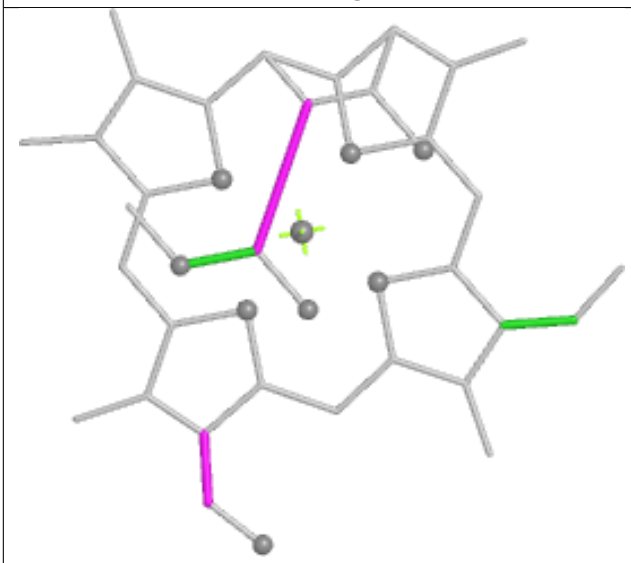
Ligand CL7 14 407



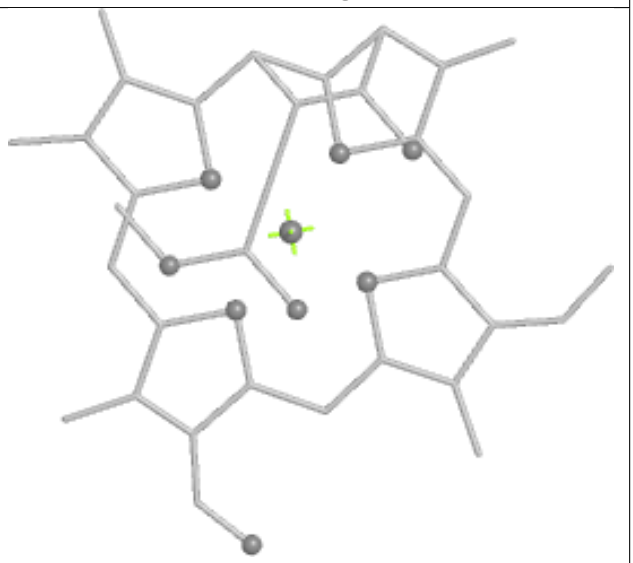
Bond lengths



Bond angles

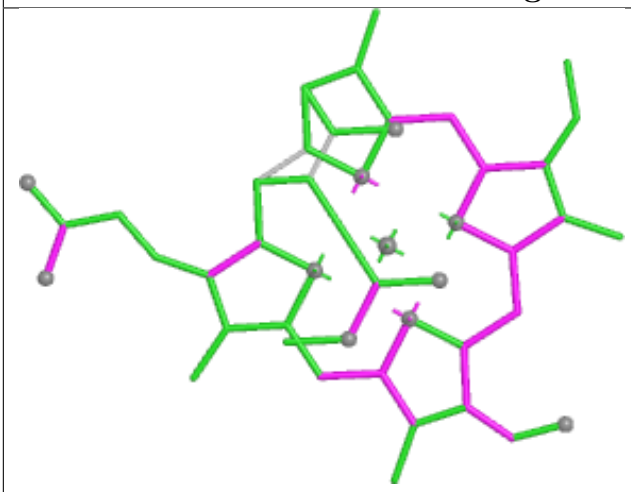


Torsions

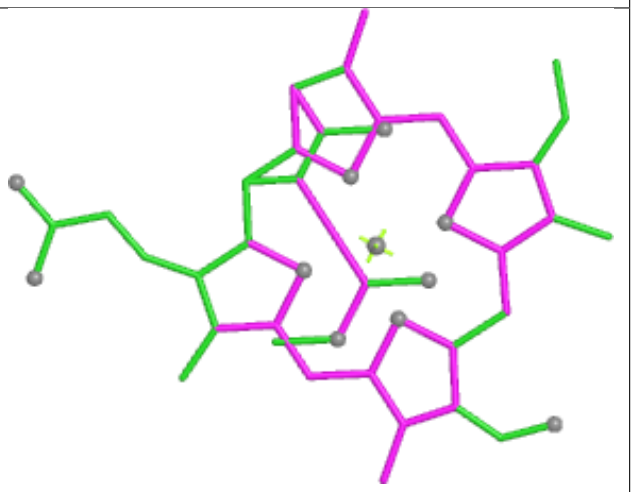


Rings

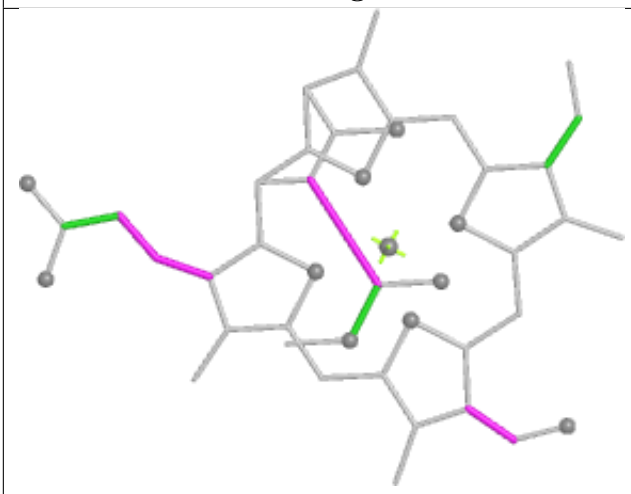
Ligand CL7 42 508



Bond lengths



Bond angles

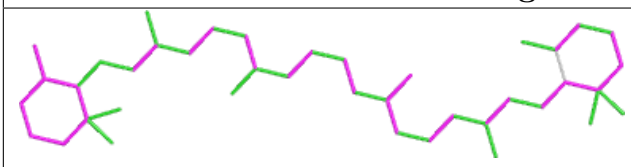


Torsions

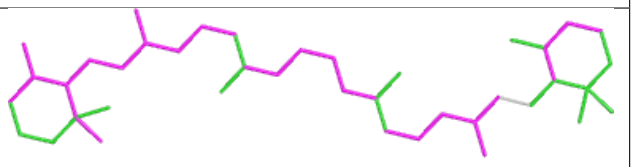


Rings

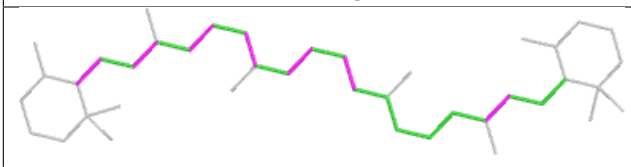
Ligand 8CT 4B 619



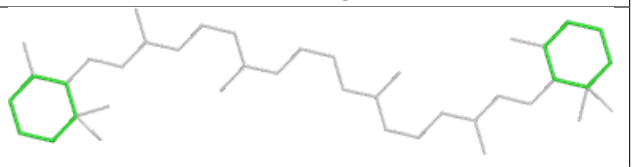
Bond lengths



Bond angles

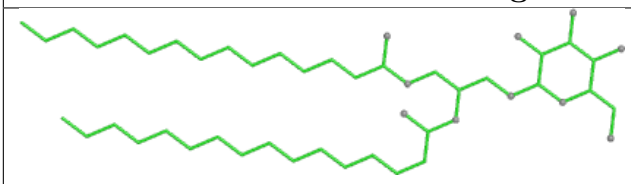


Torsions

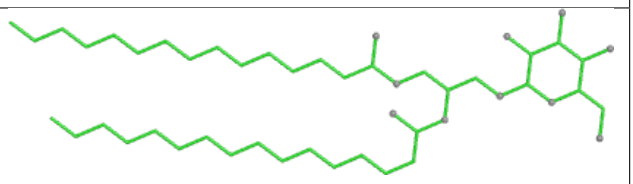


Rings

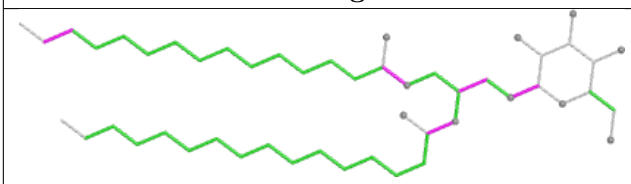
Ligand LMG 2A 405



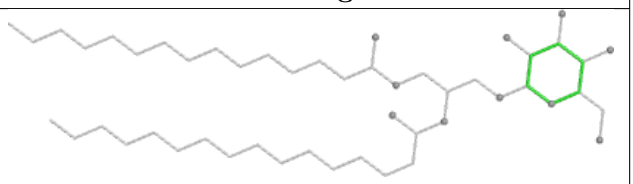
Bond lengths



Bond angles

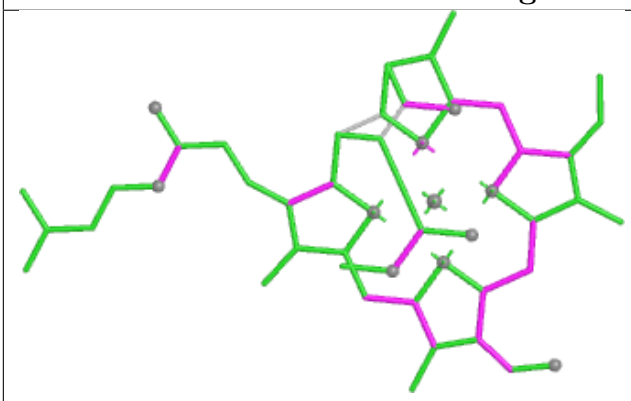


Torsions

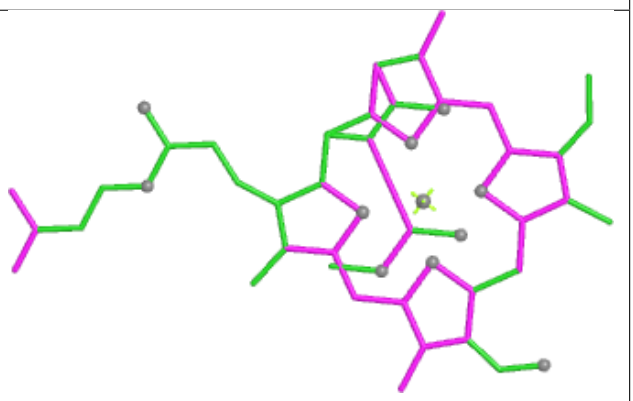


Rings

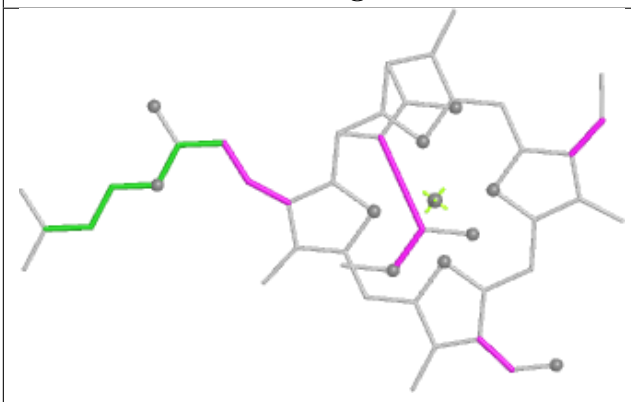
Ligand CL7 4D 402



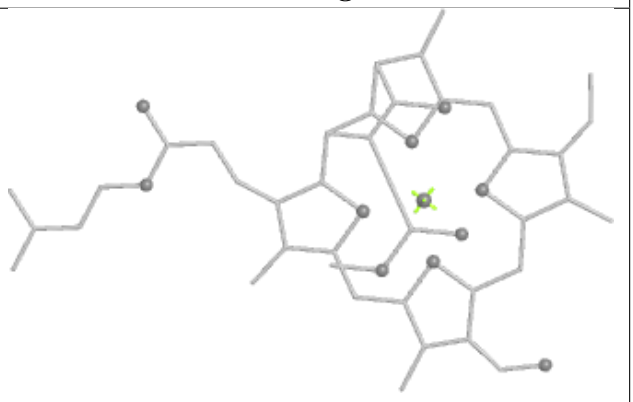
Bond lengths



Bond angles

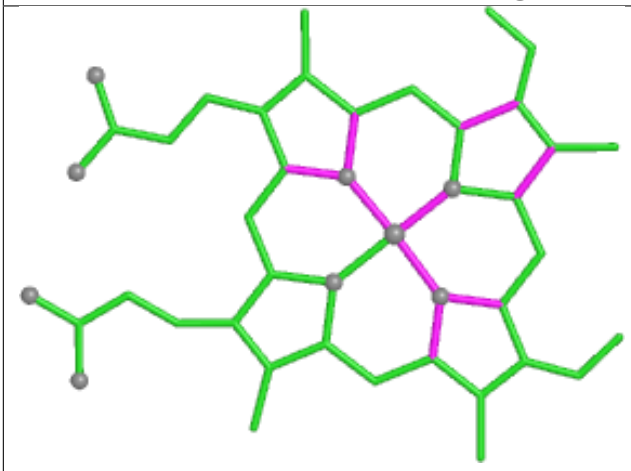


Torsions

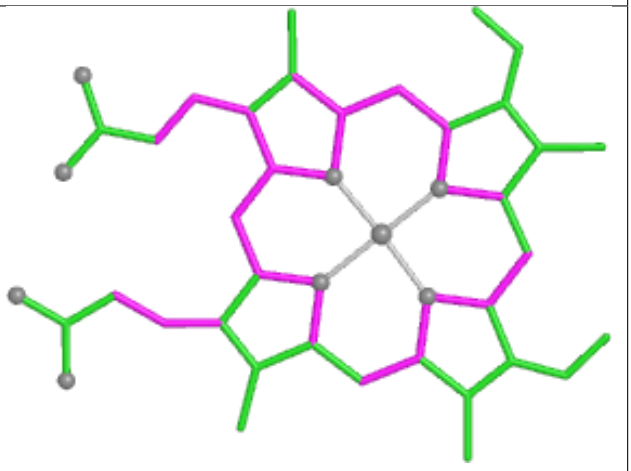


Rings

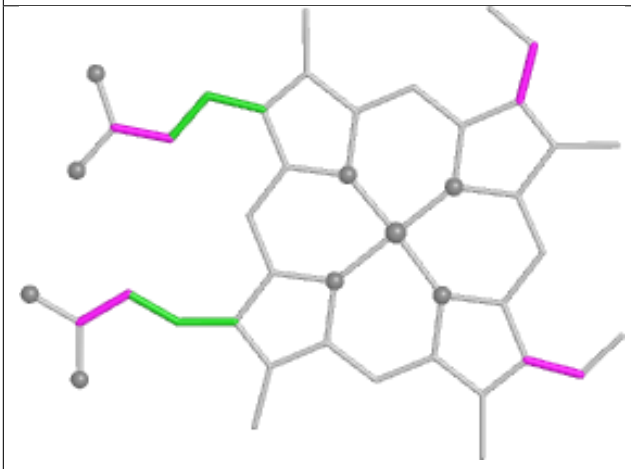
Ligand HEM 1F 101



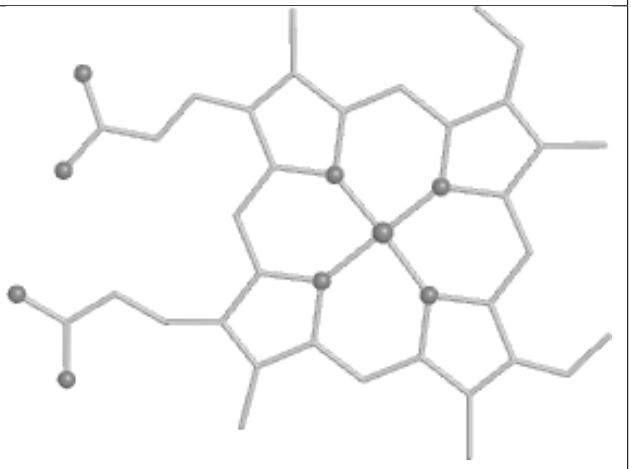
Bond lengths



Bond angles

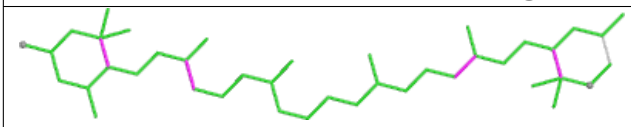


Torsions

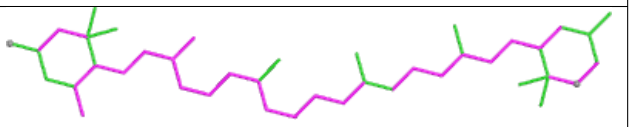


Rings

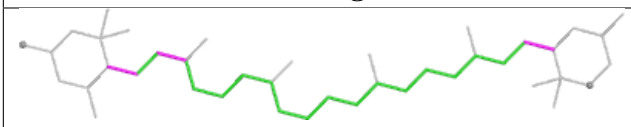
Ligand ZEX 43 423



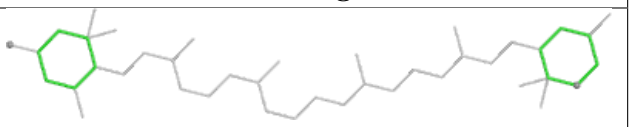
Bond lengths



Bond angles

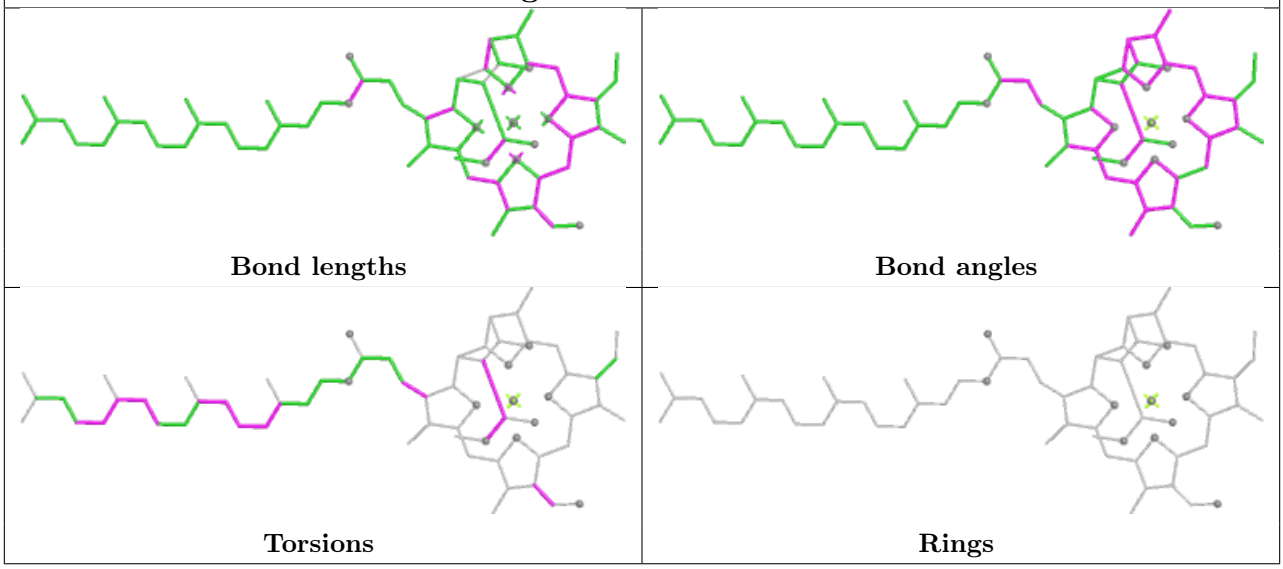


Torsions

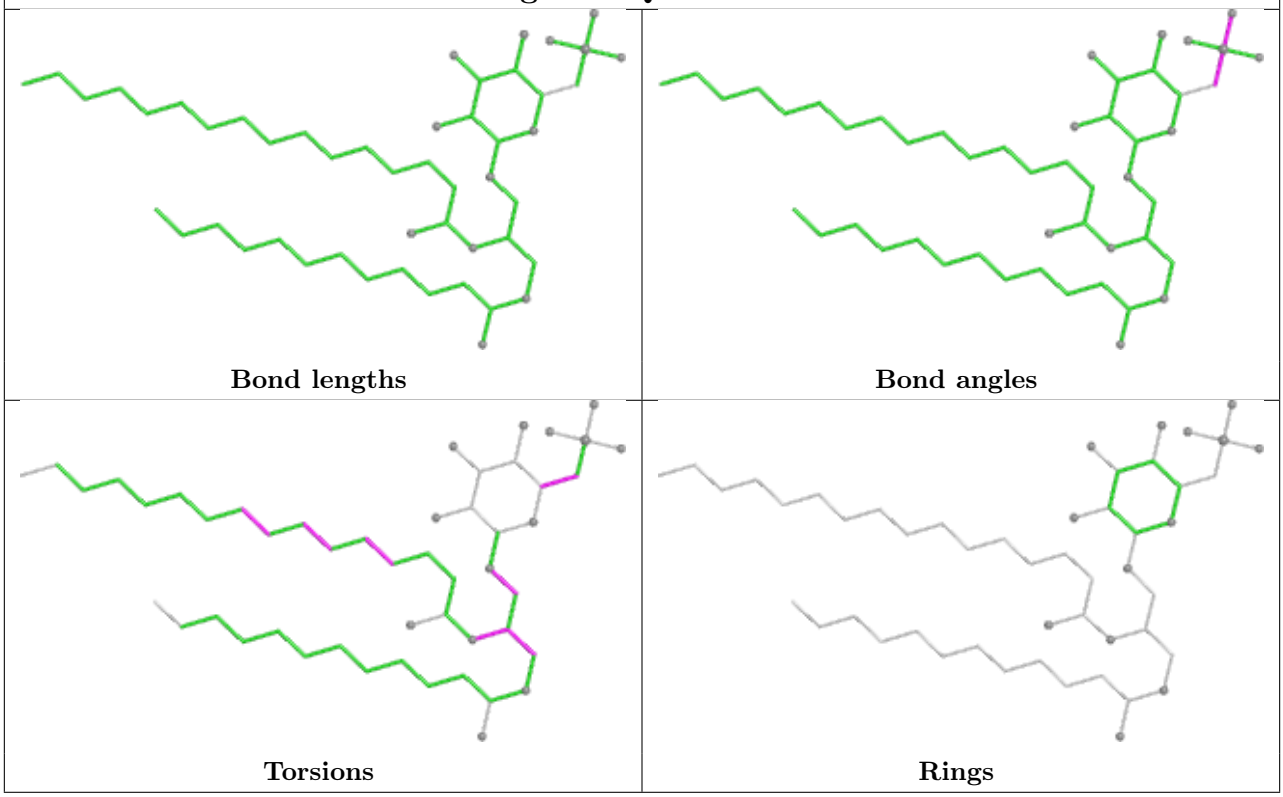


Rings

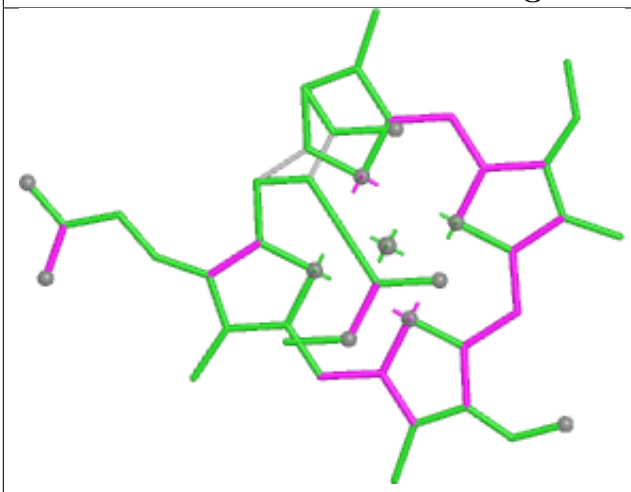
Ligand CL7 3B 605



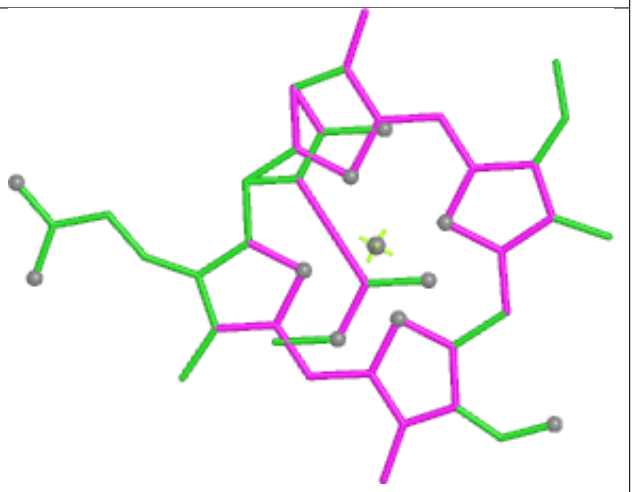
Ligand SQD 33 523



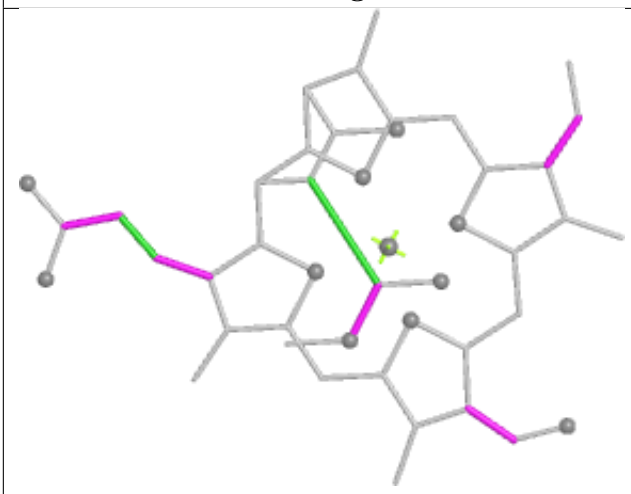
Ligand CL7 32 514



Bond lengths



Bond angles

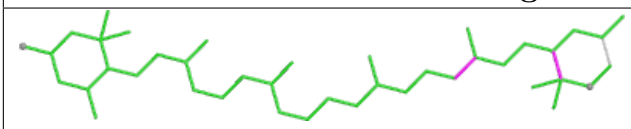


Torsions

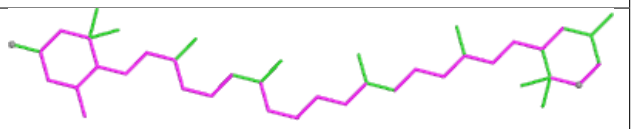


Rings

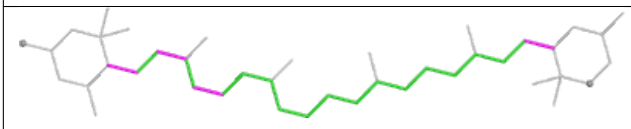
Ligand ZEX 21 422



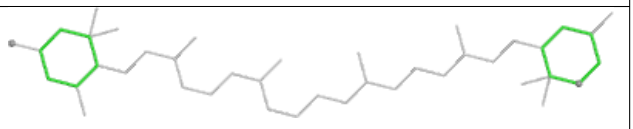
Bond lengths



Bond angles

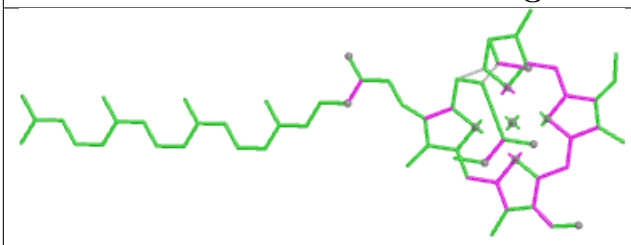


Torsions

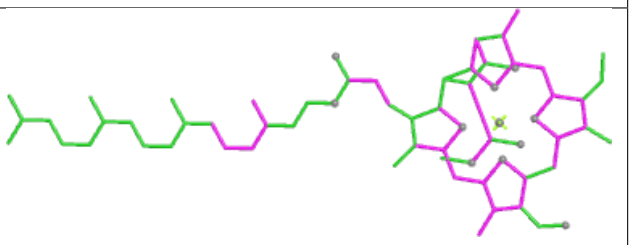


Rings

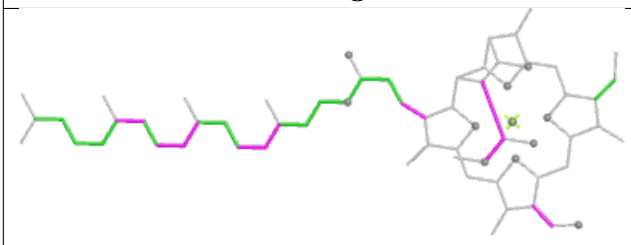
Ligand CL7 12 506



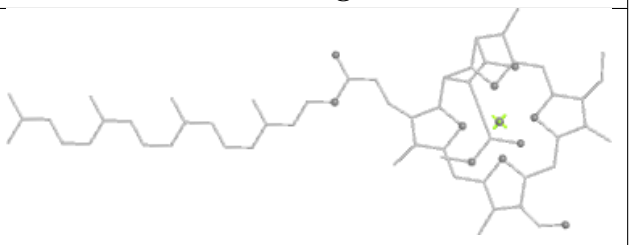
Bond lengths



Bond angles

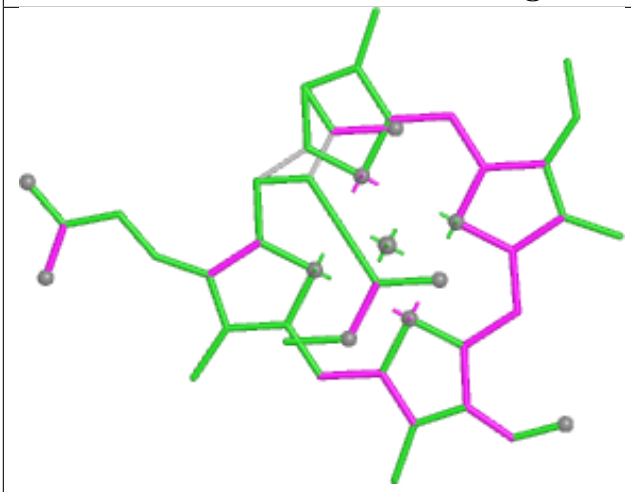


Torsions

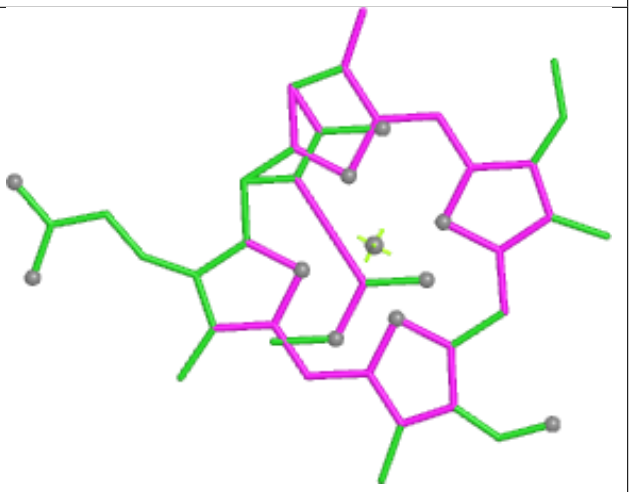


Rings

Ligand CL7 21 405



Bond lengths



Bond angles

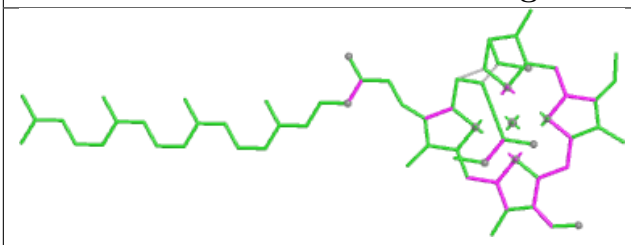


Torsions

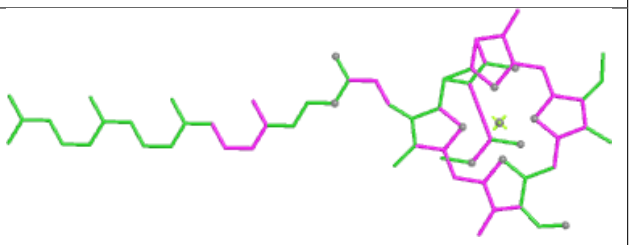


Rings

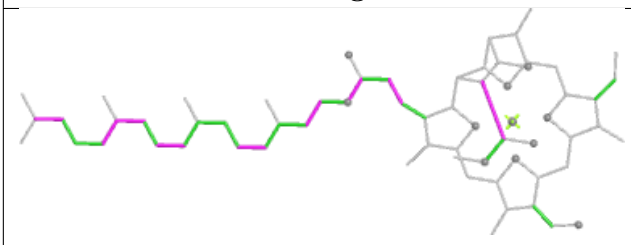
Ligand CL7 2B 611



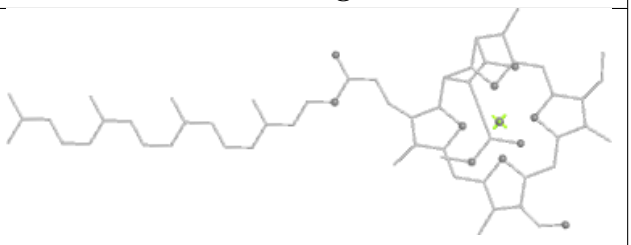
Bond lengths



Bond angles

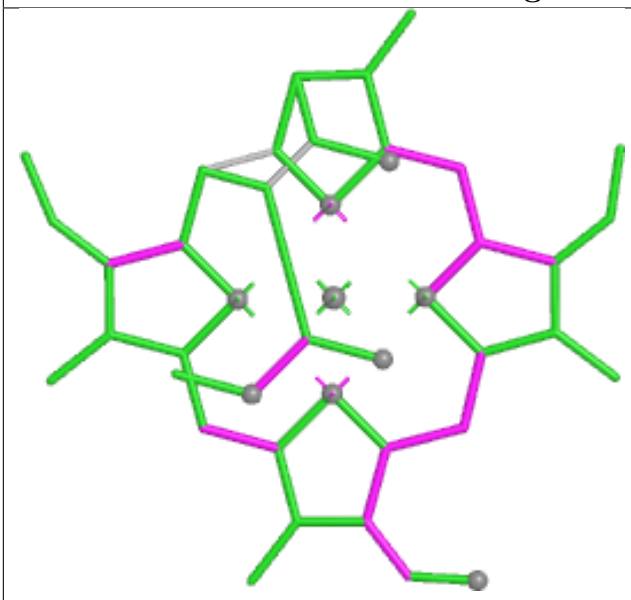


Torsions

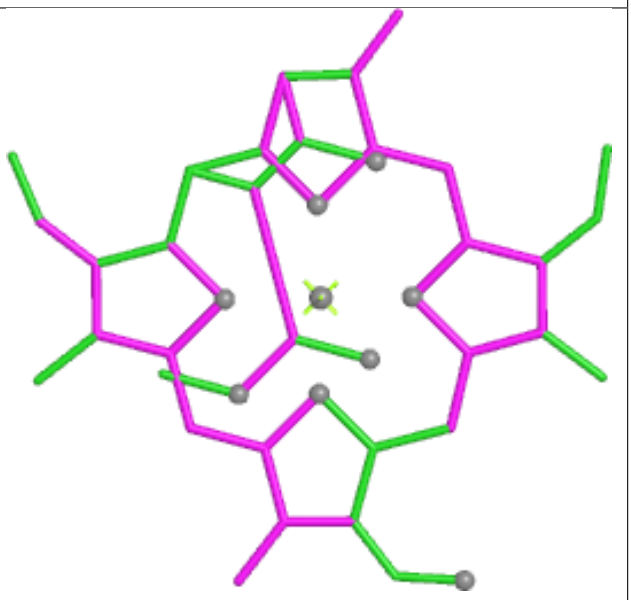


Rings

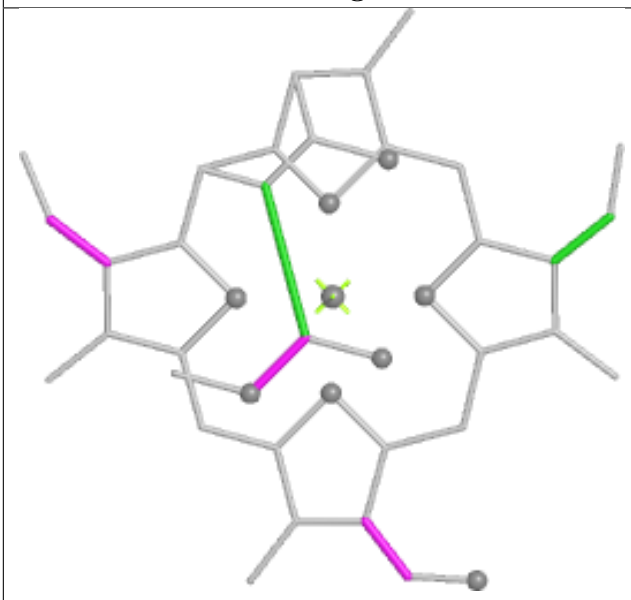
Ligand CL7 14 417



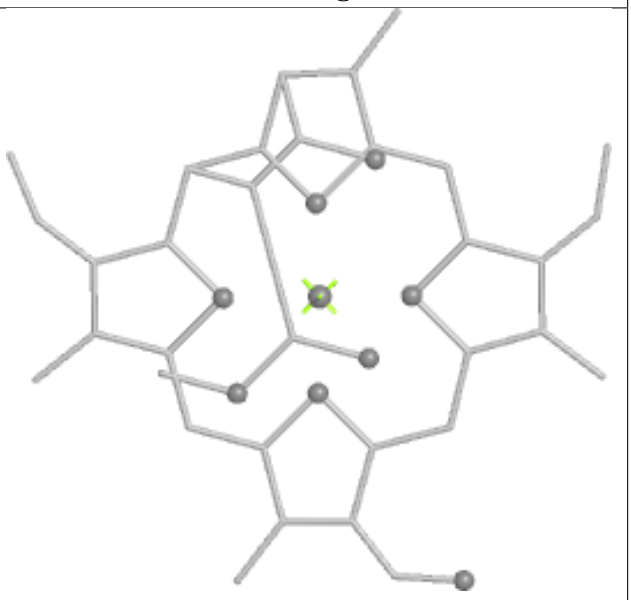
Bond lengths



Bond angles

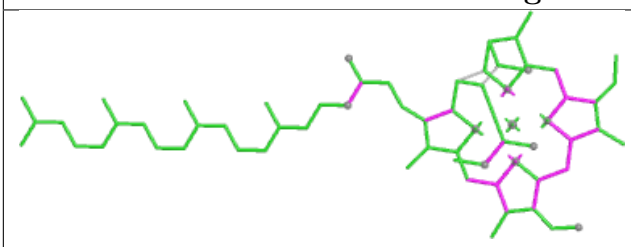


Torsions

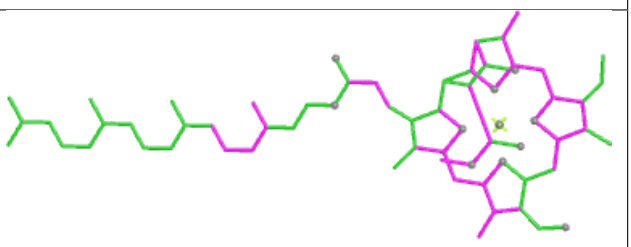


Rings

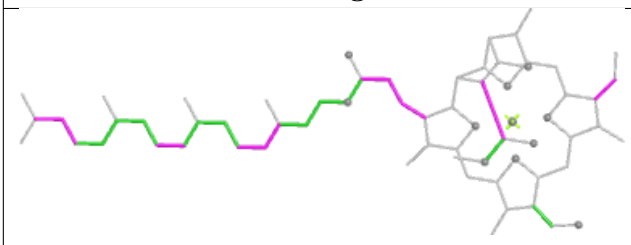
Ligand CL7 33 505



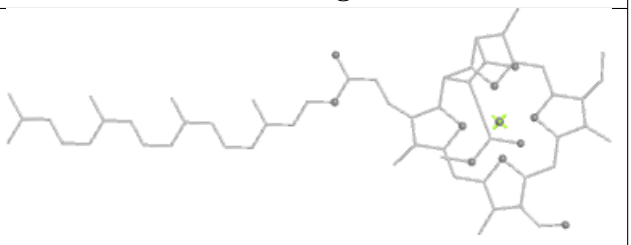
Bond lengths



Bond angles

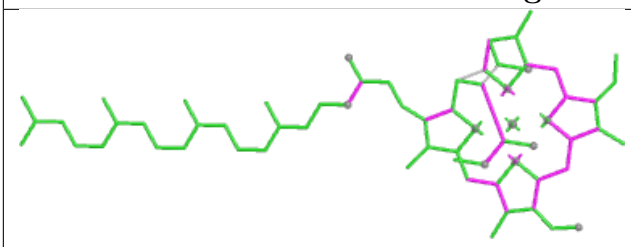


Torsions

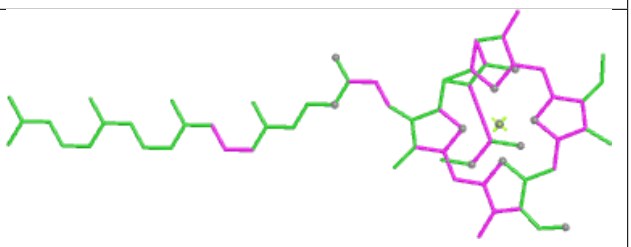


Rings

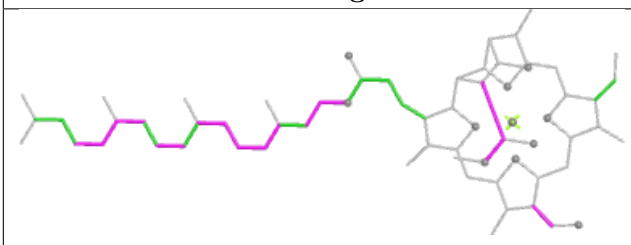
Ligand CL7 22 509



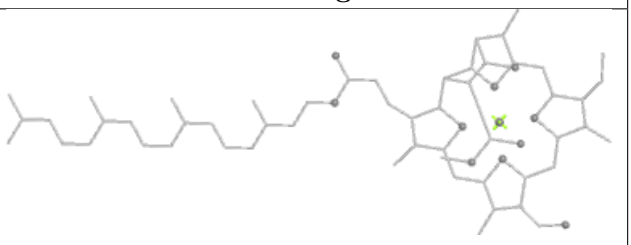
Bond lengths



Bond angles

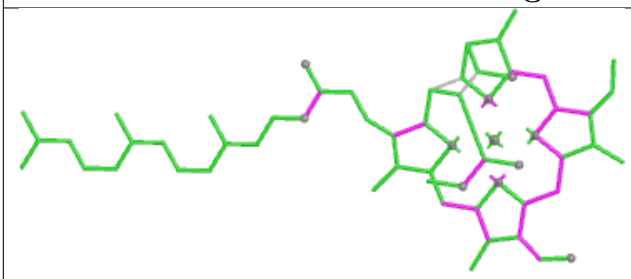


Torsions

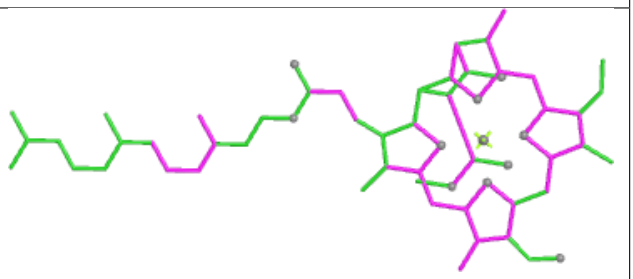


Rings

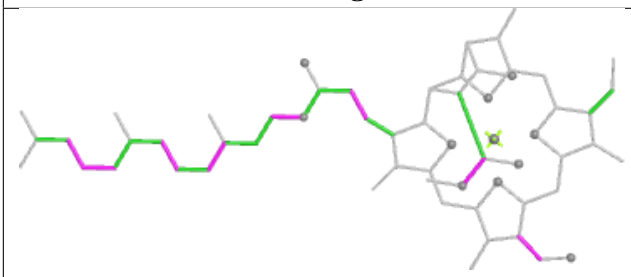
Ligand CL7 31 403



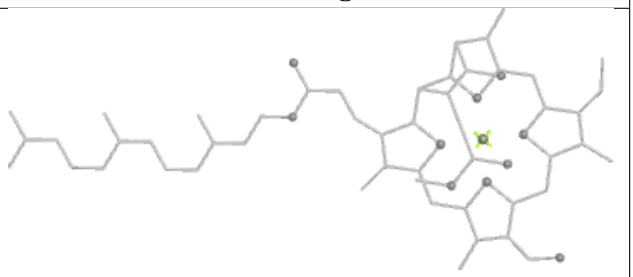
Bond lengths



Bond angles

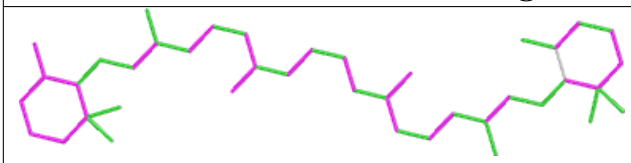


Torsions

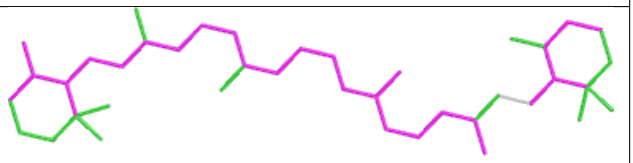


Rings

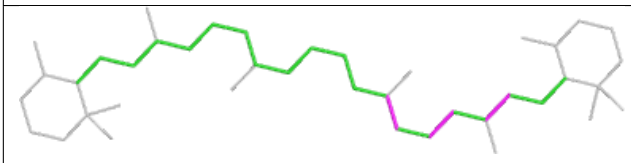
Ligand 8CT 4A 404



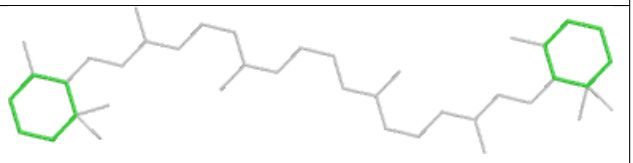
Bond lengths



Bond angles

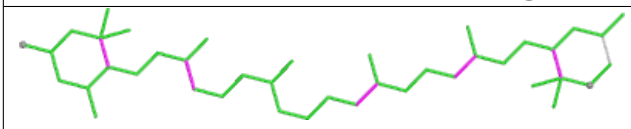


Torsions

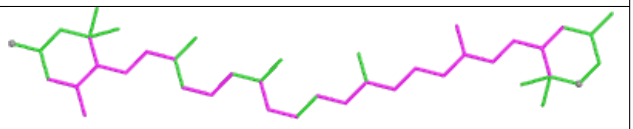


Rings

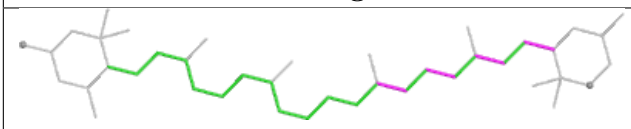
Ligand ZEX 42 522



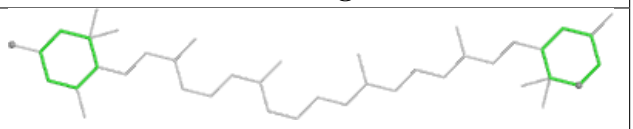
Bond lengths



Bond angles

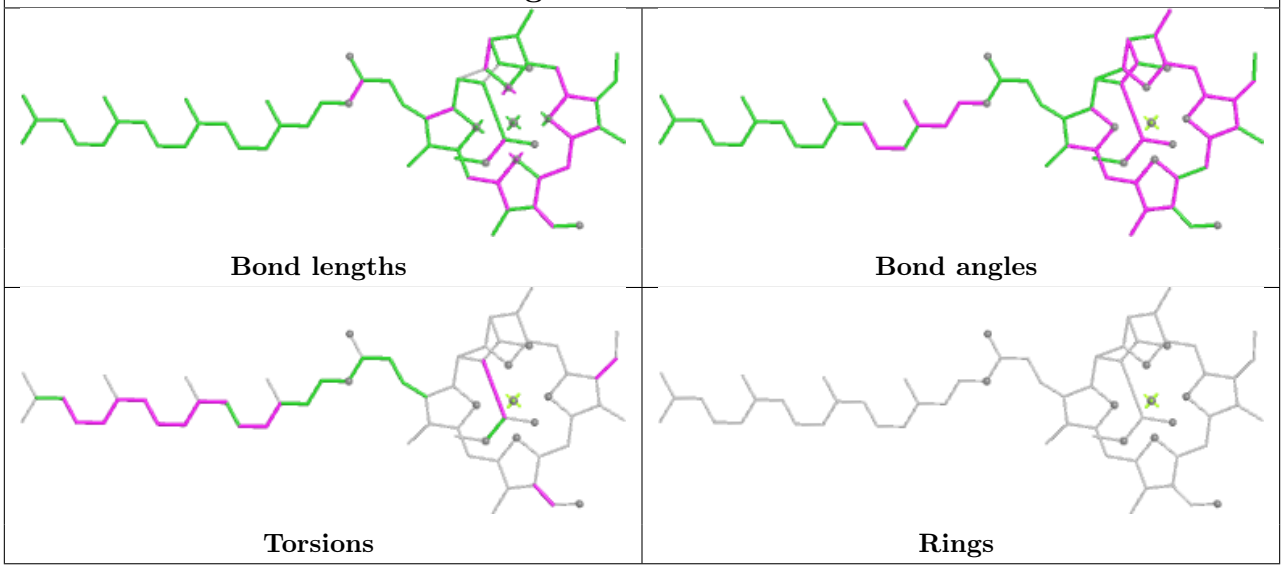


Torsions

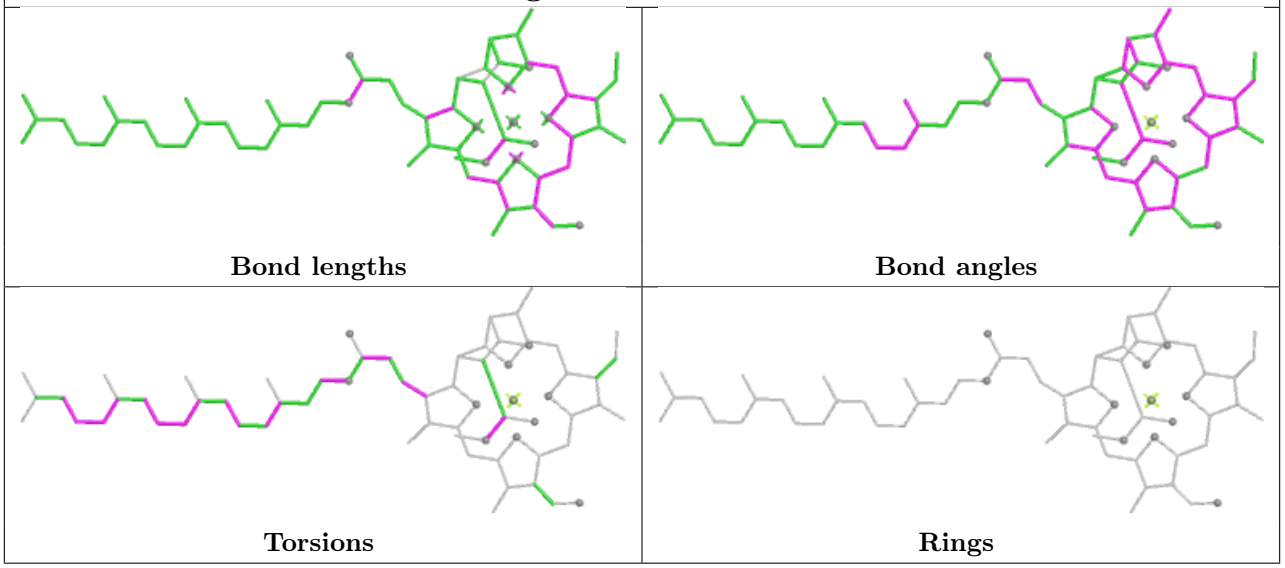


Rings

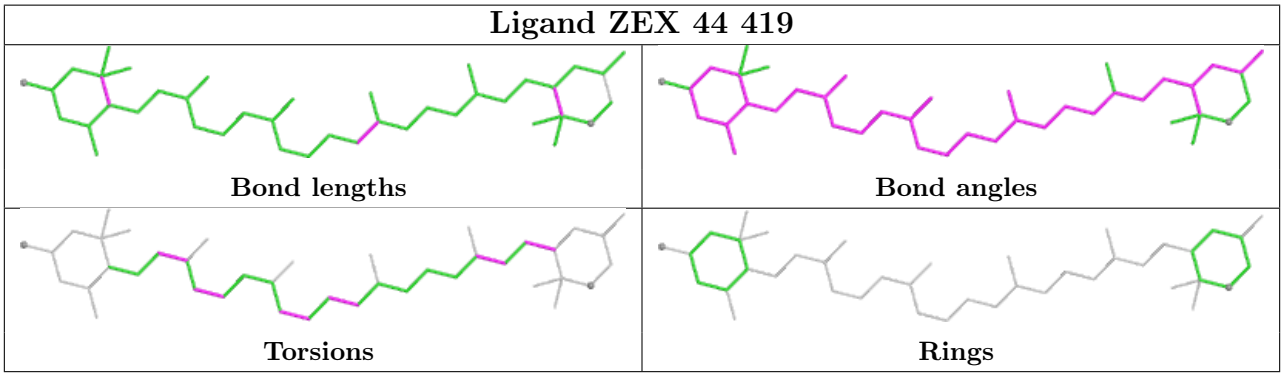
Ligand CL7 12 505

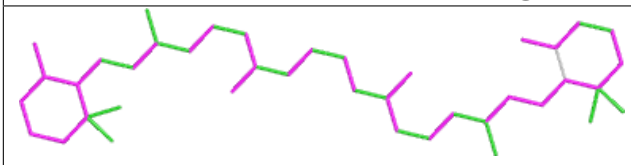
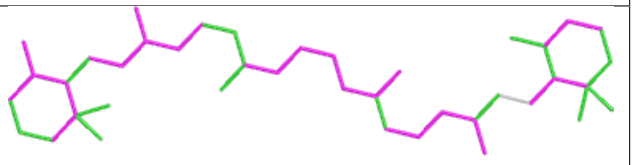
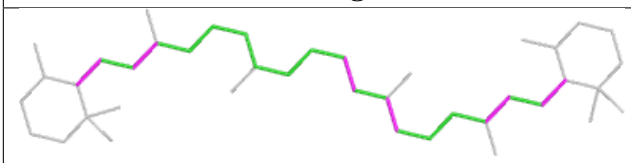
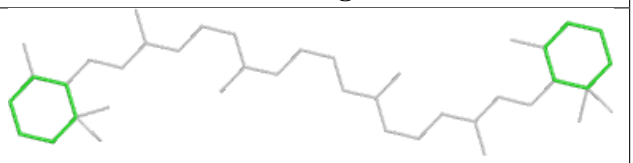


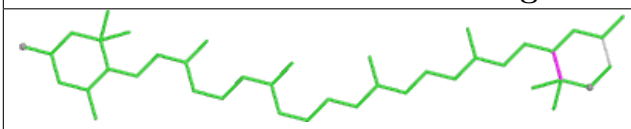
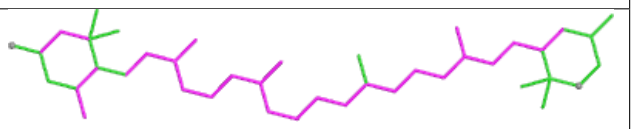
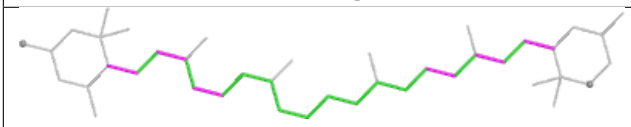
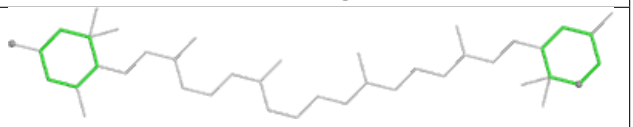
Ligand CL7 34 412



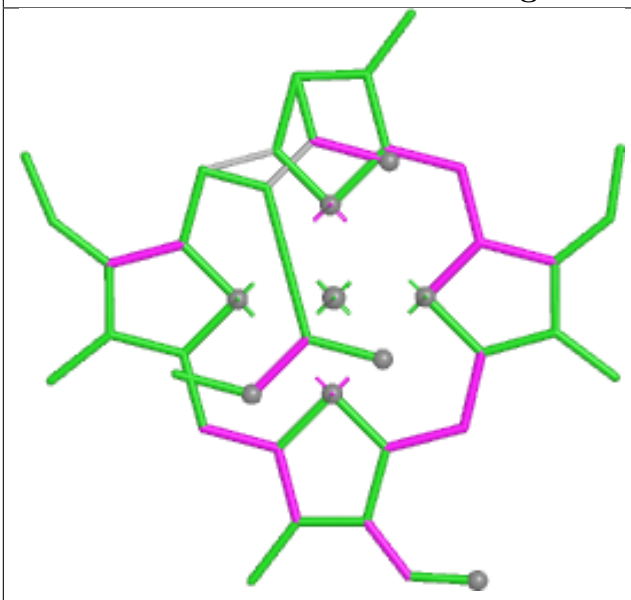
Ligand ZEX 44 419



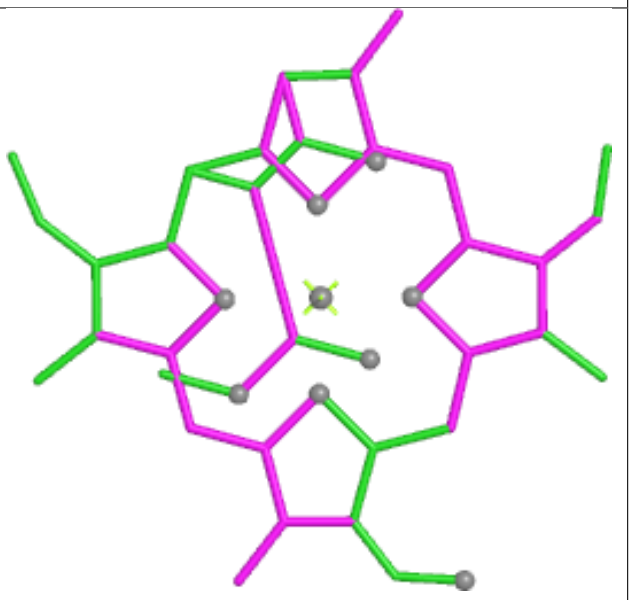
Ligand 8CT 4K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ZEX 14 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

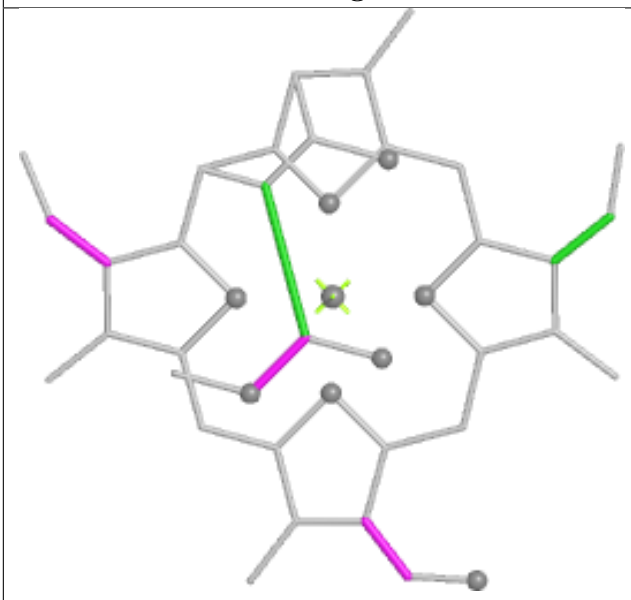
Ligand CL7 1C 511



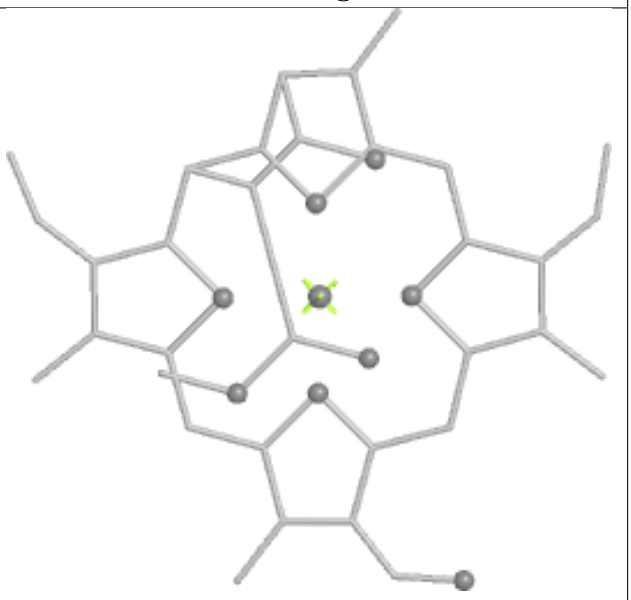
Bond lengths



Bond angles

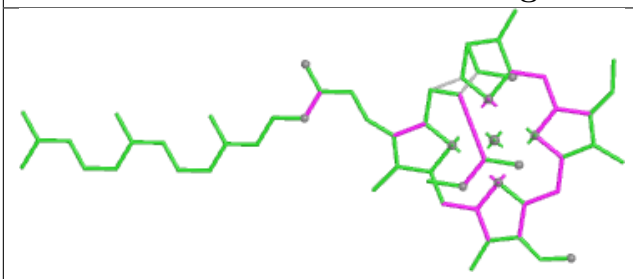


Torsions

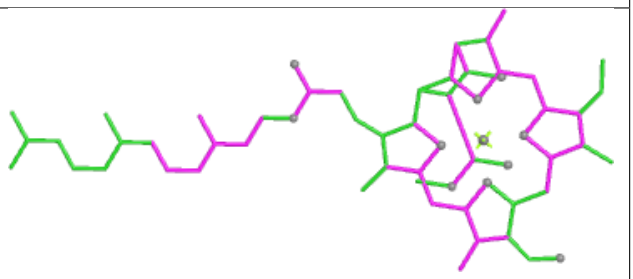


Rings

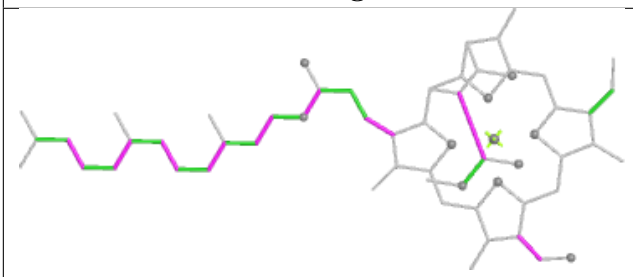
Ligand CL7 1C 506



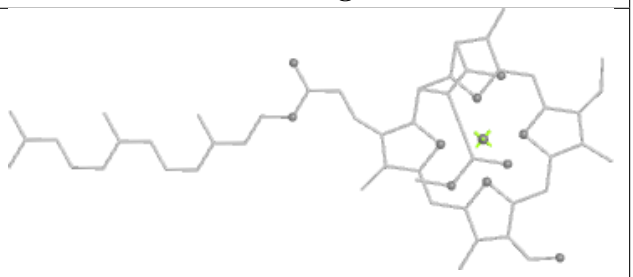
Bond lengths



Bond angles

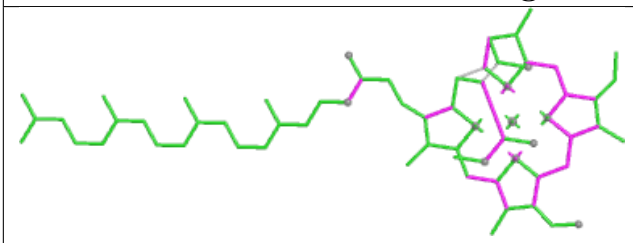


Torsions

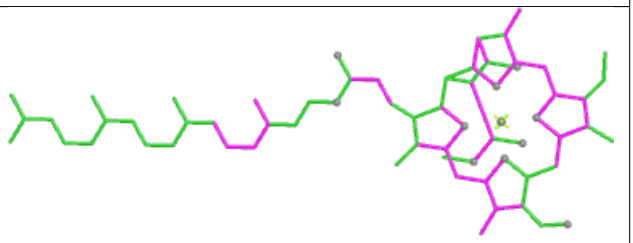


Rings

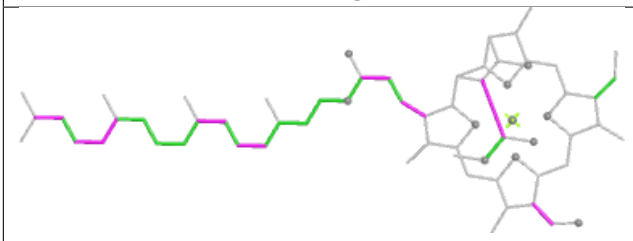
Ligand CL7 1B 609



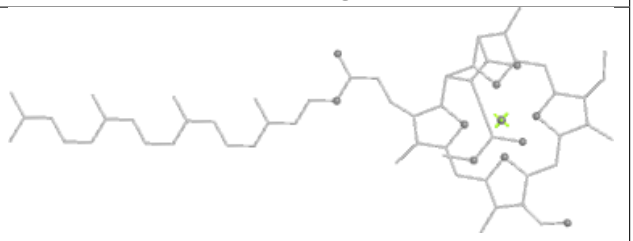
Bond lengths



Bond angles

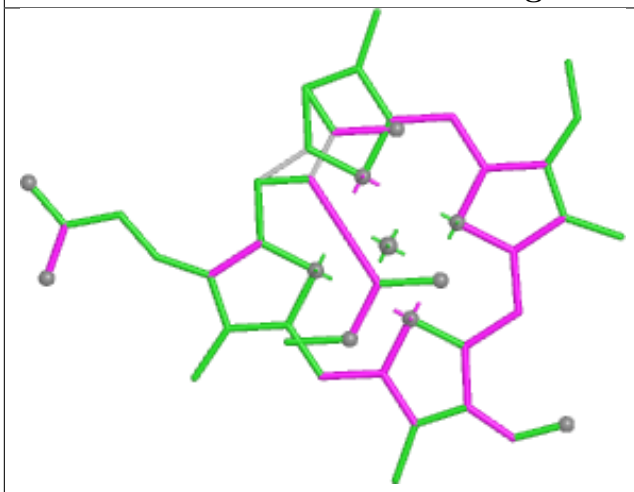


Torsions

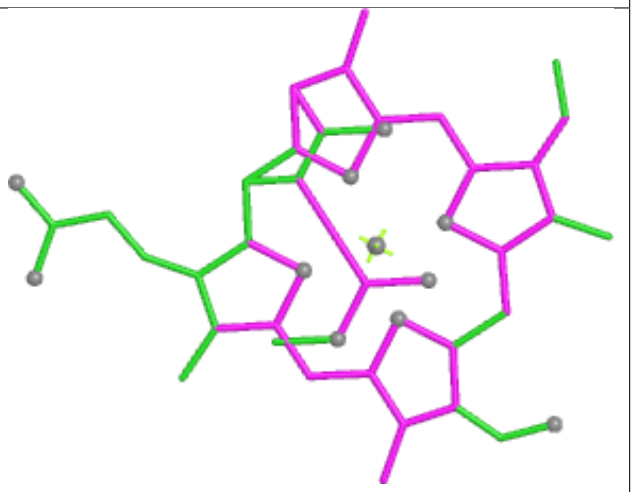


Rings

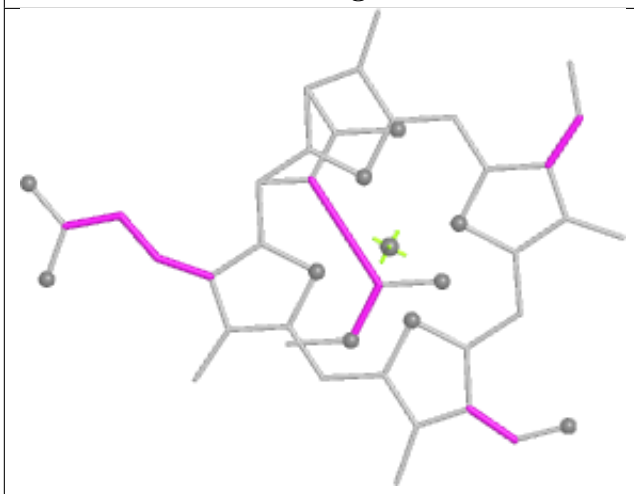
Ligand CL7 24 415



Bond lengths



Bond angles

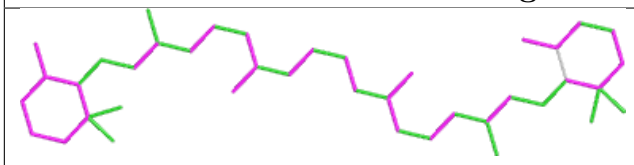


Torsions

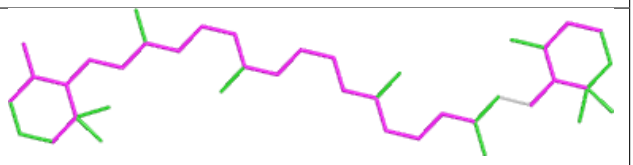


Rings

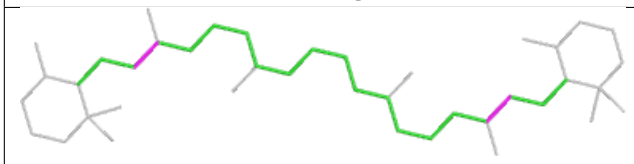
Ligand 8CT 1B 619



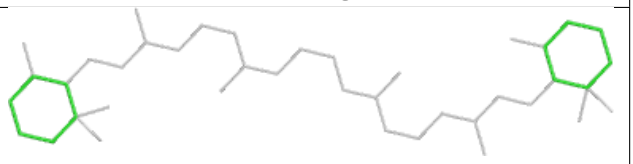
Bond lengths



Bond angles

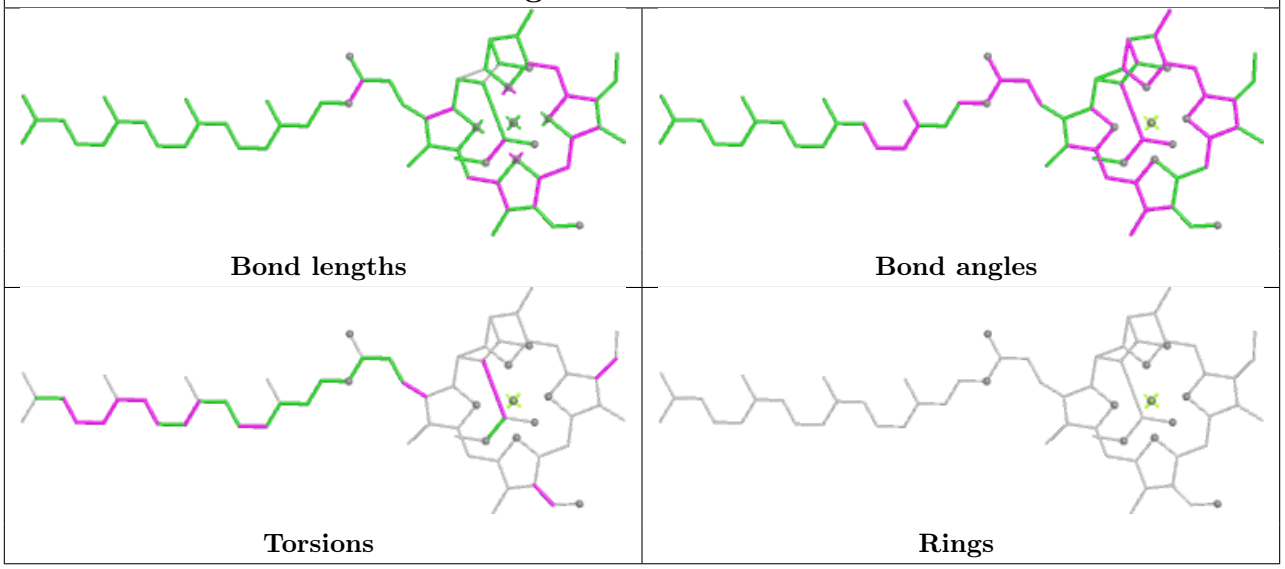


Torsions

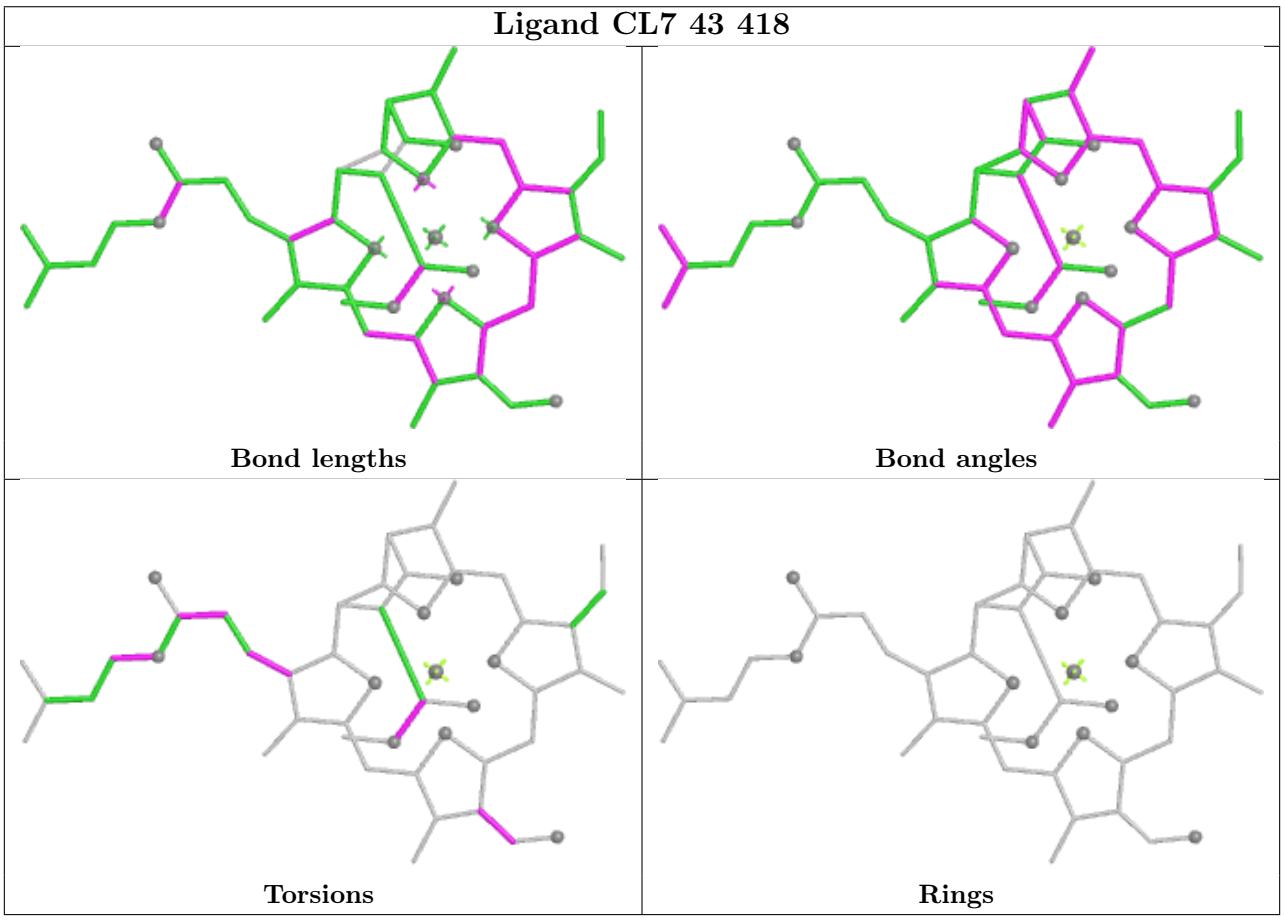


Rings

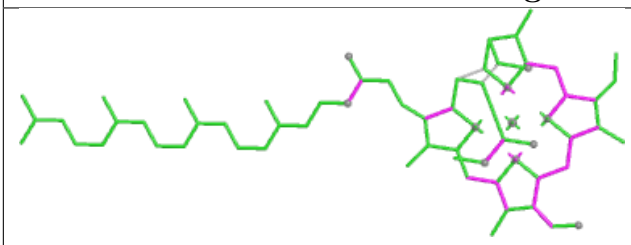
Ligand CL7 31 408



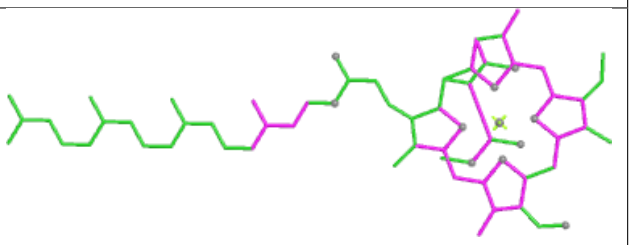
Ligand CL7 43 418



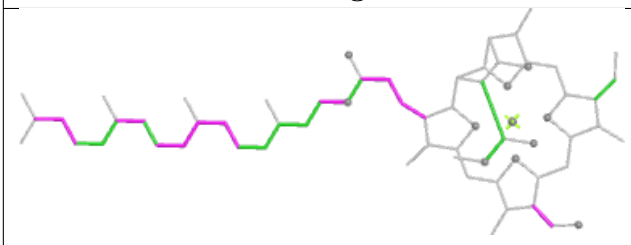
Ligand CL7 12 501



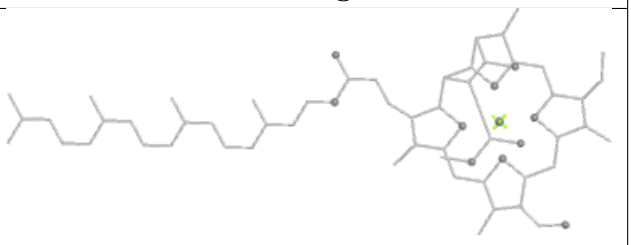
Bond lengths



Bond angles

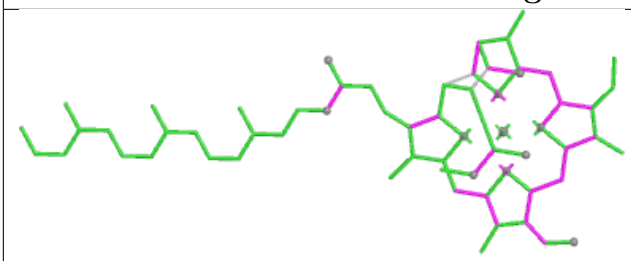


Torsions

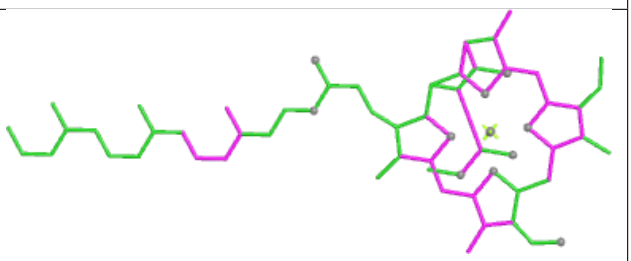


Rings

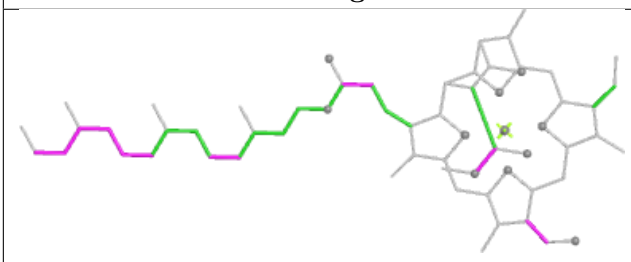
Ligand CL7 21 406



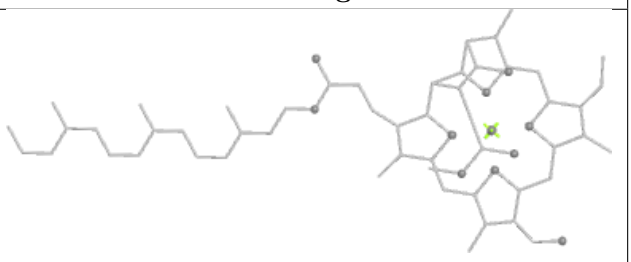
Bond lengths



Bond angles

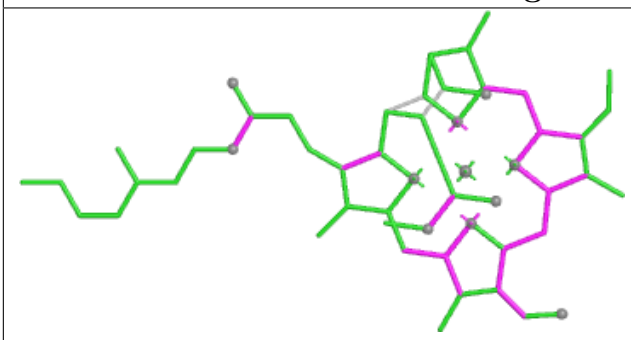


Torsions

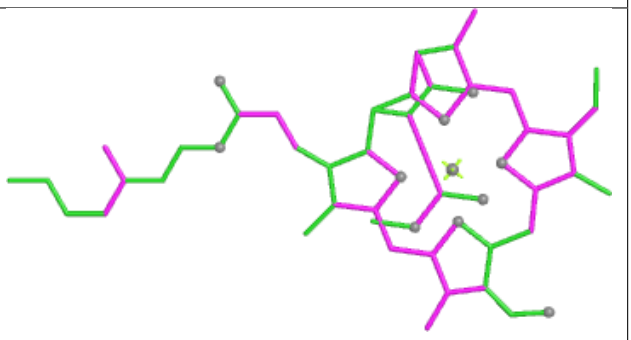


Rings

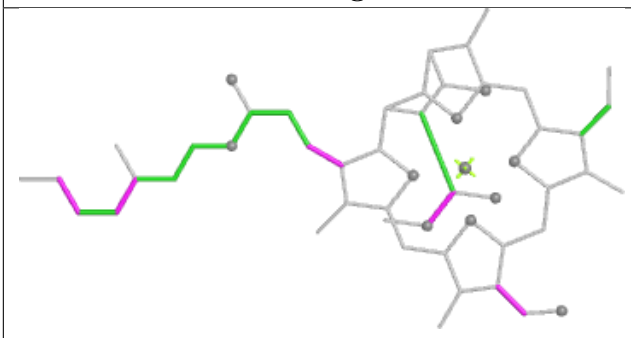
Ligand CL7 44 414



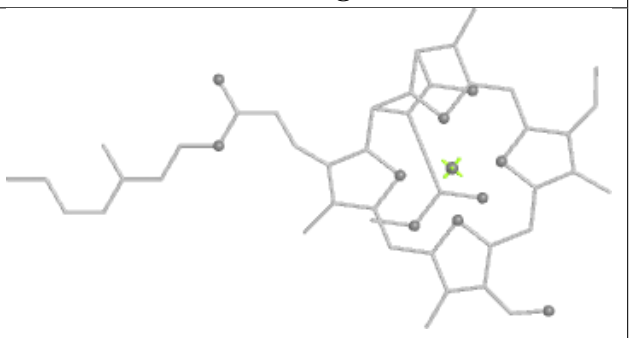
Bond lengths



Bond angles

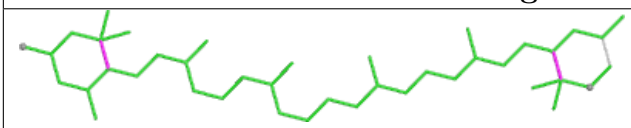


Torsions

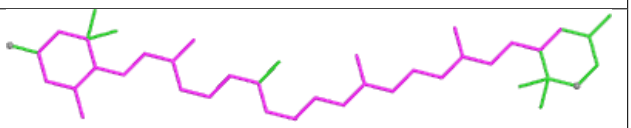


Rings

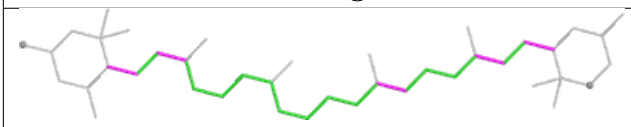
Ligand ZEX 33 520



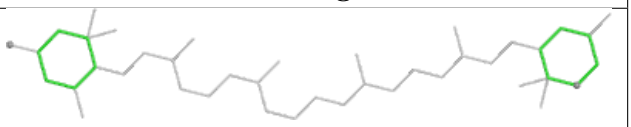
Bond lengths



Bond angles

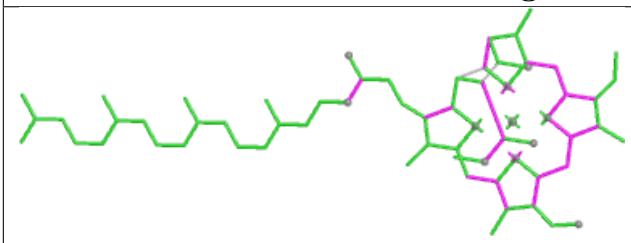


Torsions

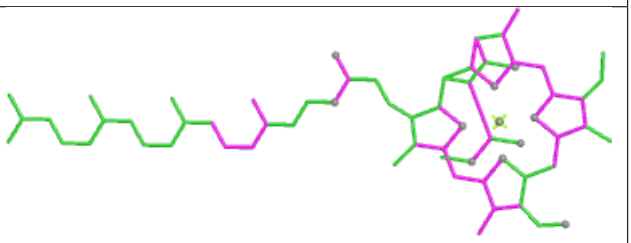


Rings

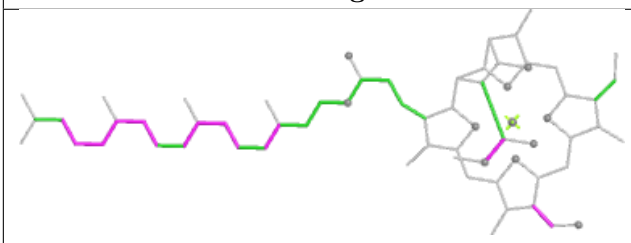
Ligand CL7 3B 611



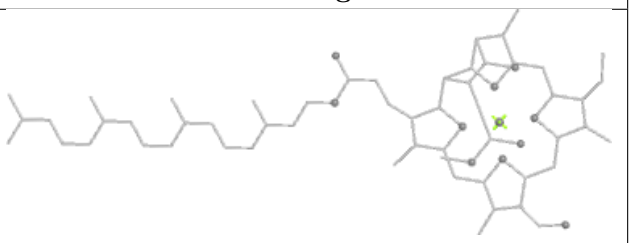
Bond lengths



Bond angles

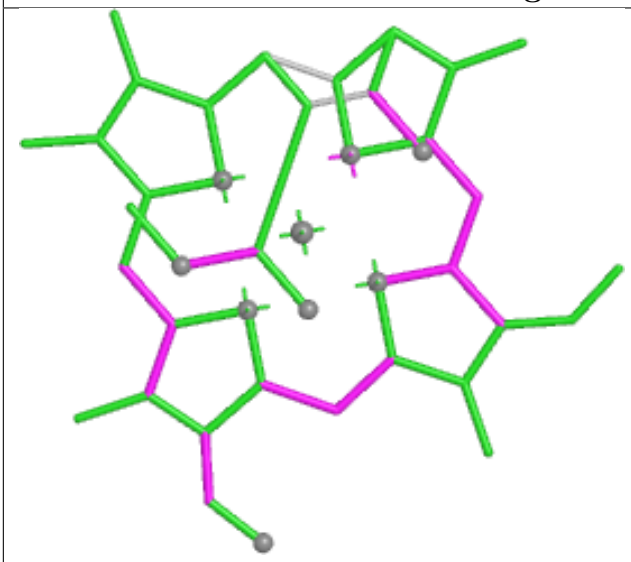


Torsions

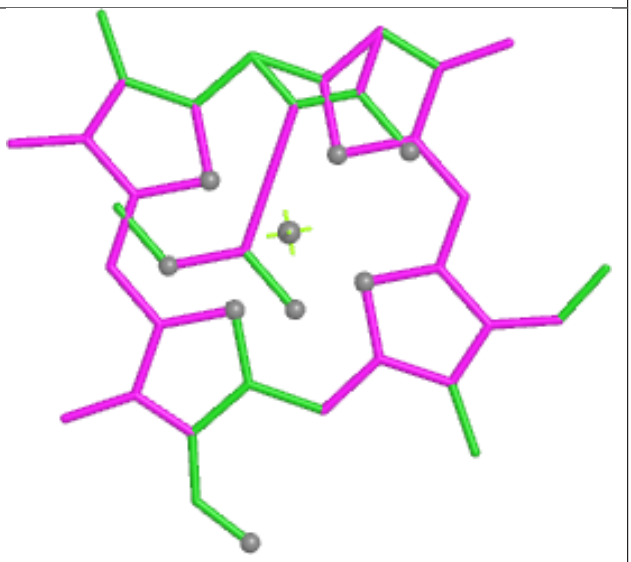


Rings

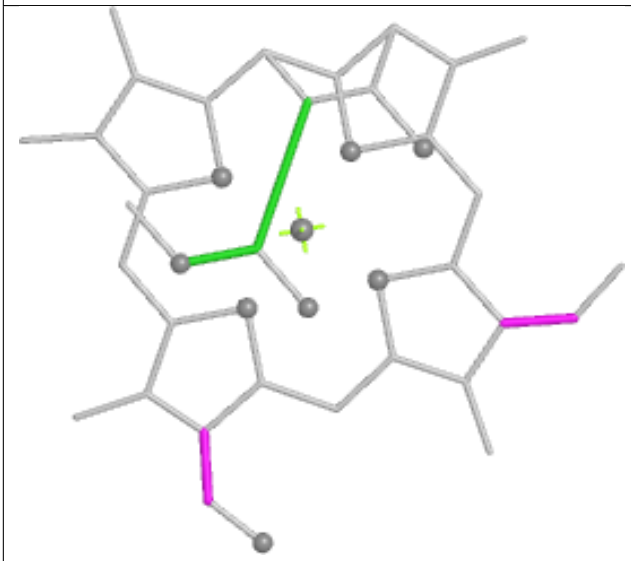
Ligand CL7 21 414



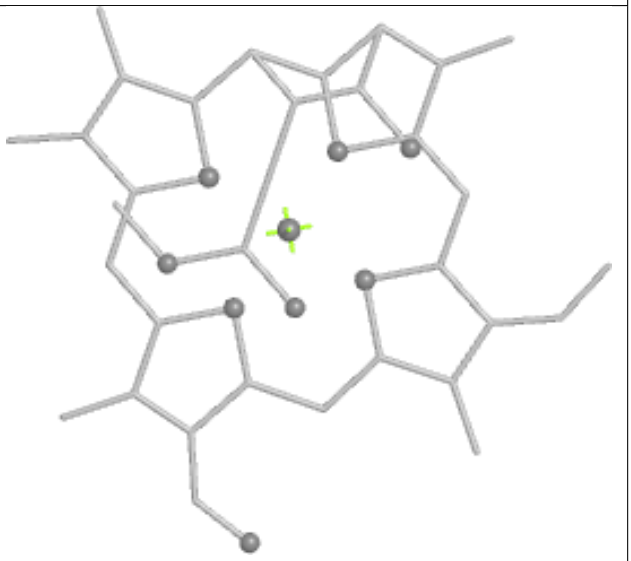
Bond lengths



Bond angles

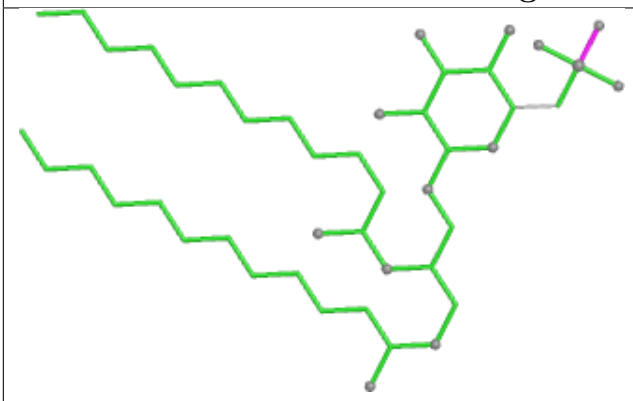


Torsions

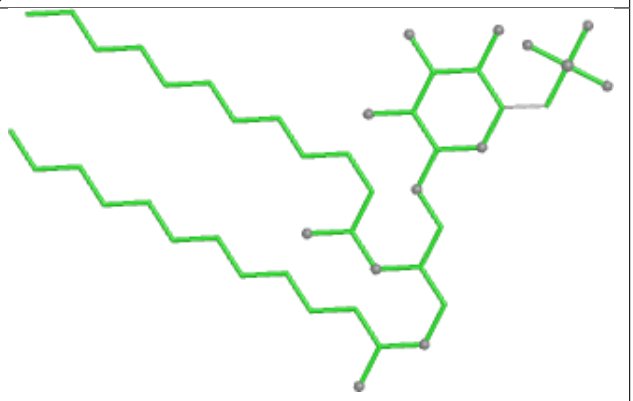


Rings

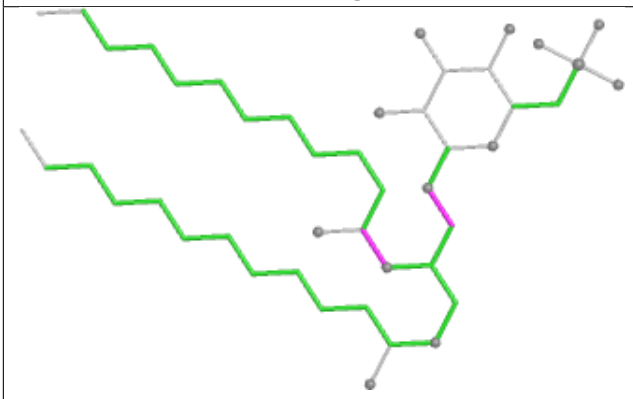
Ligand SQD 23 422



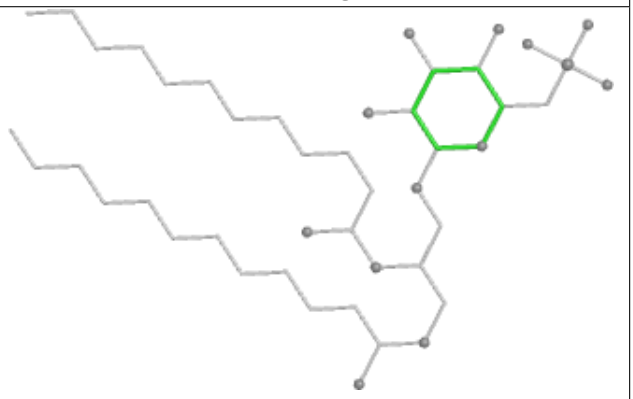
Bond lengths



Bond angles

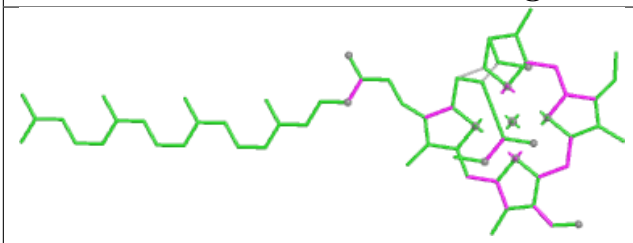


Torsions

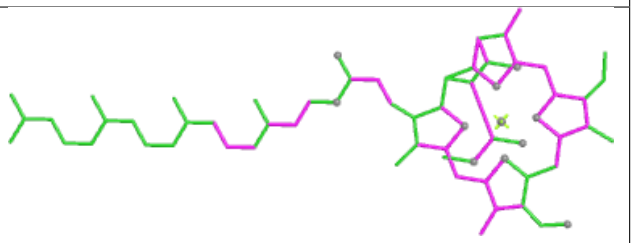


Rings

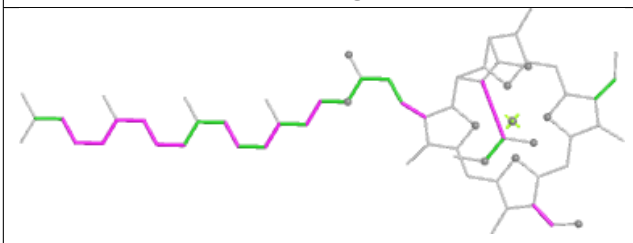
Ligand CL7 21 404



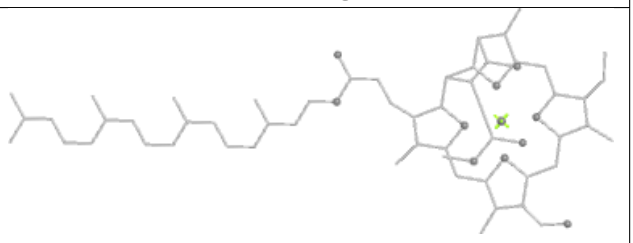
Bond lengths



Bond angles

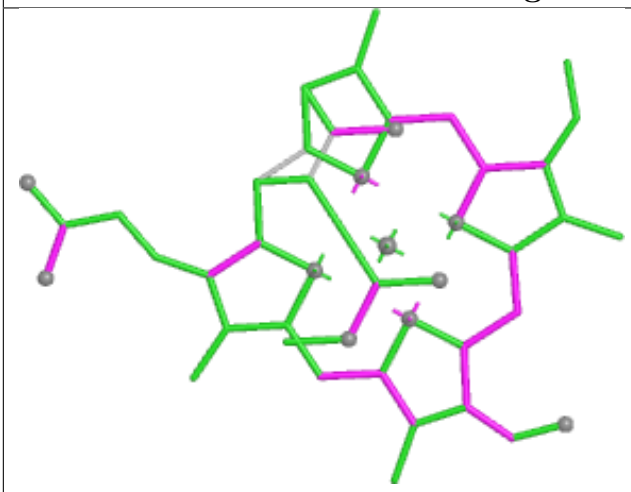


Torsions

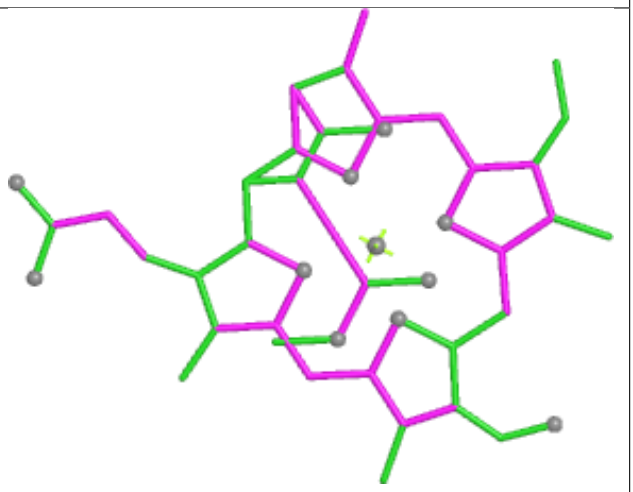


Rings

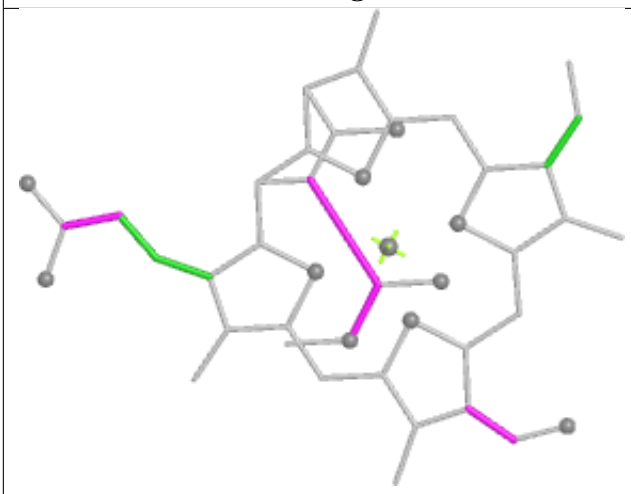
Ligand CL7 31 411



Bond lengths



Bond angles

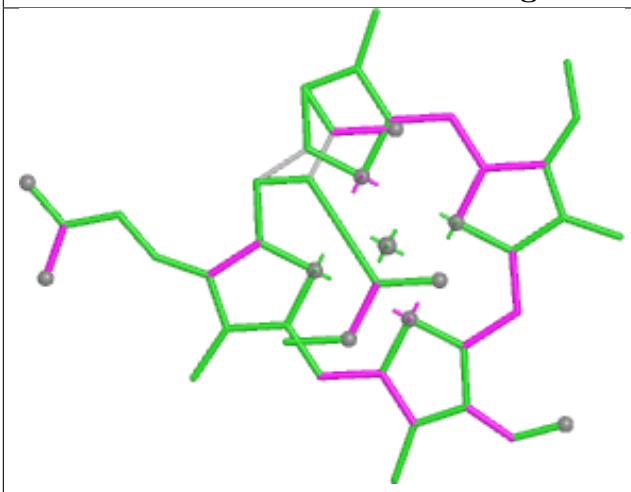


Torsions

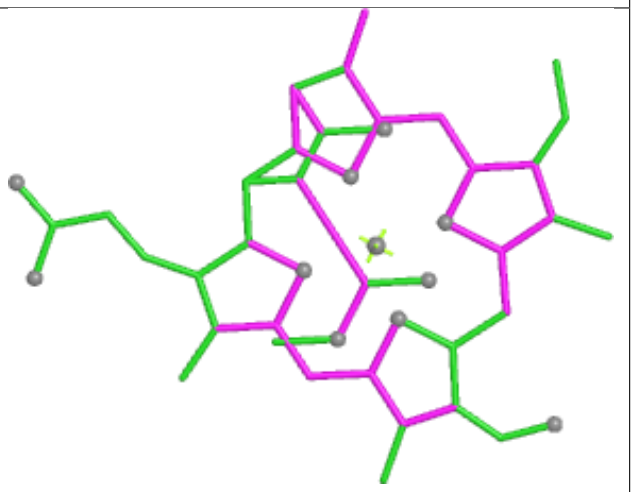


Rings

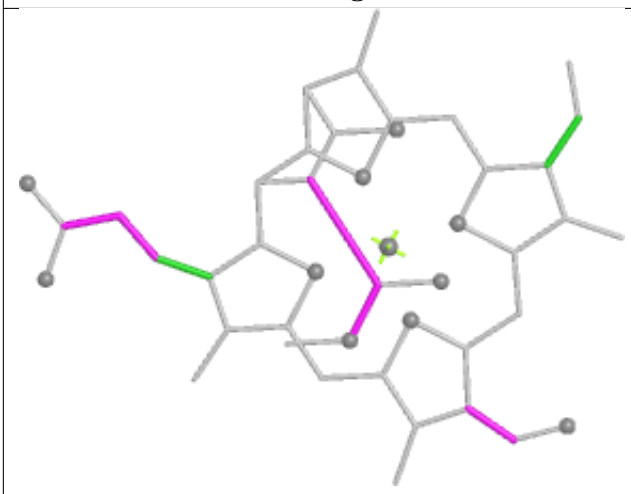
Ligand CL7 1B 622



Bond lengths



Bond angles

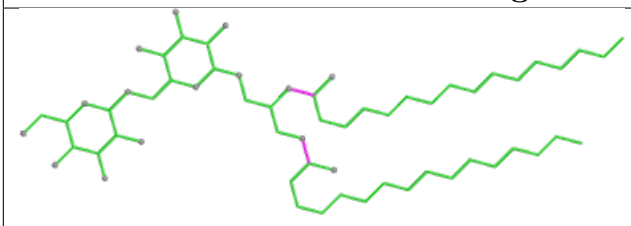


Torsions

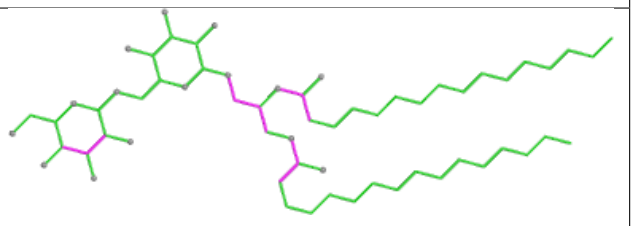


Rings

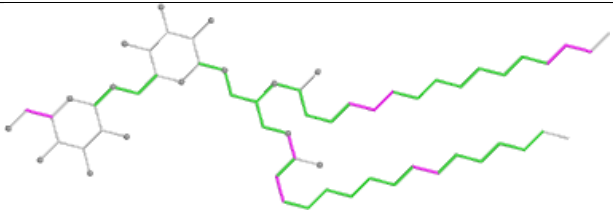
Ligand DGD 3C 516



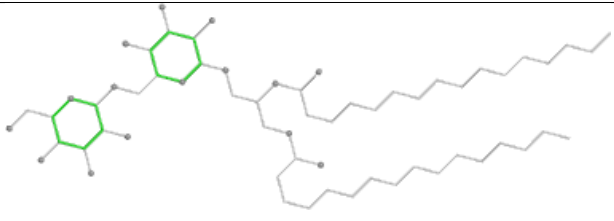
Bond lengths



Bond angles

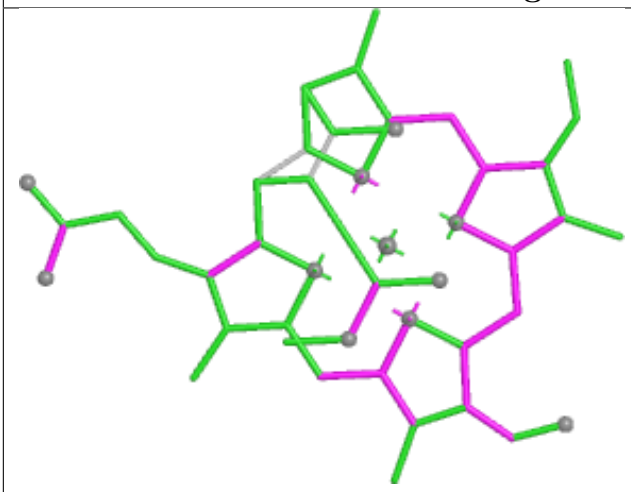


Torsions

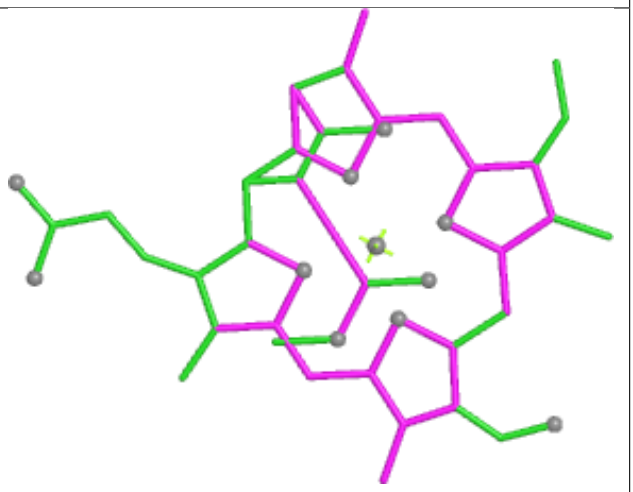


Rings

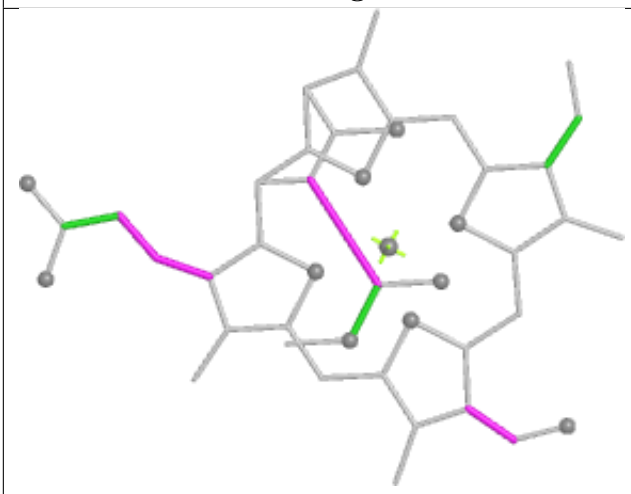
Ligand CL7 22 508



Bond lengths



Bond angles

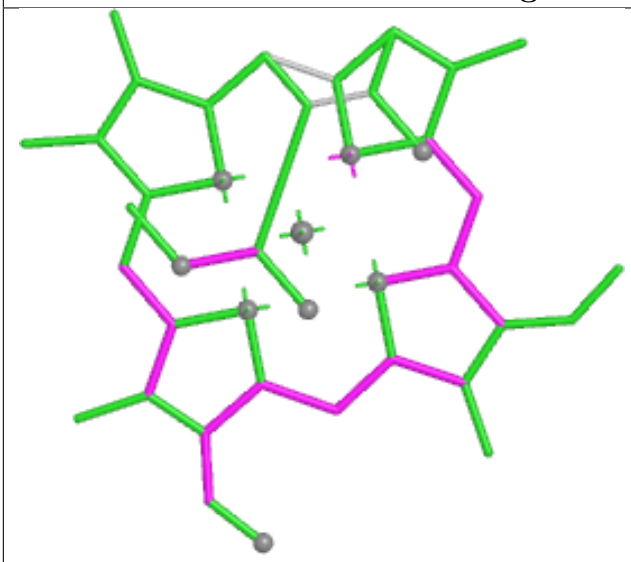


Torsions

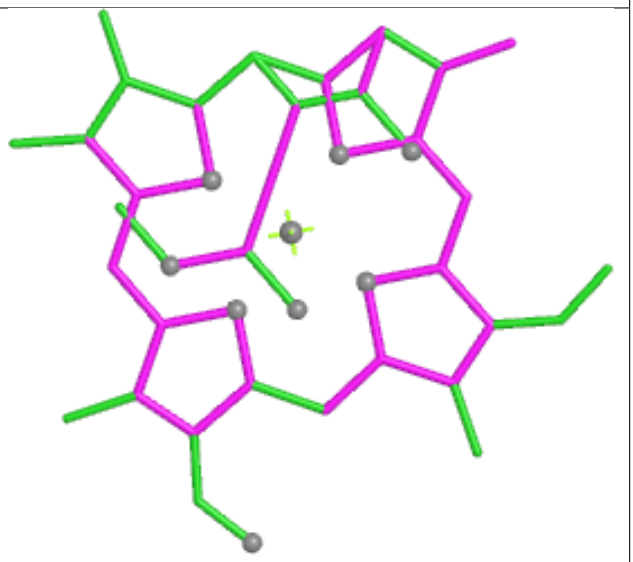


Rings

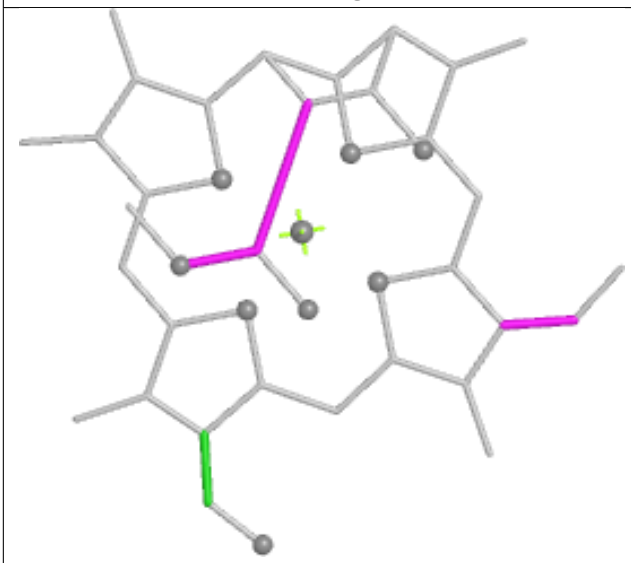
Ligand CL7 1B 601



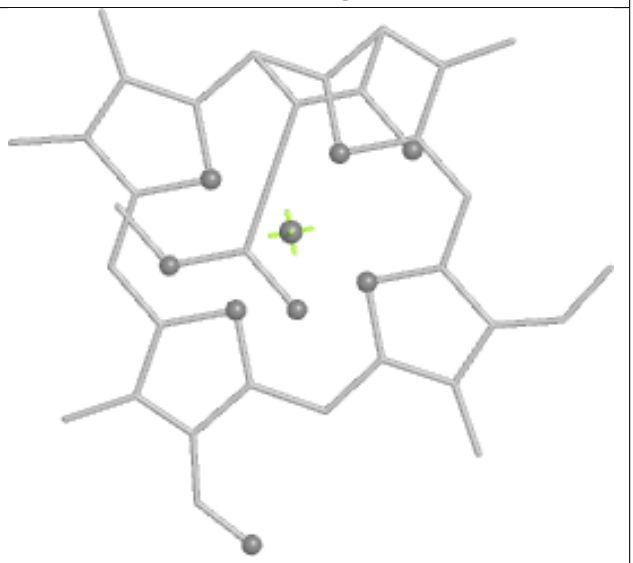
Bond lengths



Bond angles

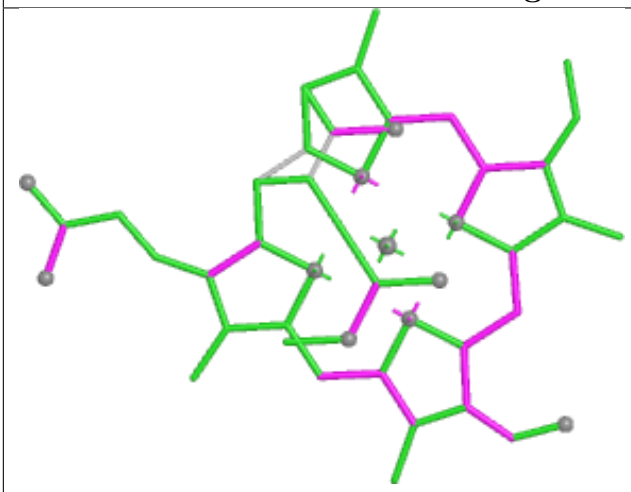


Torsions

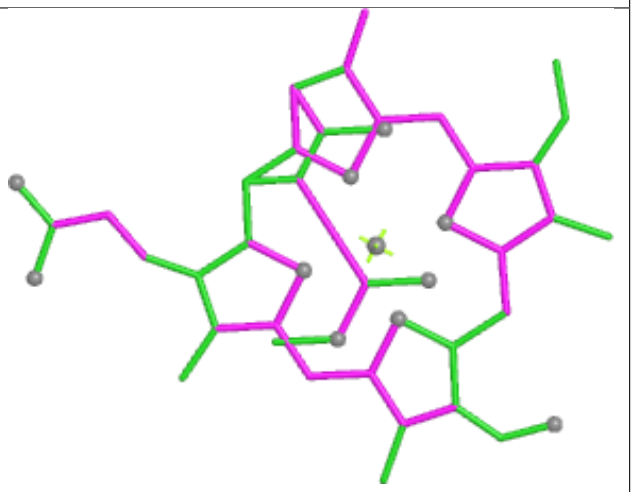


Rings

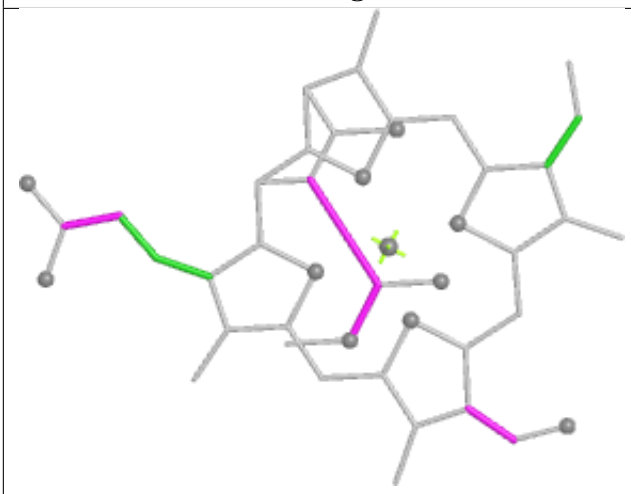
Ligand CL7 21 411



Bond lengths



Bond angles

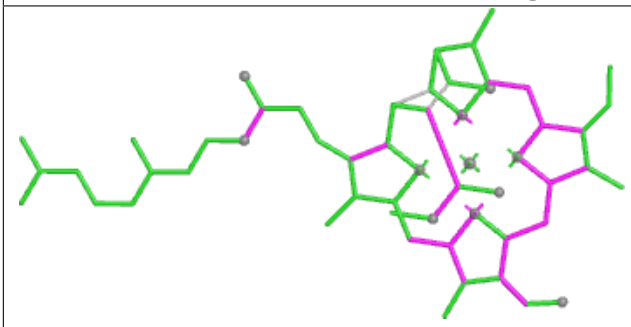


Torsions

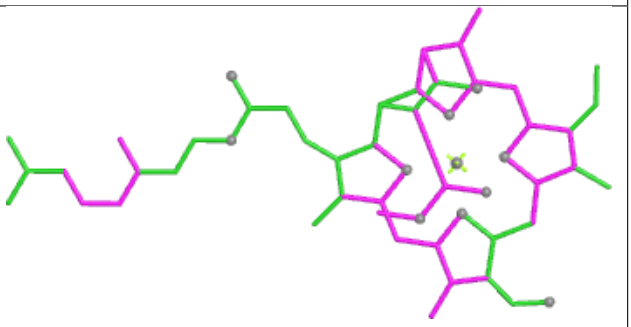


Rings

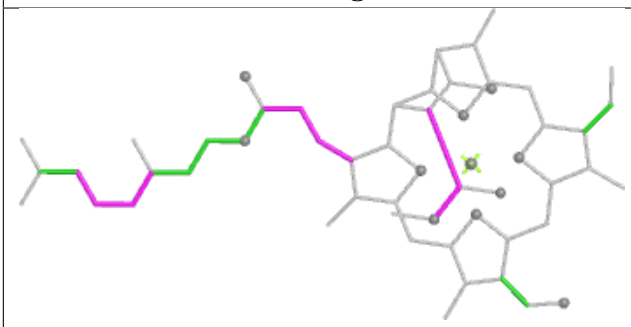
Ligand CL7 33 512



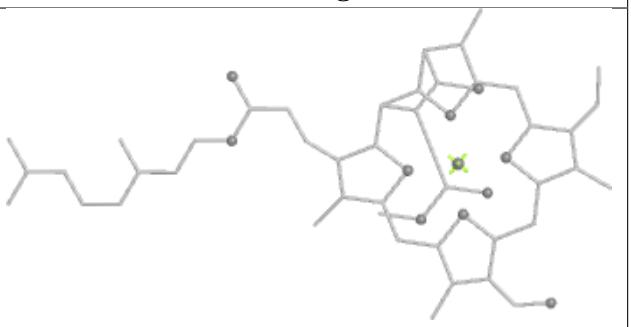
Bond lengths



Bond angles

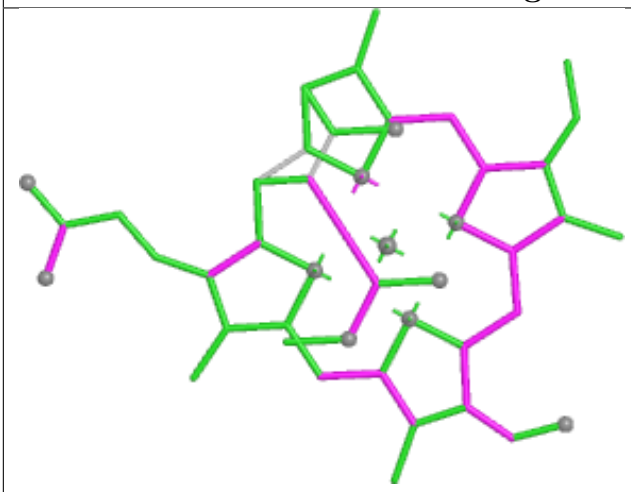


Torsions

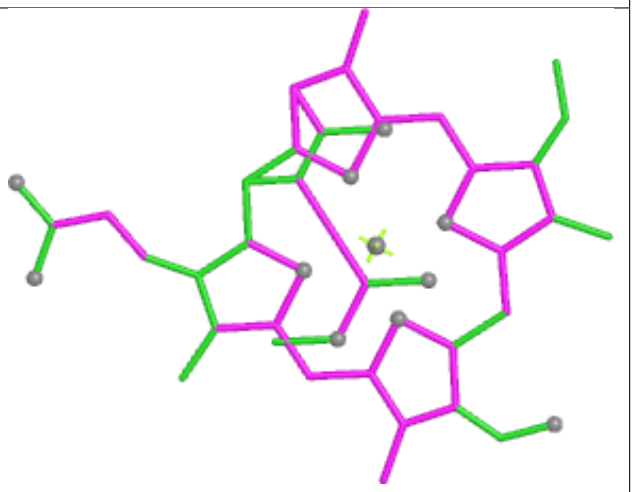


Rings

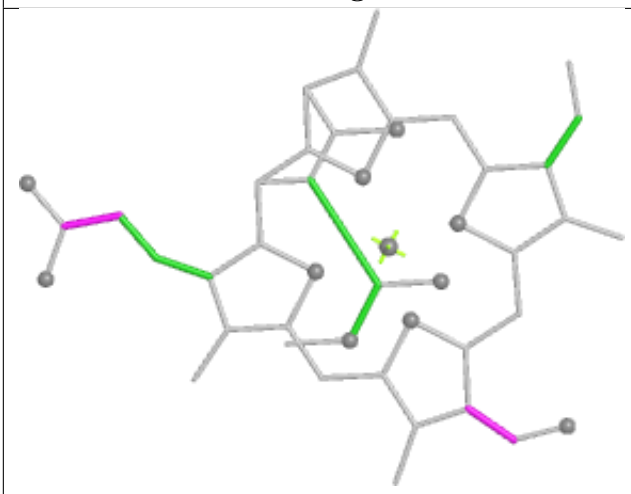
Ligand CL7 14 408



Bond lengths



Bond angles

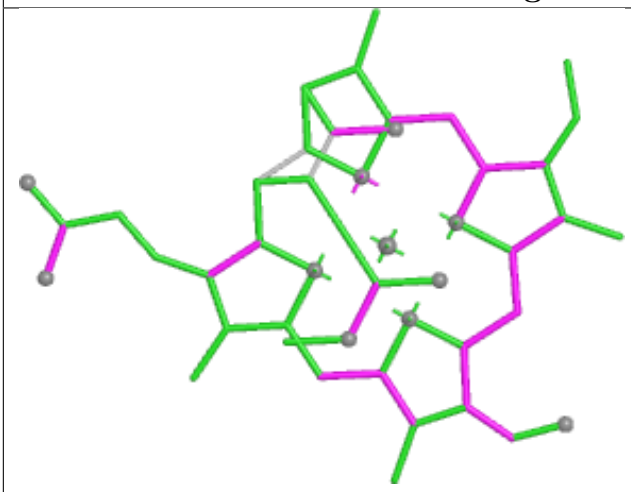


Torsions

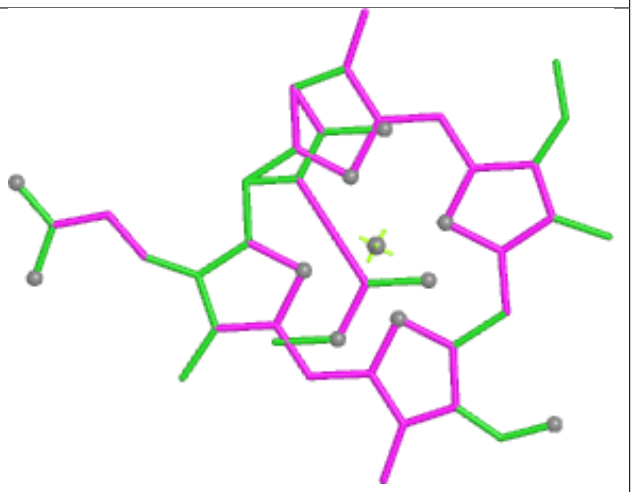


Rings

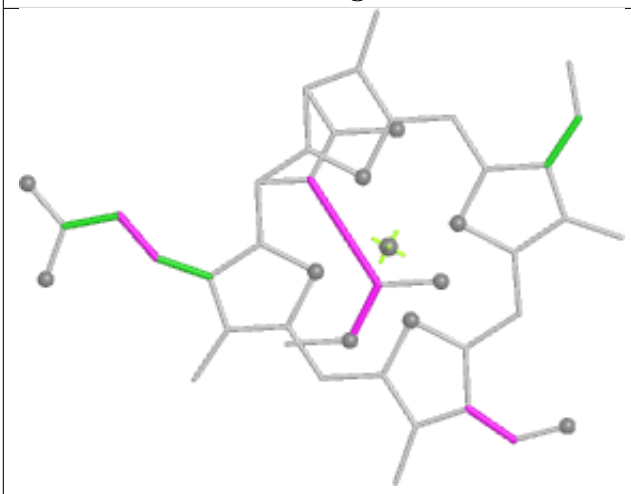
Ligand CL7 21 409



Bond lengths



Bond angles

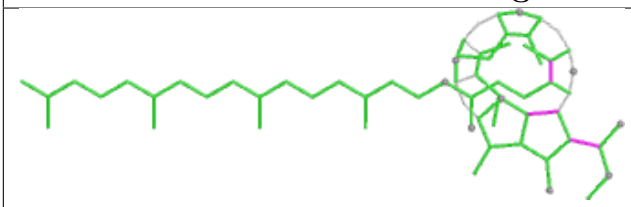


Torsions

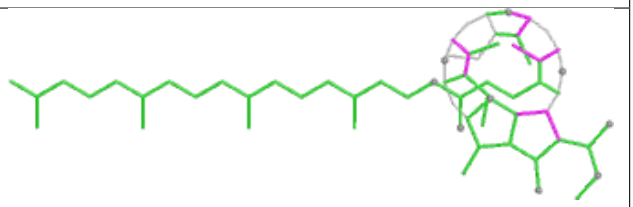


Rings

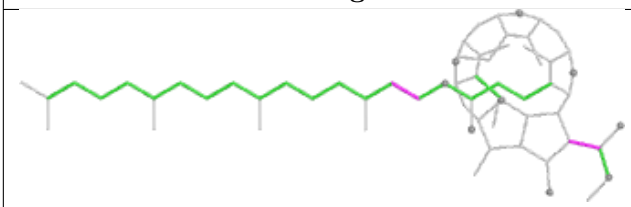
Ligand PHO 4A 402



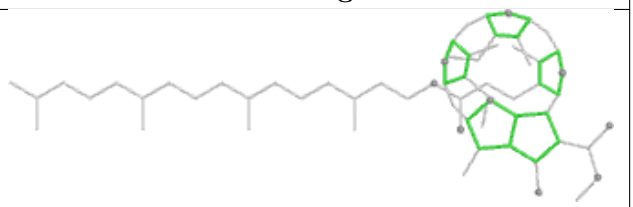
Bond lengths



Bond angles

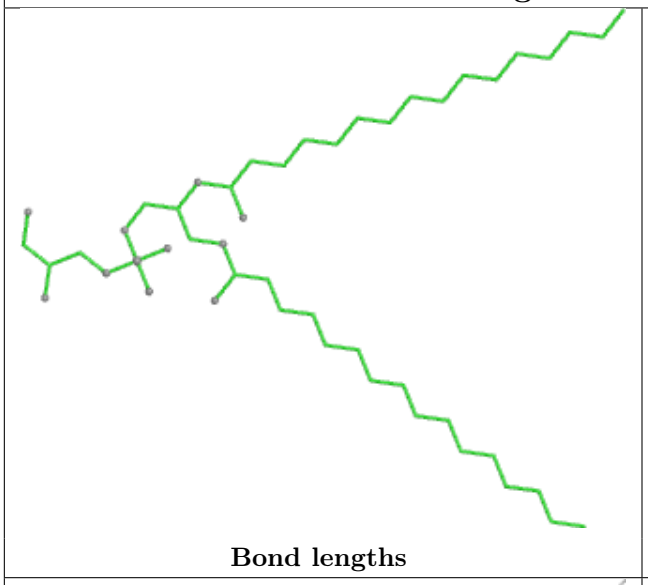


Torsions

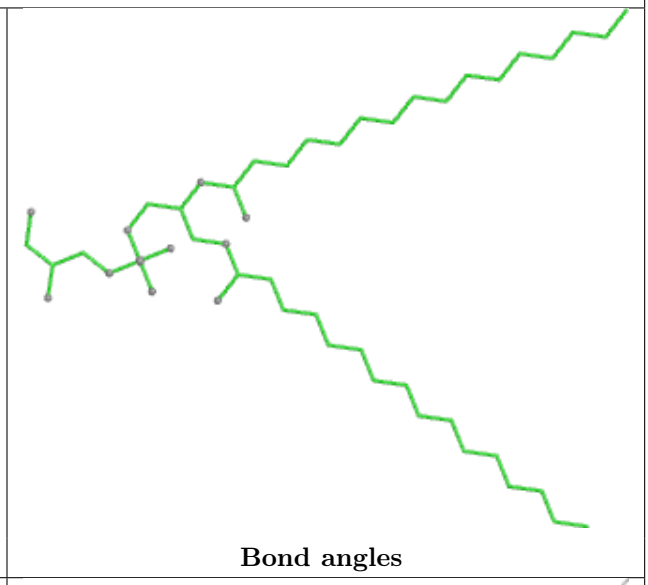


Rings

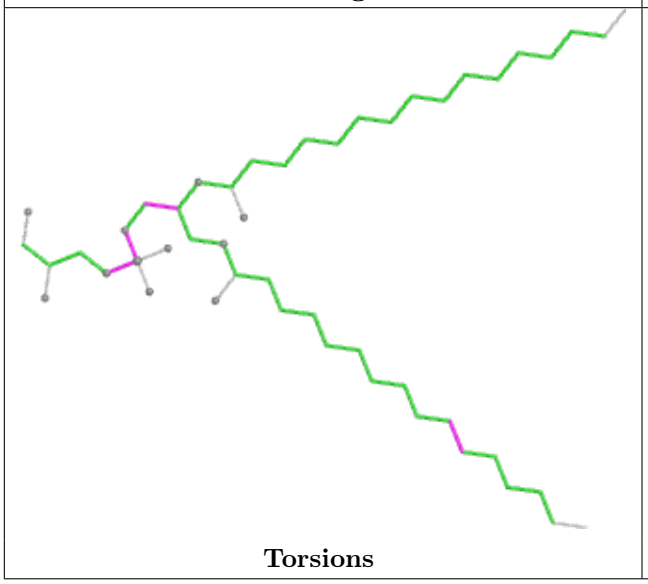
Ligand LHG 1D 409



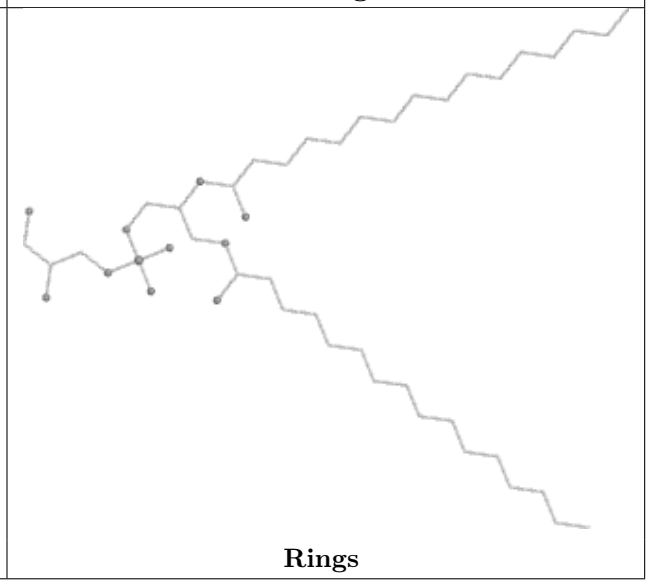
Bond lengths



Bond angles

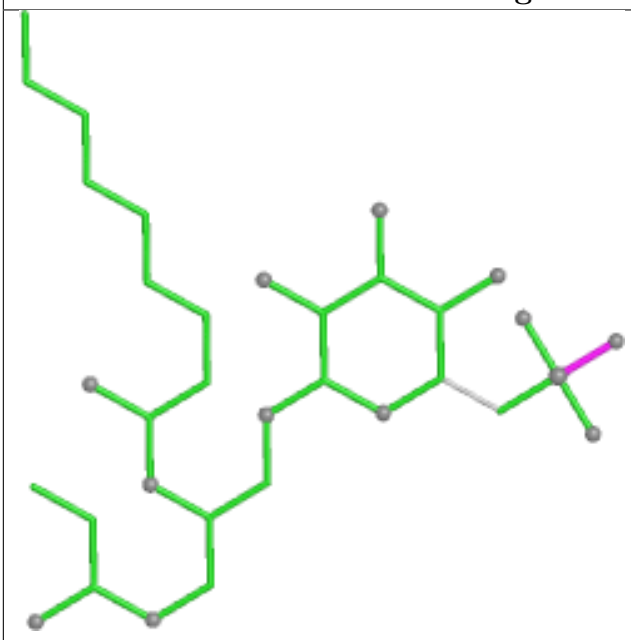


Torsions

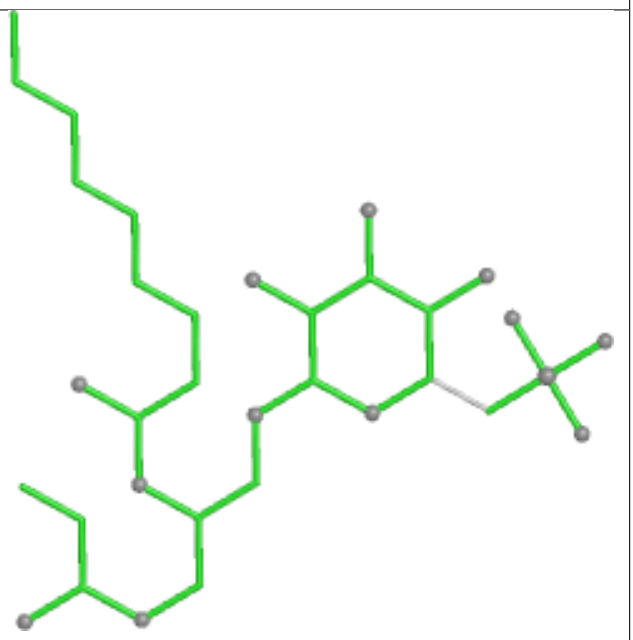


Rings

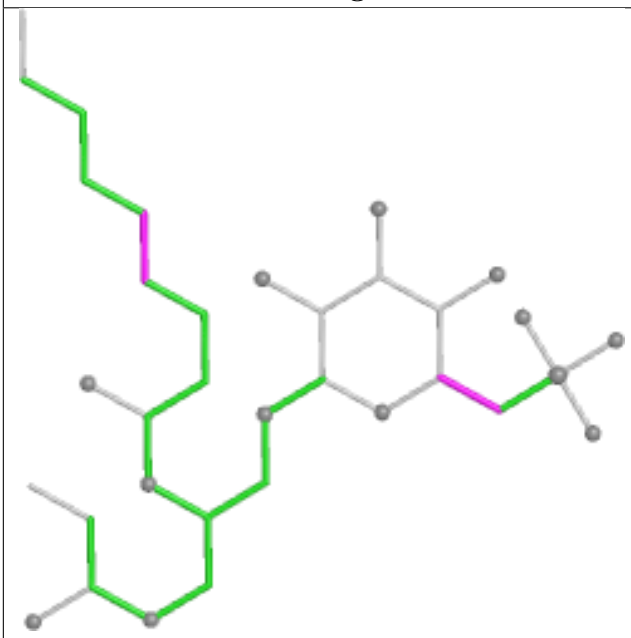
Ligand SQD 3A 406



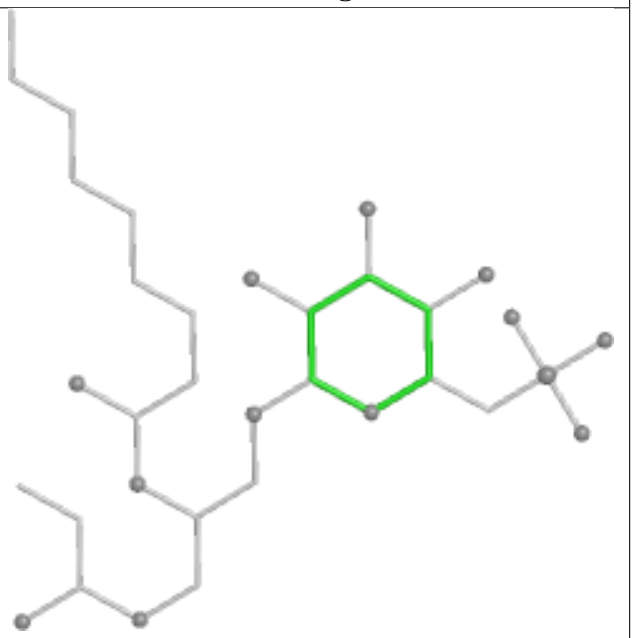
Bond lengths



Bond angles

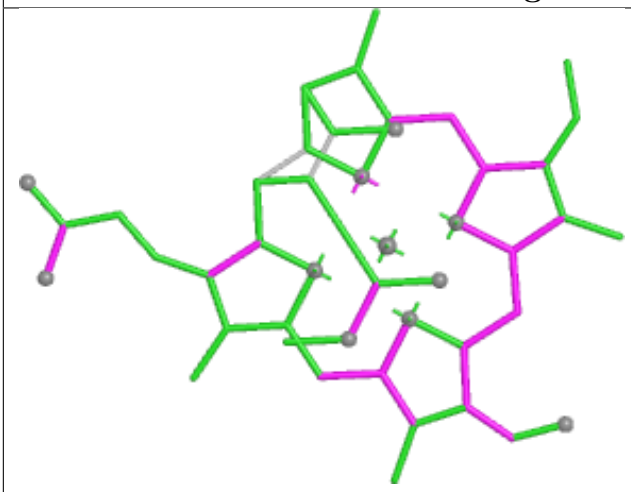


Torsions

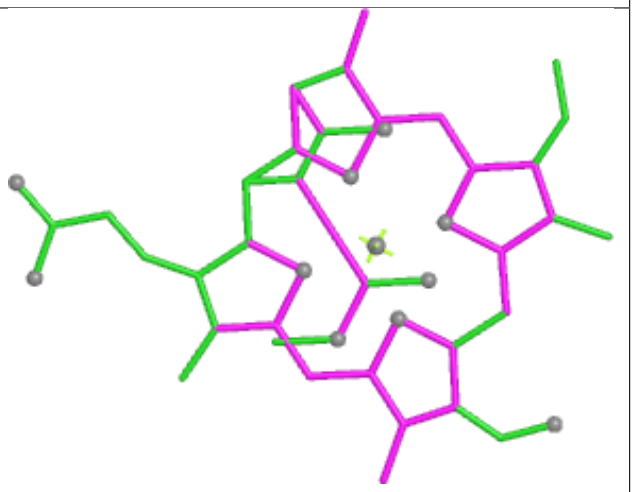


Rings

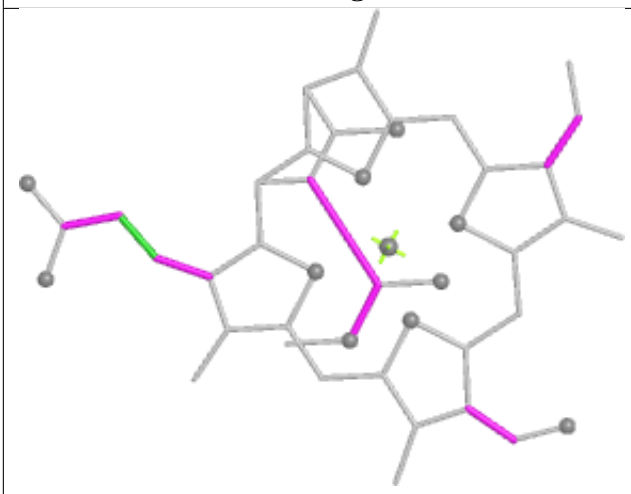
Ligand CL7 23 407



Bond lengths



Bond angles

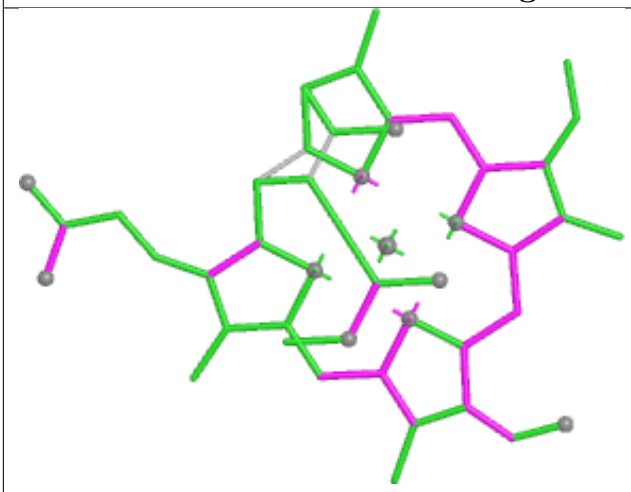


Torsions

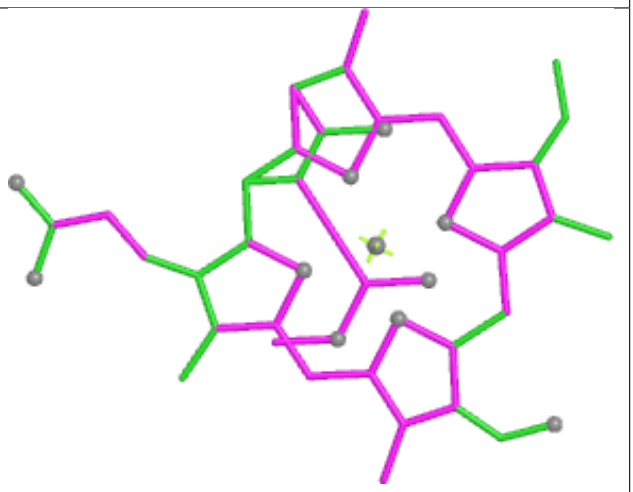


Rings

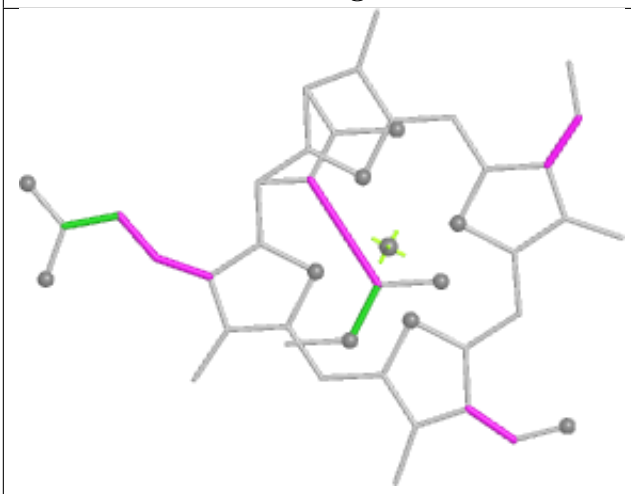
Ligand CL7 1D 405



Bond lengths



Bond angles

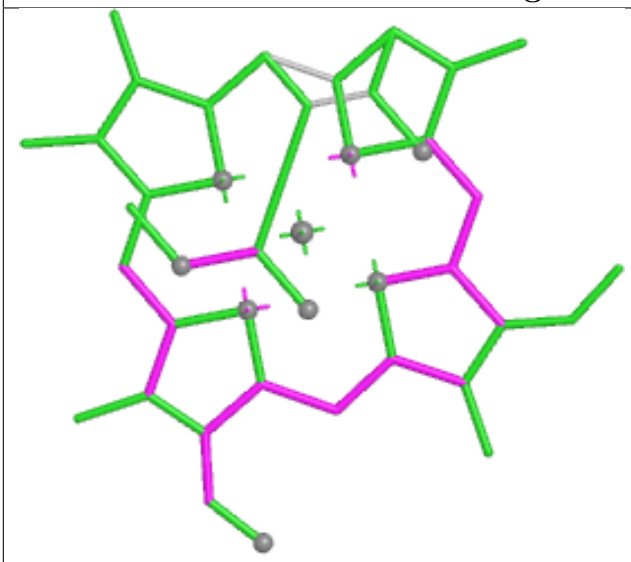


Torsions

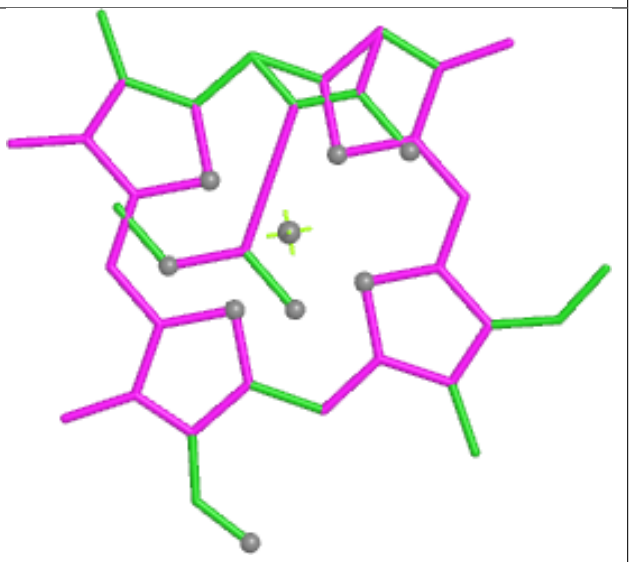


Rings

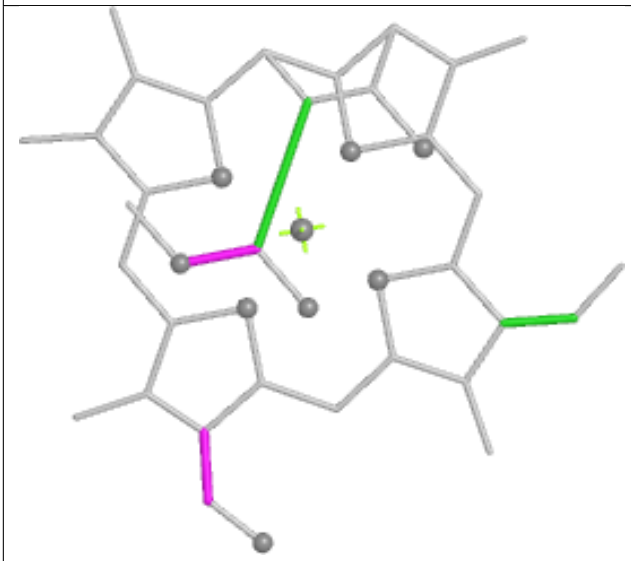
Ligand CL7 21 407



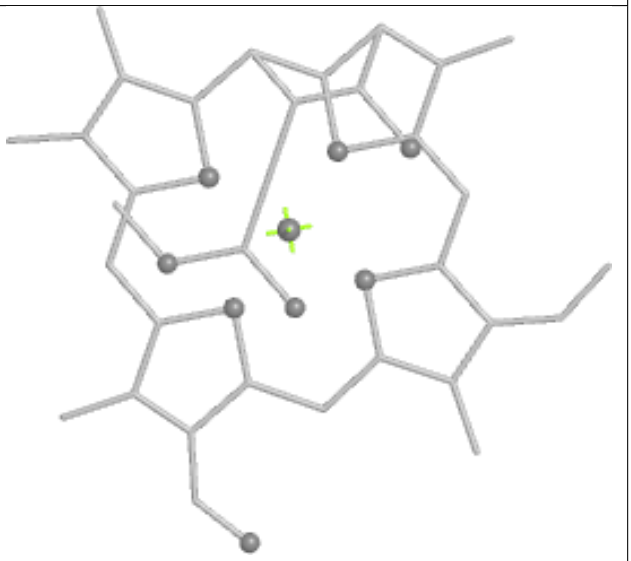
Bond lengths



Bond angles

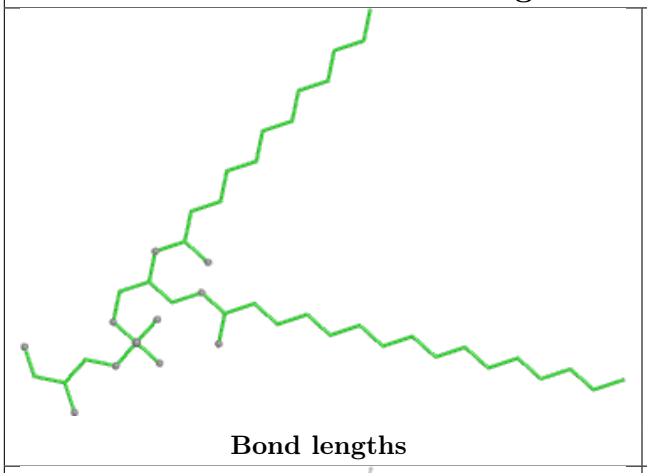


Torsions

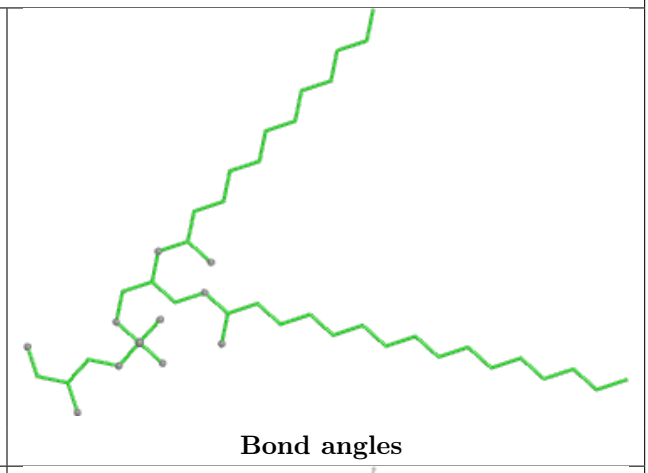


Rings

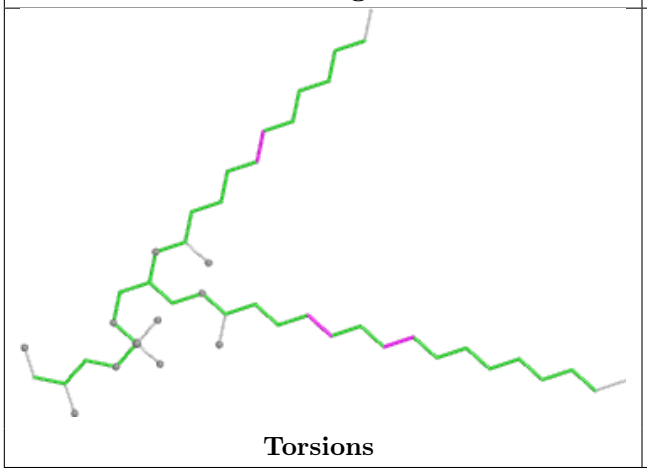
Ligand LHG 3B 623



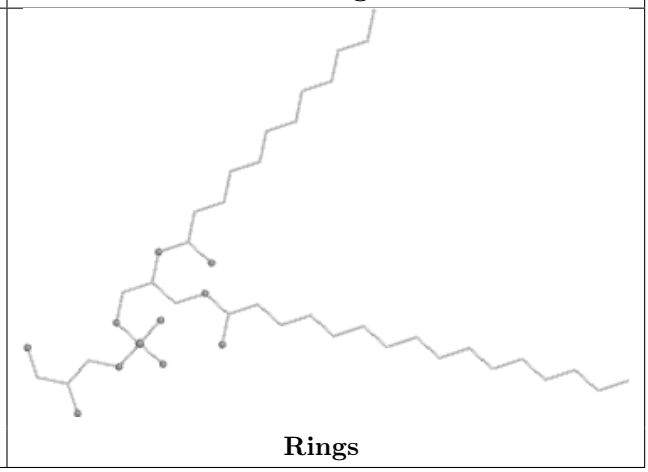
Bond lengths



Bond angles

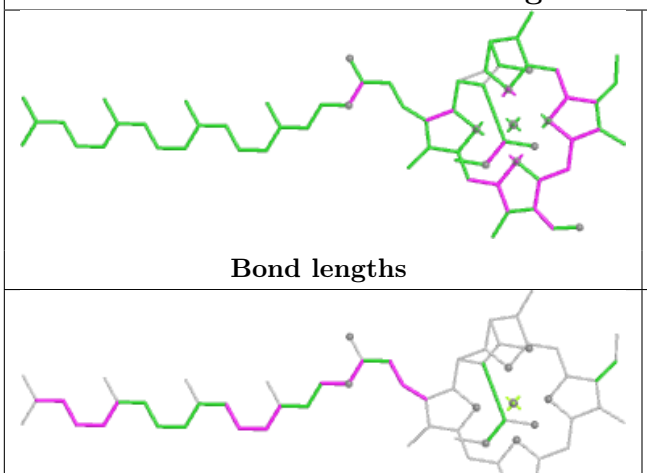


Torsions

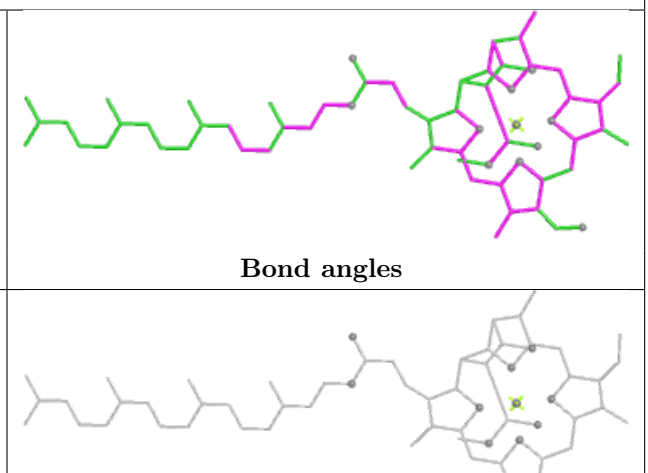


Rings

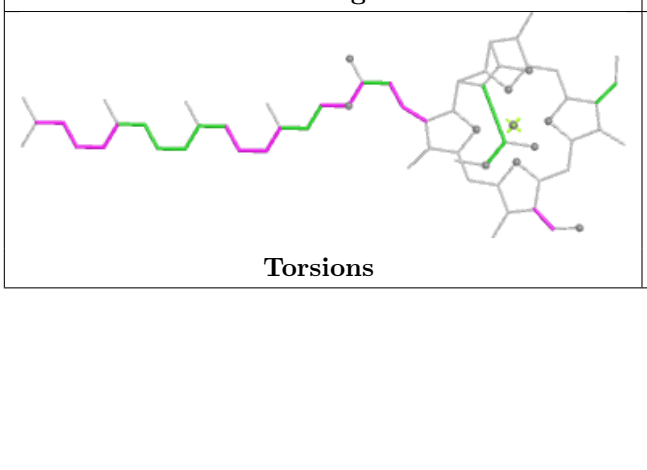
Ligand CL7 12 516



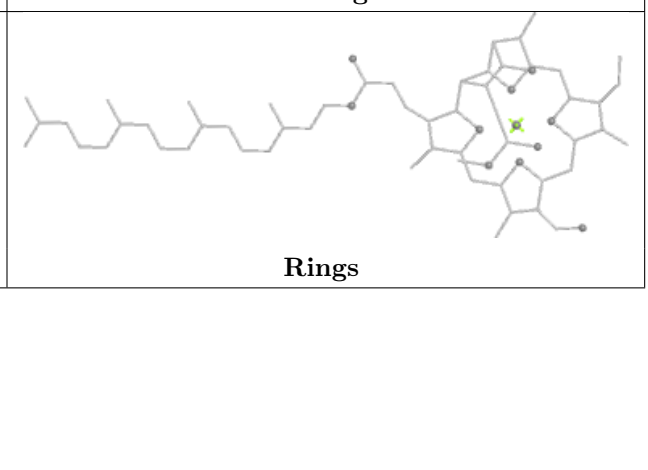
Bond lengths



Bond angles

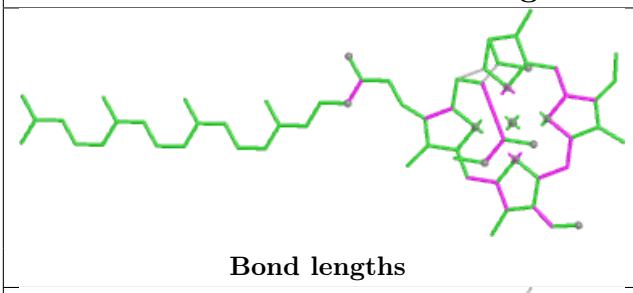


Torsions

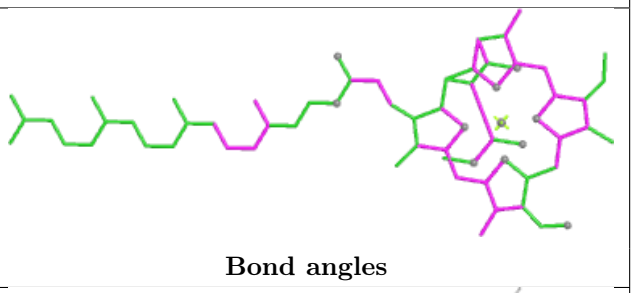


Rings

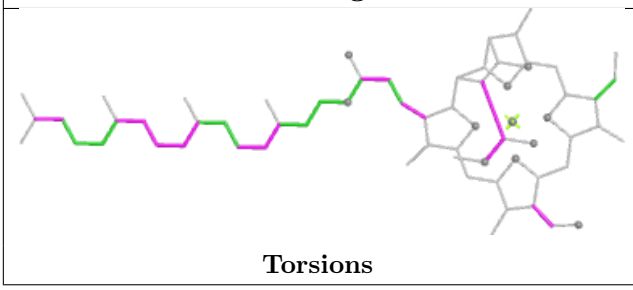
Ligand CL7 4C 503



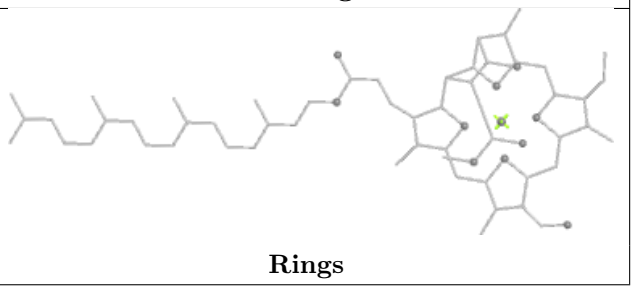
Bond lengths



Bond angles



Torsions

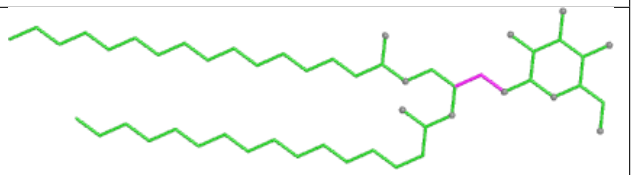


Rings

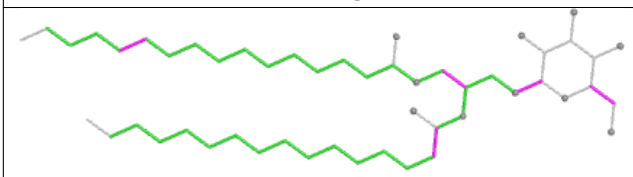
Ligand LMG 31 401



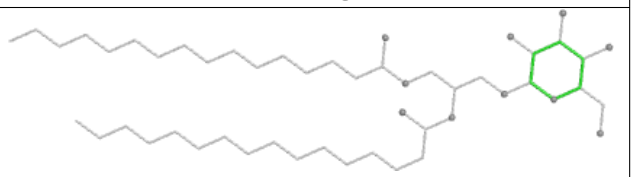
Bond lengths



Bond angles

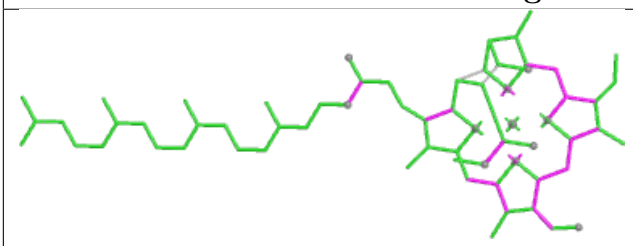


Torsions

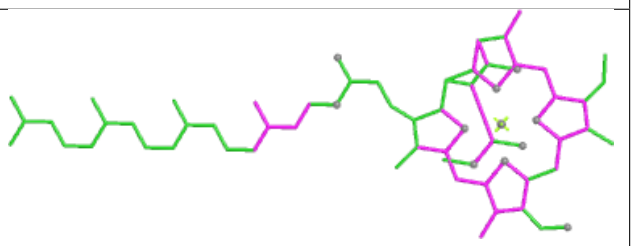


Rings

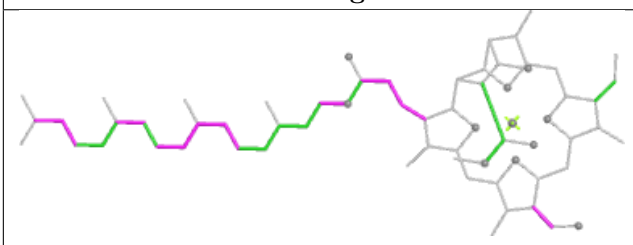
Ligand CL7 32 501



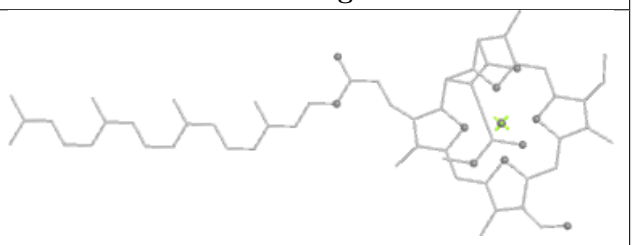
Bond lengths



Bond angles

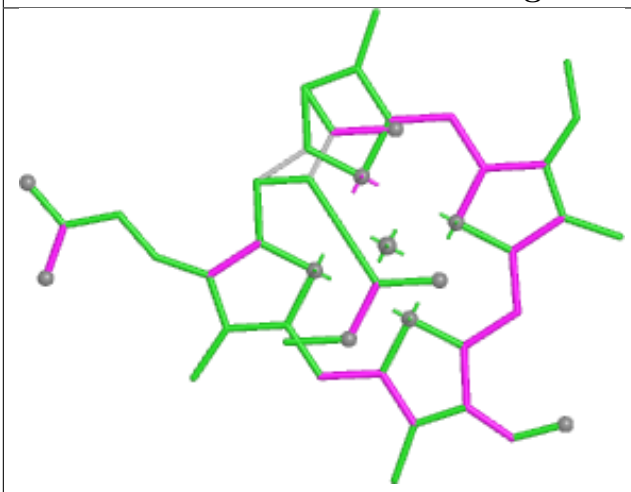


Torsions

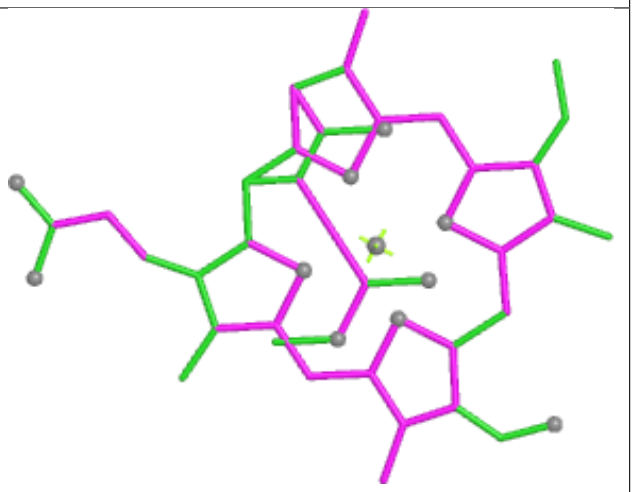


Rings

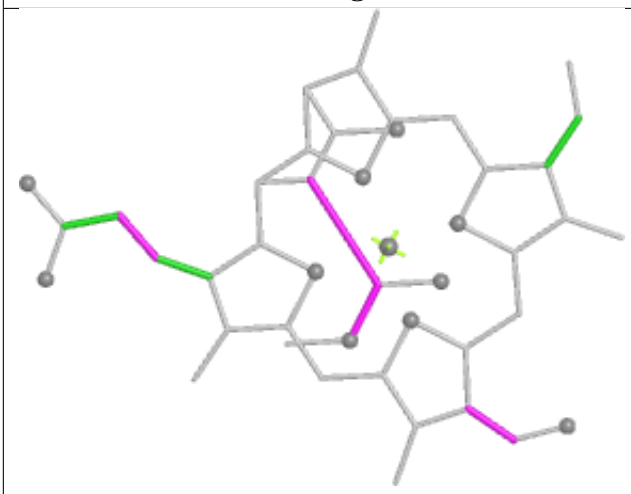
Ligand CL7 41 409



Bond lengths



Bond angles

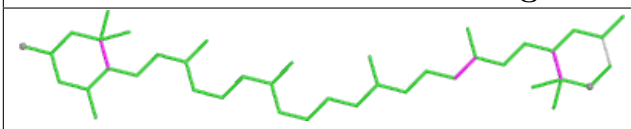


Torsions

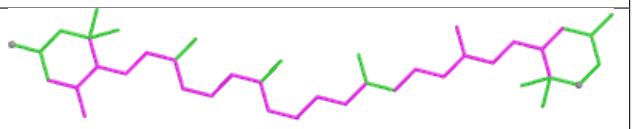


Rings

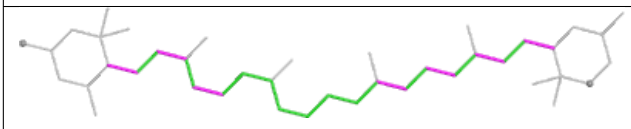
Ligand ZEX 22 524



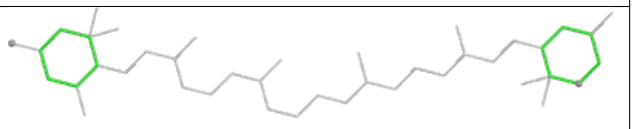
Bond lengths



Bond angles

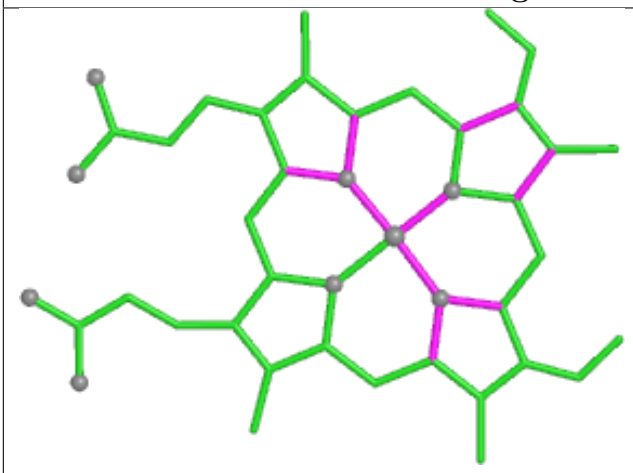


Torsions

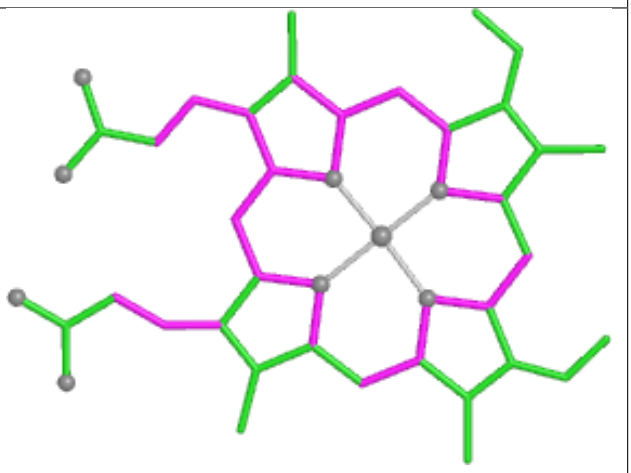


Rings

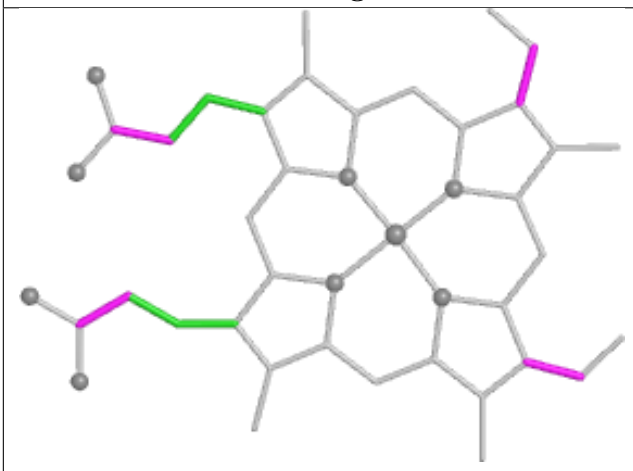
Ligand HEM 2F 101



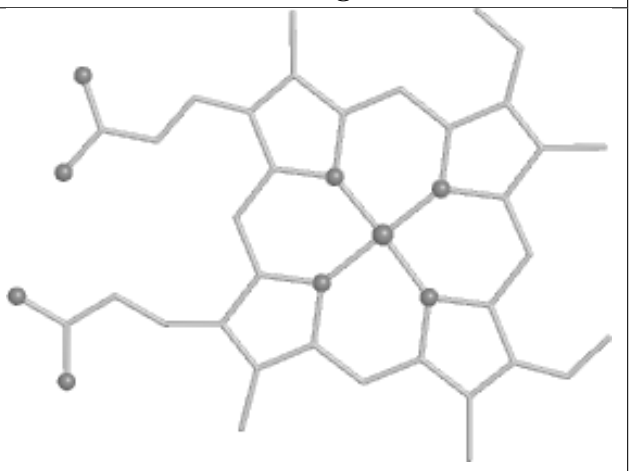
Bond lengths



Bond angles

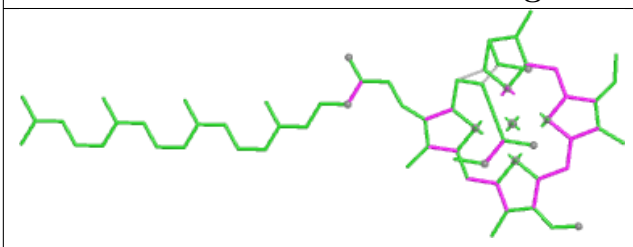


Torsions

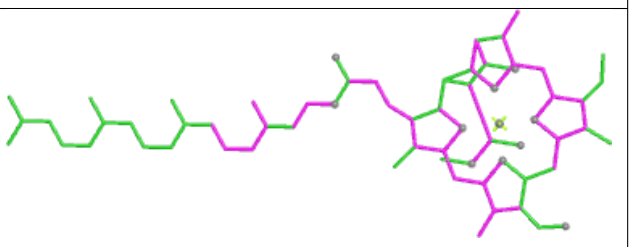


Rings

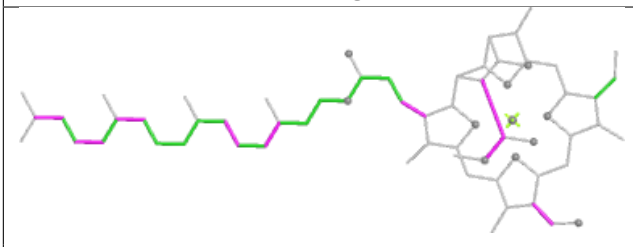
Ligand CL7 34 411



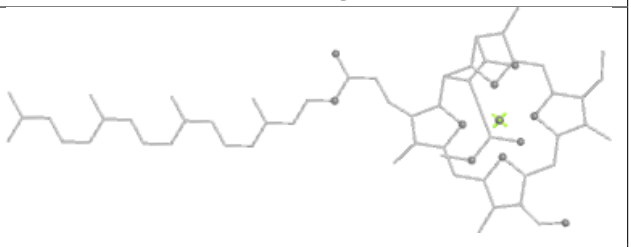
Bond lengths



Bond angles

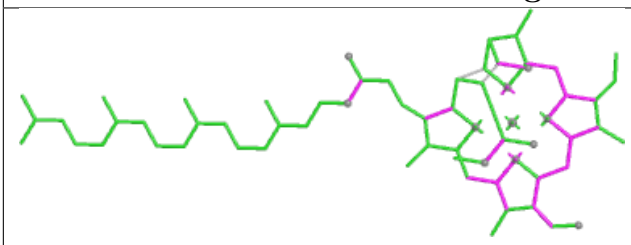


Torsions

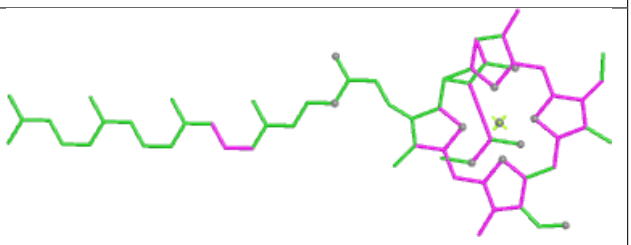


Rings

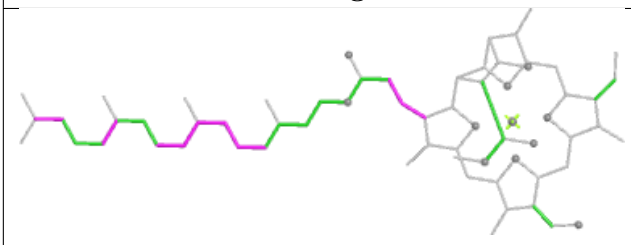
Ligand CL7 44 404



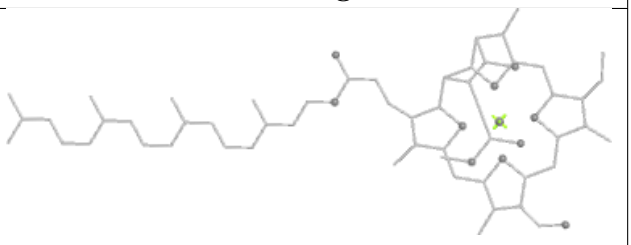
Bond lengths



Bond angles

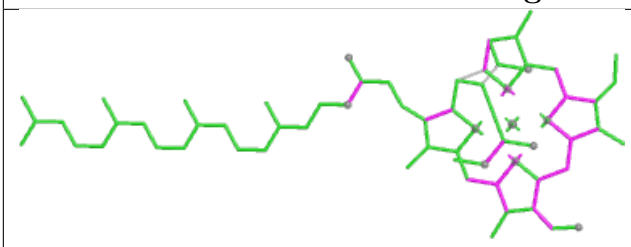


Torsions

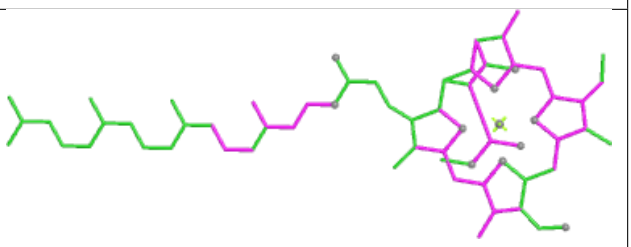


Rings

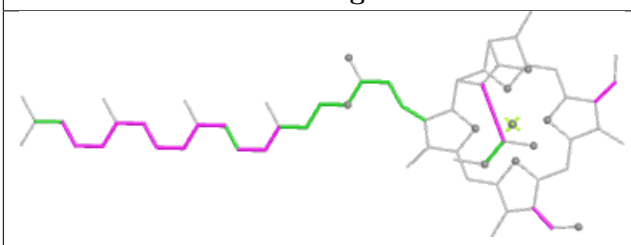
Ligand CL7 32 505



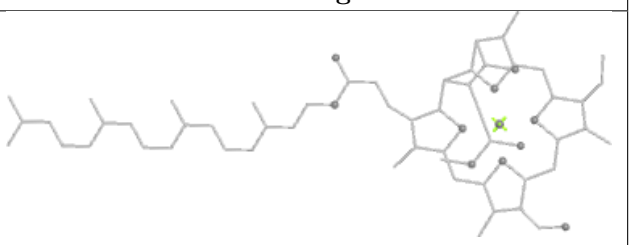
Bond lengths



Bond angles

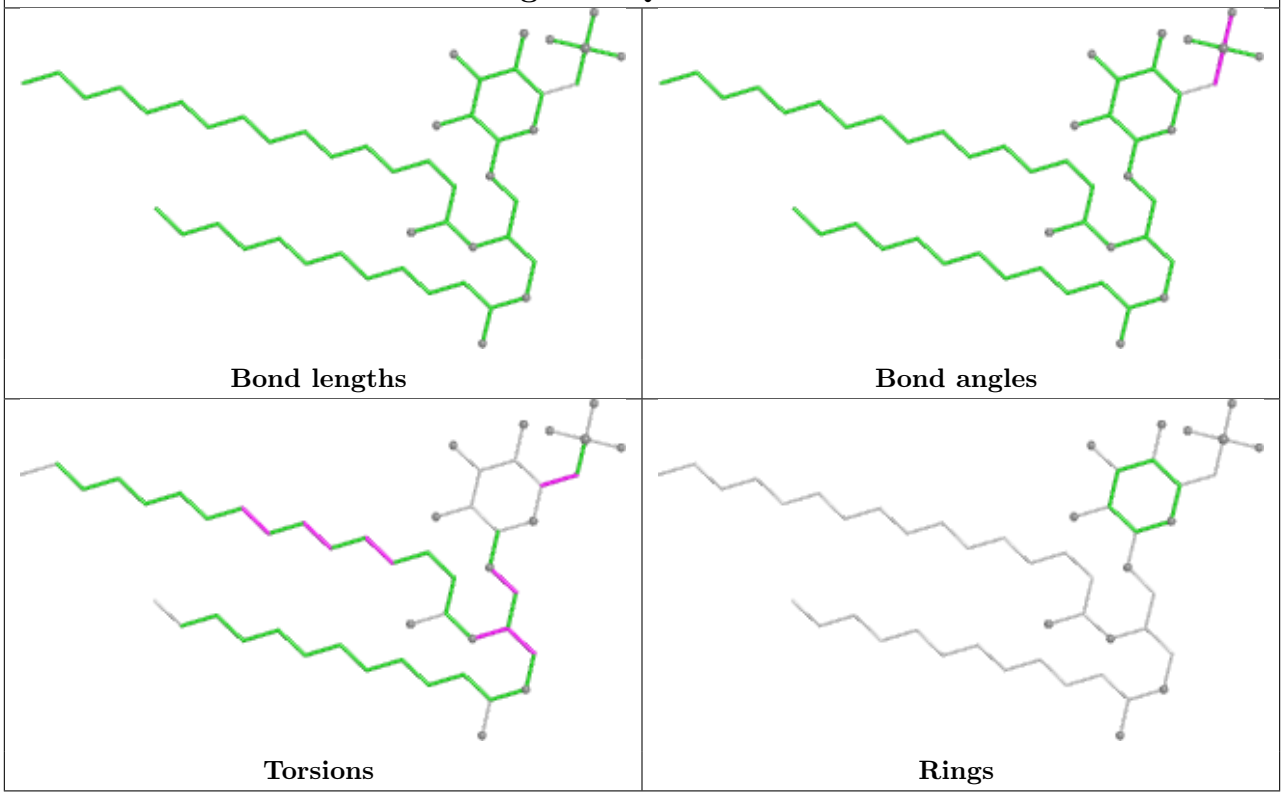


Torsions

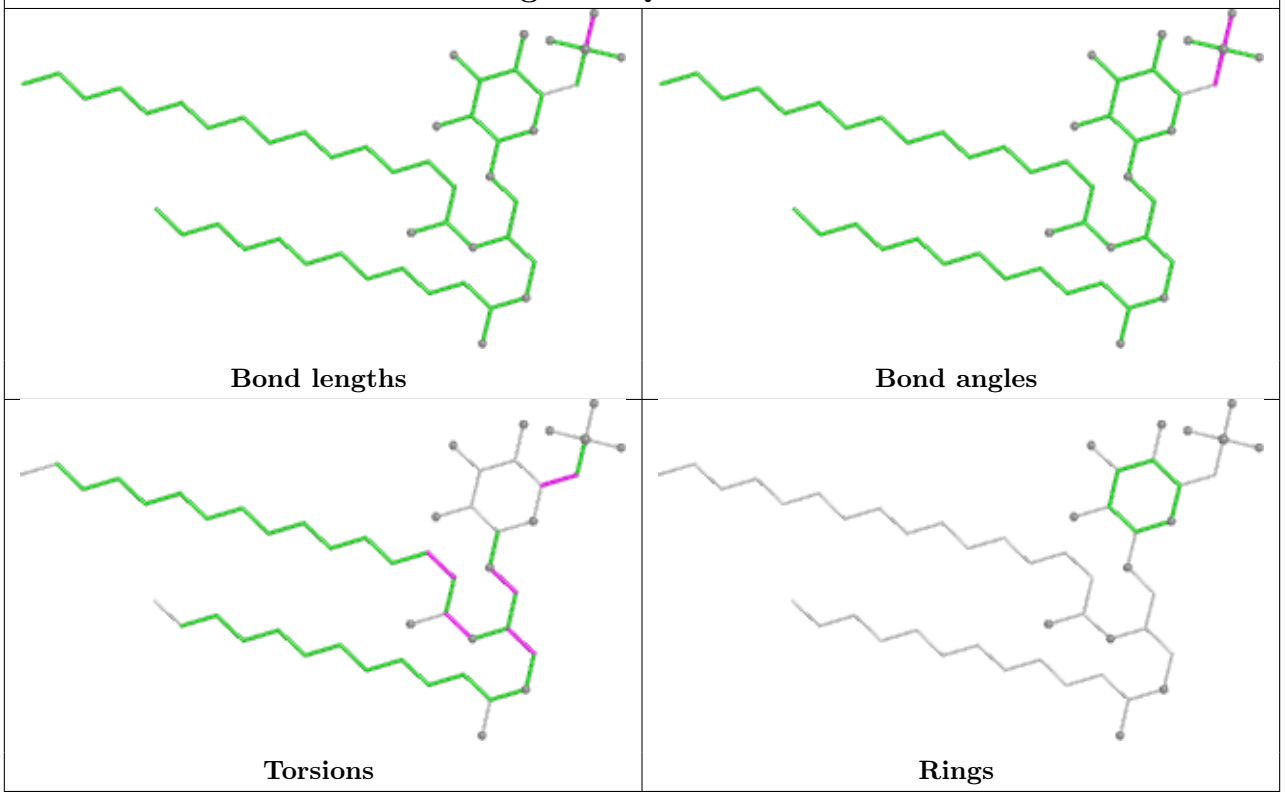


Rings

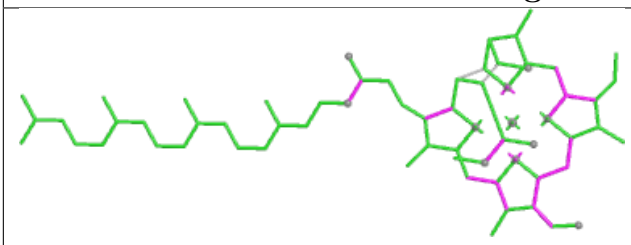
Ligand SQD 23 424



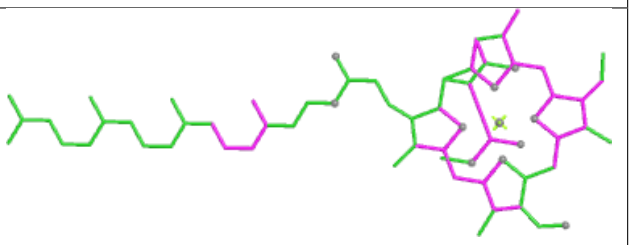
Ligand SQD 12 521



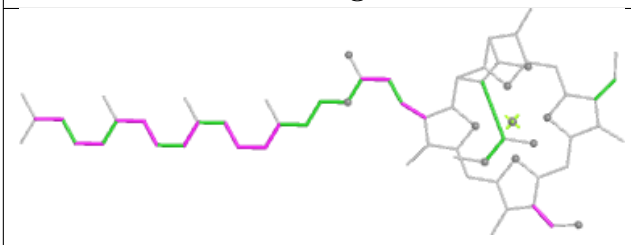
Ligand CL7 22 512



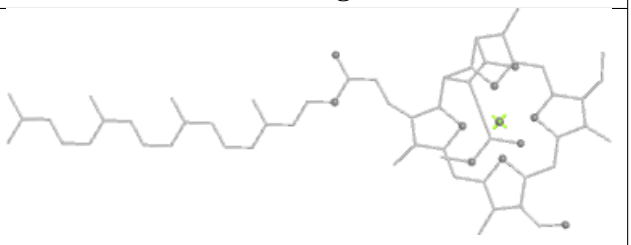
Bond lengths



Bond angles

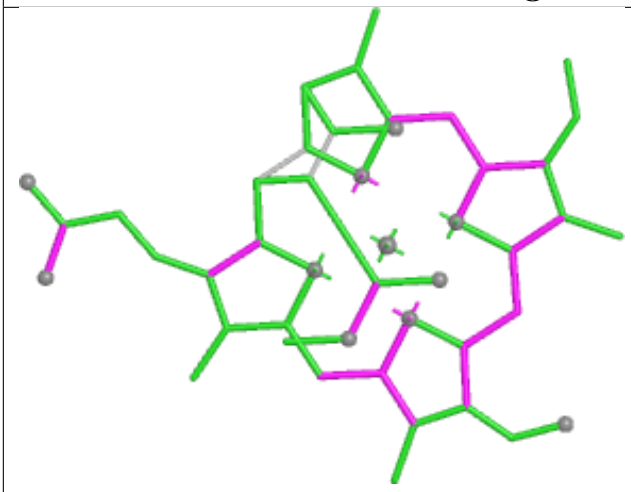


Torsions

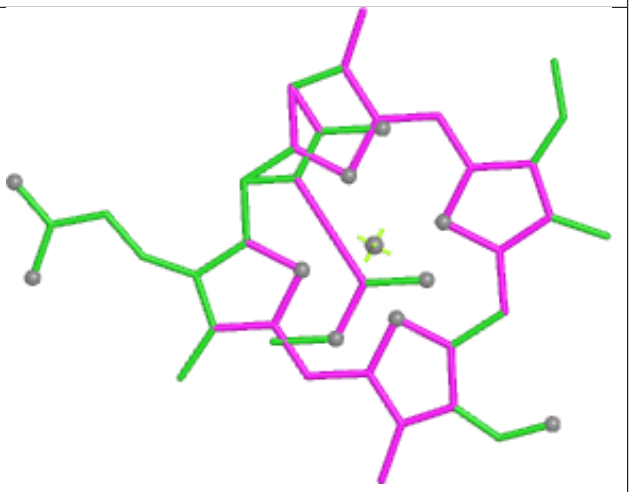


Rings

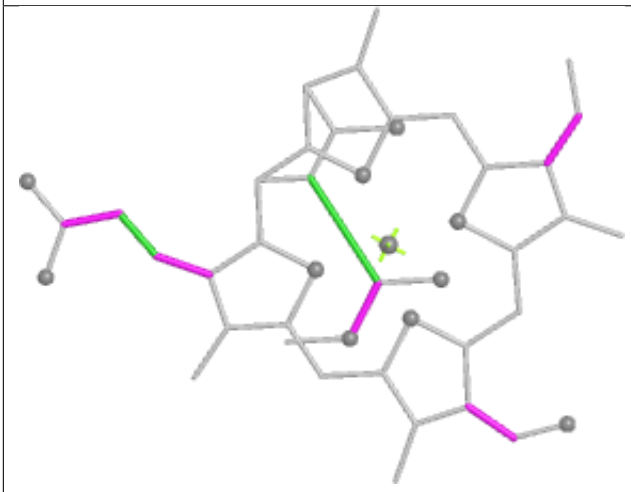
Ligand CL7 22 514



Bond lengths



Bond angles

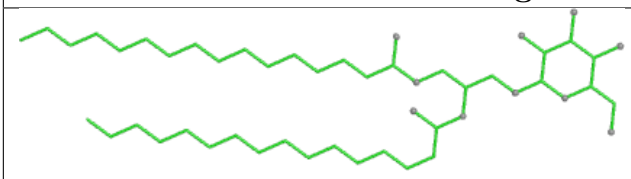


Torsions

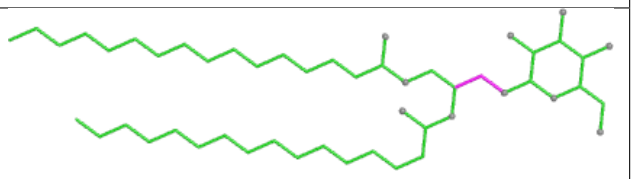


Rings

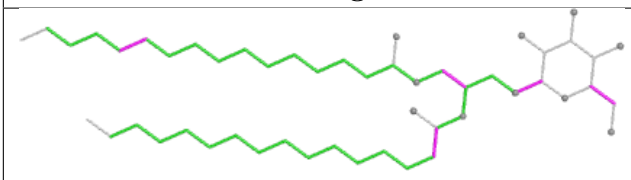
Ligand LMG 41 401



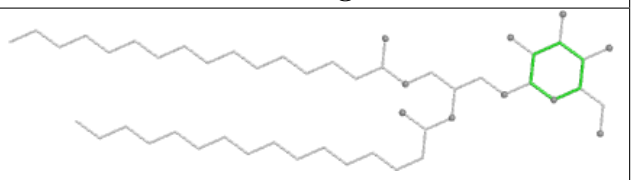
Bond lengths



Bond angles

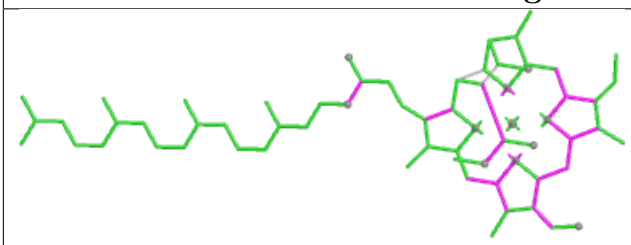


Torsions

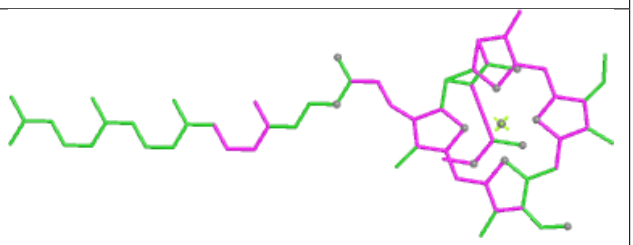


Rings

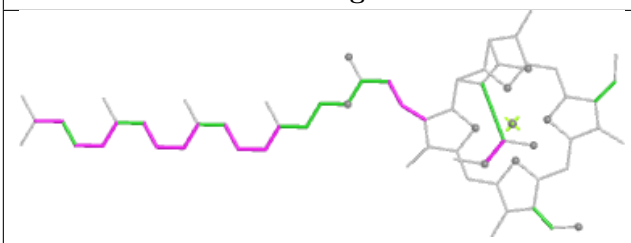
Ligand CL7 42 503



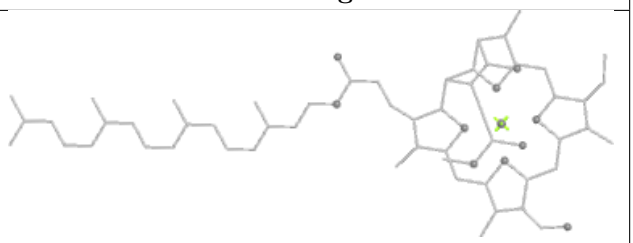
Bond lengths



Bond angles

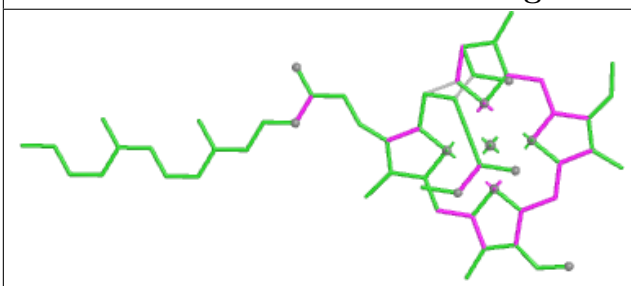


Torsions

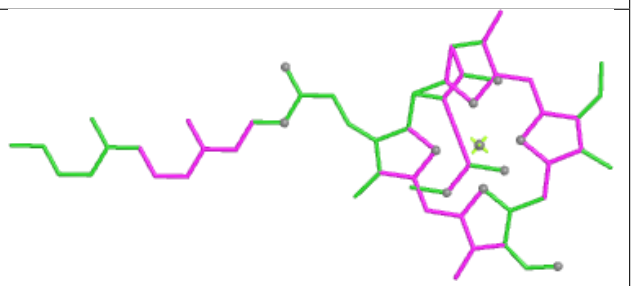


Rings

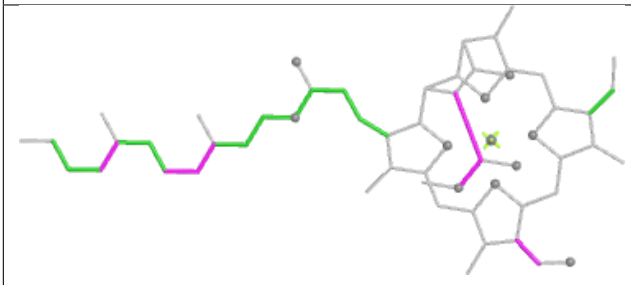
Ligand CL7 23 403



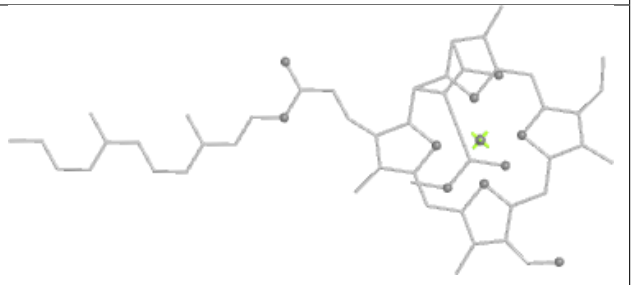
Bond lengths



Bond angles

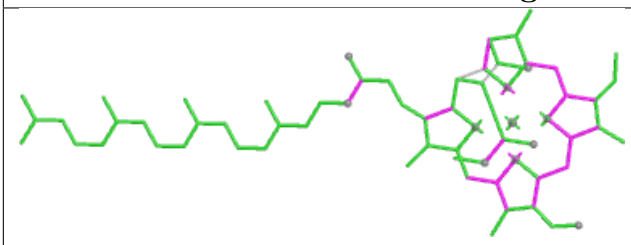


Torsions

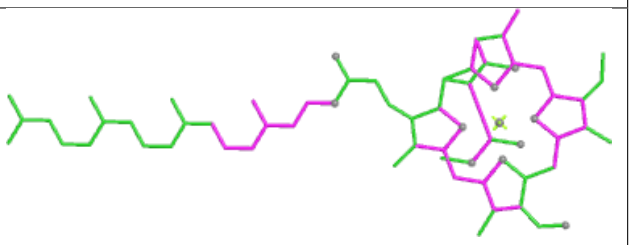


Rings

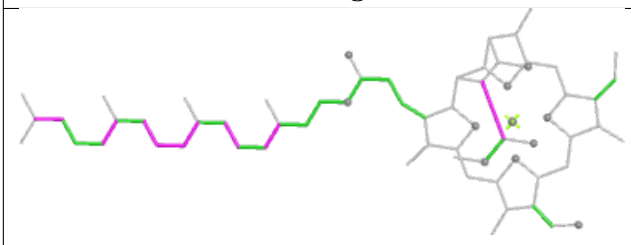
Ligand CL7 3B 603



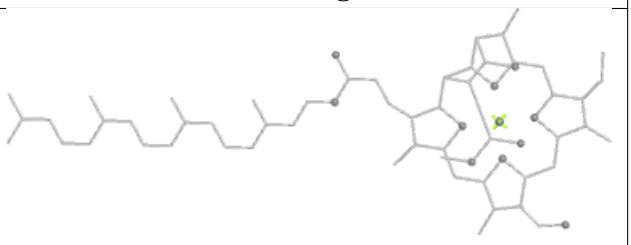
Bond lengths



Bond angles

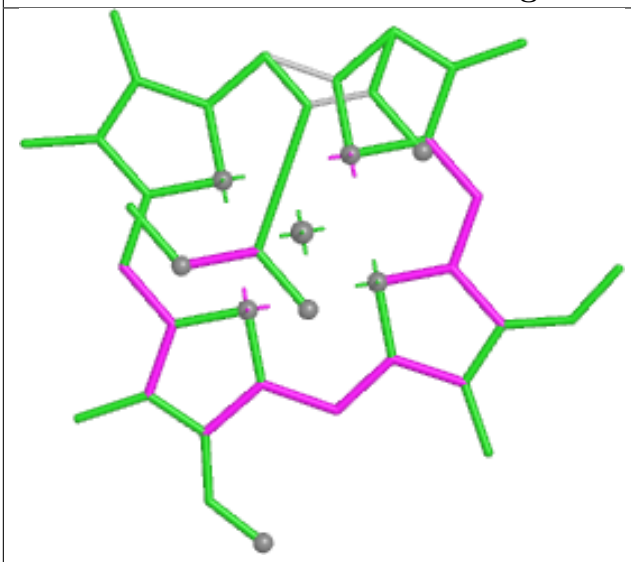


Torsions

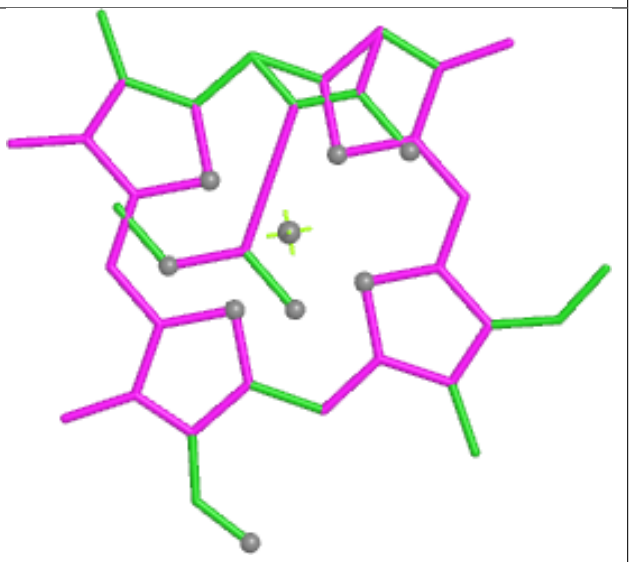


Rings

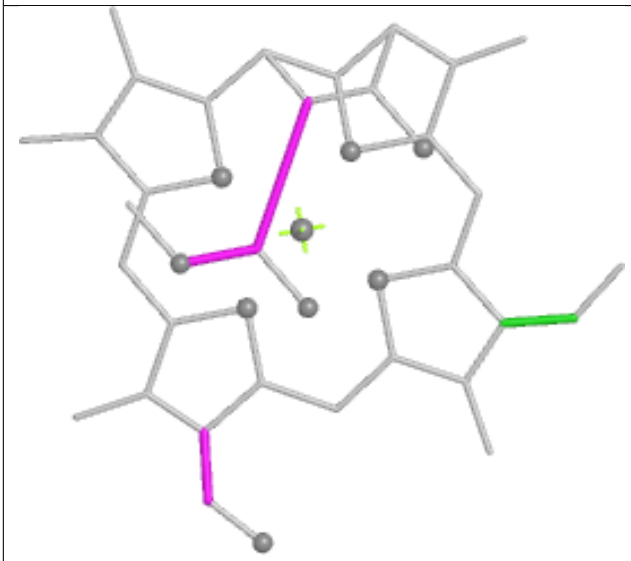
Ligand CL7 1C 517



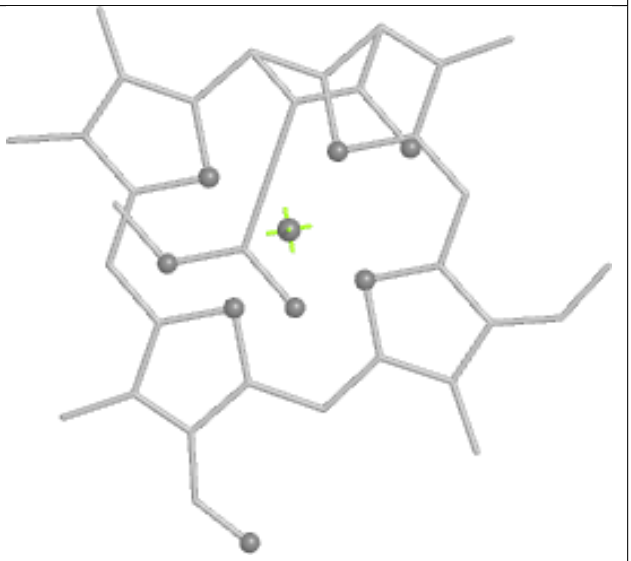
Bond lengths



Bond angles

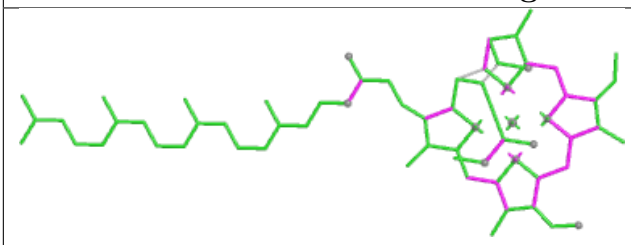


Torsions

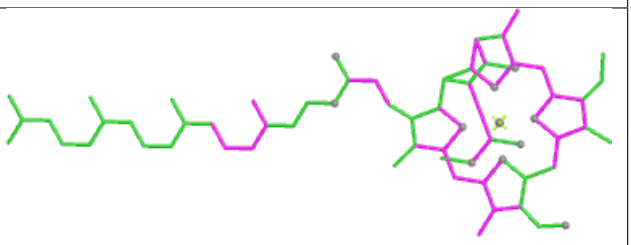


Rings

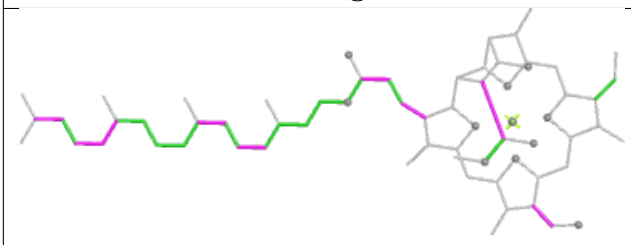
Ligand CL7 4B 610



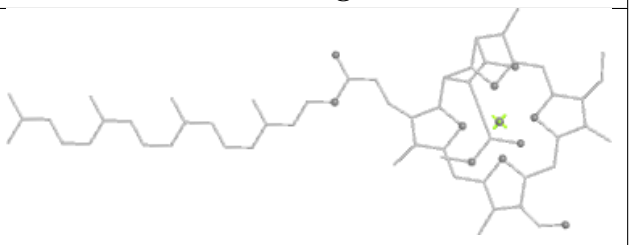
Bond lengths



Bond angles

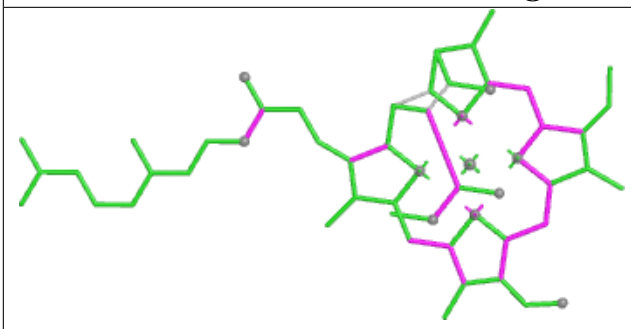


Torsions

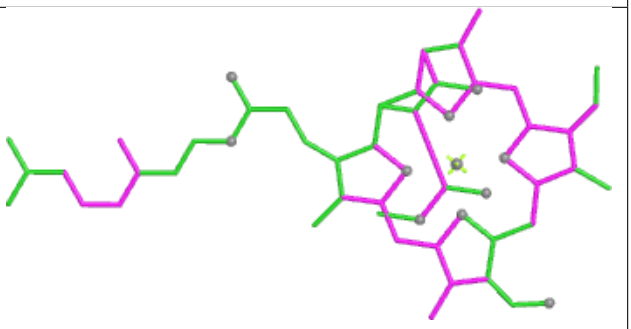


Rings

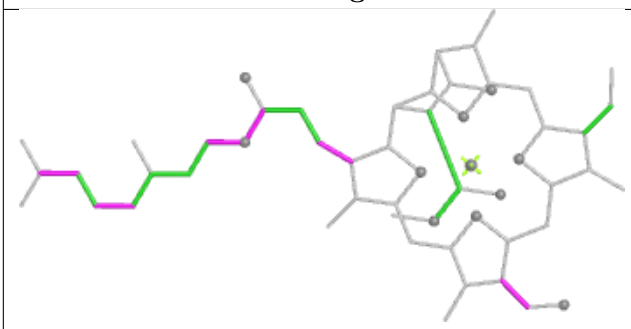
Ligand CL7 31 417



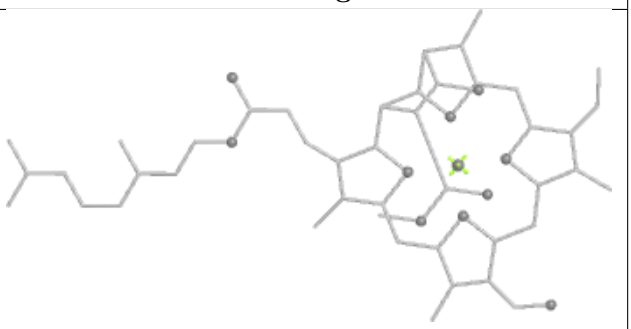
Bond lengths



Bond angles

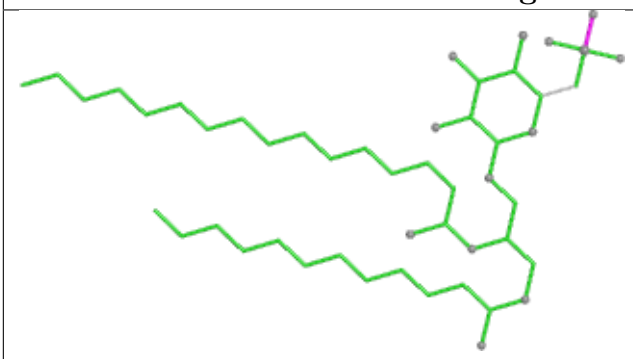


Torsions

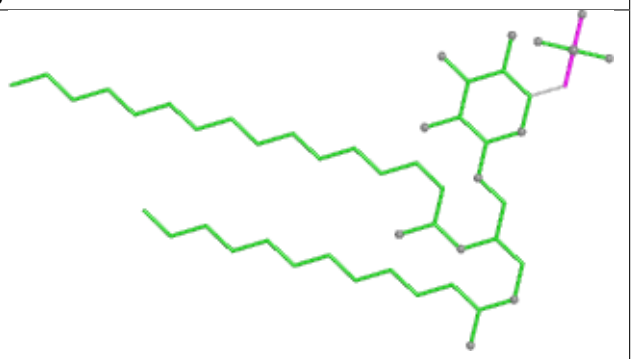


Rings

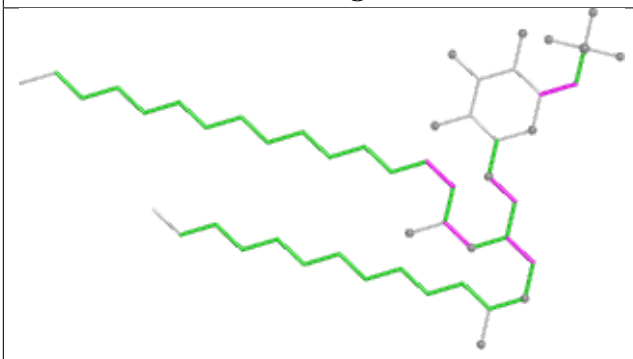
Ligand SQD 22 521



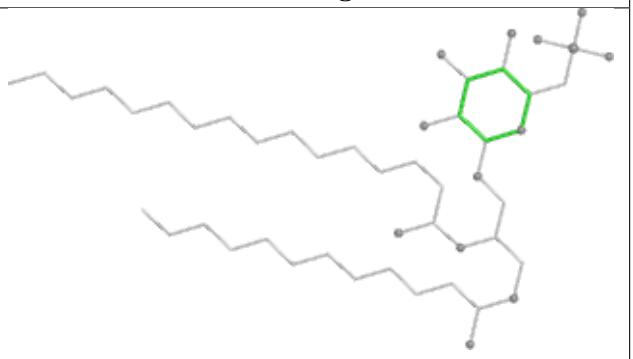
Bond lengths



Bond angles

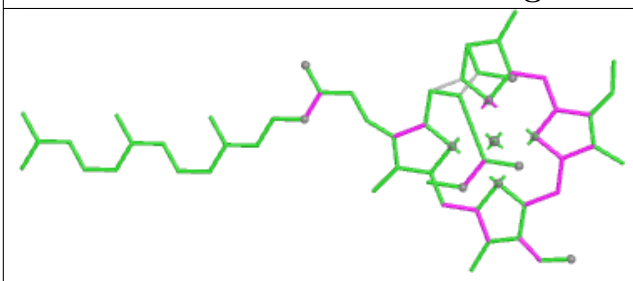


Torsions

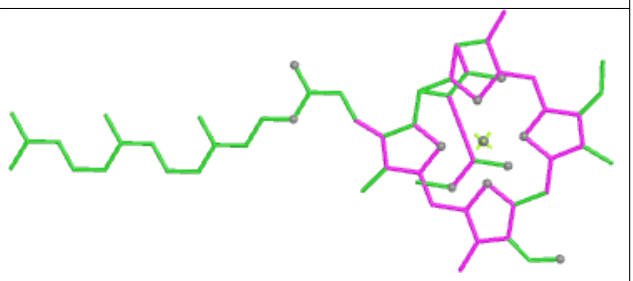


Rings

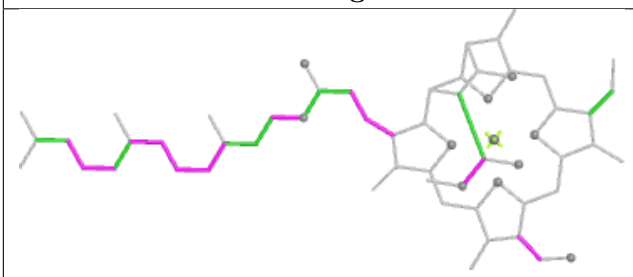
Ligand CL7 31 402



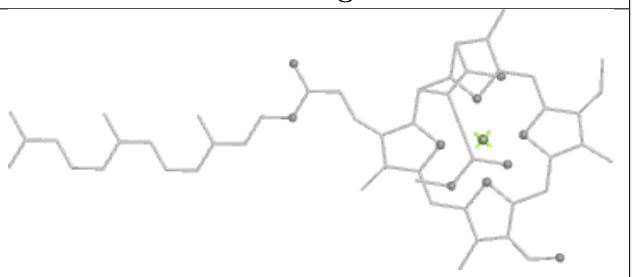
Bond lengths



Bond angles

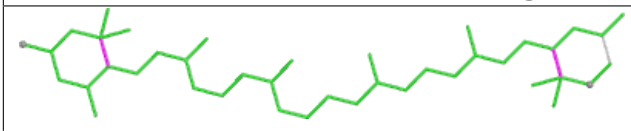


Torsions

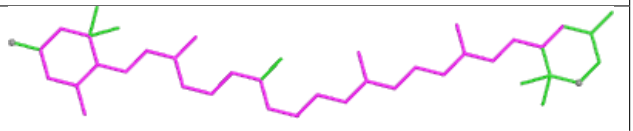


Rings

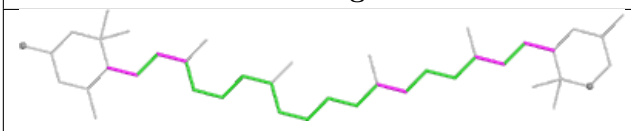
Ligand ZEX 13 520



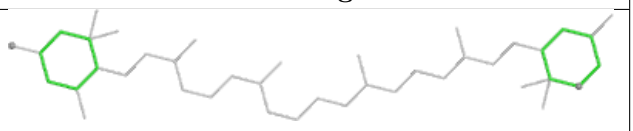
Bond lengths



Bond angles



Torsions

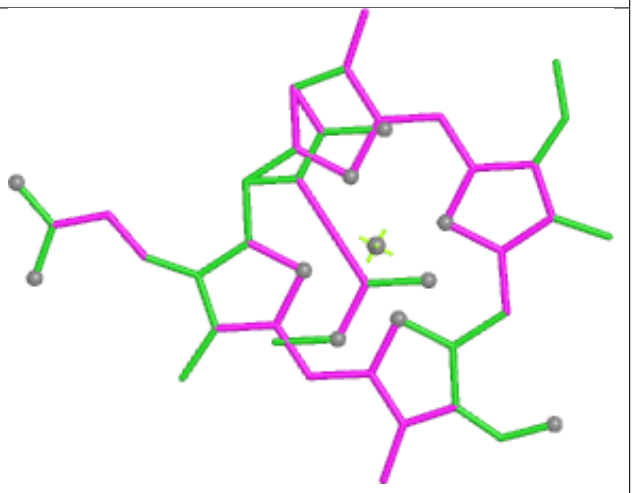


Rings

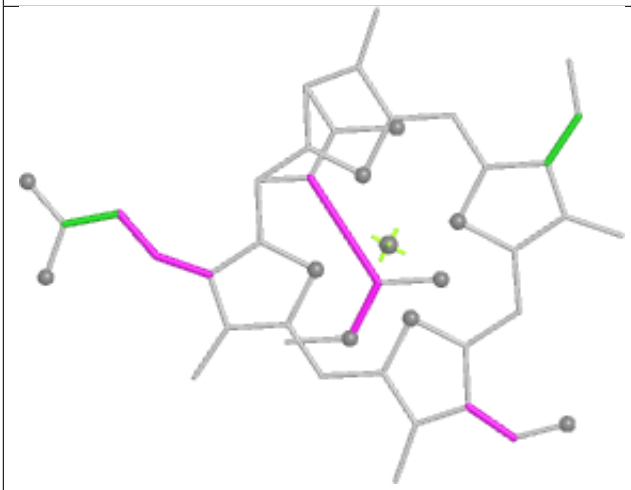
Ligand CL7 4C 513



Bond lengths



Bond angles

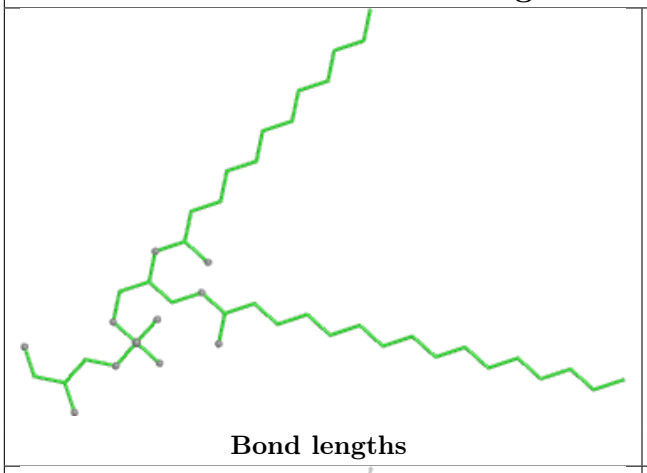


Torsions

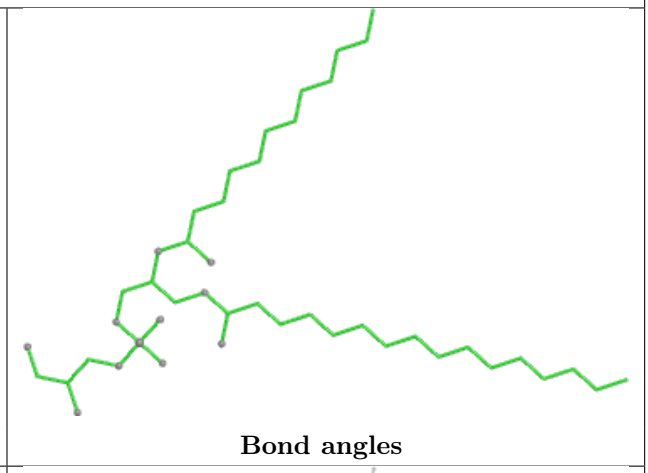


Rings

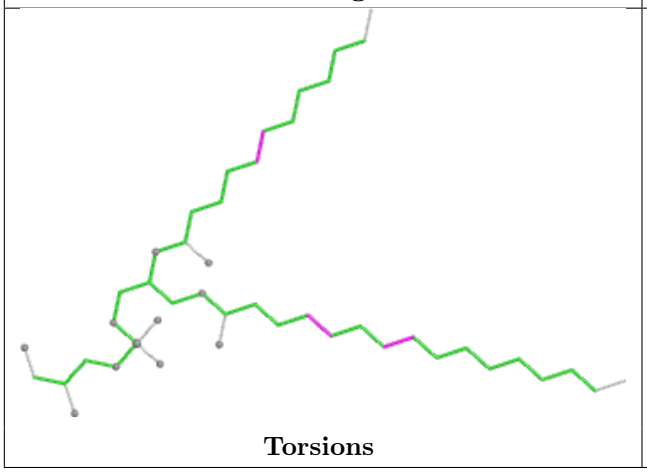
Ligand LHG 2B 624



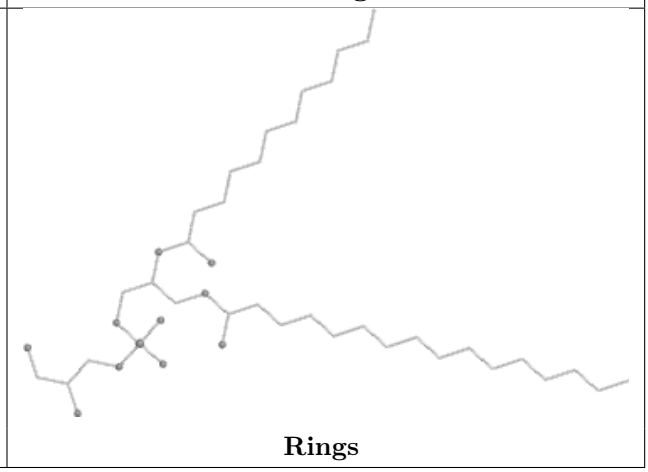
Bond lengths



Bond angles

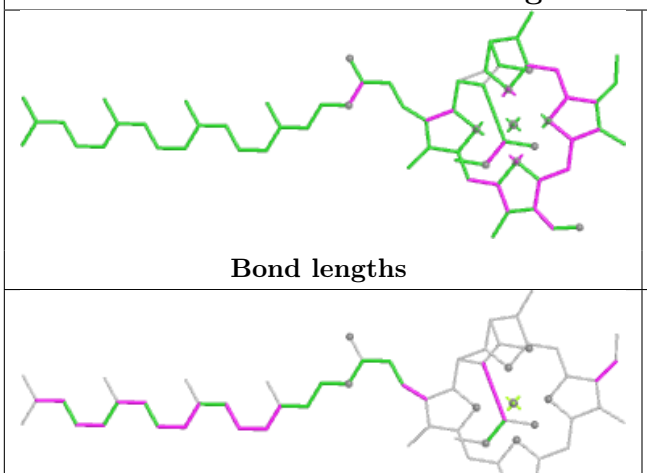


Torsions

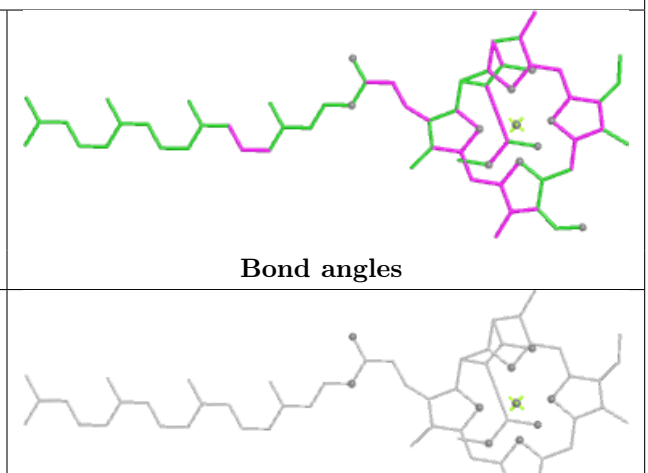


Rings

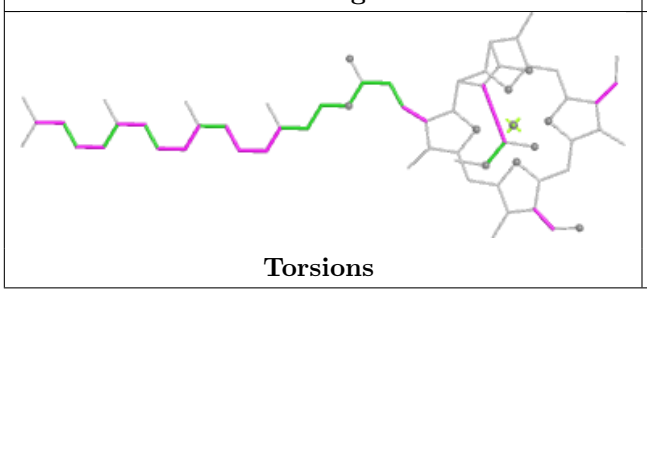
Ligand CL7 13 504



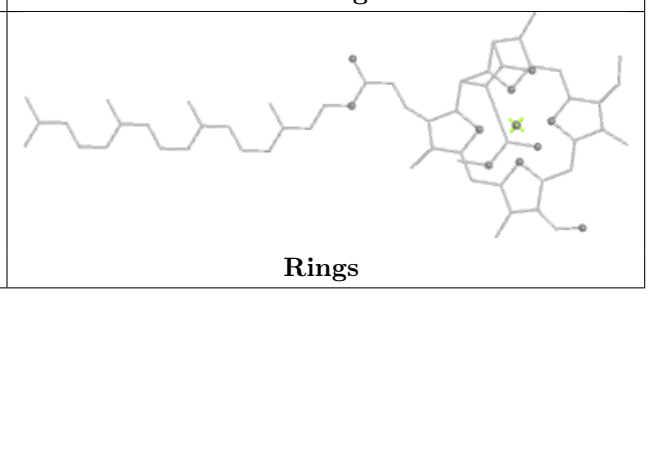
Bond lengths



Bond angles

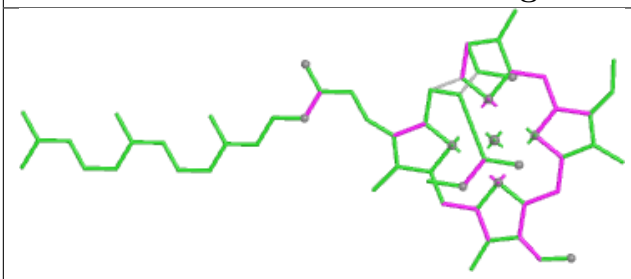


Torsions

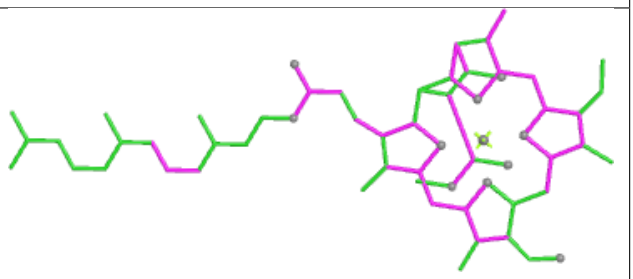


Rings

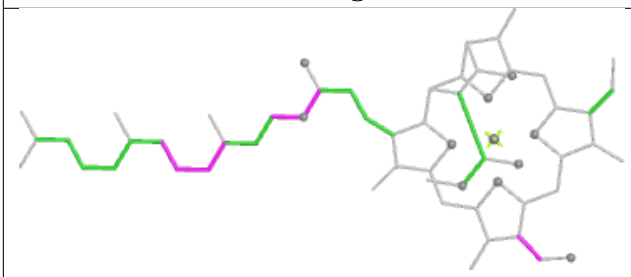
Ligand CL7 1B 602



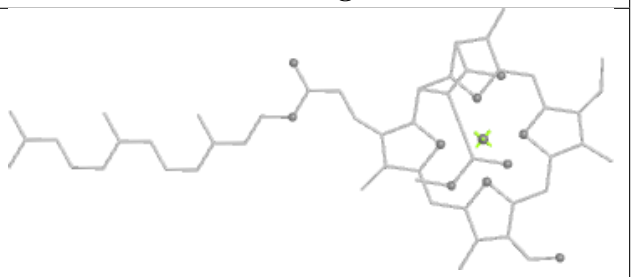
Bond lengths



Bond angles

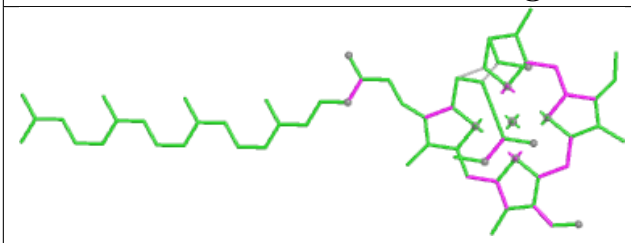


Torsions

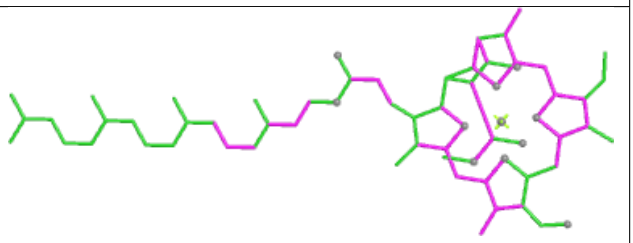


Rings

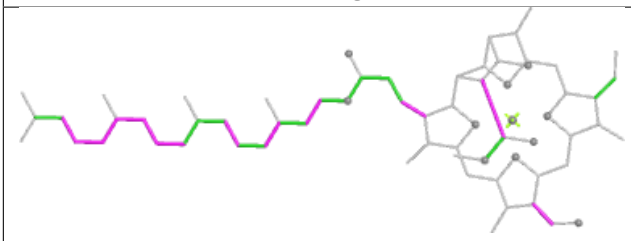
Ligand CL7 11 404



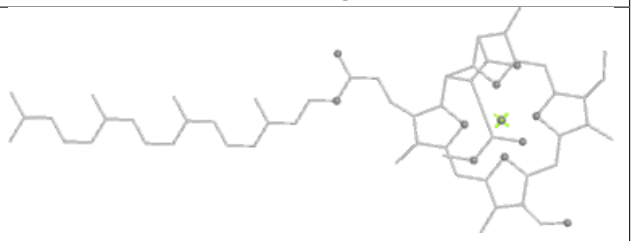
Bond lengths



Bond angles

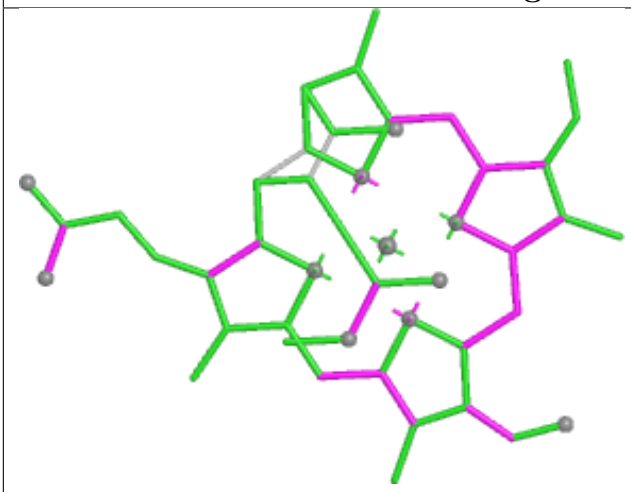


Torsions

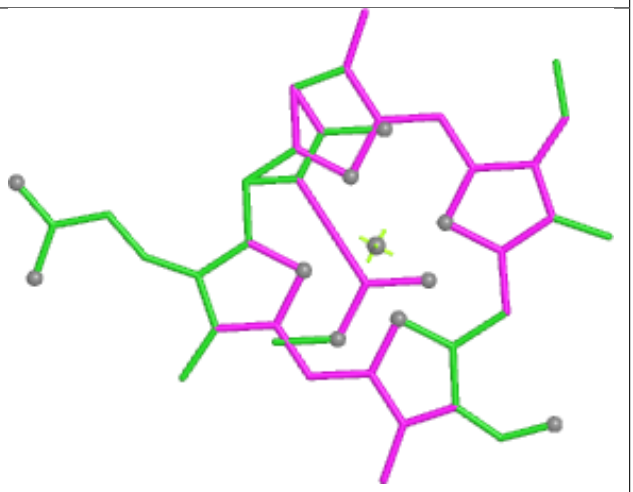


Rings

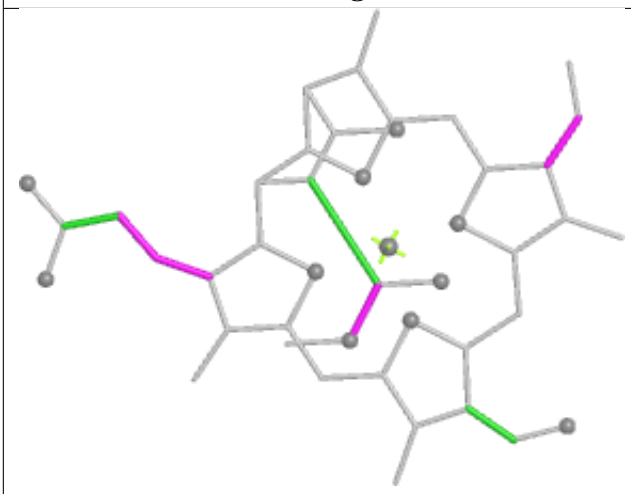
Ligand CL7 13 514



Bond lengths



Bond angles

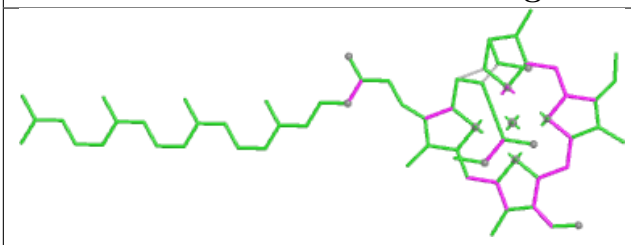


Torsions

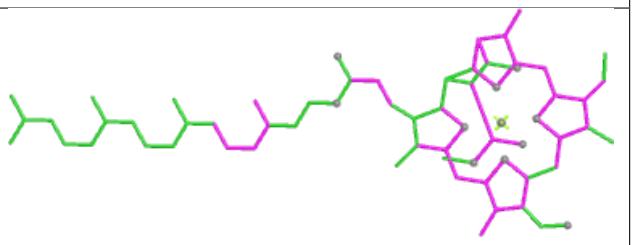


Rings

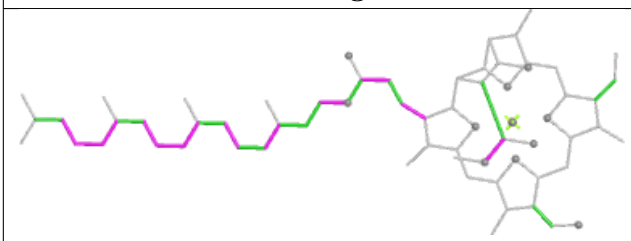
Ligand CL7 14 412



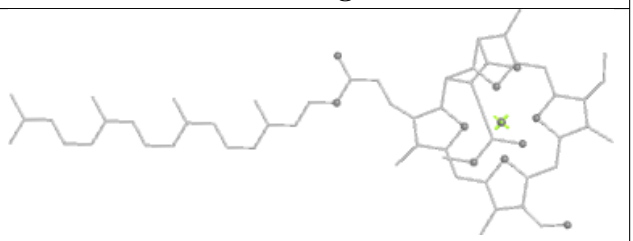
Bond lengths



Bond angles

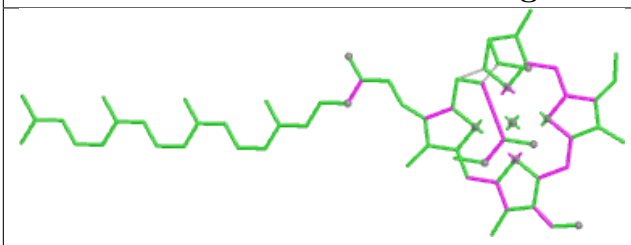


Torsions

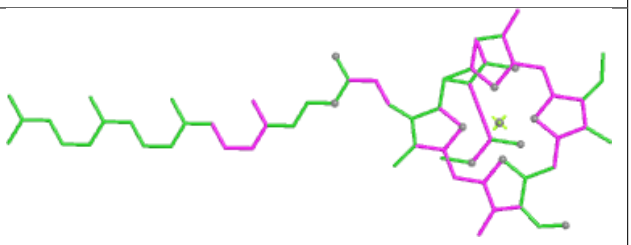


Rings

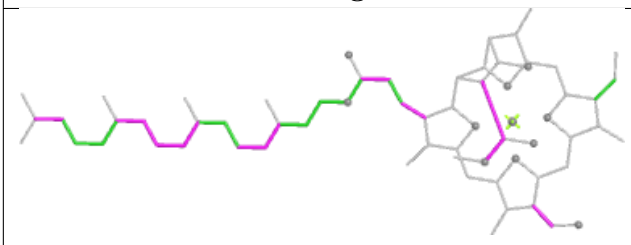
Ligand CL7 2C 503



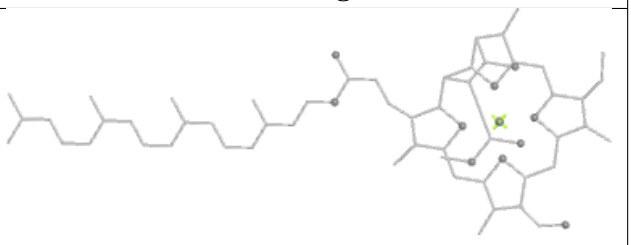
Bond lengths



Bond angles

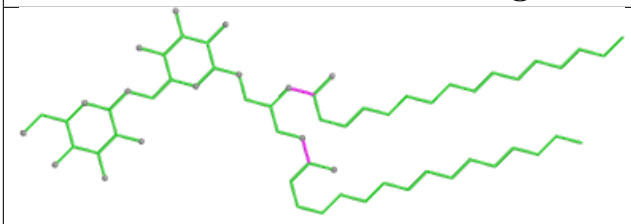


Torsions

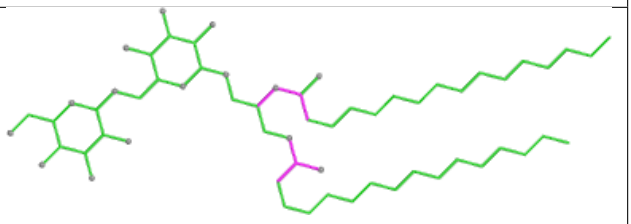


Rings

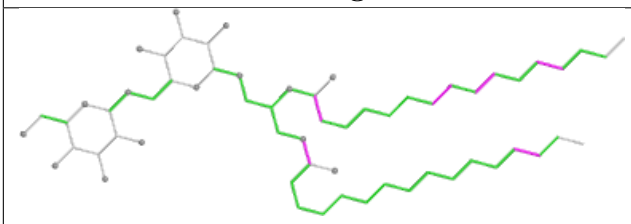
Ligand DGD 4B 625



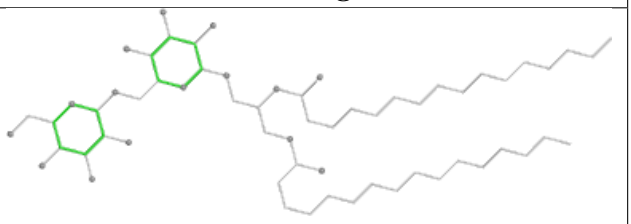
Bond lengths



Bond angles

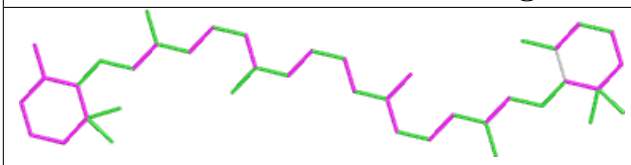


Torsions

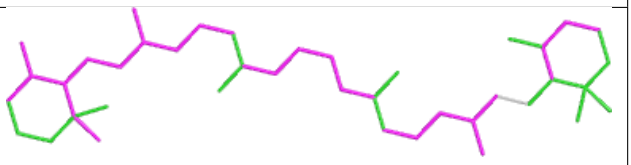


Rings

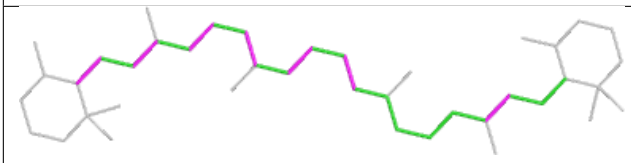
Ligand 8CT 1B 618



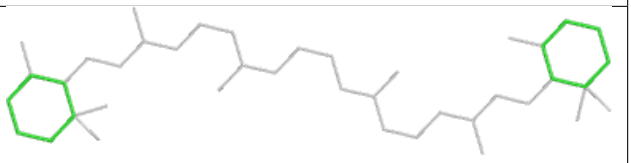
Bond lengths



Bond angles

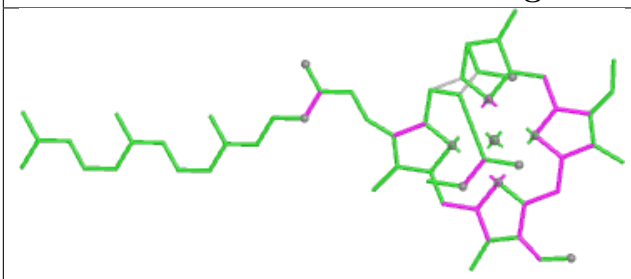


Torsions

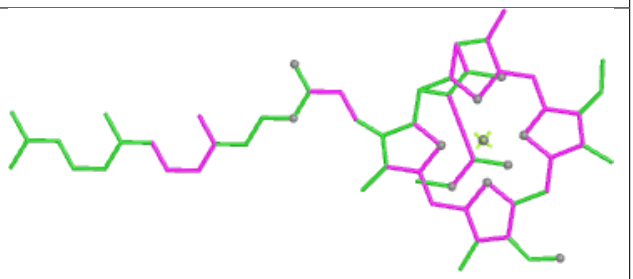


Rings

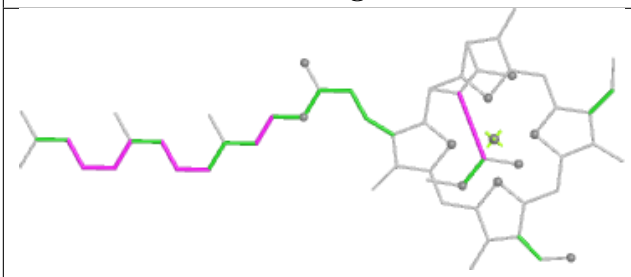
Ligand CL7 24 413



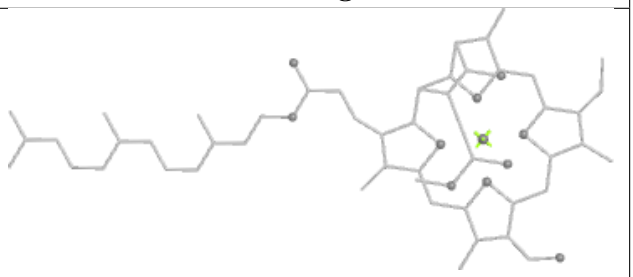
Bond lengths



Bond angles

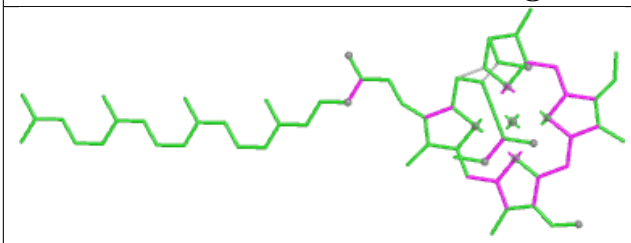


Torsions

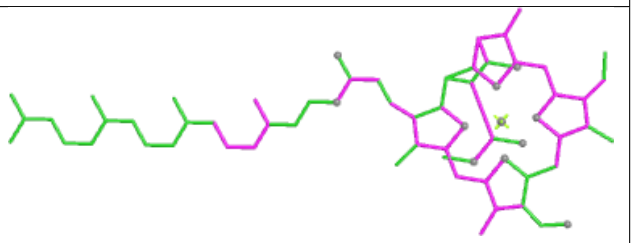


Rings

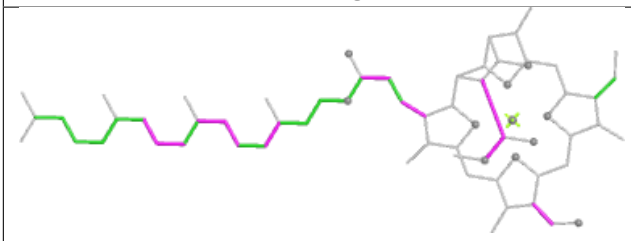
Ligand CL7 33 510



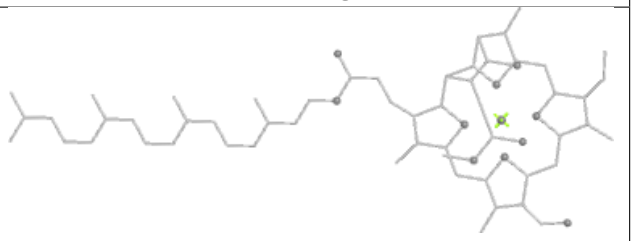
Bond lengths



Bond angles

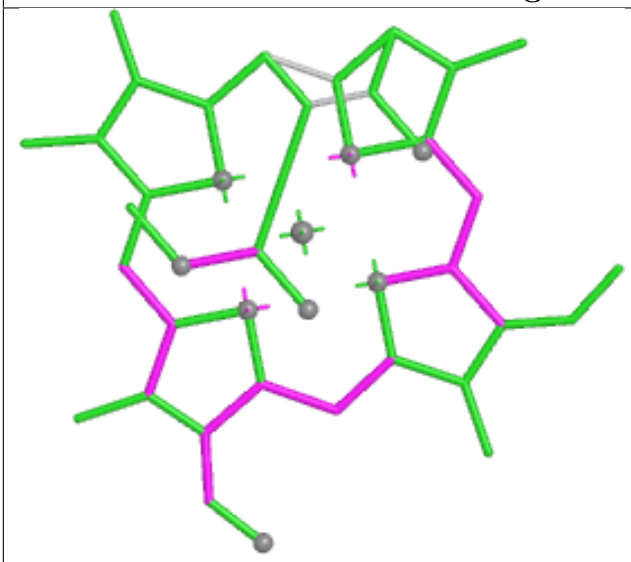


Torsions

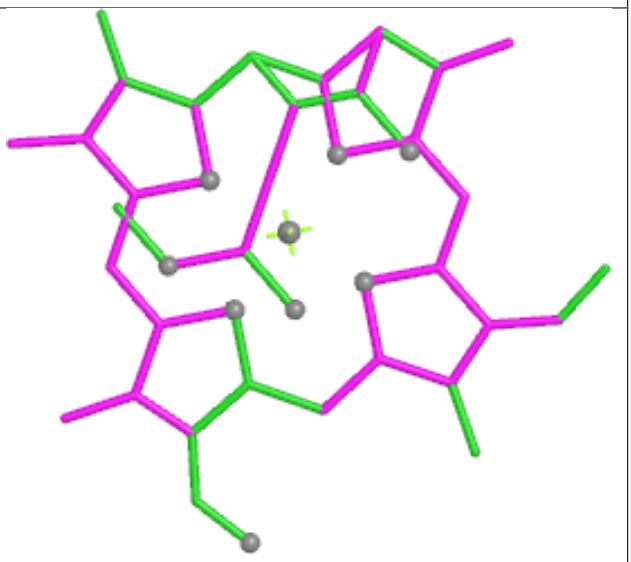


Rings

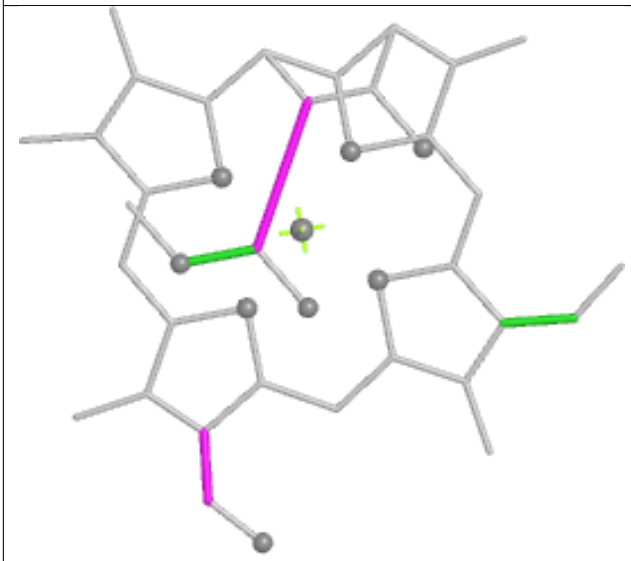
Ligand CL7 34 407



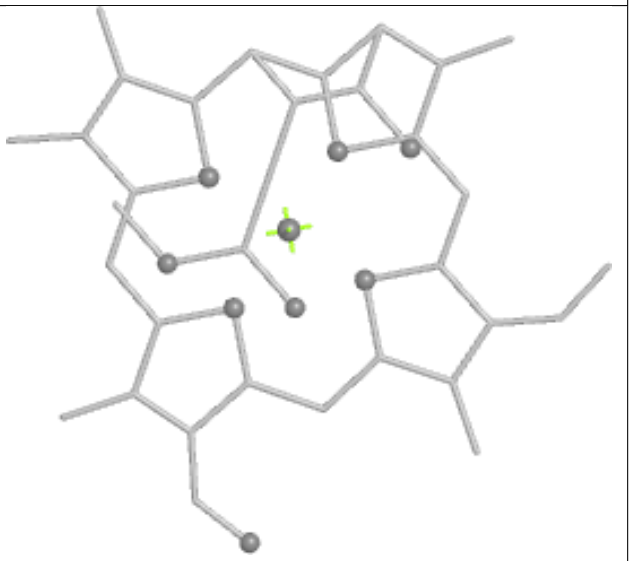
Bond lengths



Bond angles

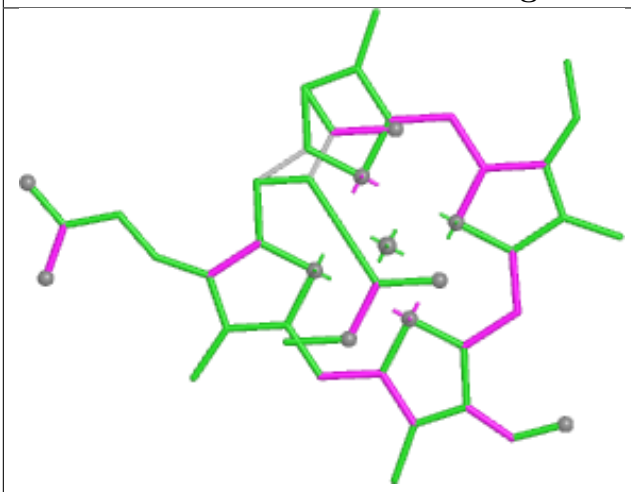


Torsions

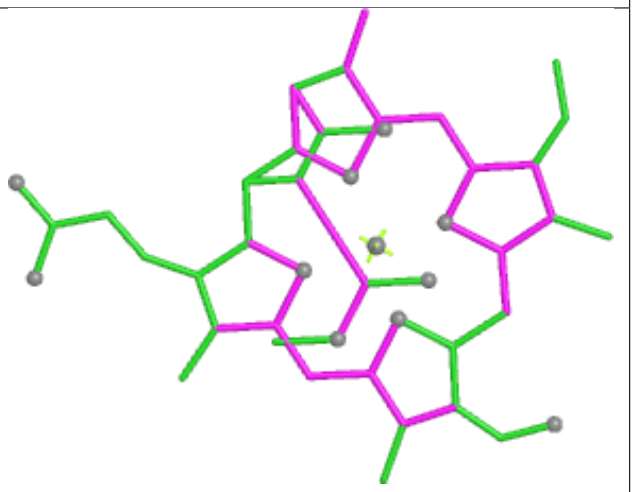


Rings

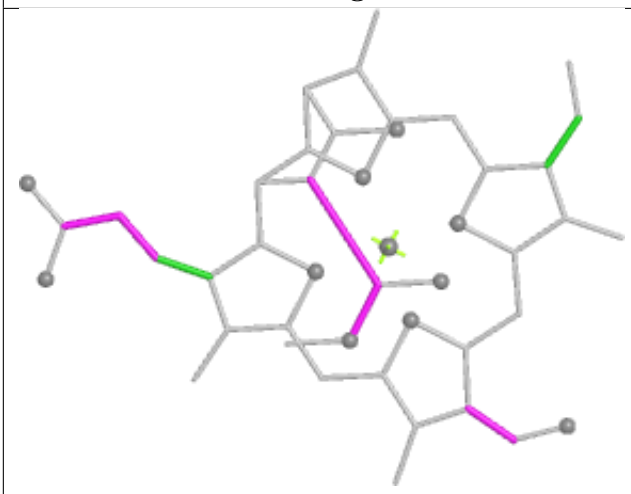
Ligand CL7 3B 622



Bond lengths



Bond angles

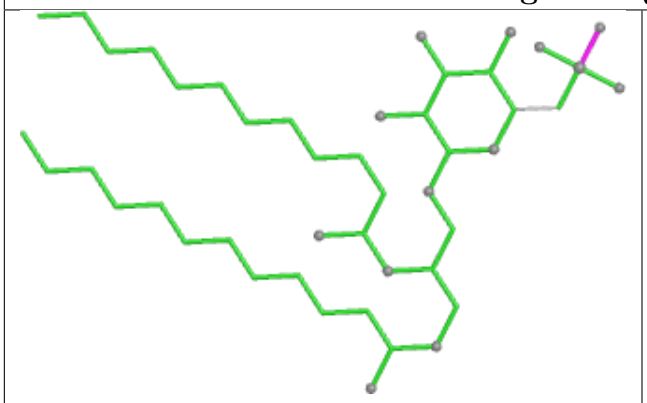


Torsions

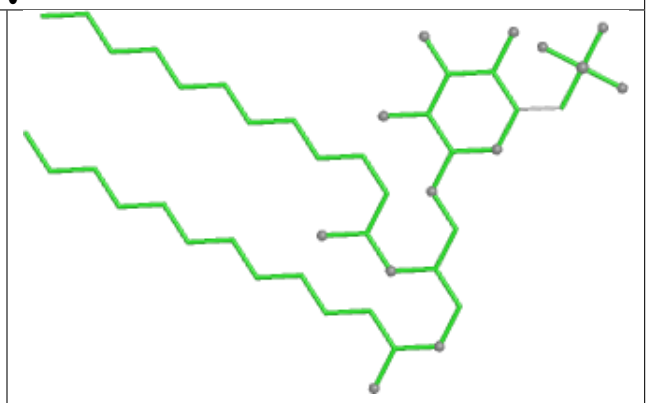


Rings

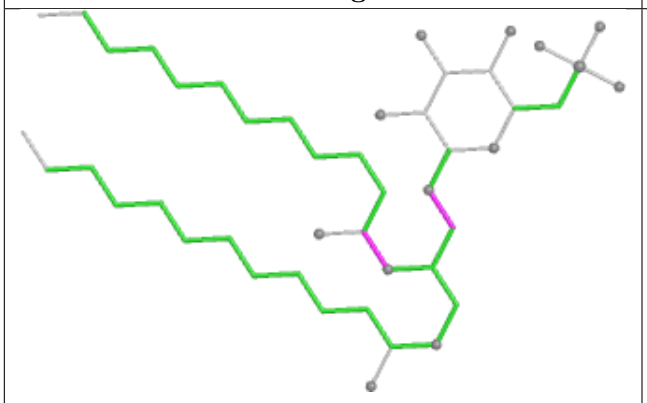
Ligand SQD 13 521



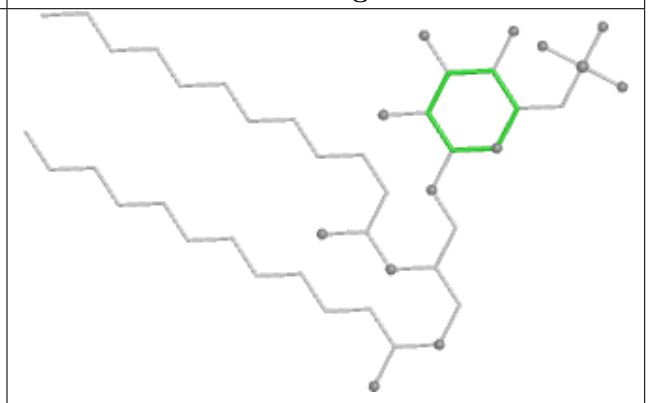
Bond lengths



Bond angles

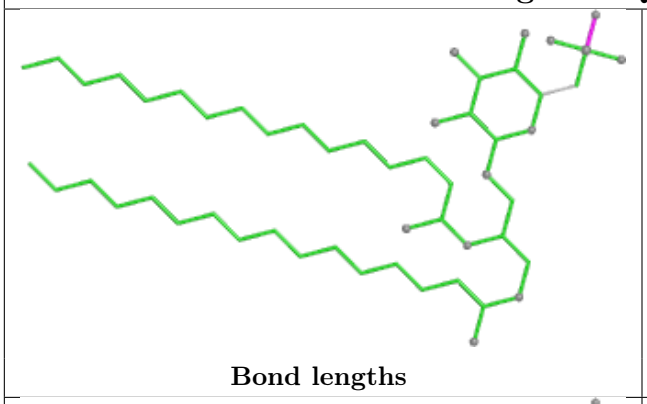


Torsions

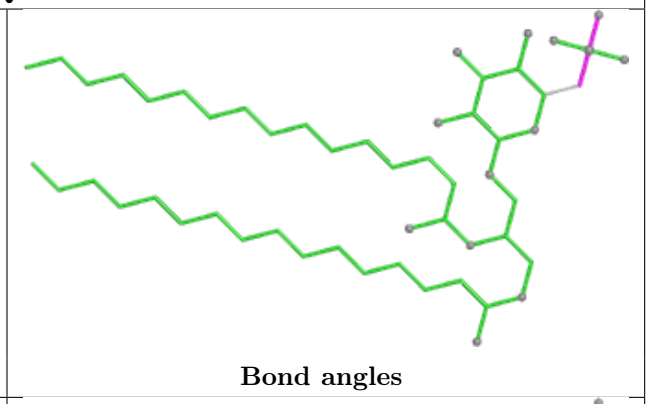


Rings

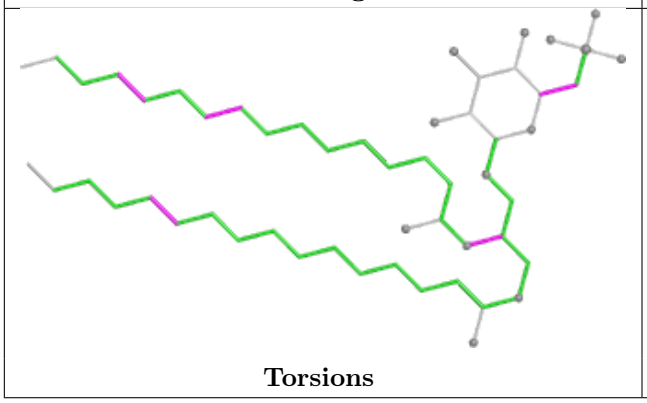
Ligand SQD 1B 620



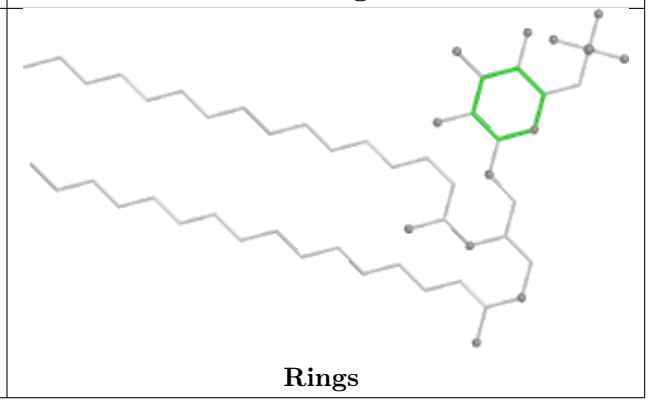
Bond lengths



Bond angles

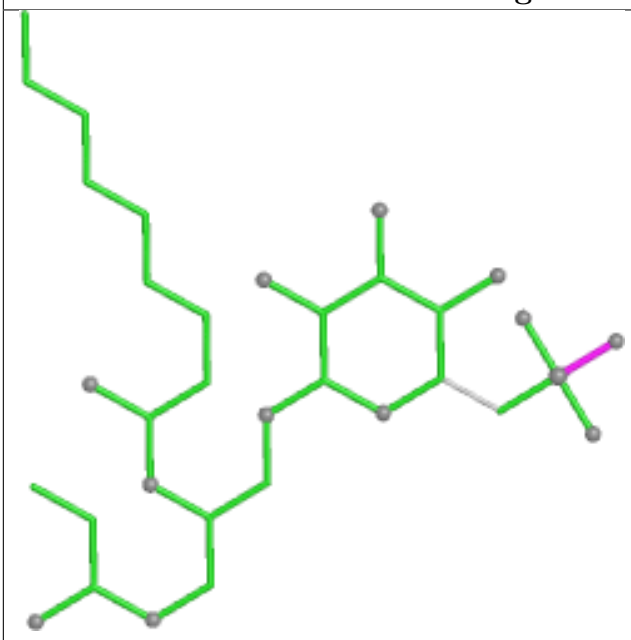


Torsions

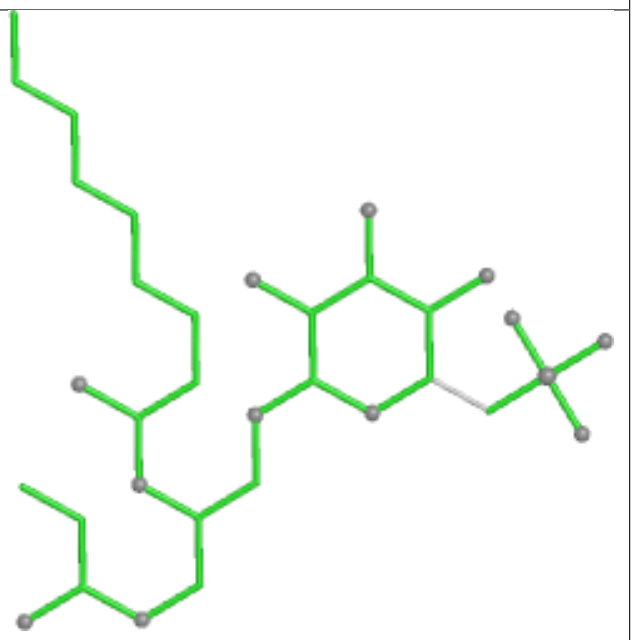


Rings

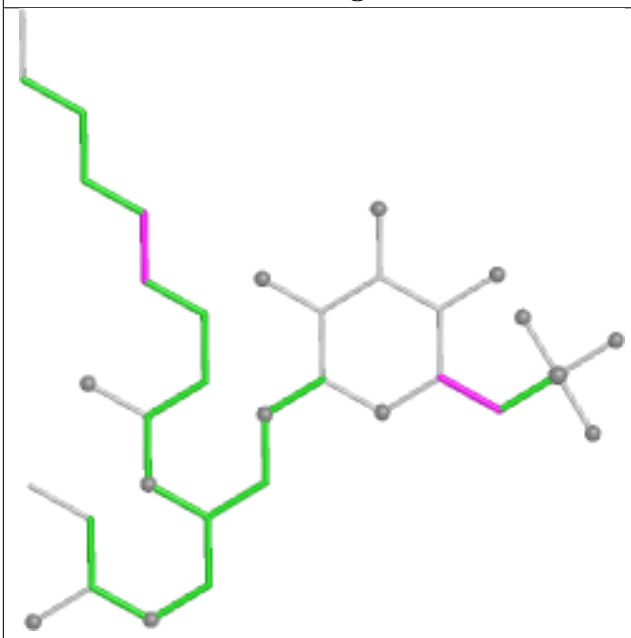
Ligand SQD 1A 406



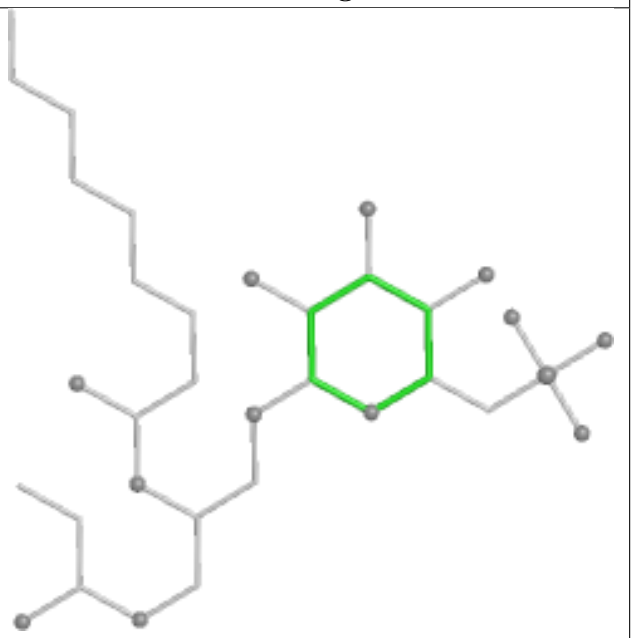
Bond lengths



Bond angles

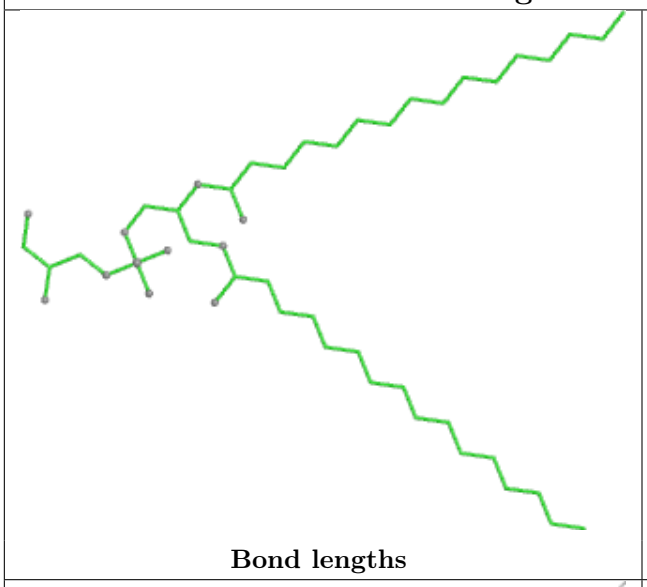


Torsions

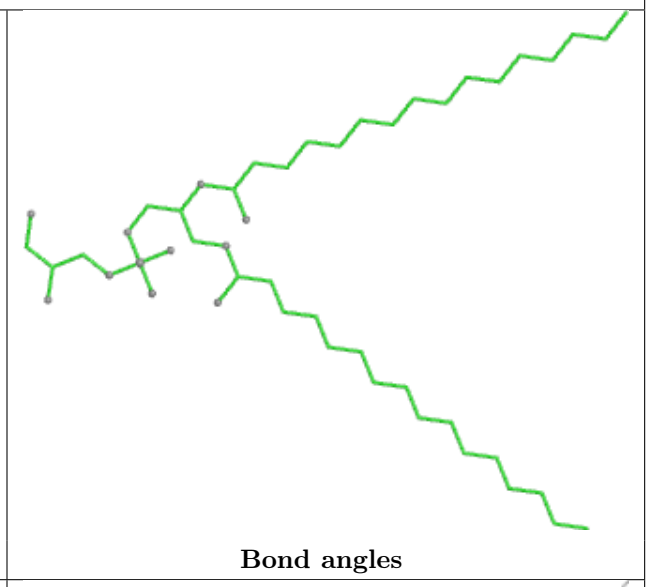


Rings

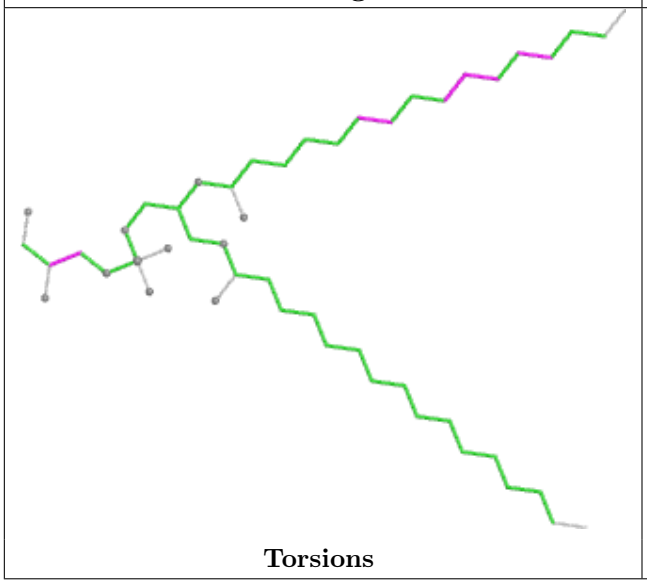
Ligand LHG 1B 625



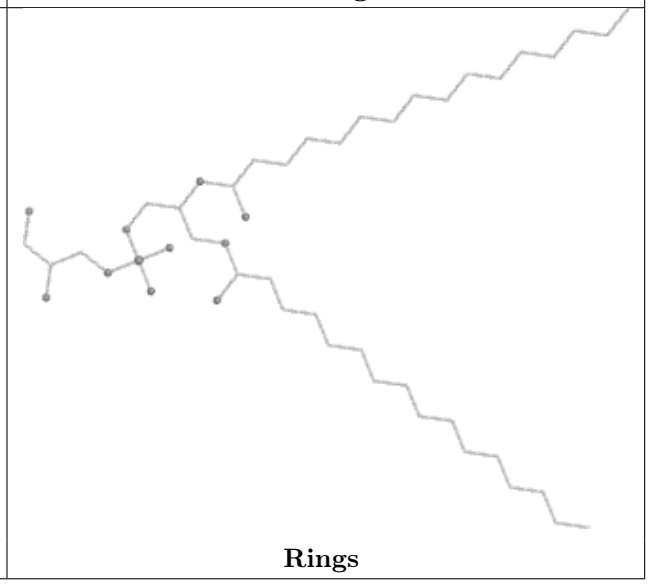
Bond lengths



Bond angles

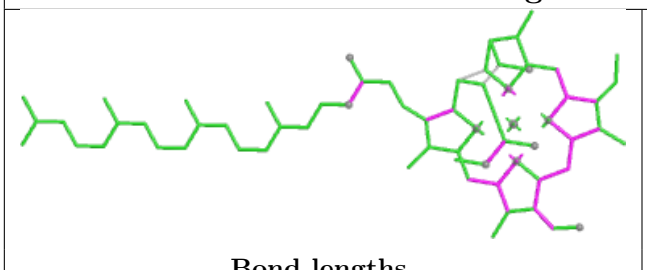


Torsions

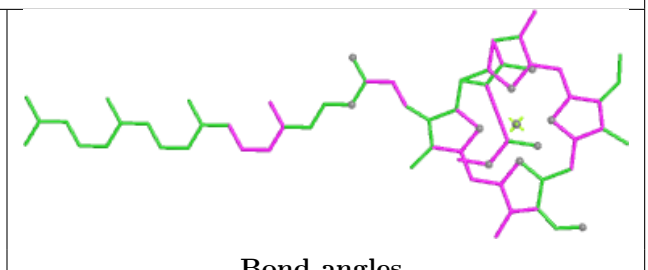


Rings

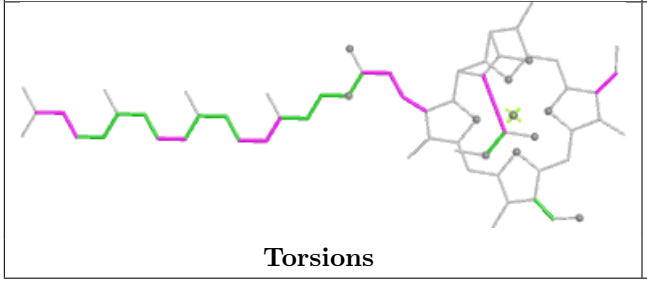
Ligand CL7 23 406



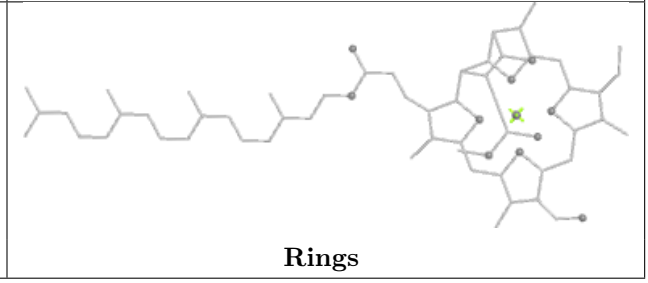
Bond lengths



Bond angles

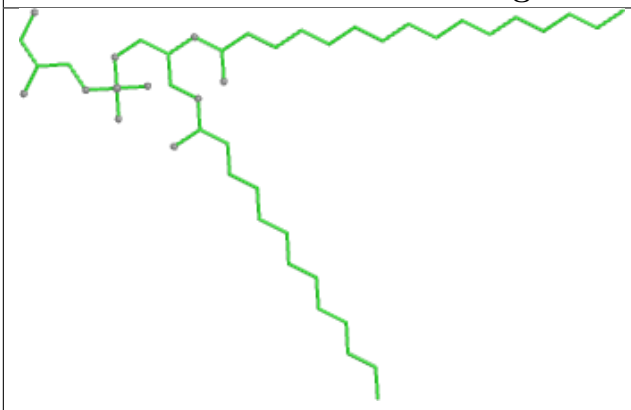


Torsions

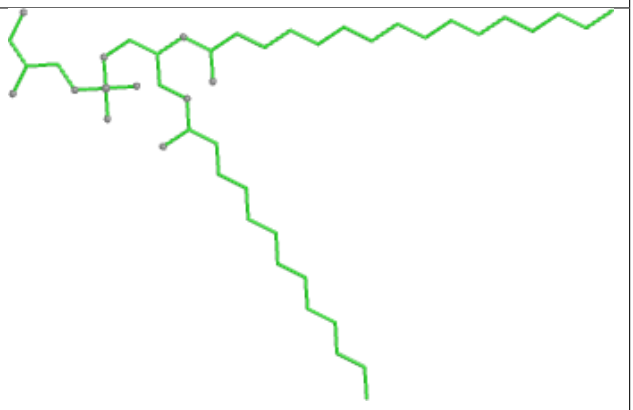


Rings

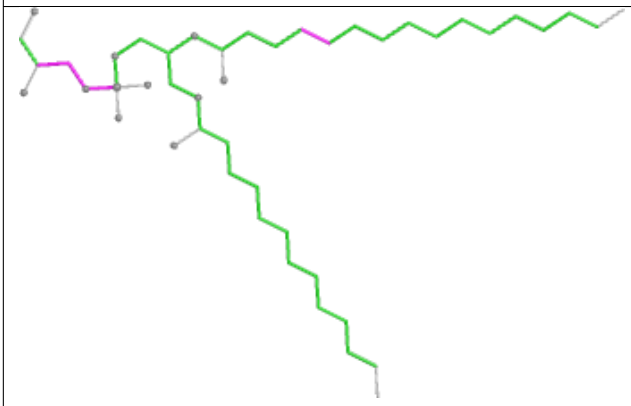
Ligand LHG 2A 408



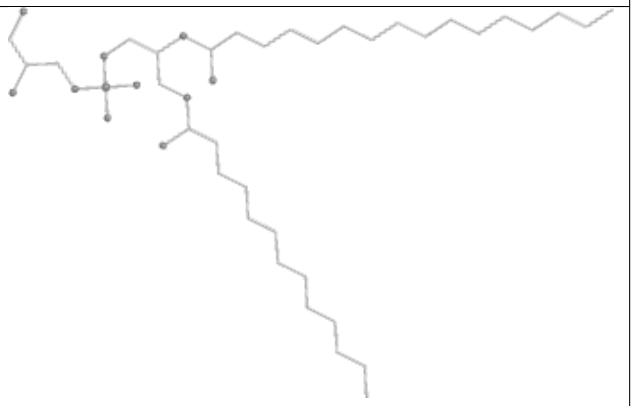
Bond lengths



Bond angles

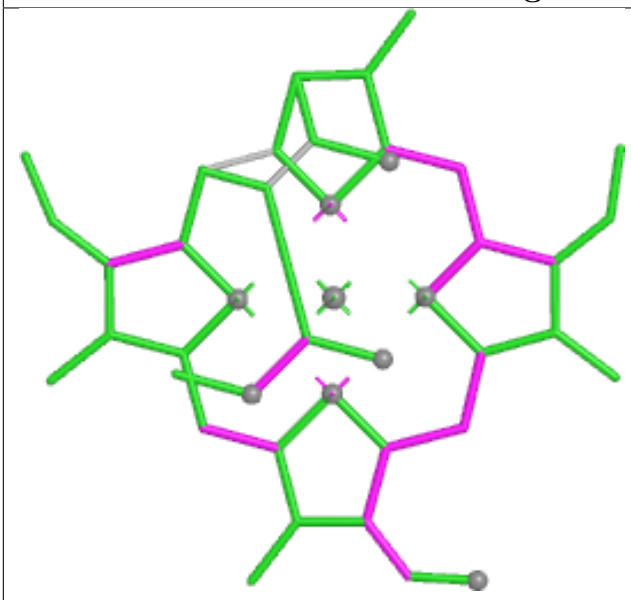


Torsions

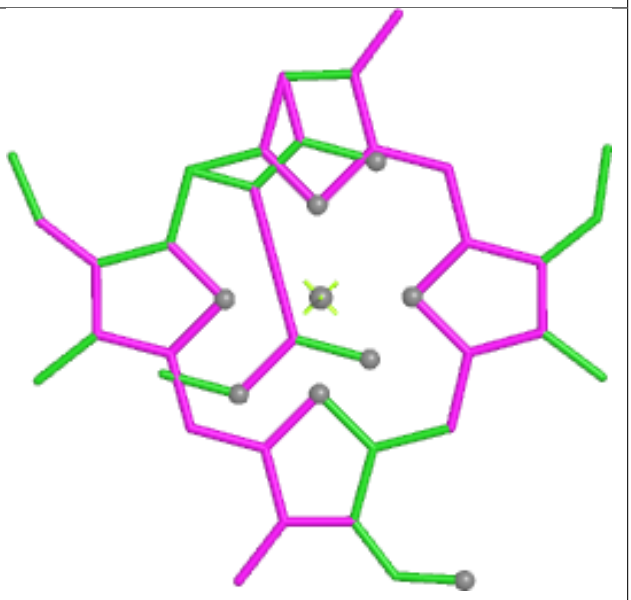


Rings

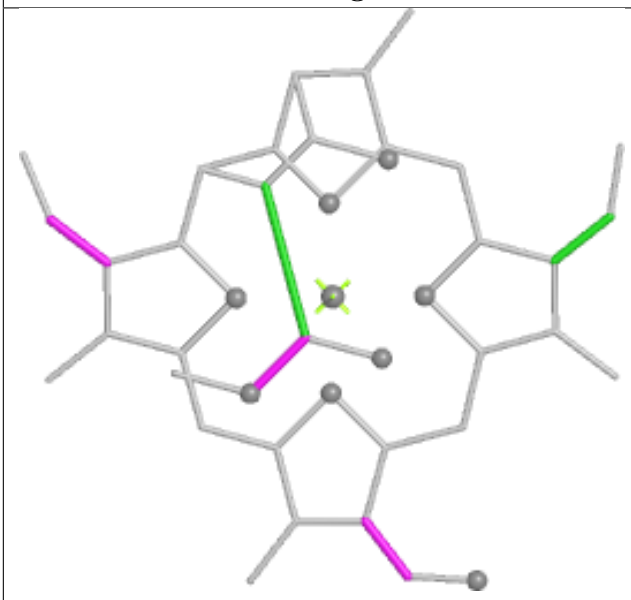
Ligand CL7 24 417



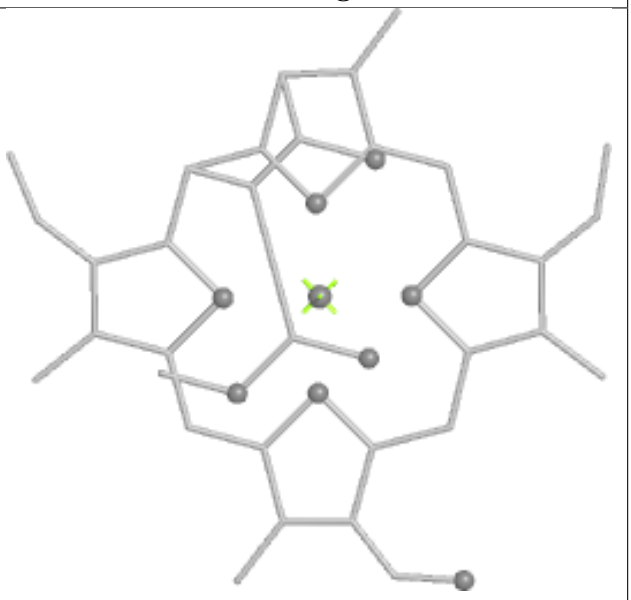
Bond lengths



Bond angles

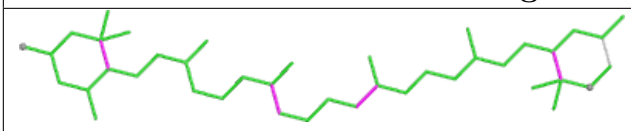


Torsions

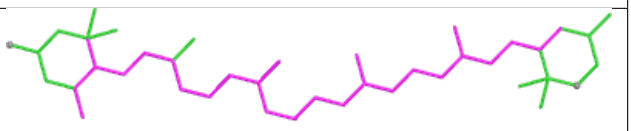


Rings

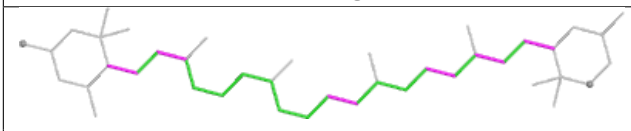
Ligand ZEX 24 403



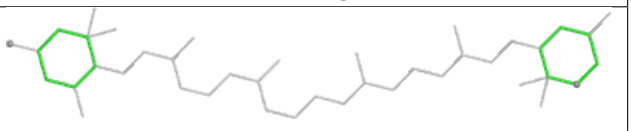
Bond lengths



Bond angles

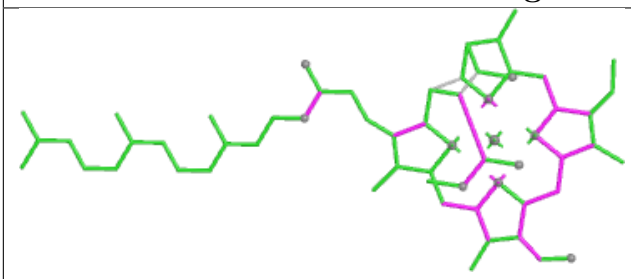


Torsions

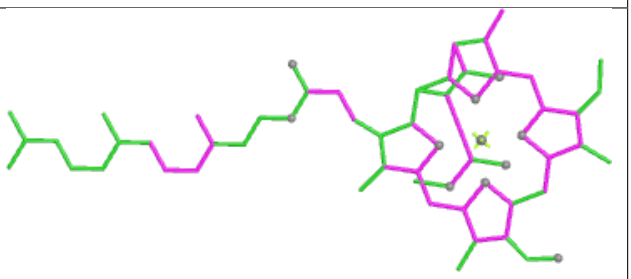


Rings

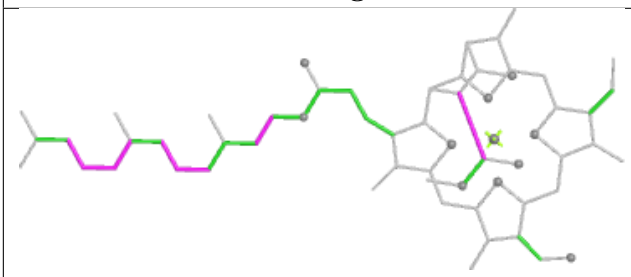
Ligand CL7 14 413



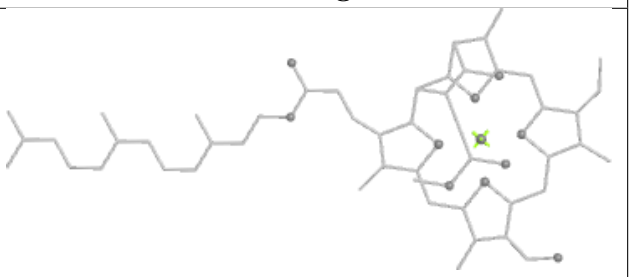
Bond lengths



Bond angles



Torsions

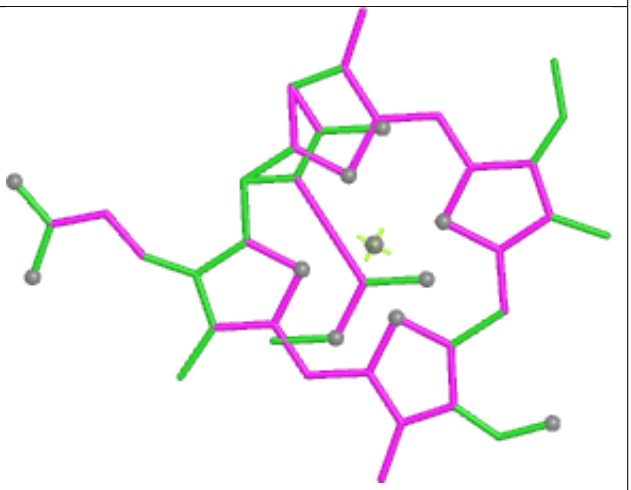


Rings

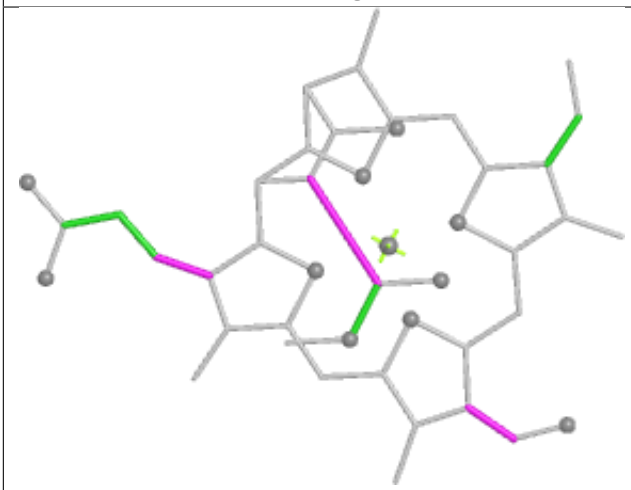
Ligand CL7 42 515



Bond lengths



Bond angles

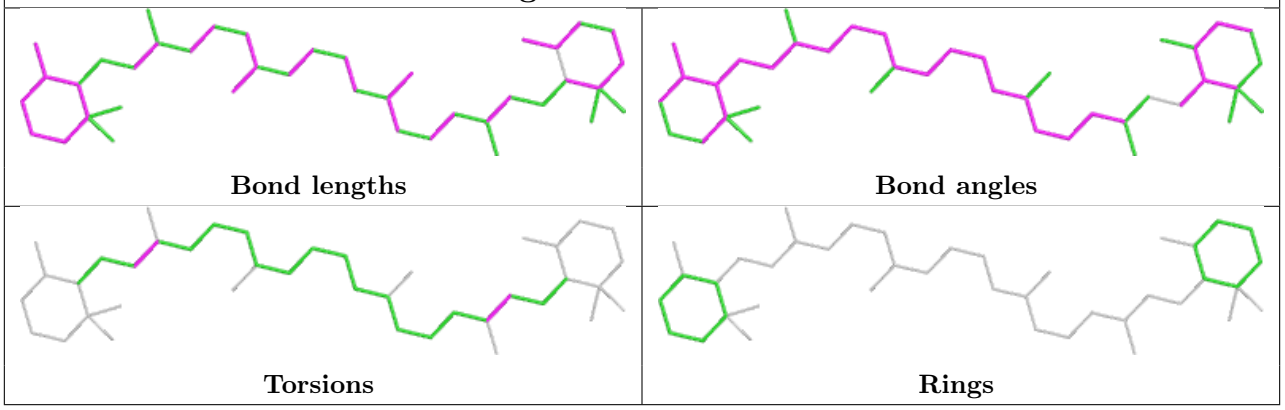


Torsions

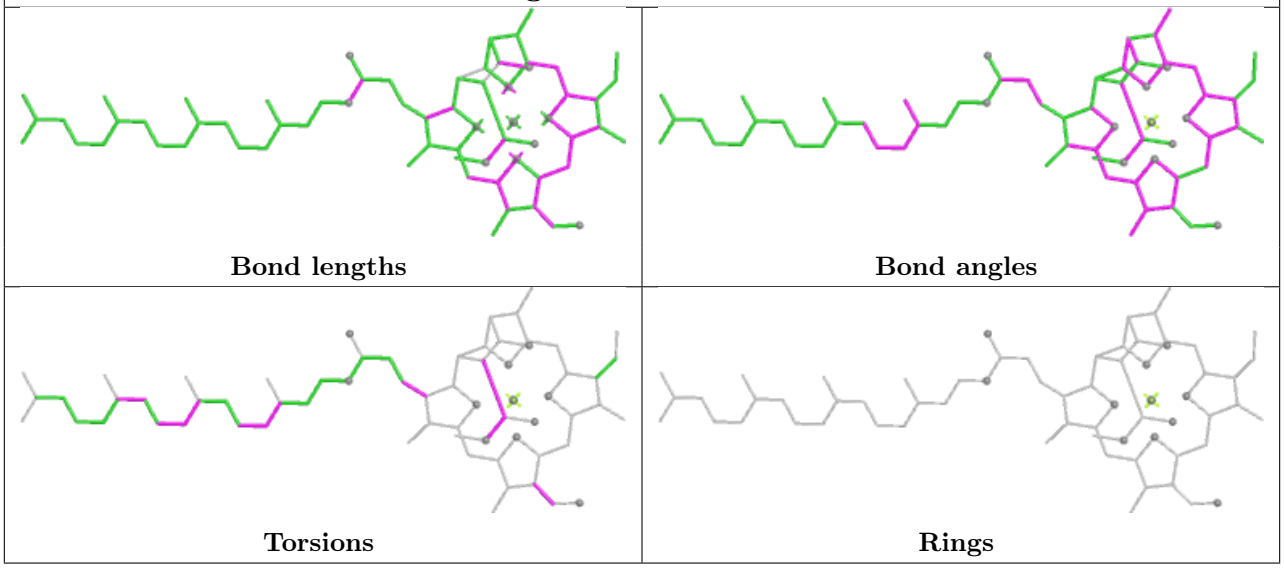


Rings

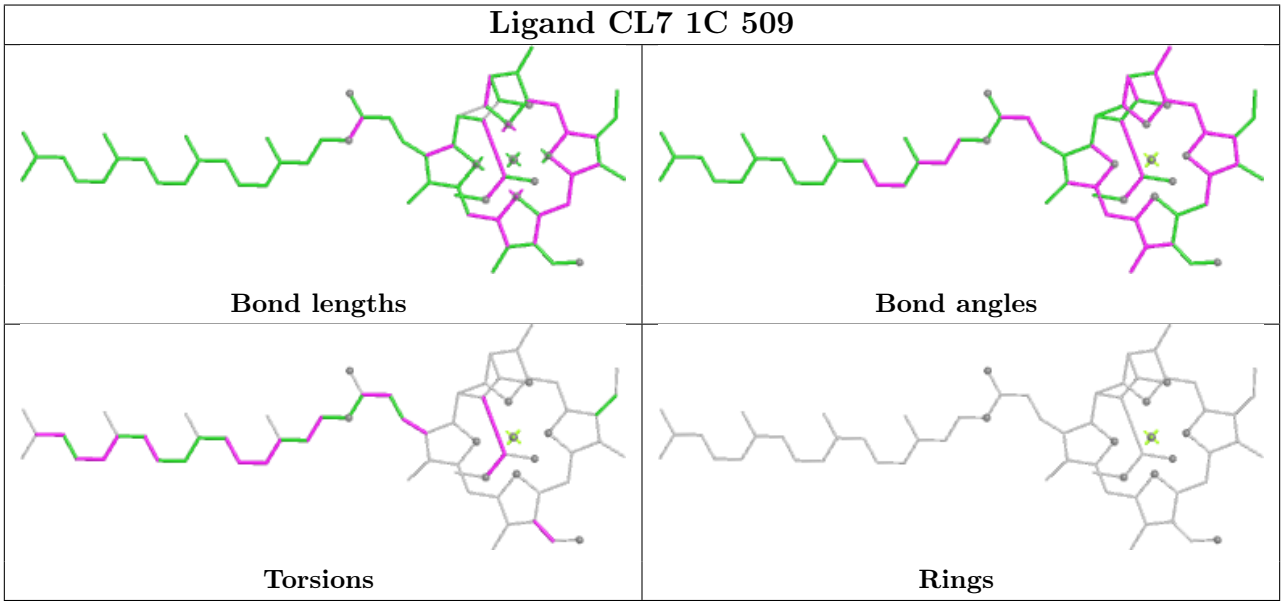
Ligand 8CT 4B 620



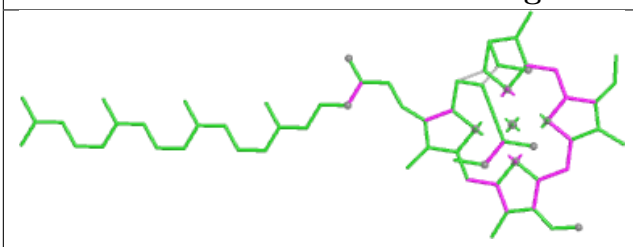
Ligand CL7 22 506



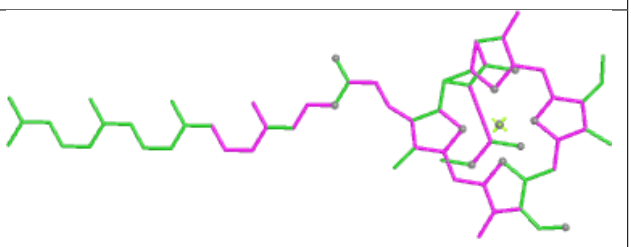
Ligand CL7 1C 509



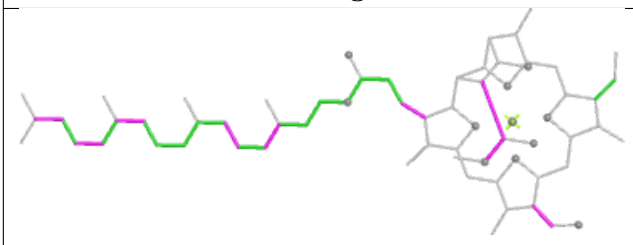
Ligand CL7 14 411



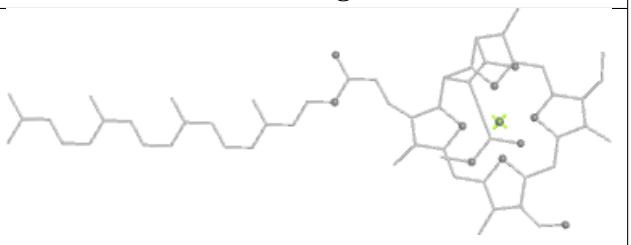
Bond lengths



Bond angles

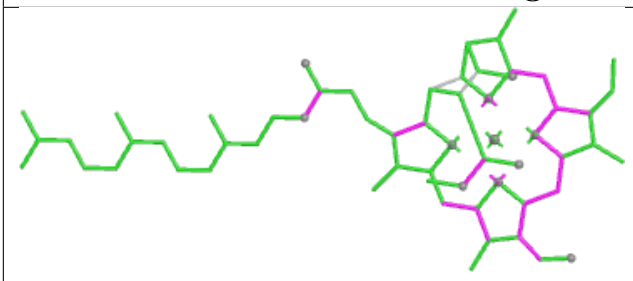


Torsions

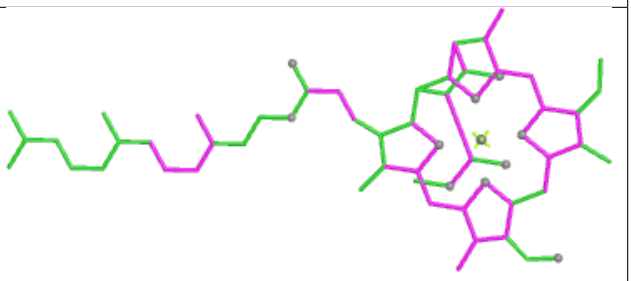


Rings

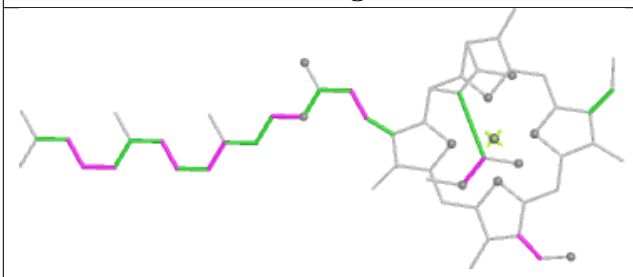
Ligand CL7 41 403



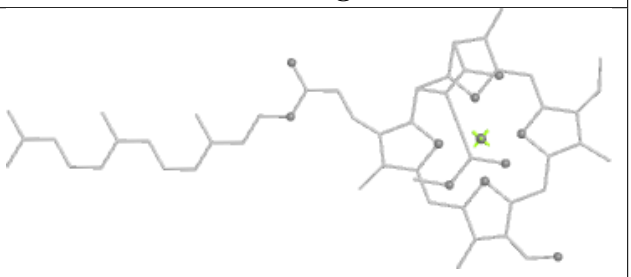
Bond lengths



Bond angles

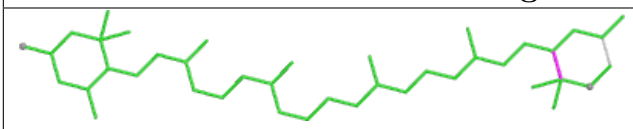


Torsions

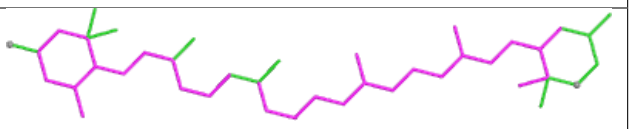


Rings

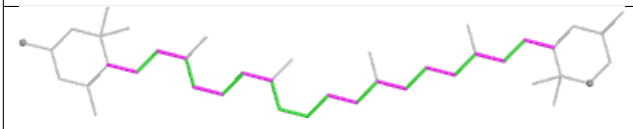
Ligand ZEX 41 421



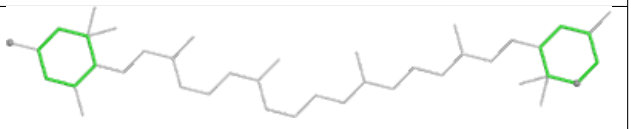
Bond lengths



Bond angles

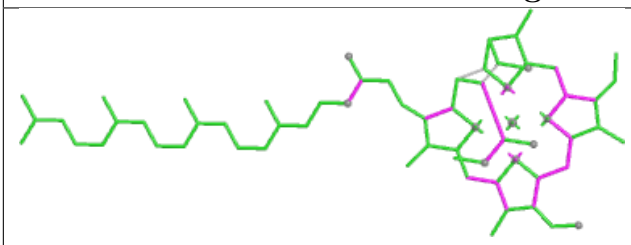


Torsions

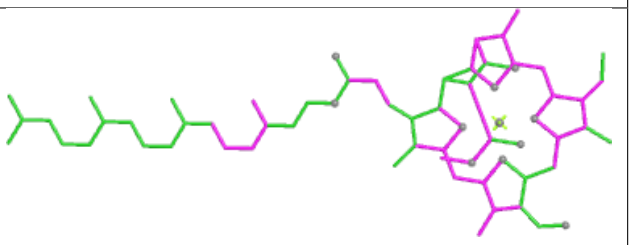


Rings

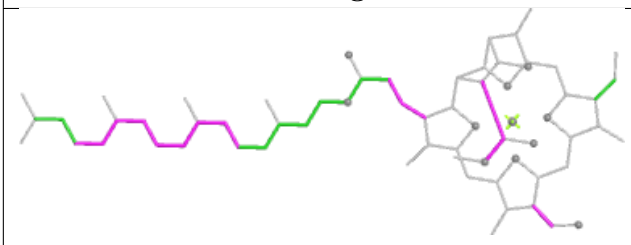
Ligand CL7 43 404



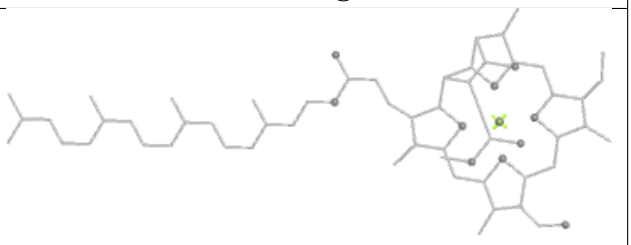
Bond lengths



Bond angles

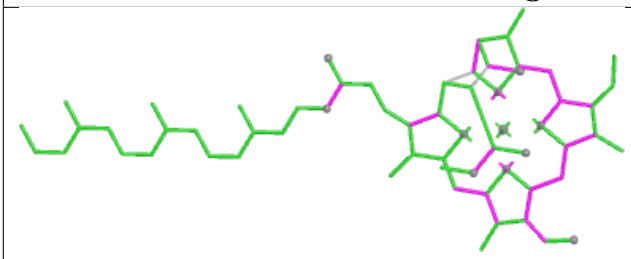


Torsions

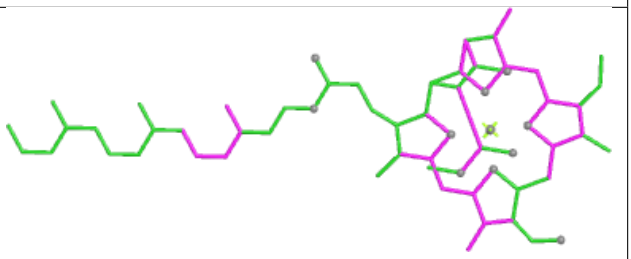


Rings

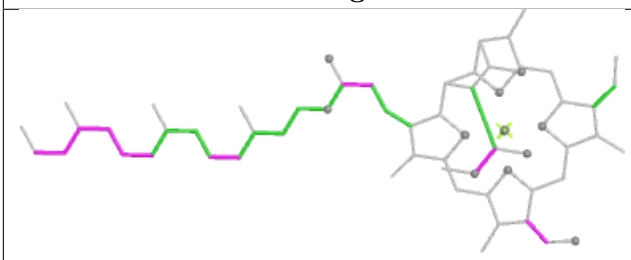
Ligand CL7 11 406



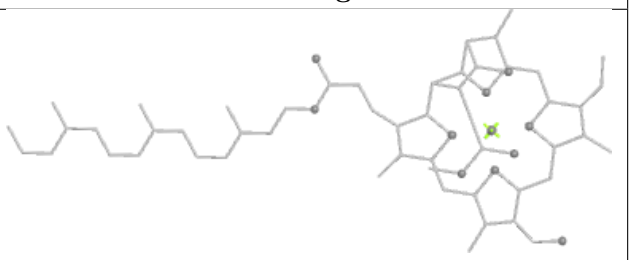
Bond lengths



Bond angles

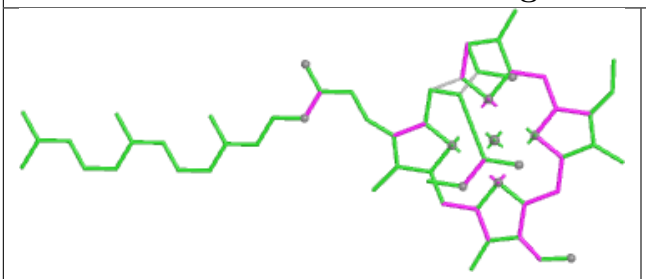


Torsions

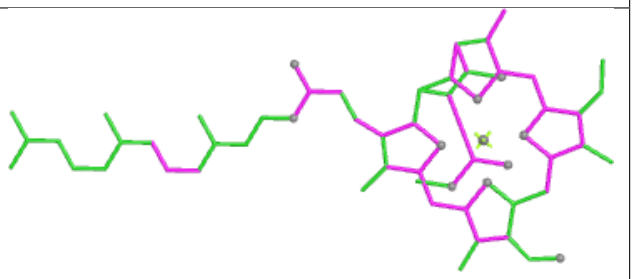


Rings

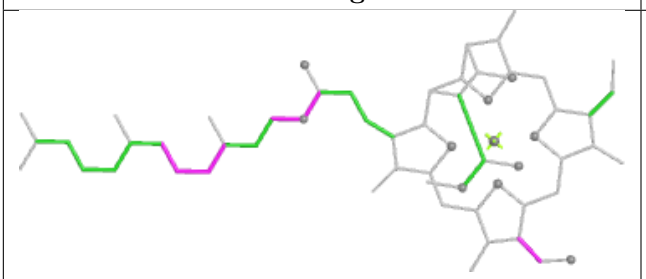
Ligand CL7 4B 603



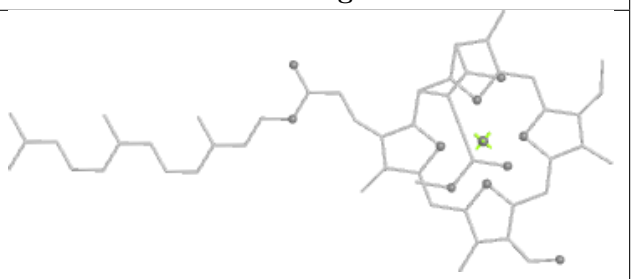
Bond lengths



Bond angles

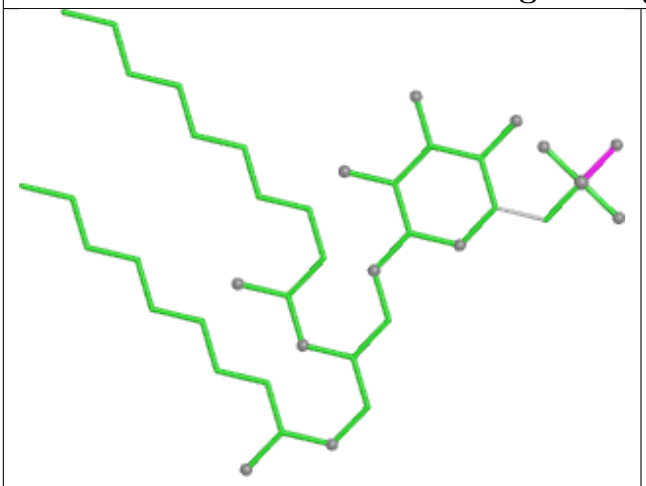


Torsions

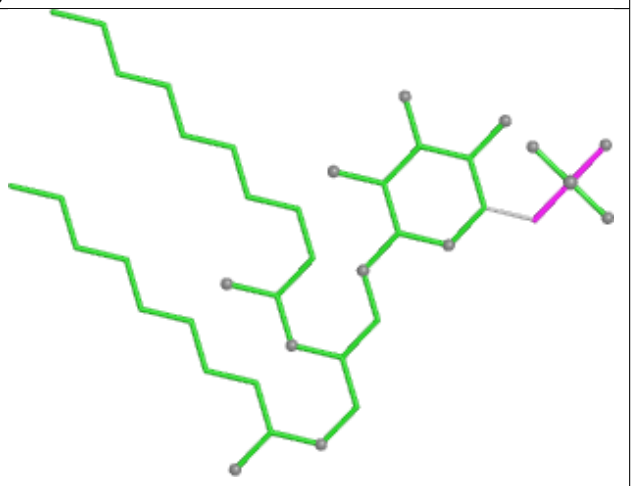


Rings

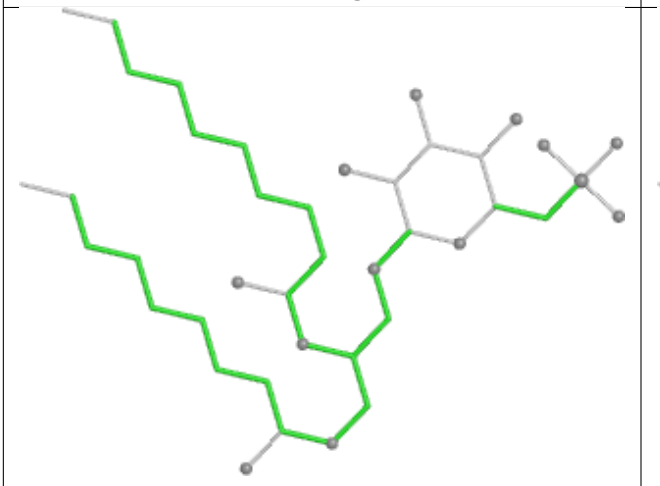
Ligand SQD 42 523



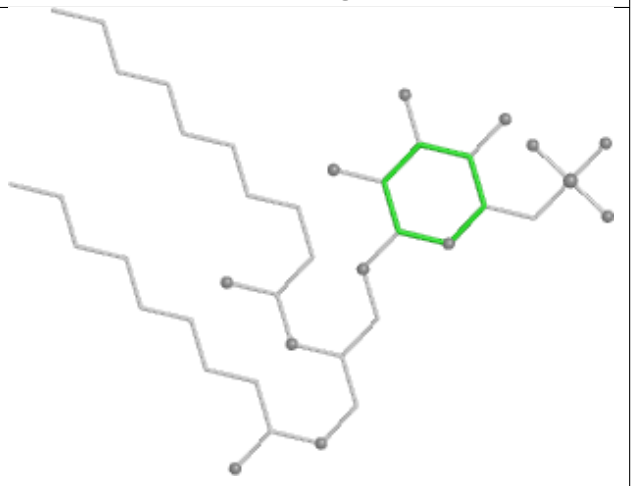
Bond lengths



Bond angles

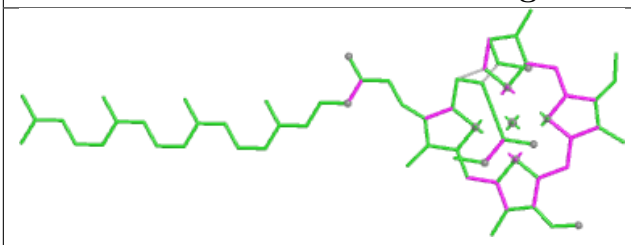


Torsions

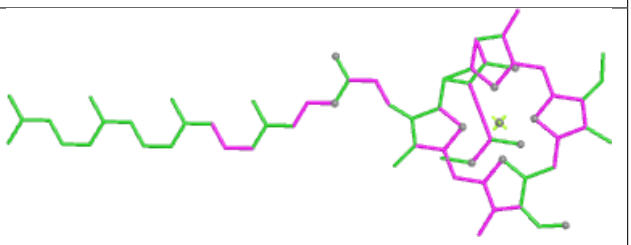


Rings

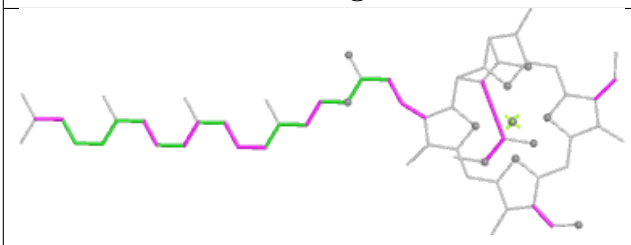
Ligand CL7 3A 407



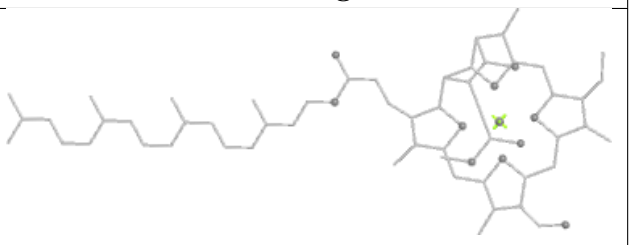
Bond lengths



Bond angles

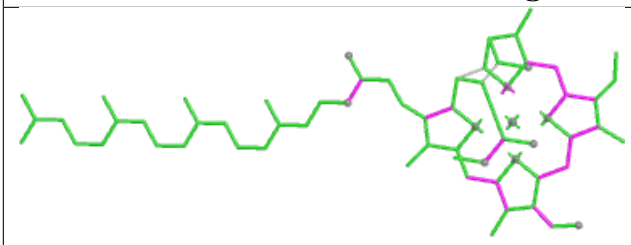


Torsions

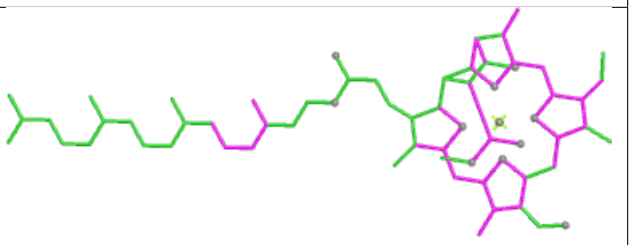


Rings

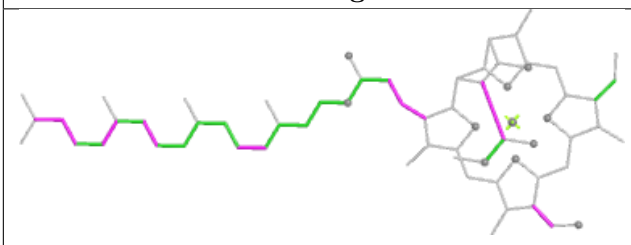
Ligand CL7 22 518



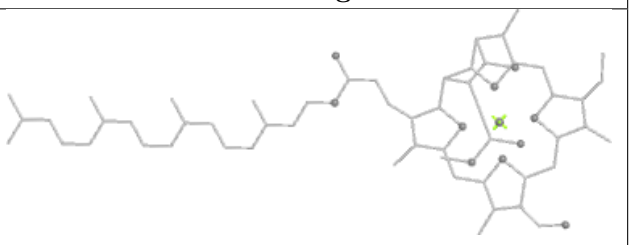
Bond lengths



Bond angles

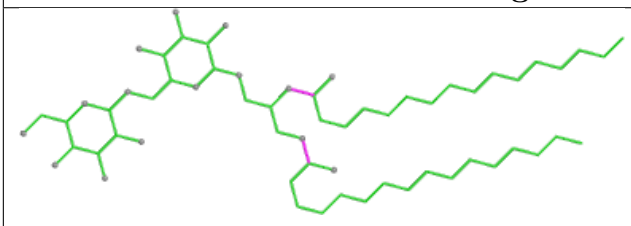


Torsions

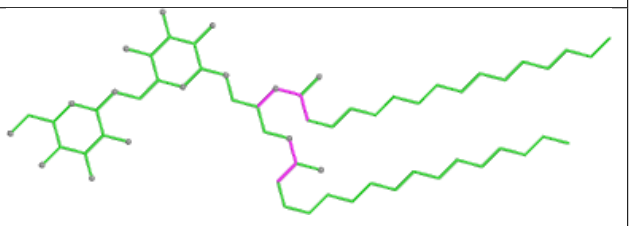


Rings

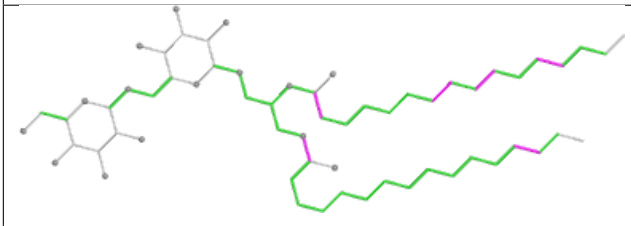
Ligand DGD 1B 624



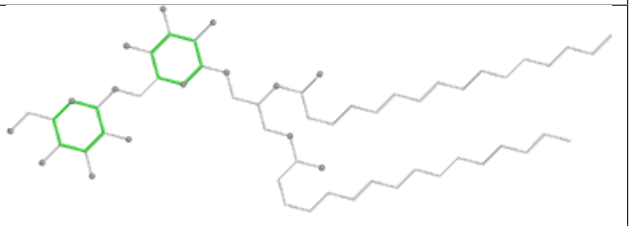
Bond lengths



Bond angles

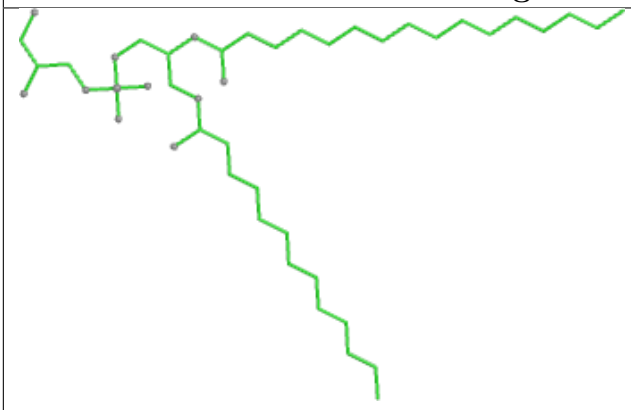


Torsions

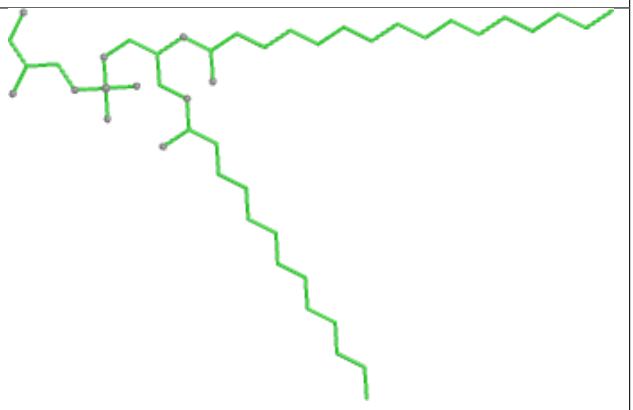


Rings

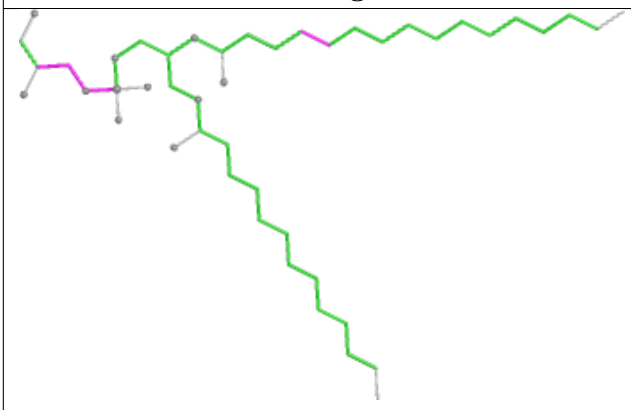
Ligand LHG 1A 408



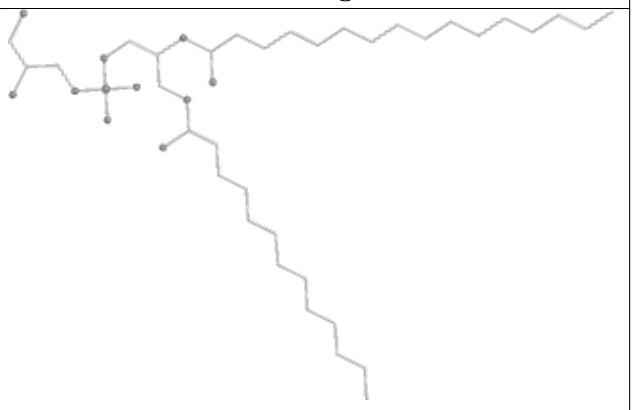
Bond lengths



Bond angles



Torsions

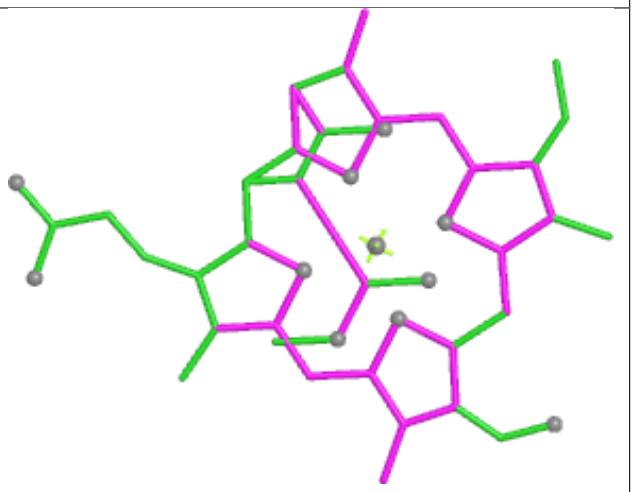


Rings

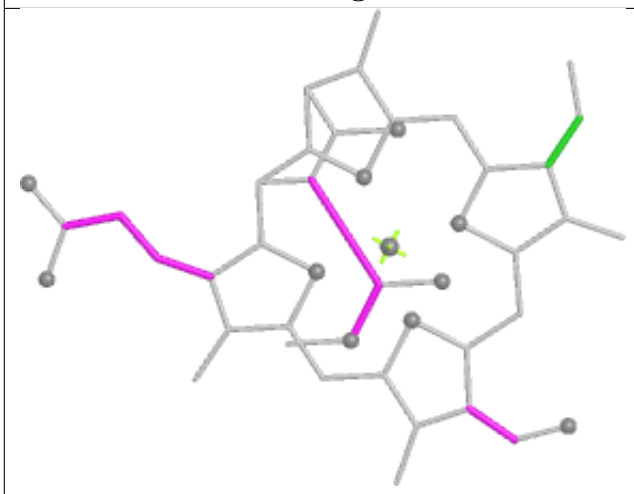
Ligand CL7 44 410



Bond lengths



Bond angles

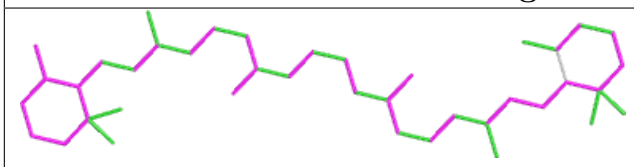


Torsions

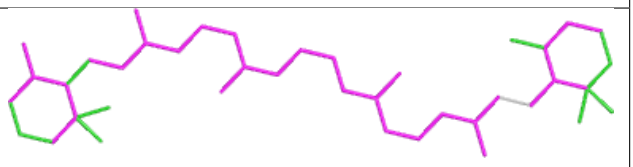


Rings

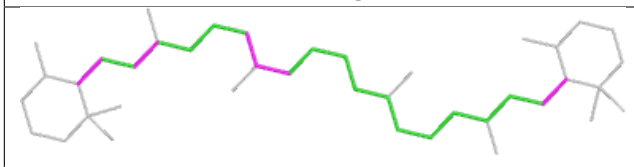
Ligand 8CT 1B 626



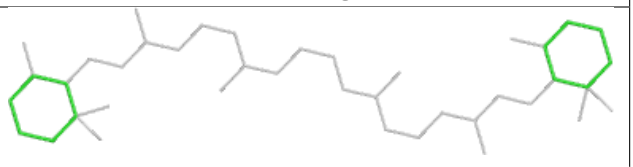
Bond lengths



Bond angles

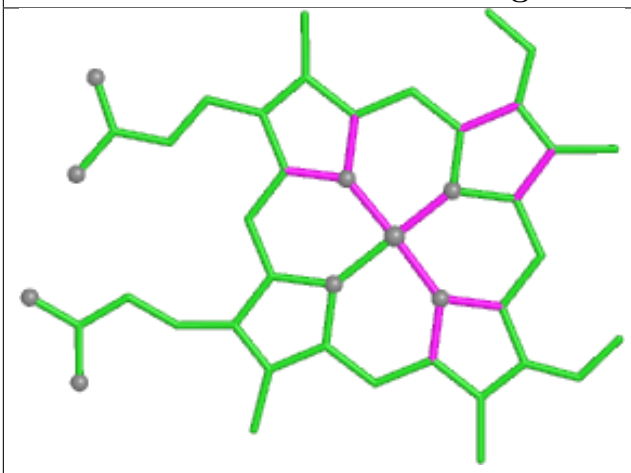


Torsions

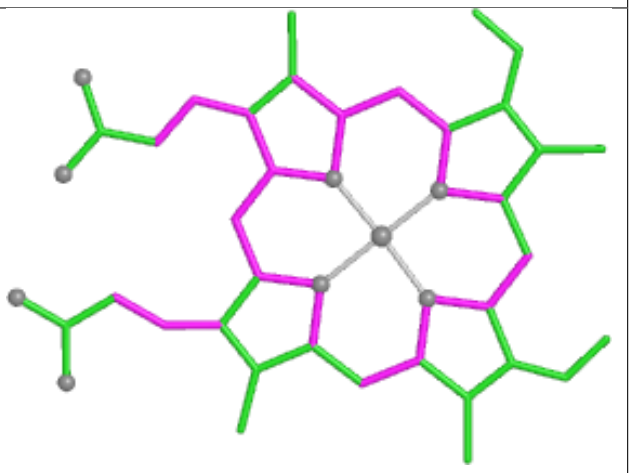


Rings

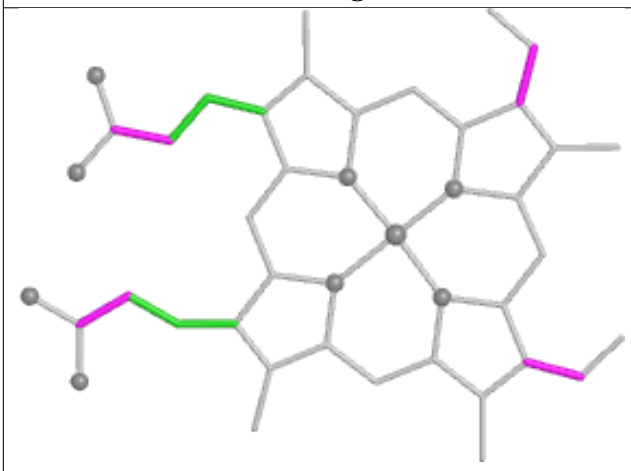
Ligand HEM 3F 101



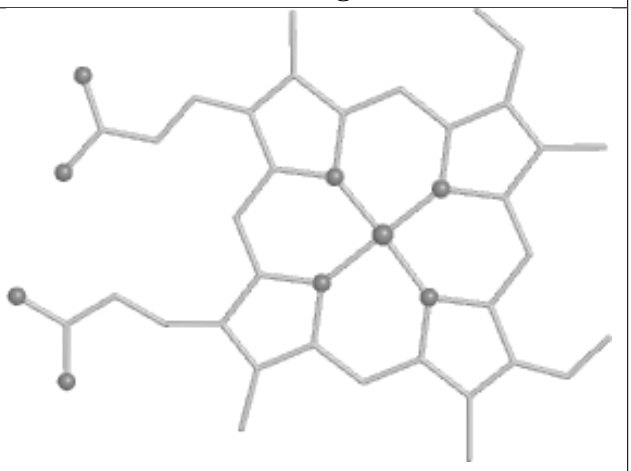
Bond lengths



Bond angles

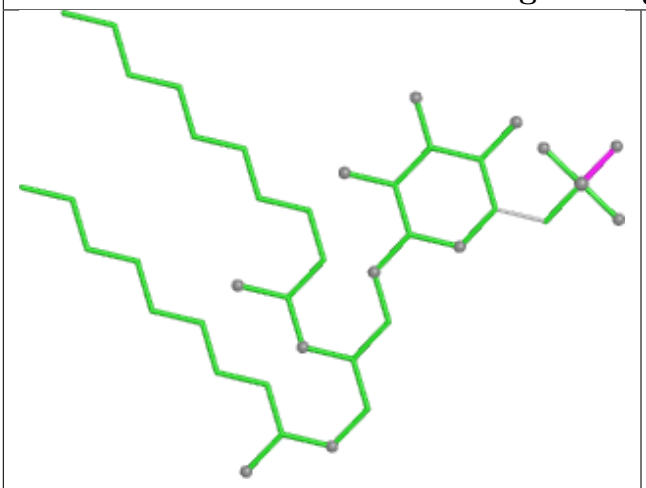


Torsions

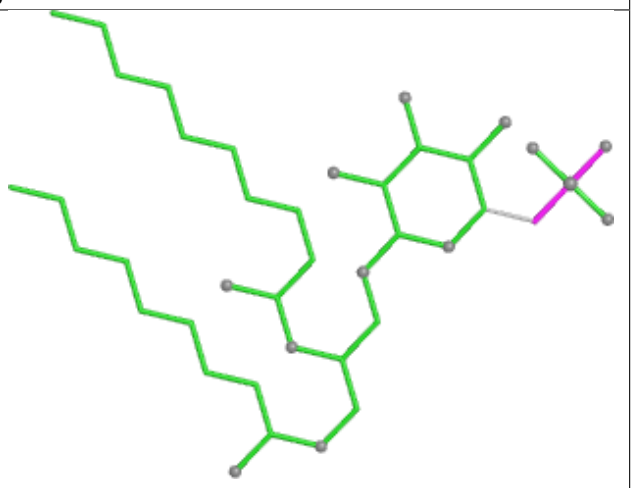


Rings

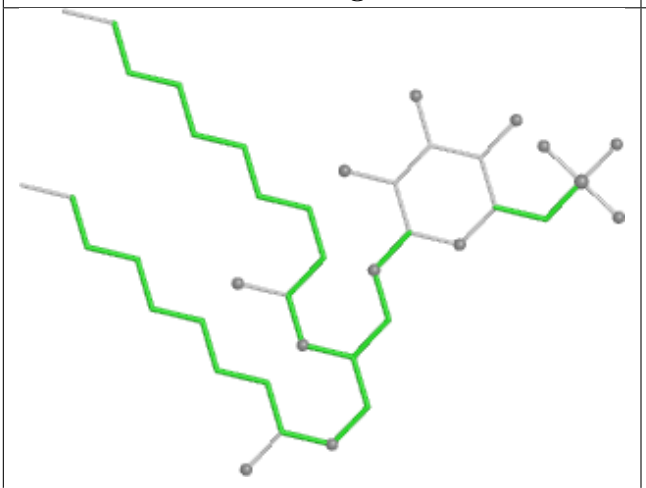
Ligand SQD 12 523



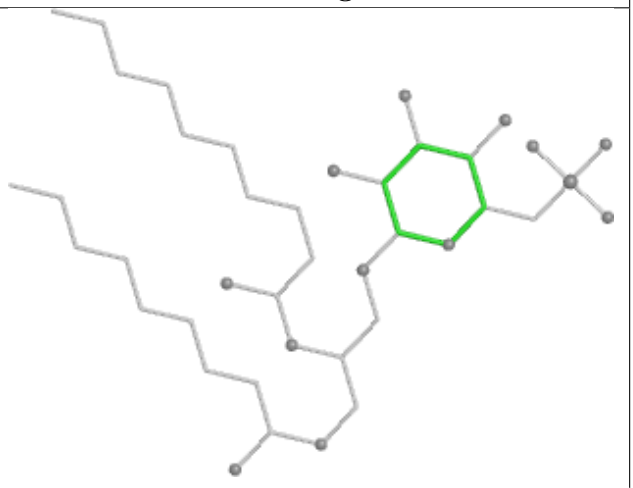
Bond lengths



Bond angles

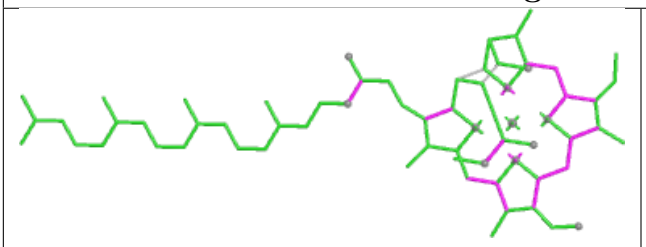


Torsions

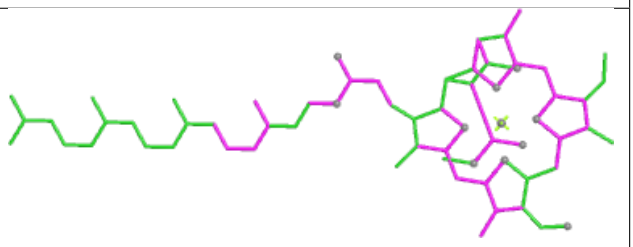


Rings

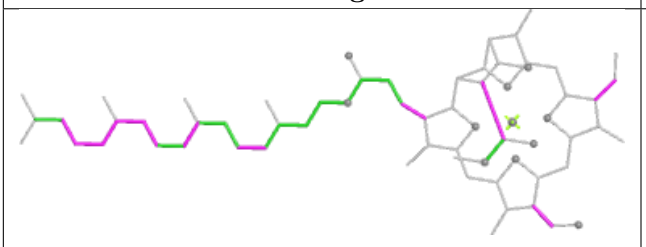
Ligand CL7 41 408



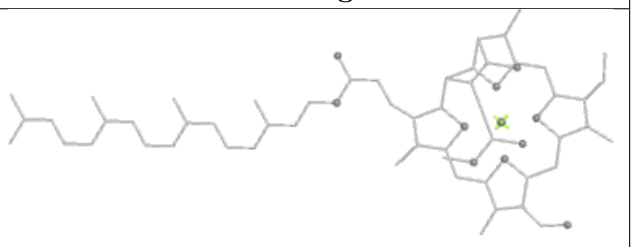
Bond lengths



Bond angles

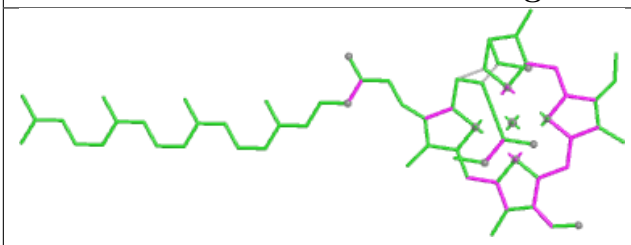


Torsions

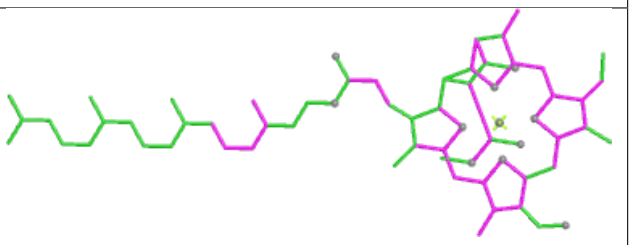


Rings

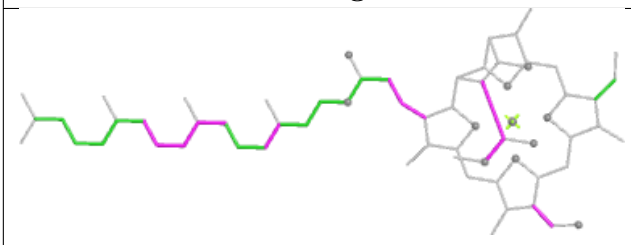
Ligand CL7 42 502



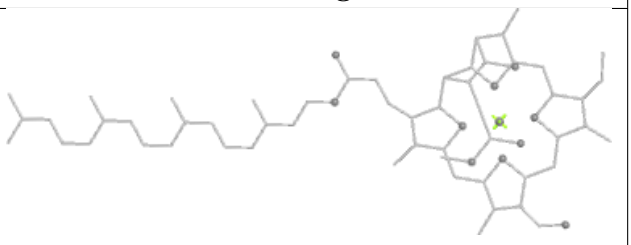
Bond lengths



Bond angles

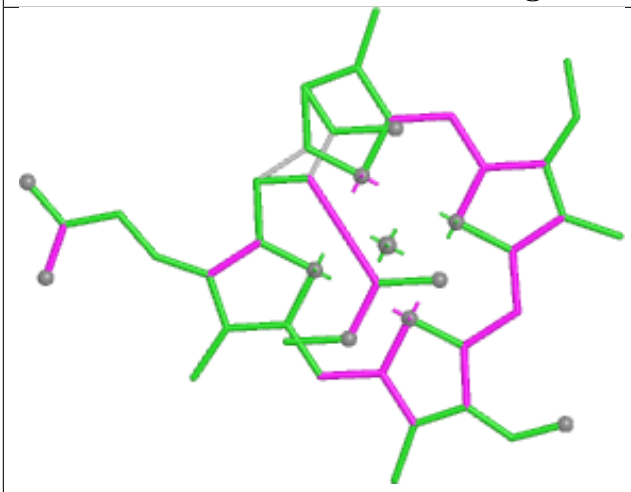


Torsions



Rings

Ligand CL7 23 414



Bond lengths



Bond angles

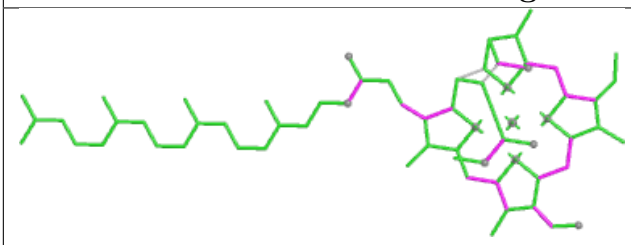


Torsions

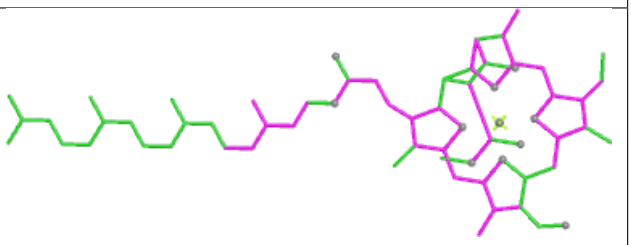


Rings

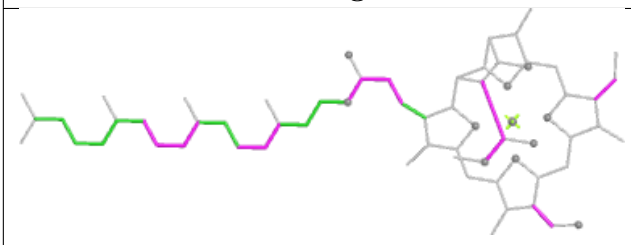
Ligand CL7 1A 401



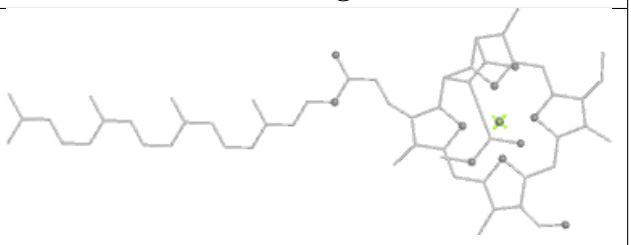
Bond lengths



Bond angles

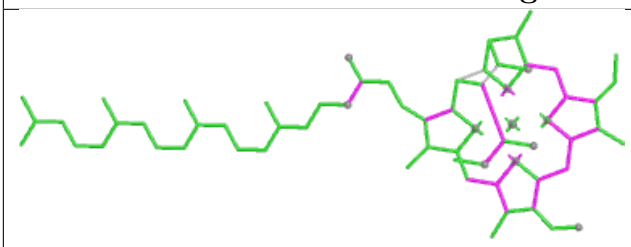


Torsions

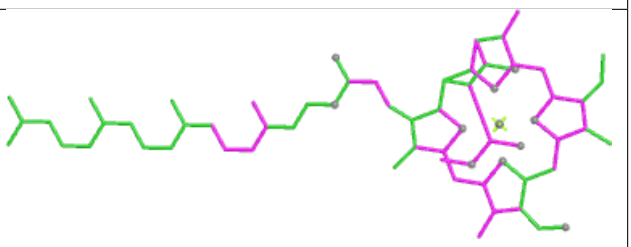


Rings

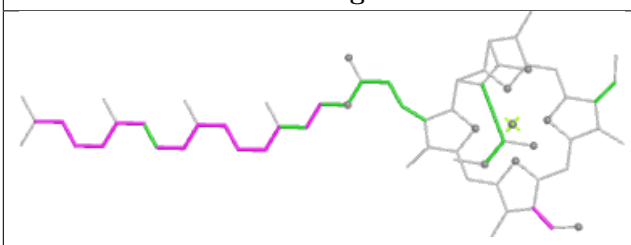
Ligand CL7 1C 507



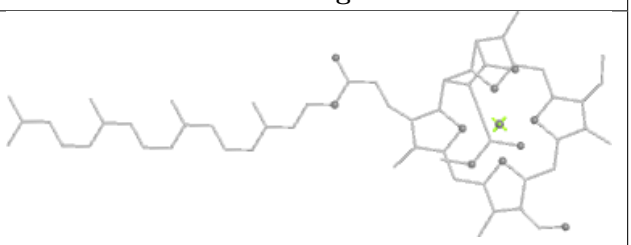
Bond lengths



Bond angles

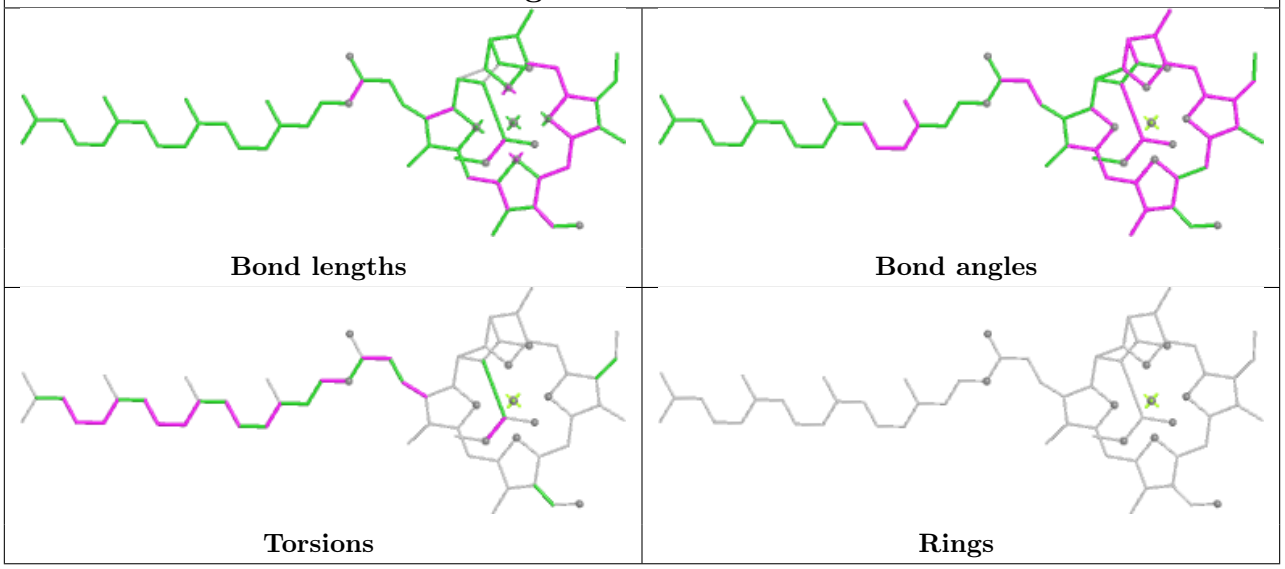


Torsions

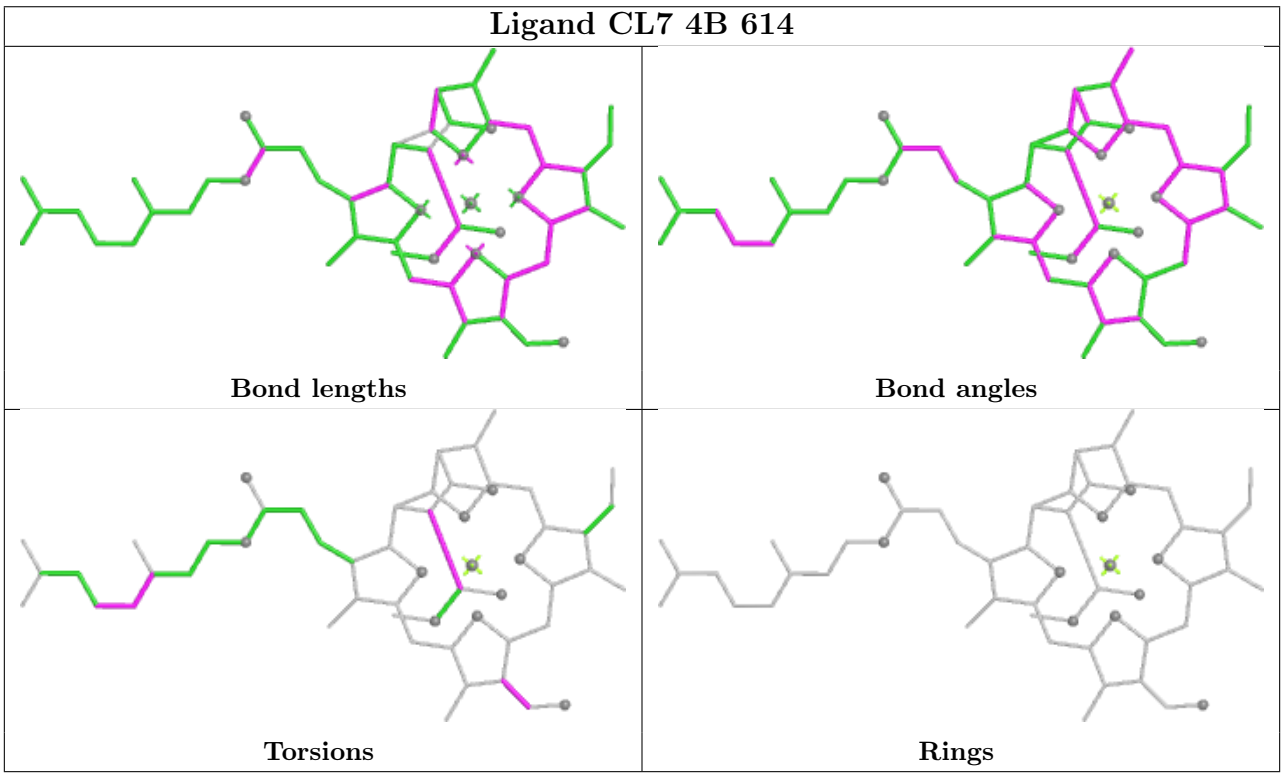


Rings

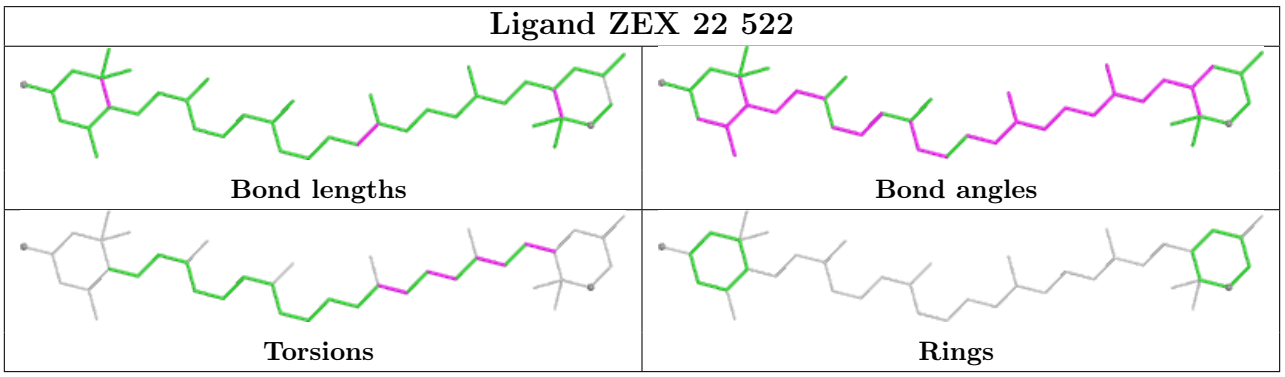
Ligand CL7 24 412



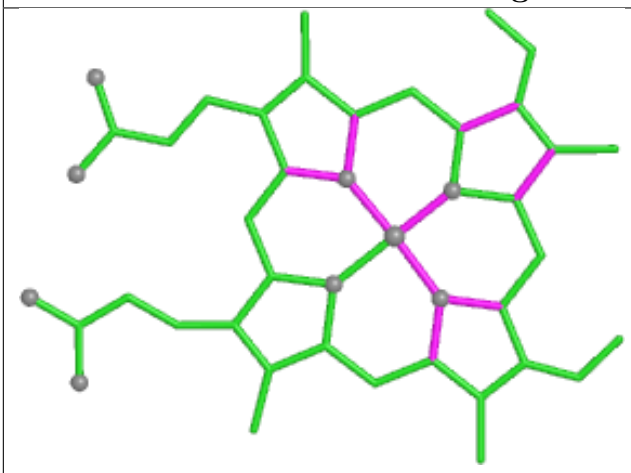
Ligand CL7 4B 614



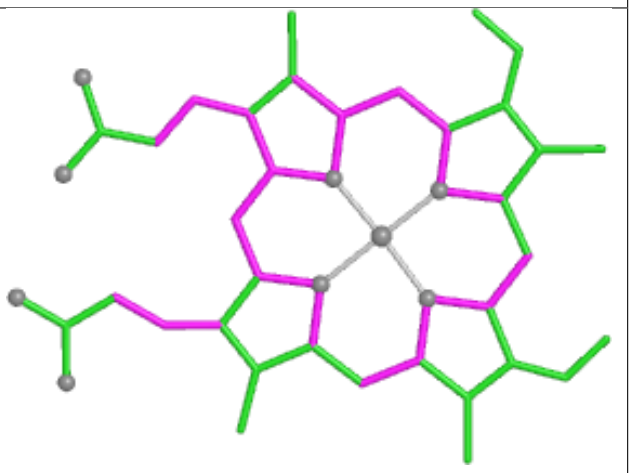
Ligand ZEX 22 522



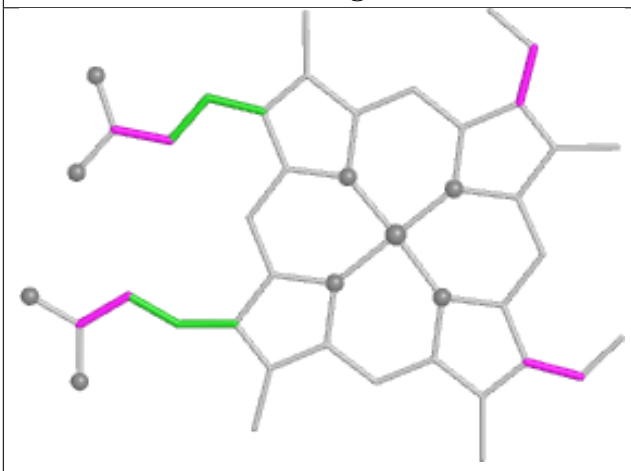
Ligand HEM 4F 101



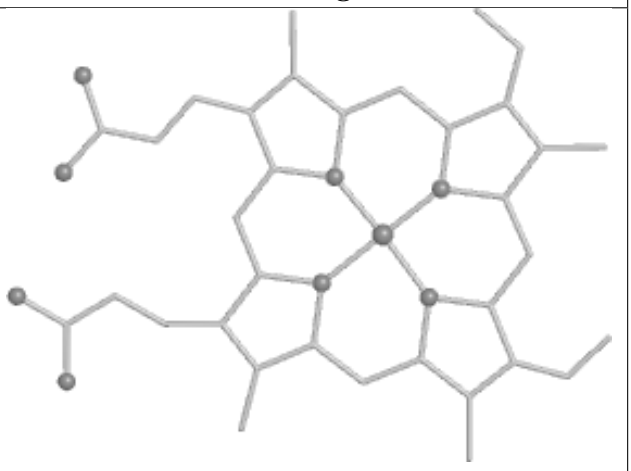
Bond lengths



Bond angles

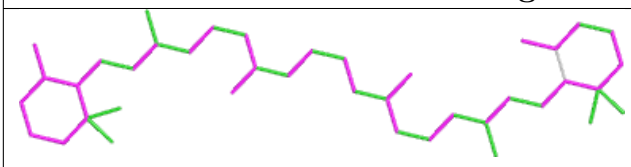


Torsions

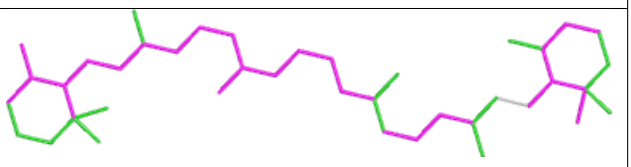


Rings

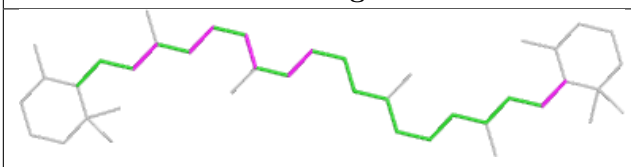
Ligand 8CT 3B 617



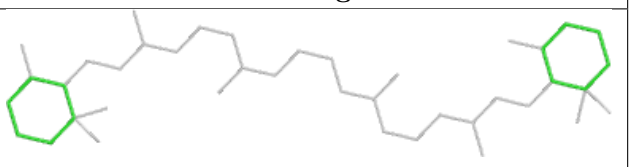
Bond lengths



Bond angles

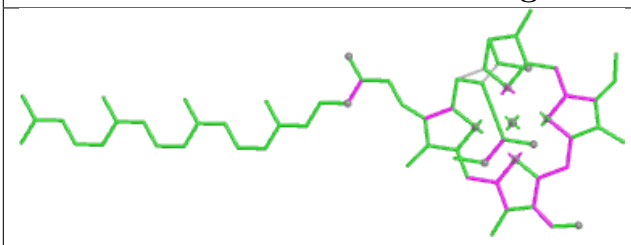


Torsions

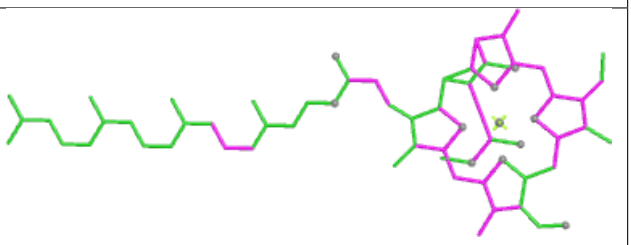


Rings

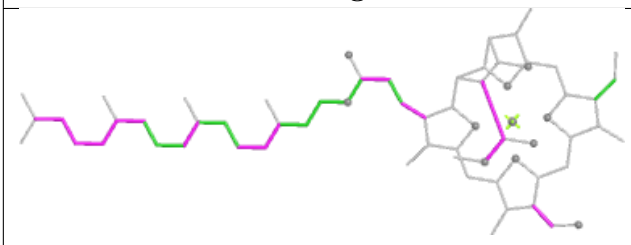
Ligand CL7 4C 501



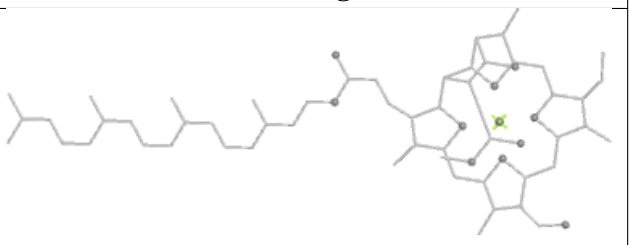
Bond lengths



Bond angles

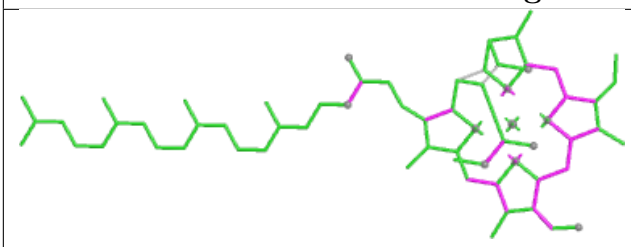


Torsions

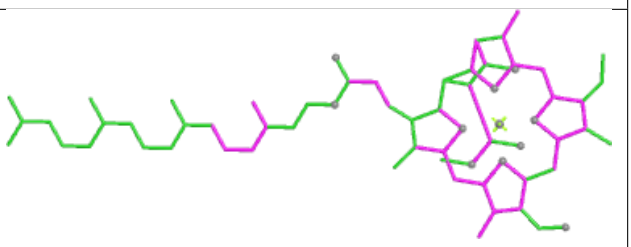


Rings

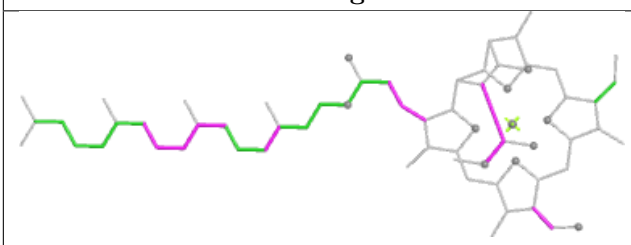
Ligand CL7 12 502



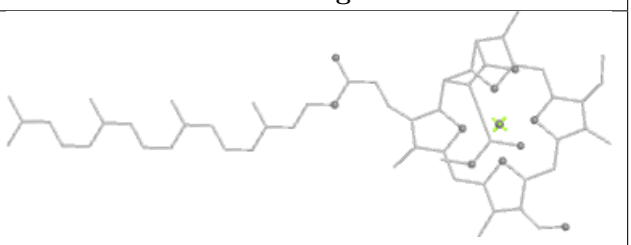
Bond lengths



Bond angles

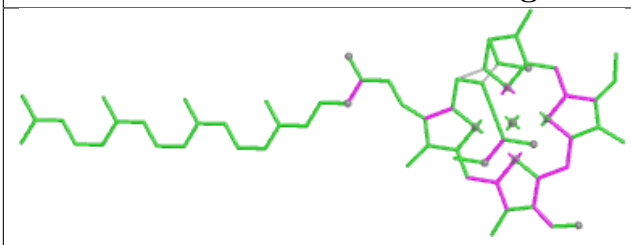


Torsions

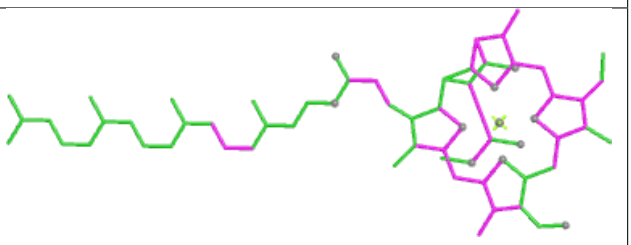


Rings

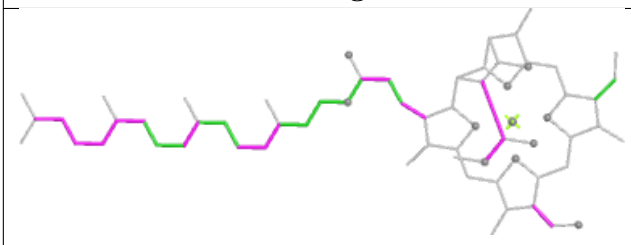
Ligand CL7 3C 501



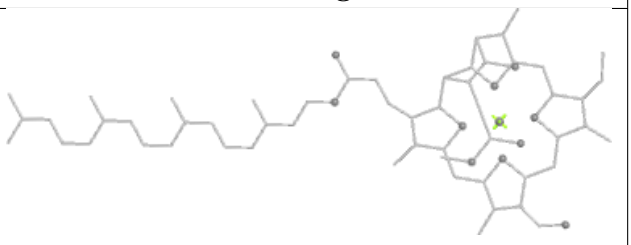
Bond lengths



Bond angles

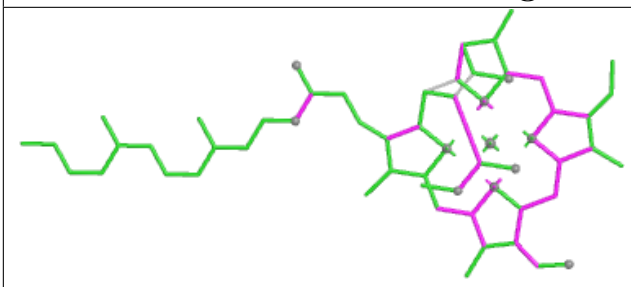


Torsions

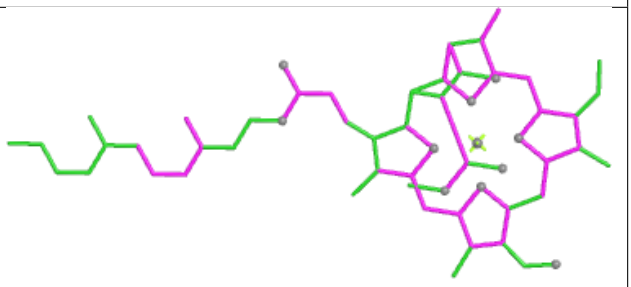


Rings

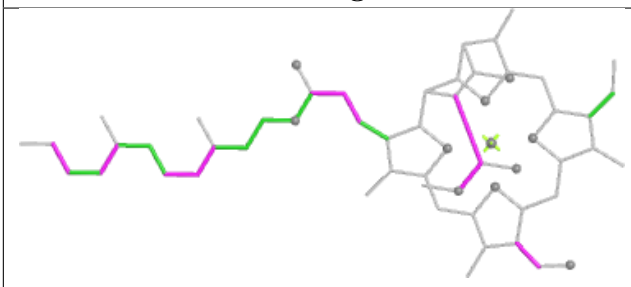
Ligand CL7 2D 404



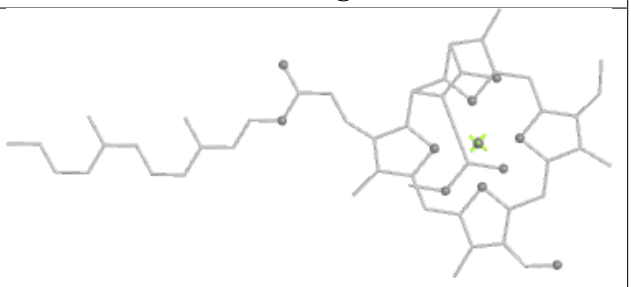
Bond lengths



Bond angles

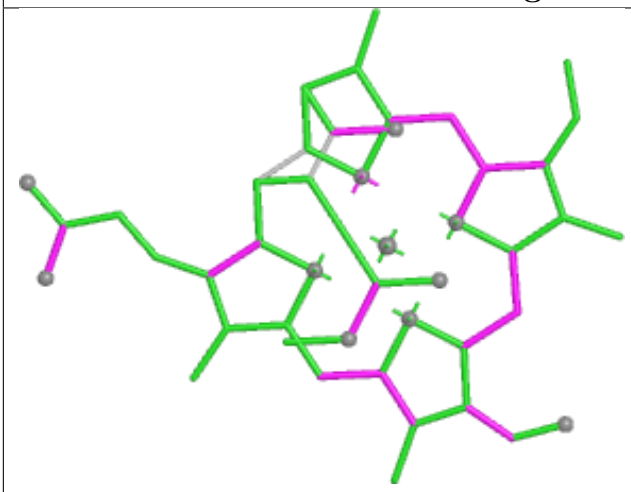


Torsions

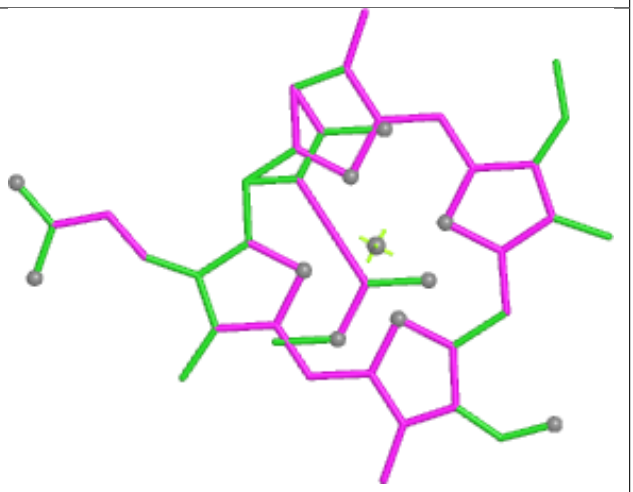


Rings

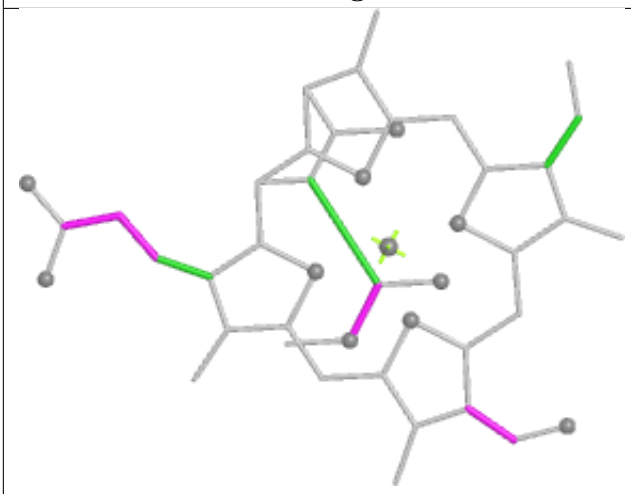
Ligand CL7 13 518



Bond lengths



Bond angles

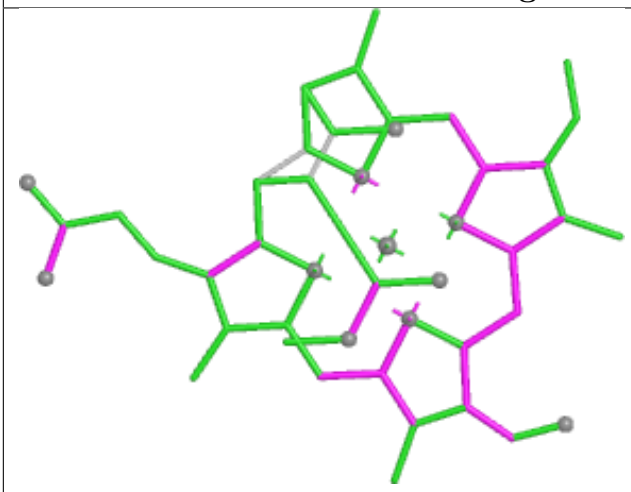


Torsions

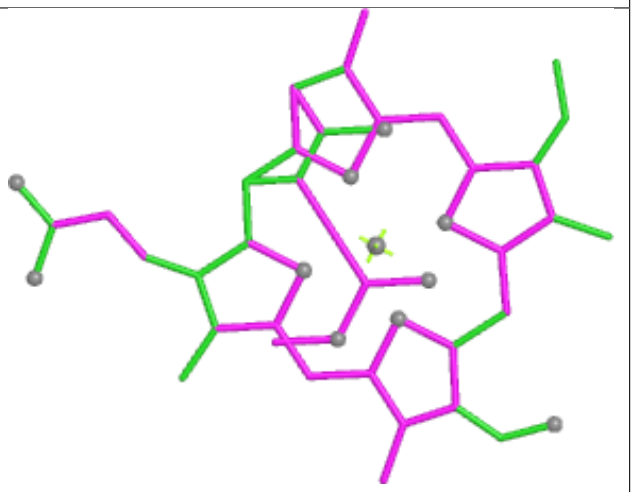


Rings

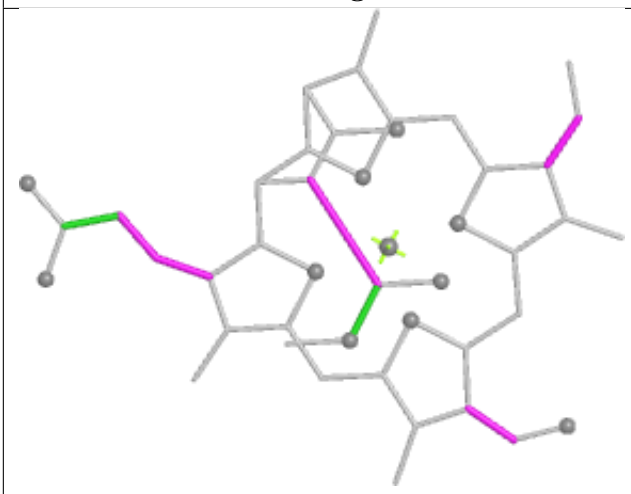
Ligand CL7 2D 405



Bond lengths



Bond angles

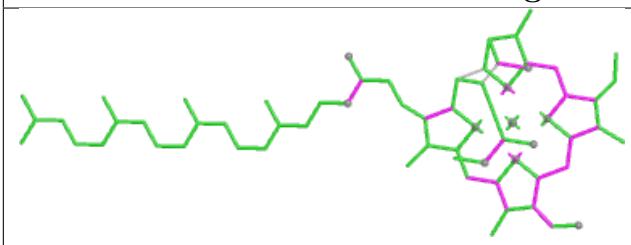


Torsions

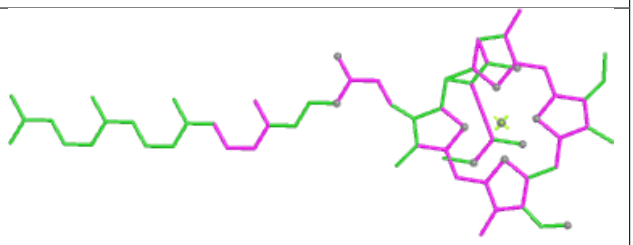


Rings

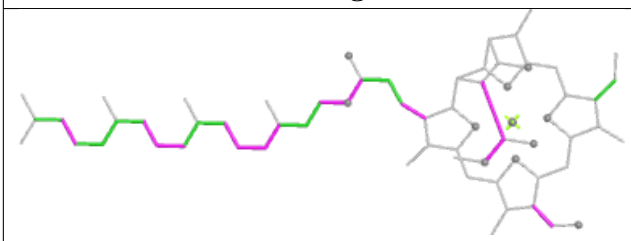
Ligand CL7 11 410



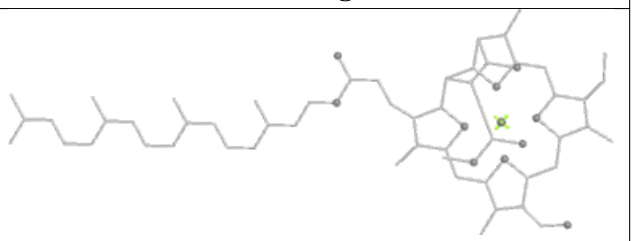
Bond lengths



Bond angles

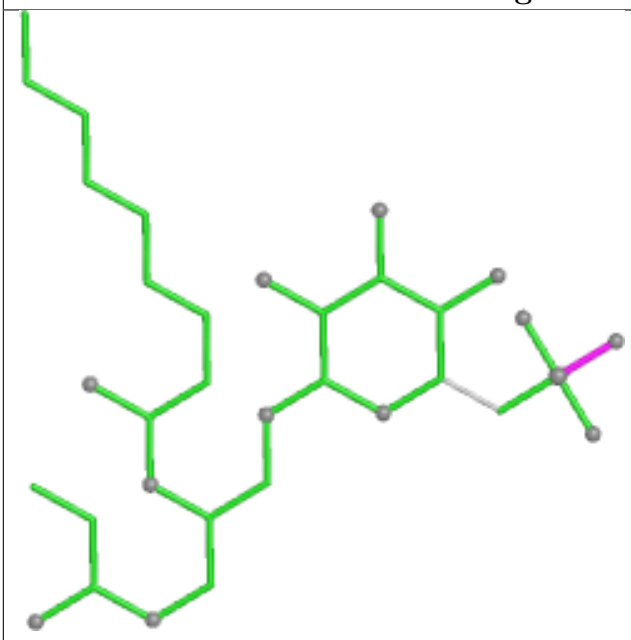


Torsions

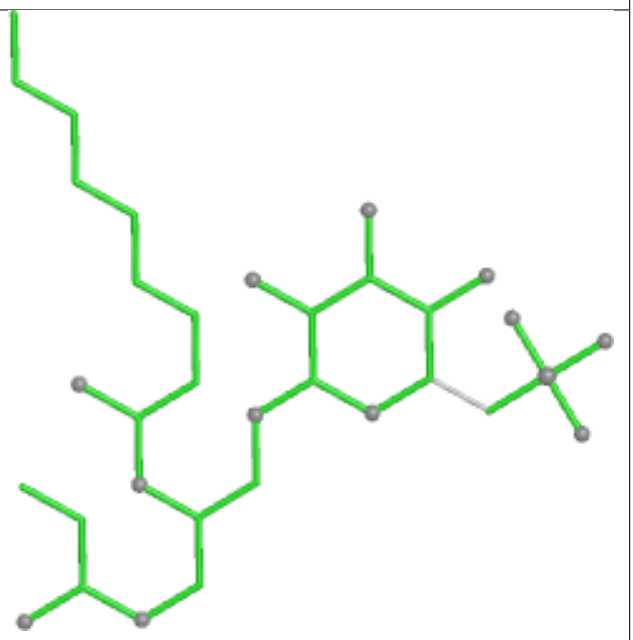


Rings

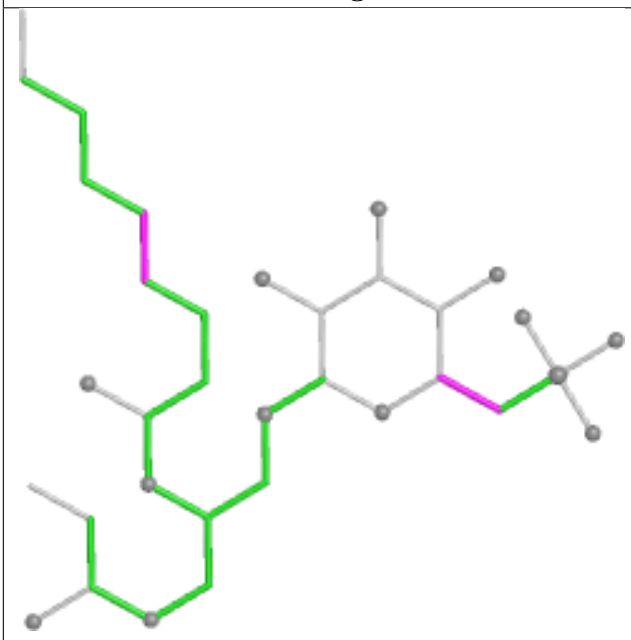
Ligand SQD 2A 406



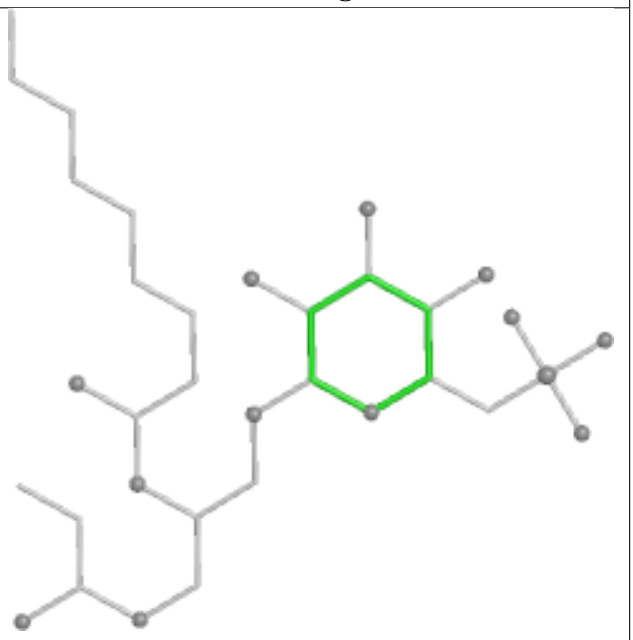
Bond lengths



Bond angles

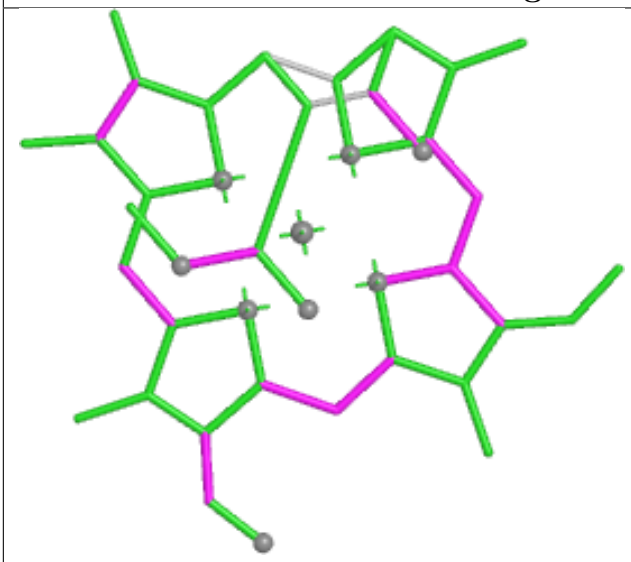


Torsions

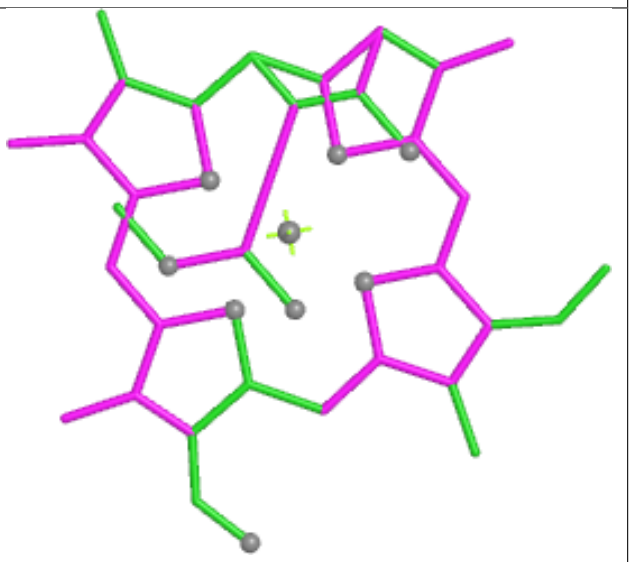


Rings

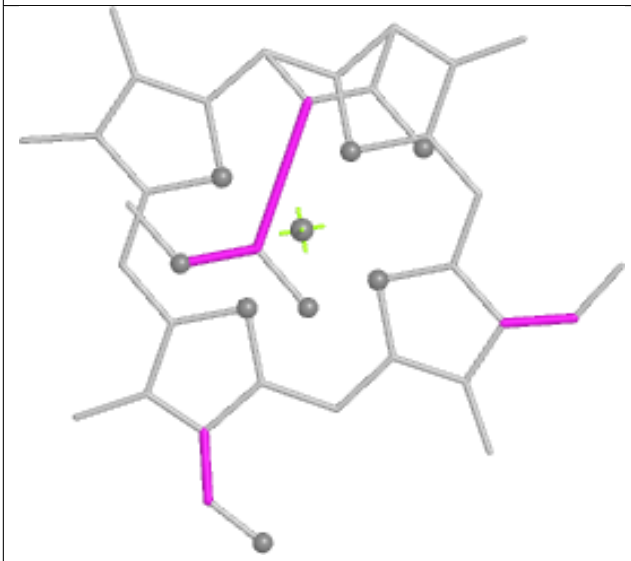
Ligand CL7 21 415



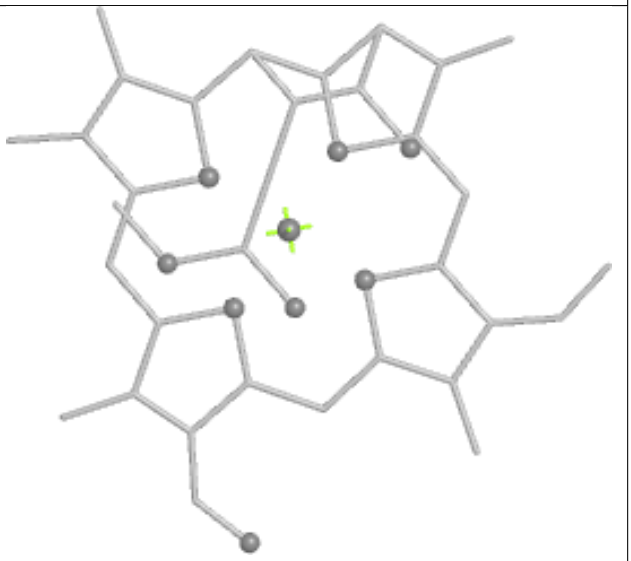
Bond lengths



Bond angles

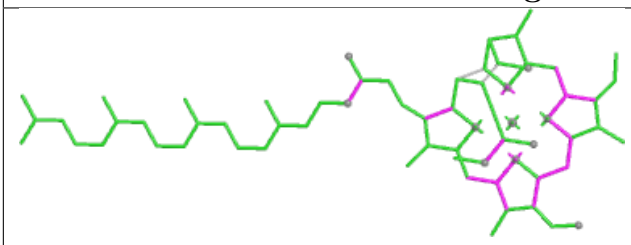


Torsions

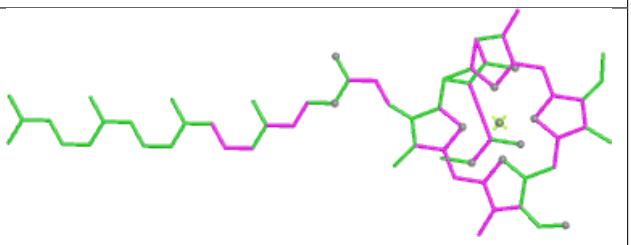


Rings

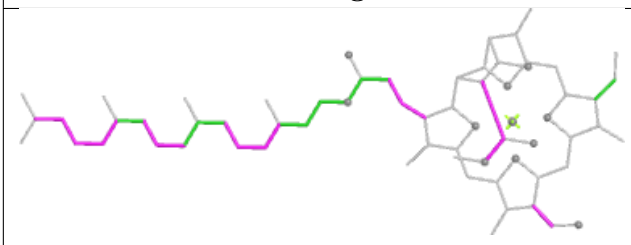
Ligand CL7 22 517



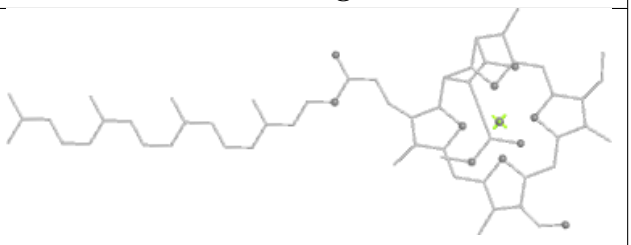
Bond lengths



Bond angles

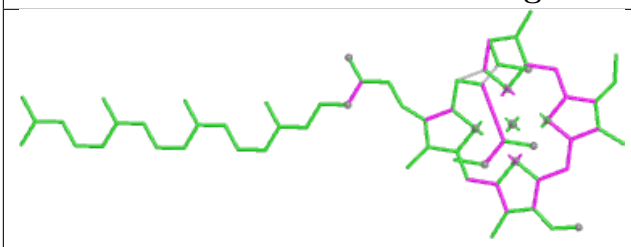


Torsions

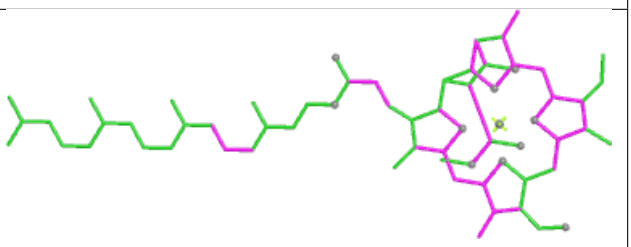


Rings

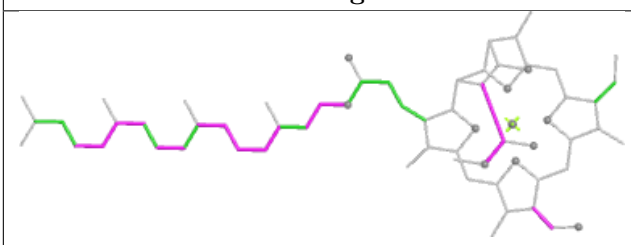
Ligand CL7 12 509



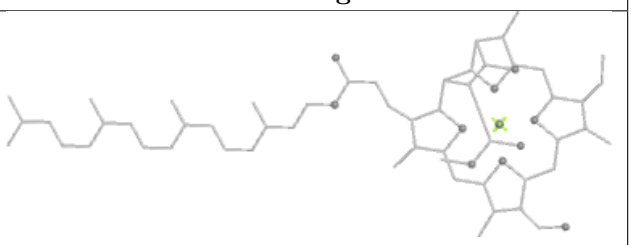
Bond lengths



Bond angles

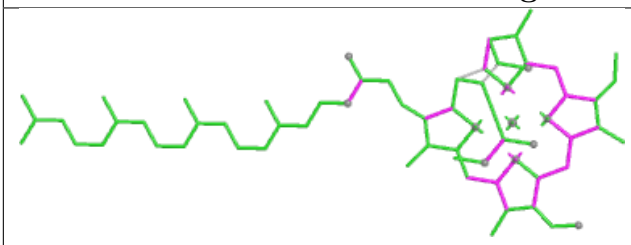


Torsions

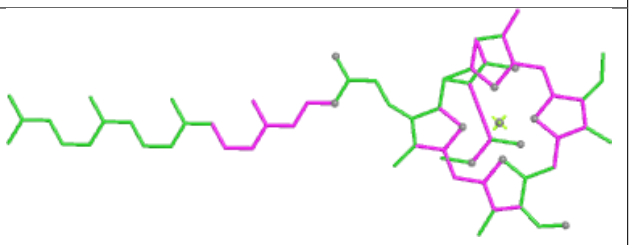


Rings

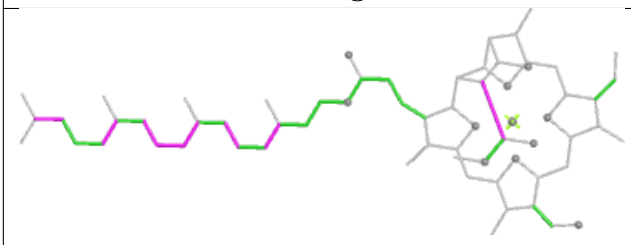
Ligand CL7 4B 604



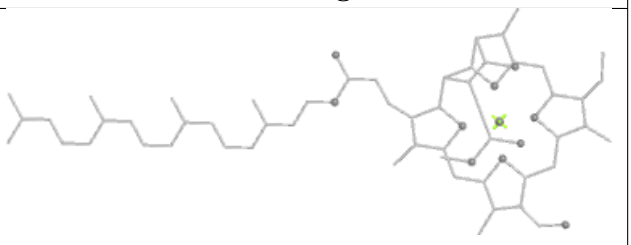
Bond lengths



Bond angles



Torsions



Rings

Ligand PL9 3D 407



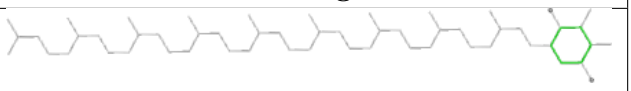
Bond lengths



Bond angles

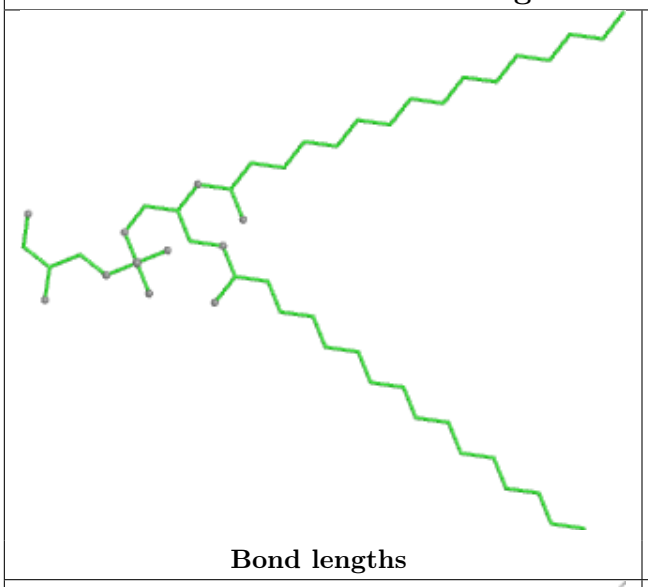


Torsions

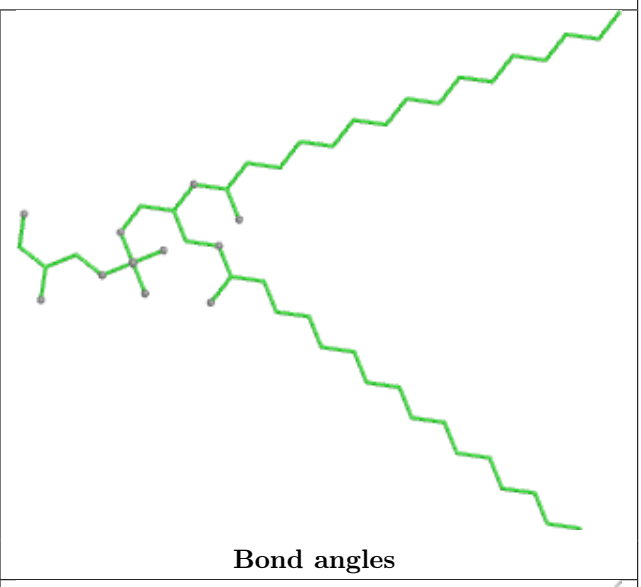


Rings

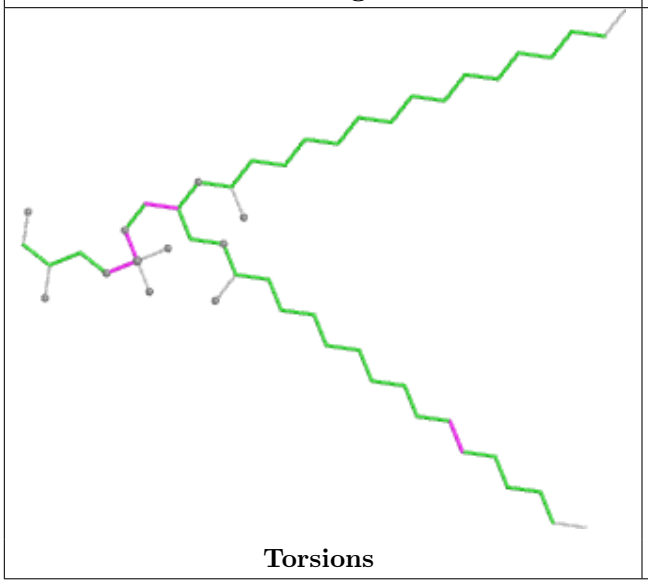
Ligand LHG 2D 409



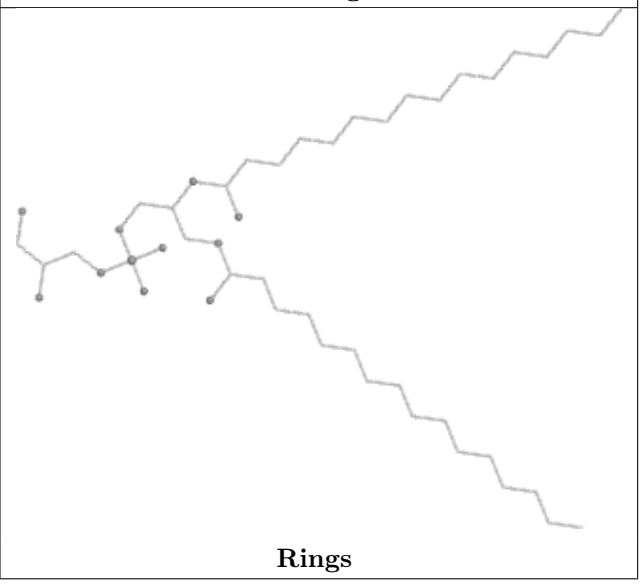
Bond lengths



Bond angles

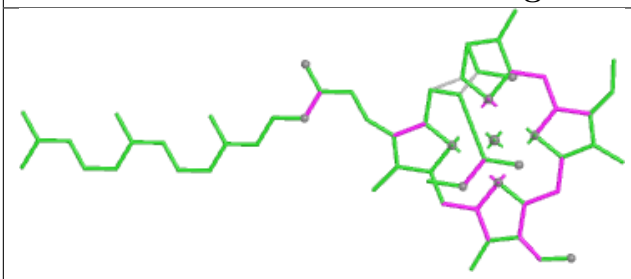


Torsions

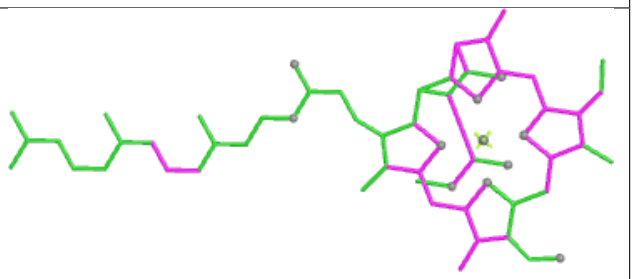


Rings

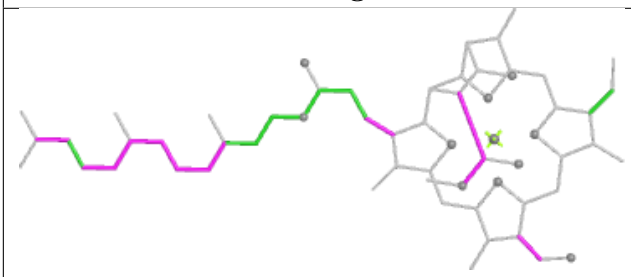
Ligand CL7 12 511



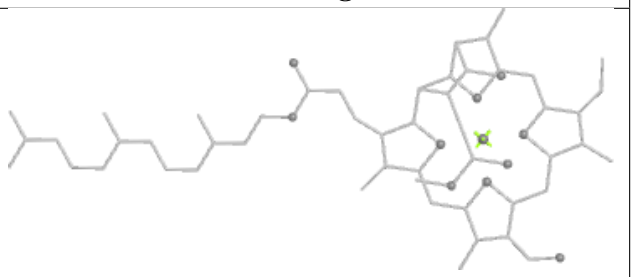
Bond lengths



Bond angles

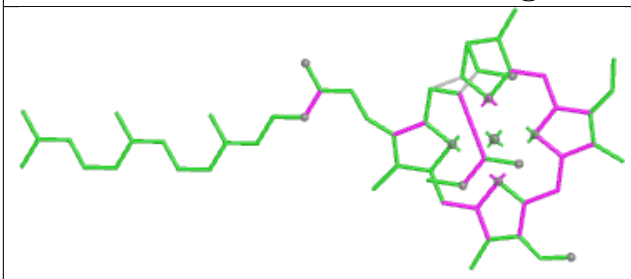


Torsions

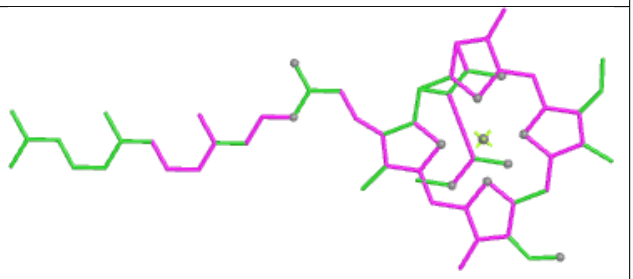


Rings

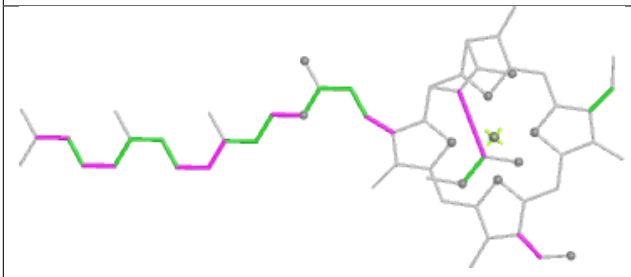
Ligand CL7 1B 614



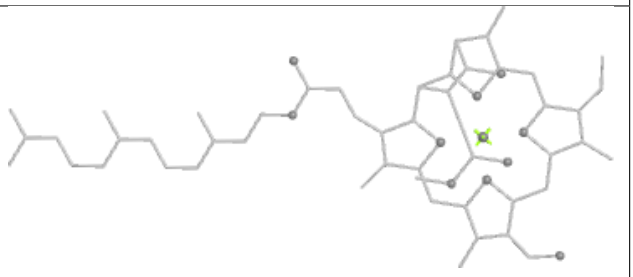
Bond lengths



Bond angles

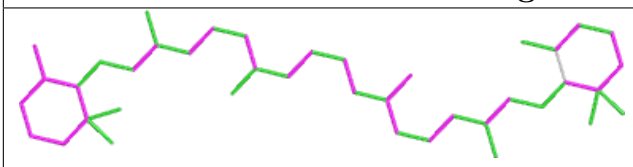


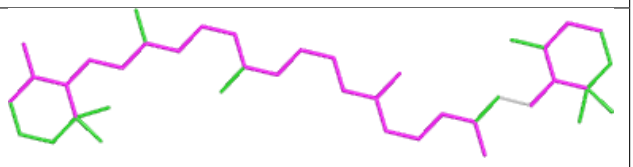
Torsions

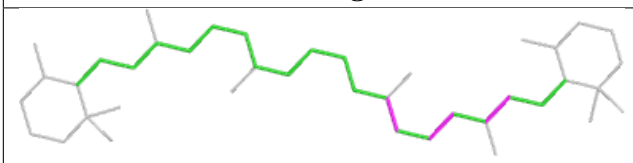


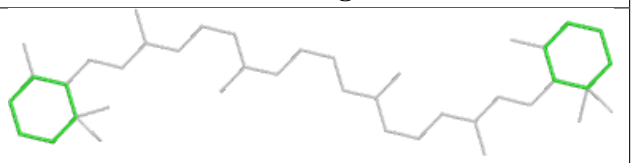
Rings

Ligand 8CT 2A 404

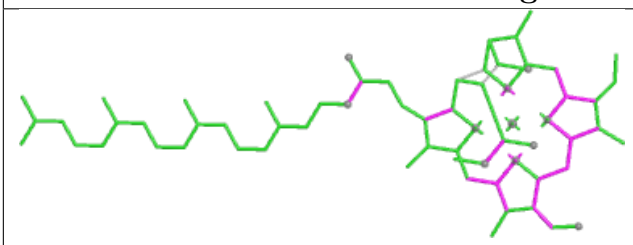

Bond lengths

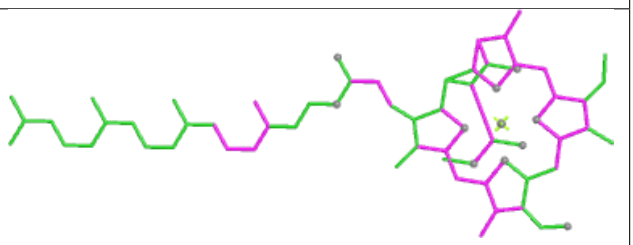

Bond angles

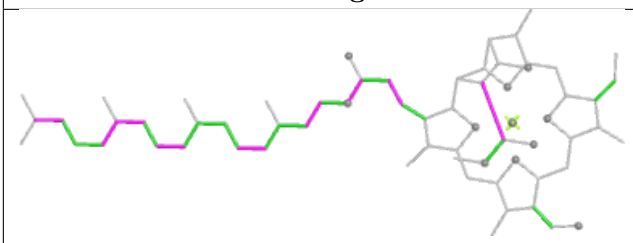

Torsions

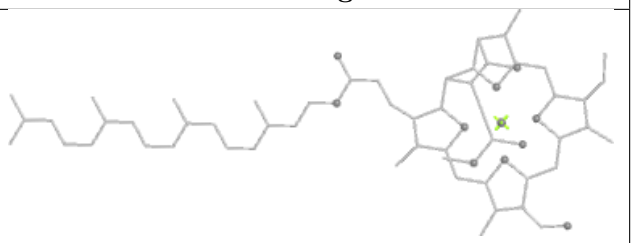

Rings

Ligand CL7 4B 611

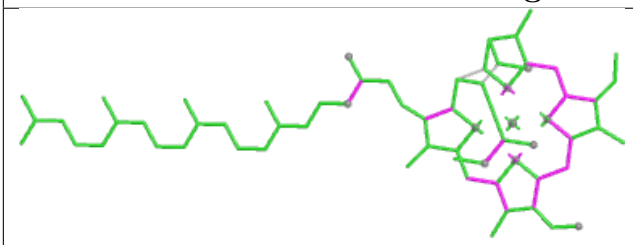

Bond lengths

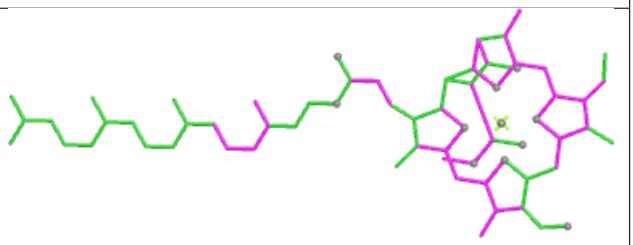

Bond angles

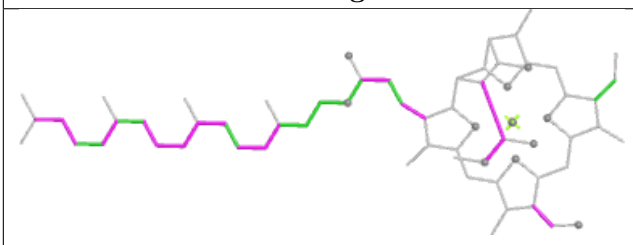

Torsions

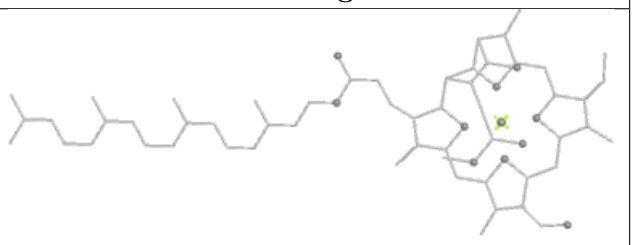

Rings

Ligand CL7 41 418

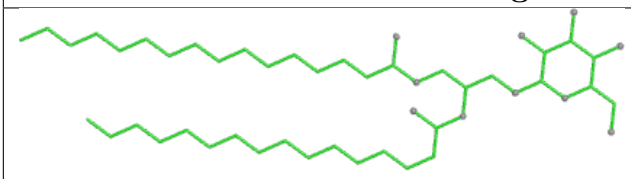

Bond lengths


Bond angles

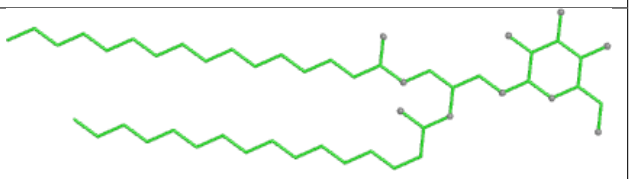

Torsions


Rings

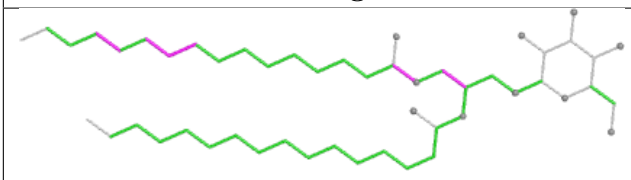
Ligand LMG 2B 622



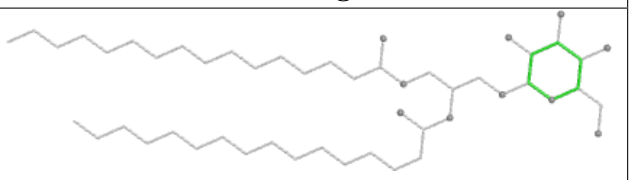
Bond lengths



Bond angles

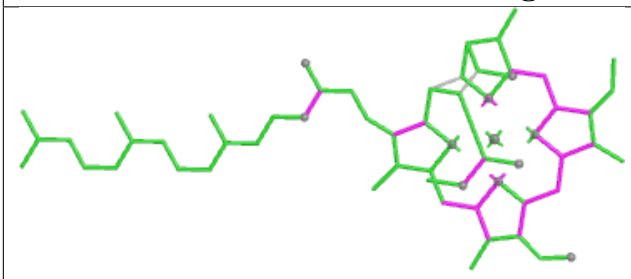


Torsions

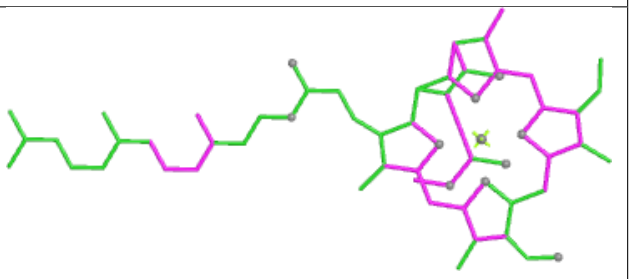


Rings

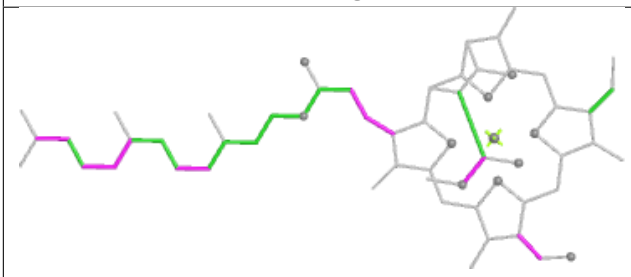
Ligand CL7 1B 607



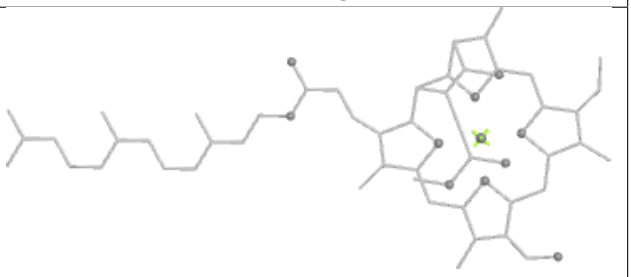
Bond lengths



Bond angles

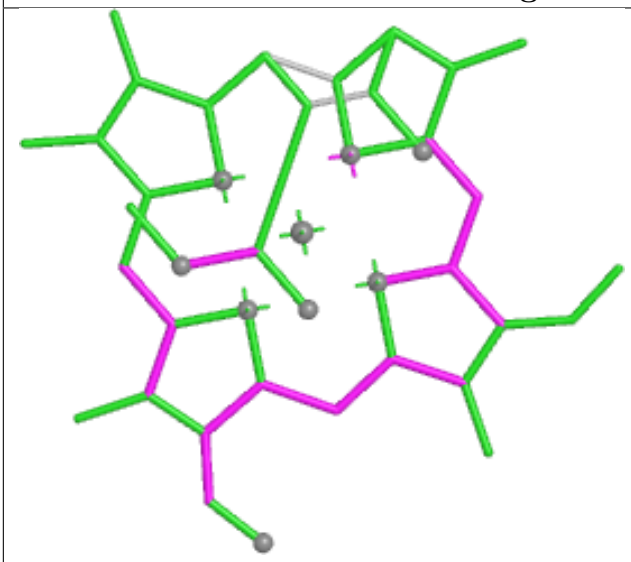


Torsions

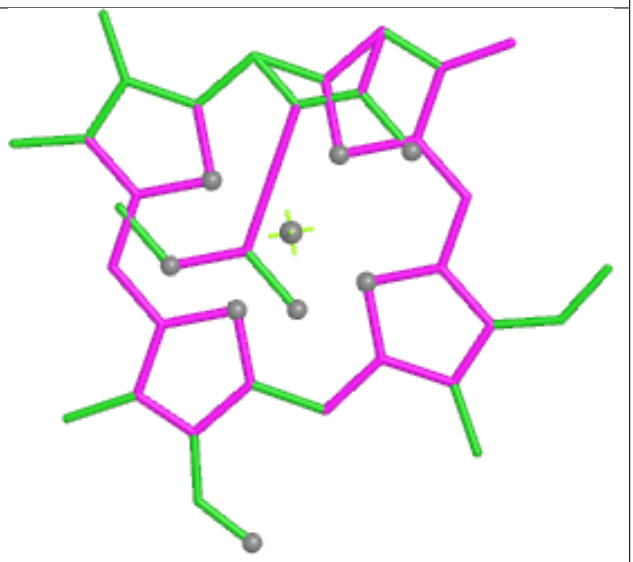


Rings

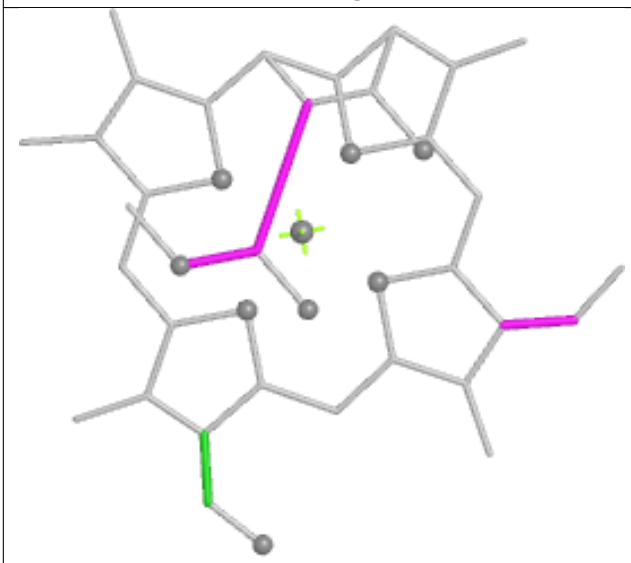
Ligand CL7 3B 601



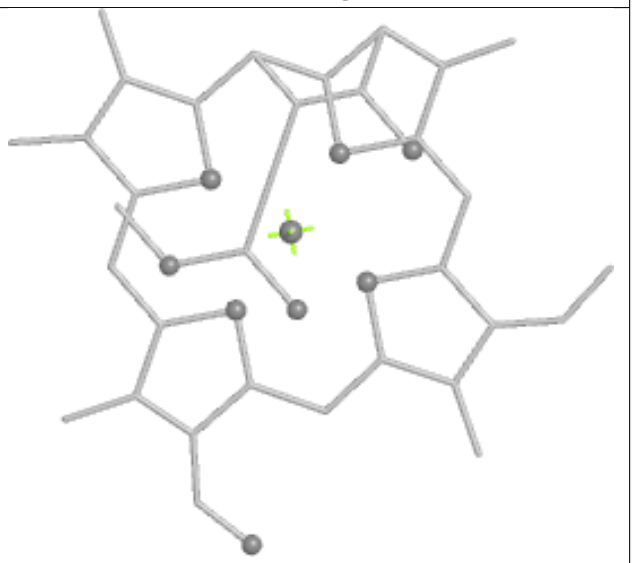
Bond lengths



Bond angles

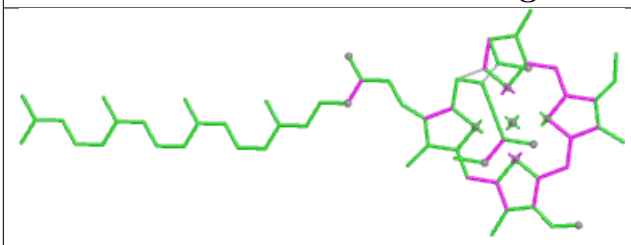


Torsions

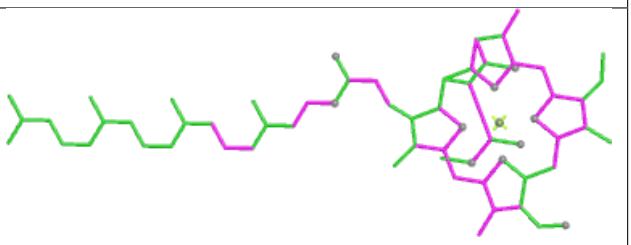


Rings

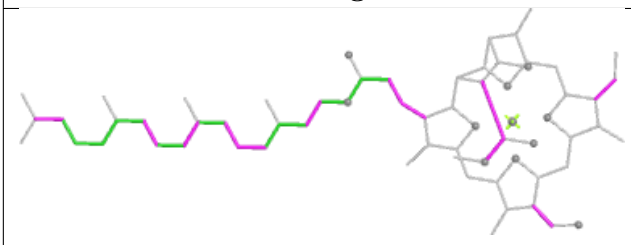
Ligand CL7 4A 407



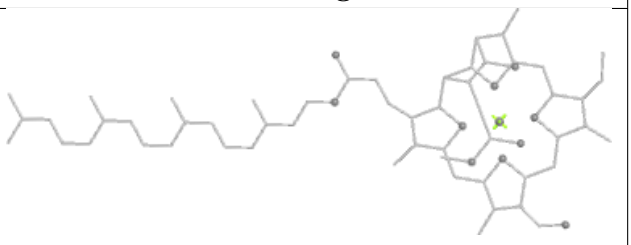
Bond lengths



Bond angles

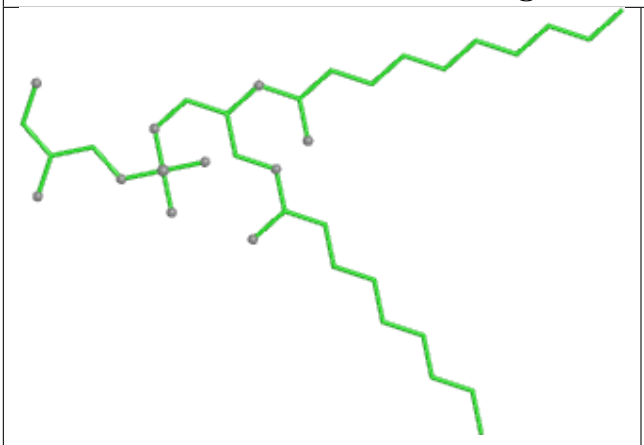


Torsions

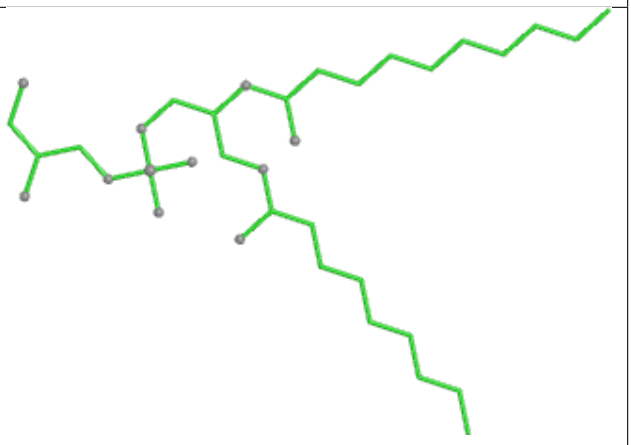


Rings

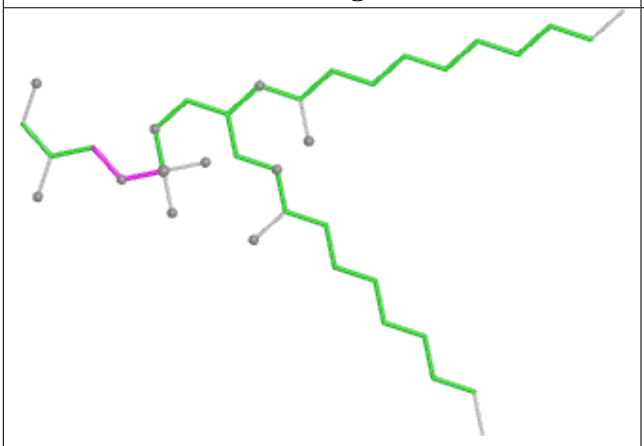
Ligand LHG 43 425



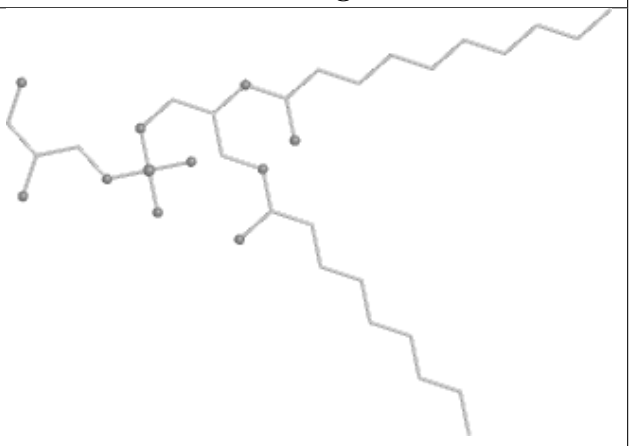
Bond lengths



Bond angles

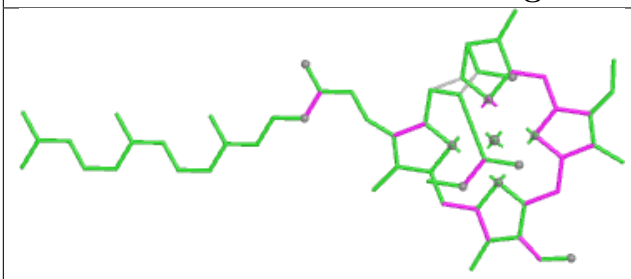


Torsions

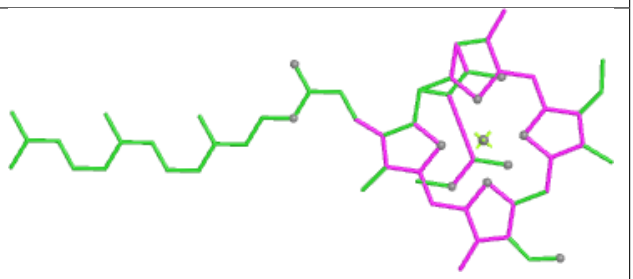


Rings

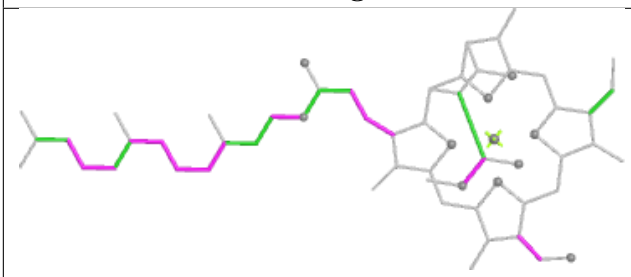
Ligand CL7 41 402



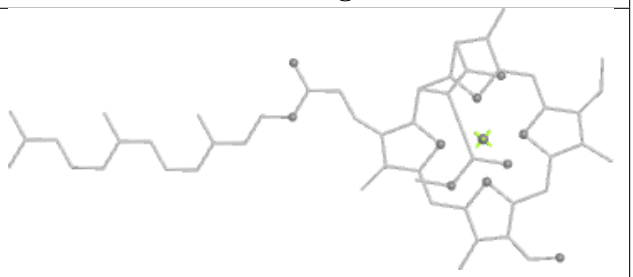
Bond lengths



Bond angles

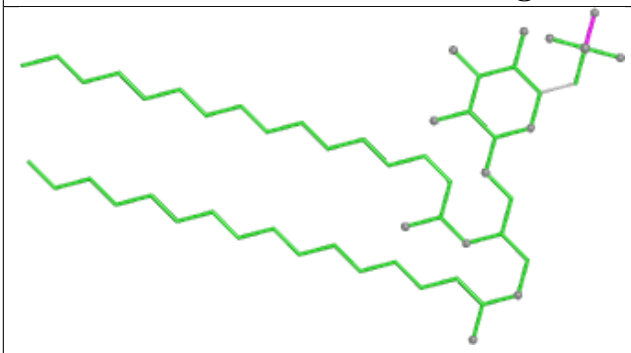


Torsions

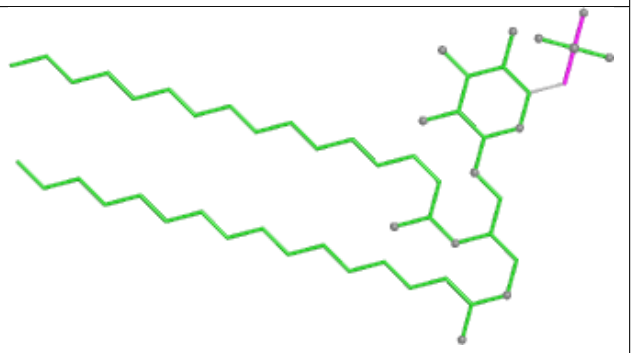


Rings

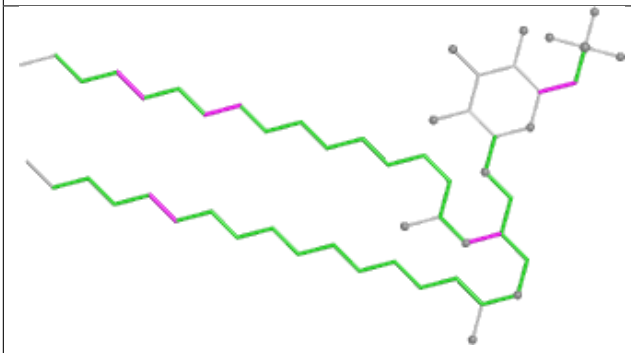
Ligand SQD 4B 621



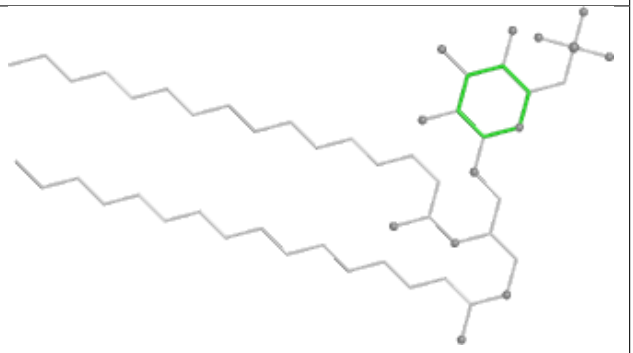
Bond lengths



Bond angles

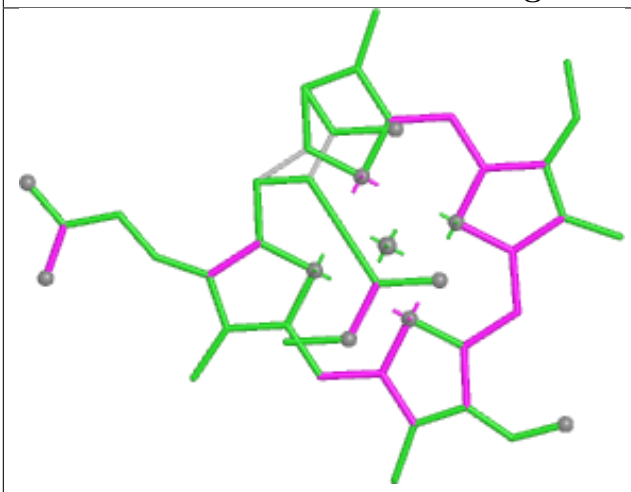


Torsions

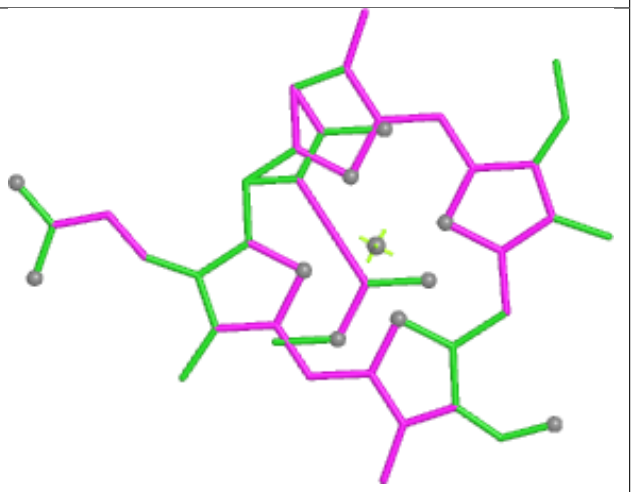


Rings

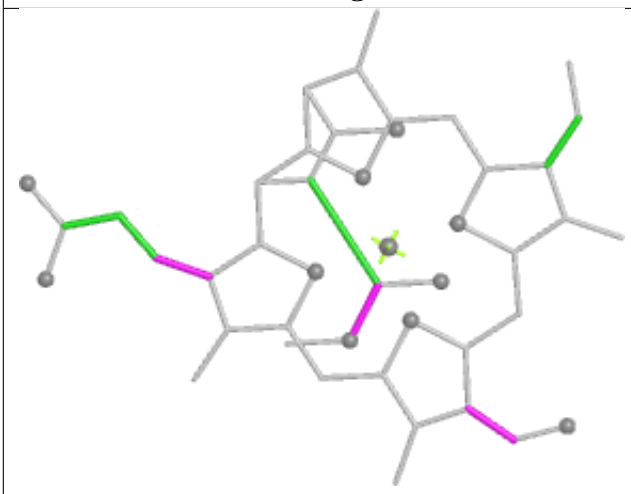
Ligand CL7 12 504



Bond lengths



Bond angles

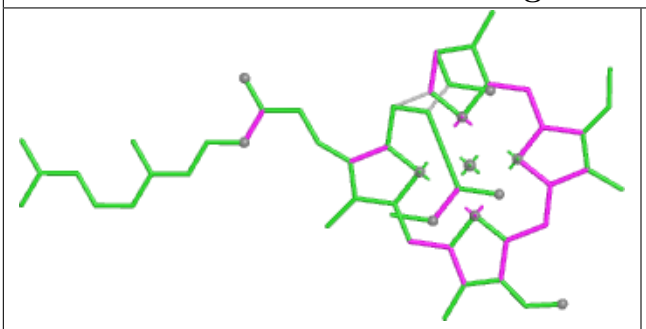


Torsions

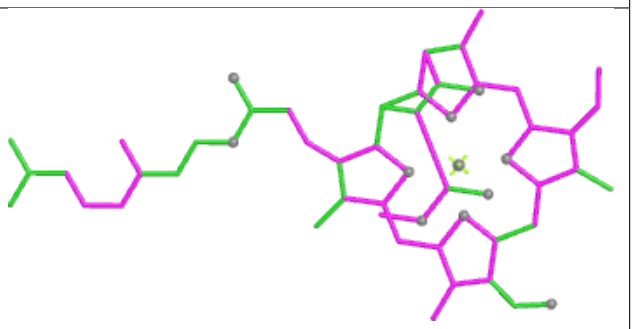


Rings

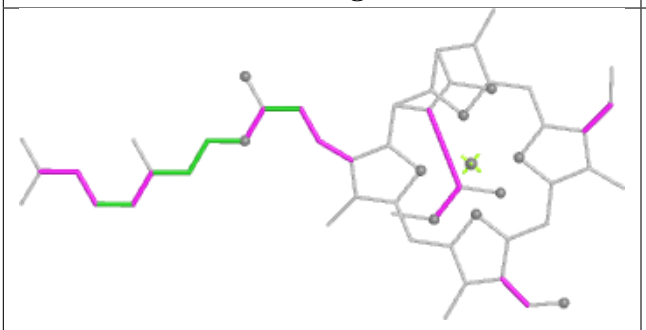
Ligand CL7 23 417



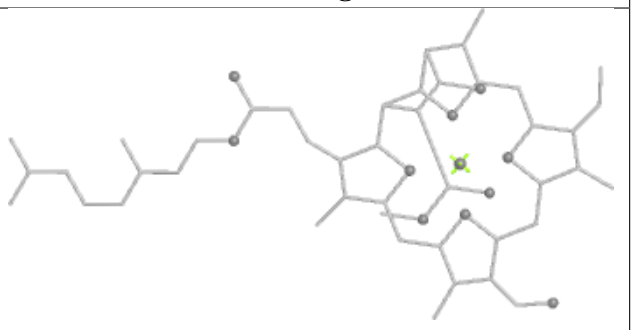
Bond lengths



Bond angles

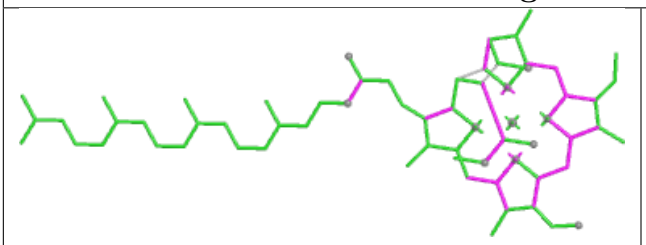


Torsions

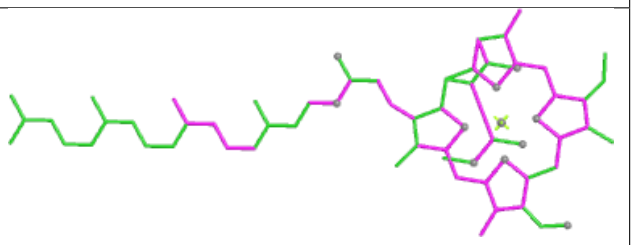


Rings

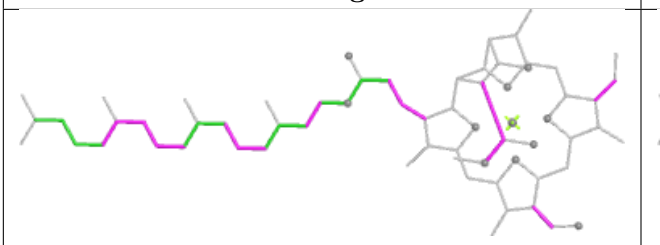
Ligand CL7 2C 505



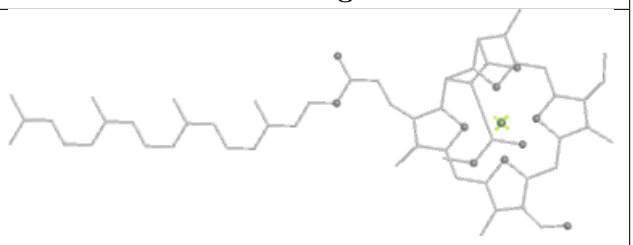
Bond lengths



Bond angles

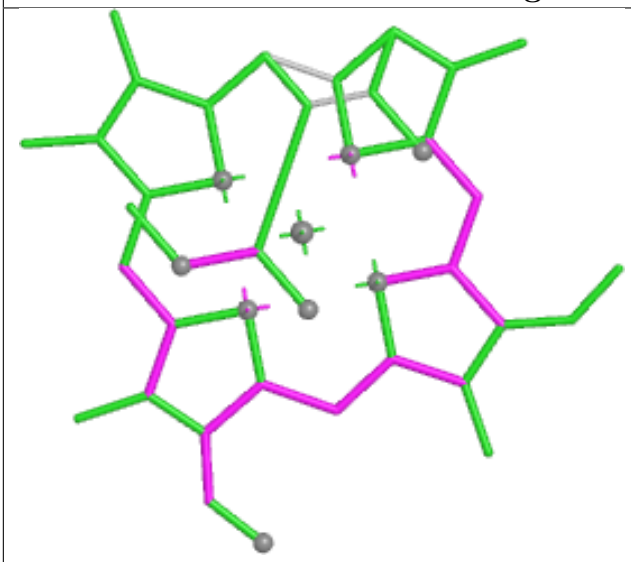


Torsions

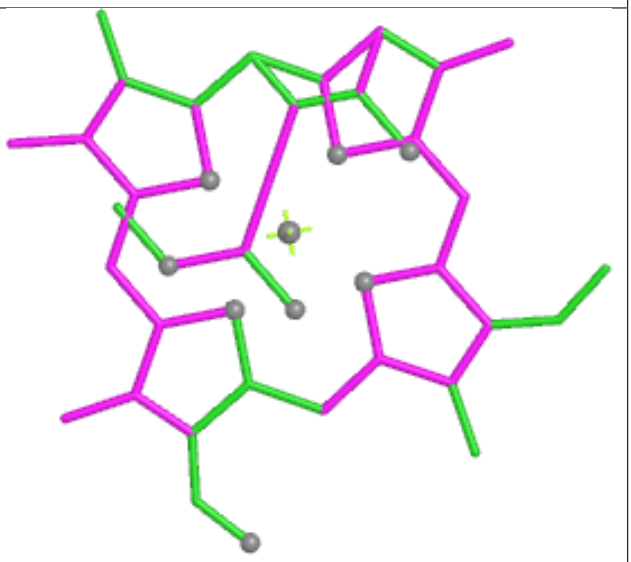


Rings

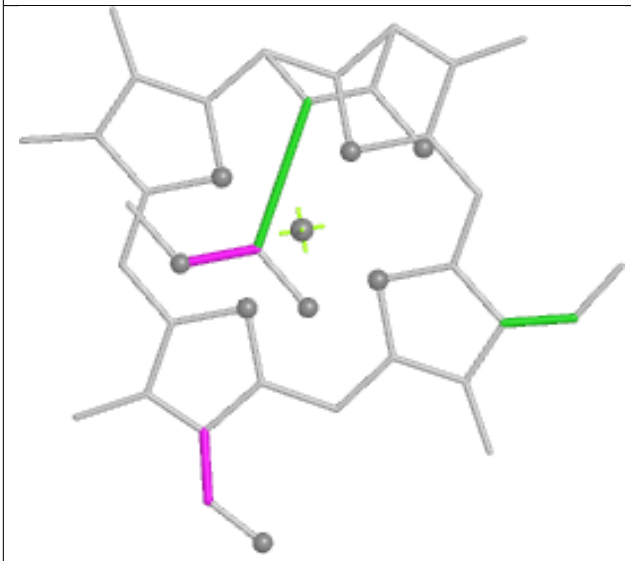
Ligand CL7 31 407



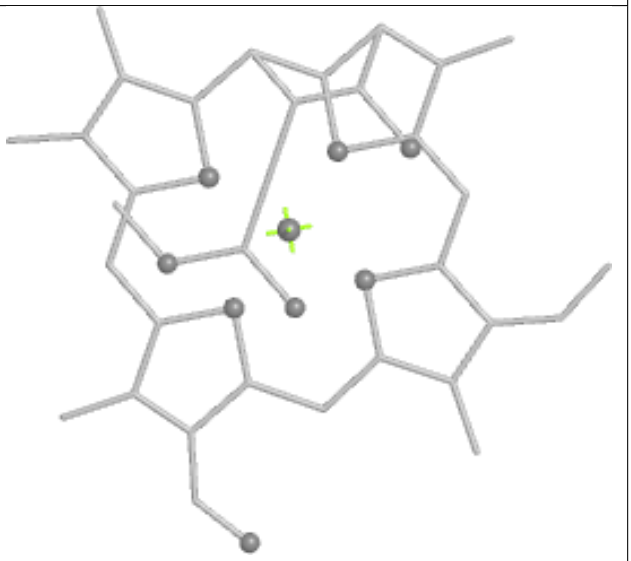
Bond lengths



Bond angles

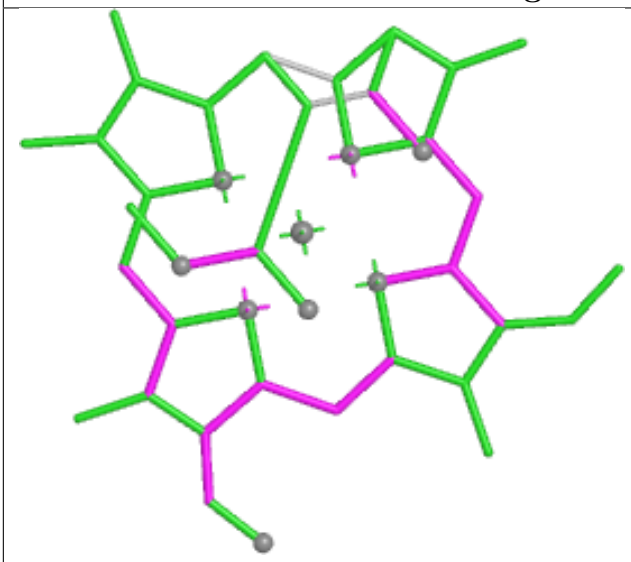


Torsions

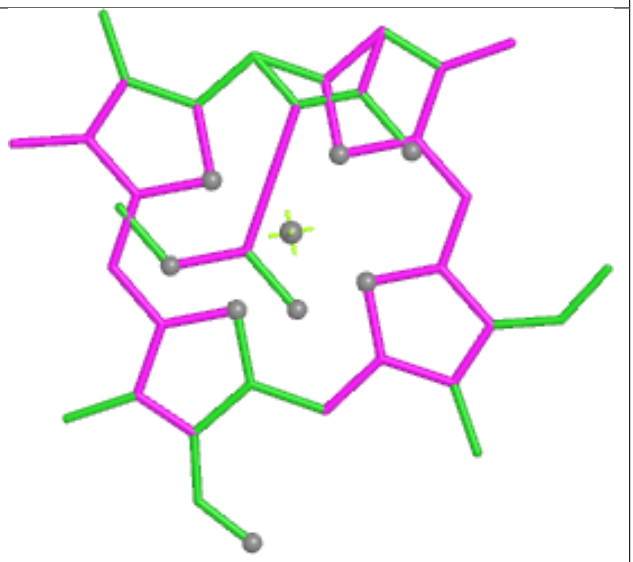


Rings

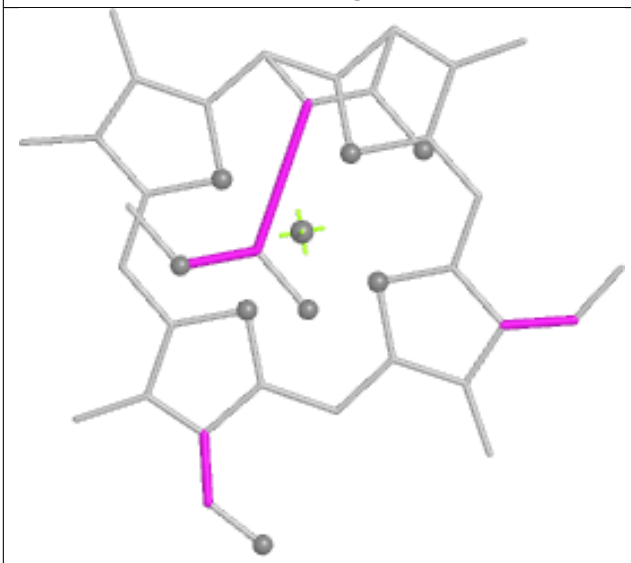
Ligand CL7 44 416



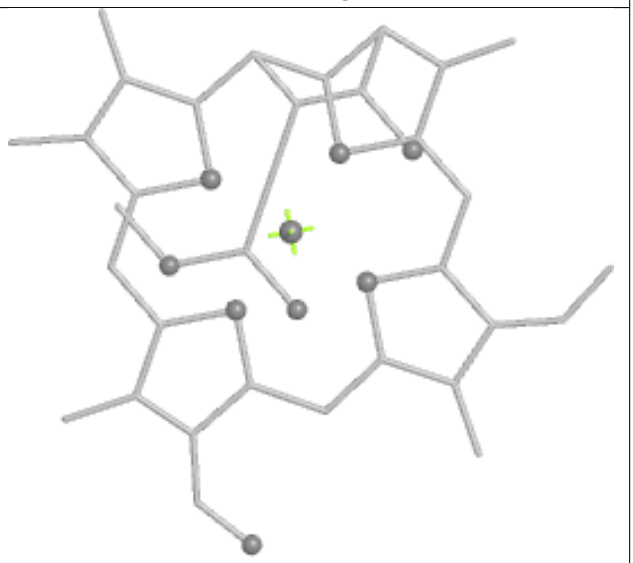
Bond lengths



Bond angles

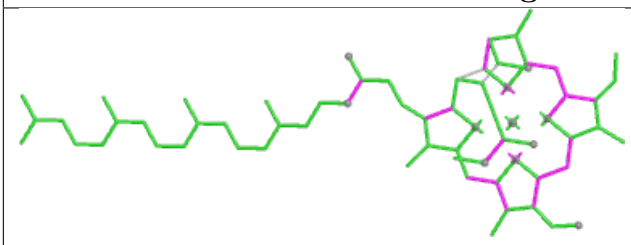


Torsions

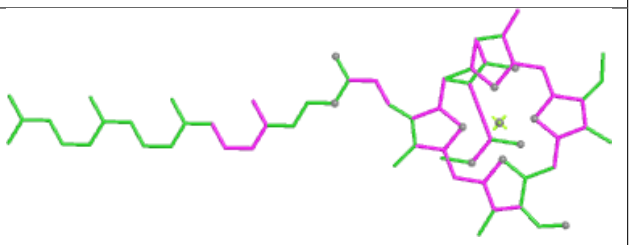


Rings

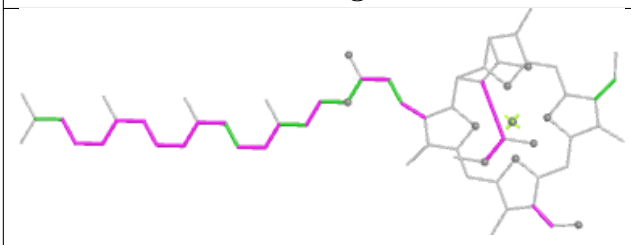
Ligand CL7 2C 510



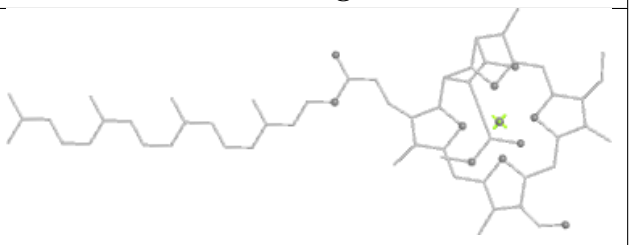
Bond lengths



Bond angles

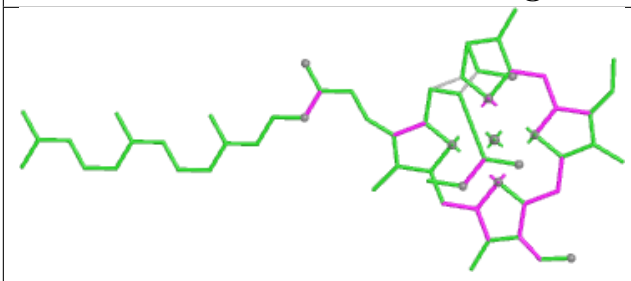


Torsions

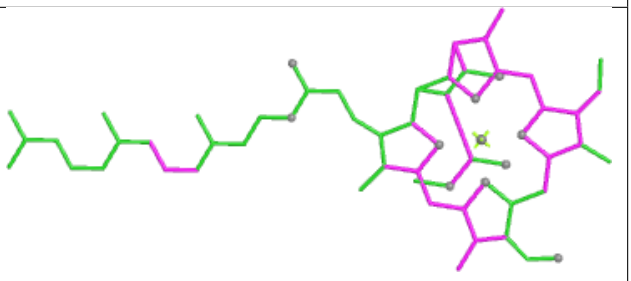


Rings

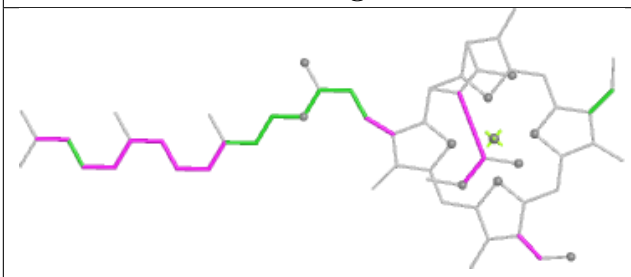
Ligand CL7 22 511



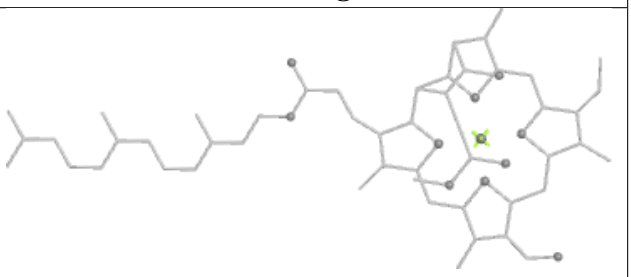
Bond lengths



Bond angles

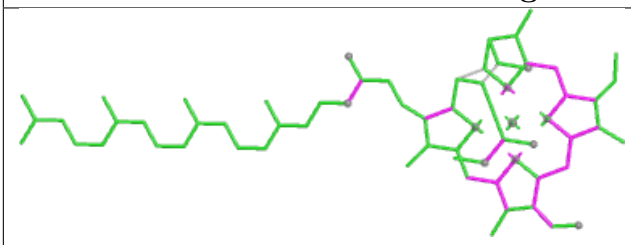


Torsions

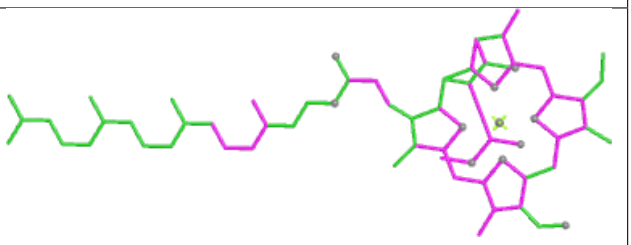


Rings

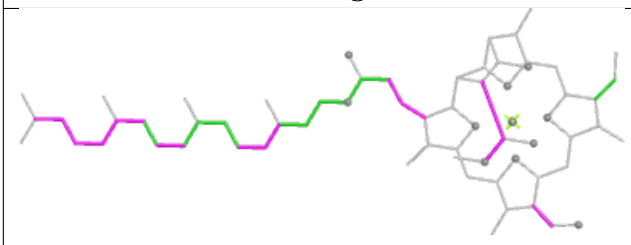
Ligand CL7 1B 604



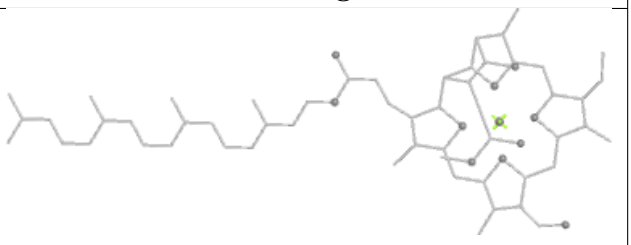
Bond lengths



Bond angles

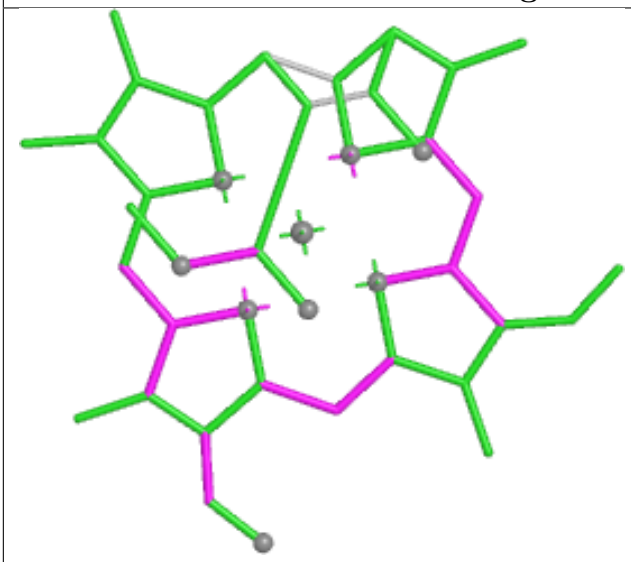


Torsions

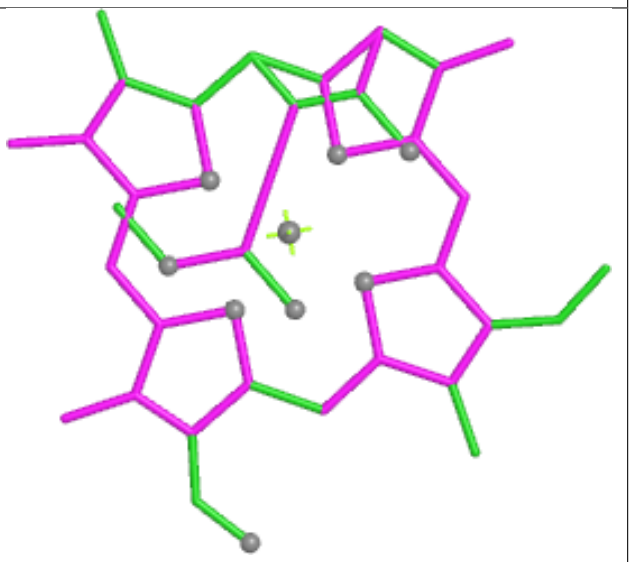


Rings

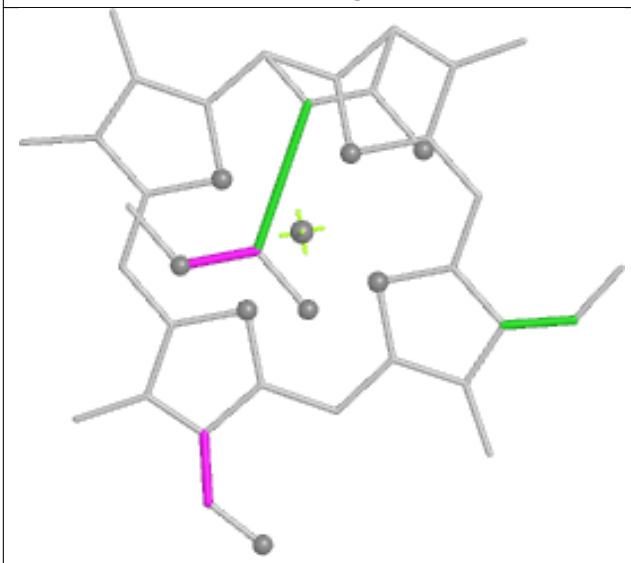
Ligand CL7 1C 512



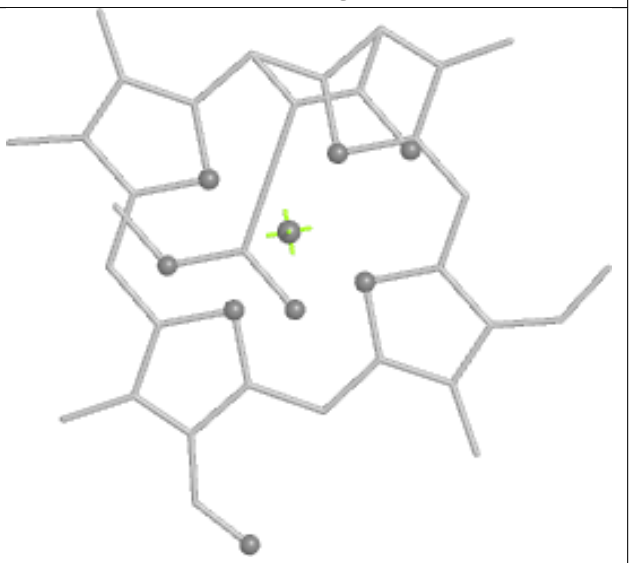
Bond lengths



Bond angles

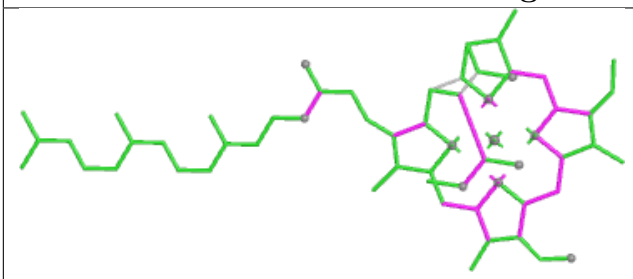


Torsions

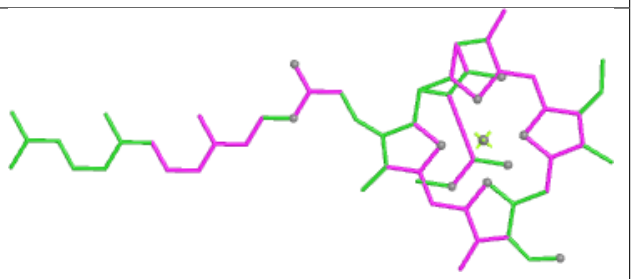


Rings

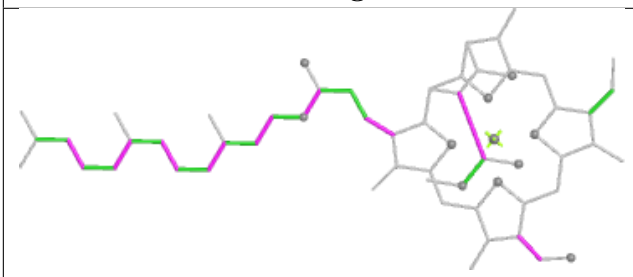
Ligand CL7 3C 506



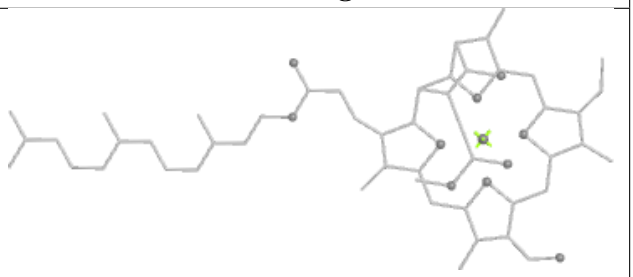
Bond lengths



Bond angles

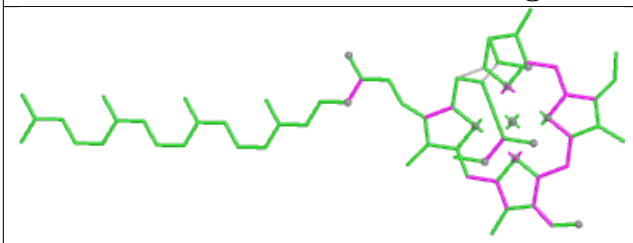


Torsions

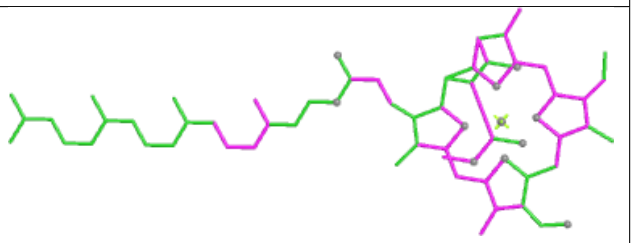


Rings

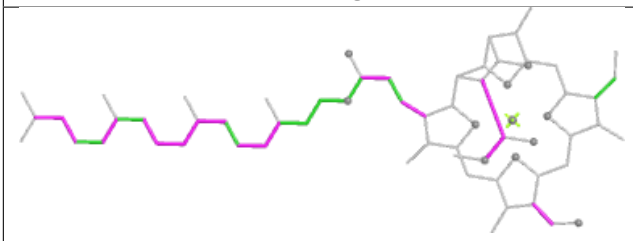
Ligand CL7 11 418



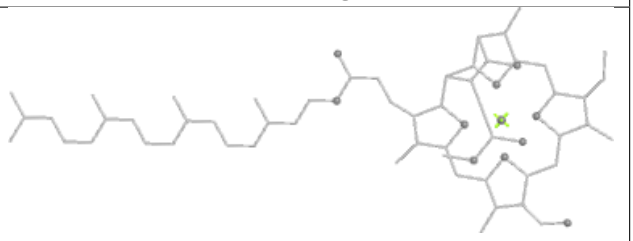
Bond lengths



Bond angles

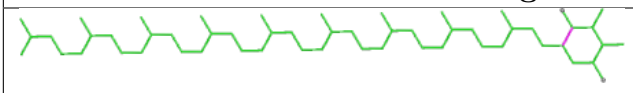


Torsions



Rings

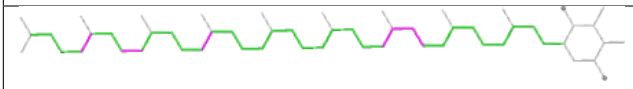
Ligand PL9 2D 407



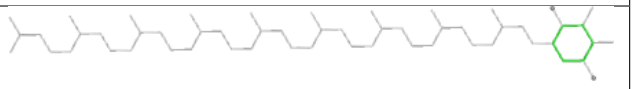
Bond lengths



Bond angles

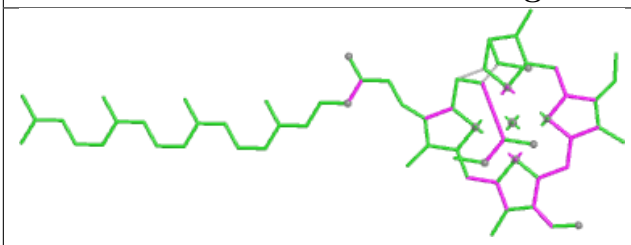


Torsions

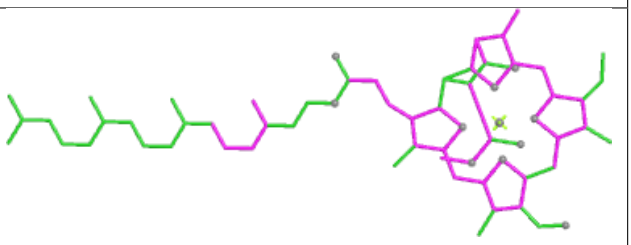


Rings

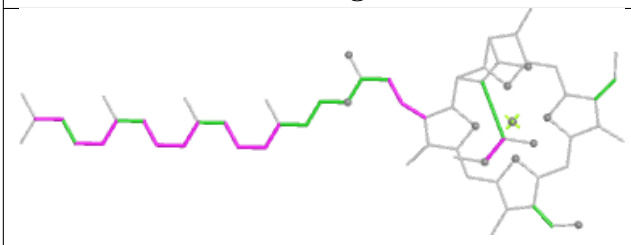
Ligand CL7 12 503



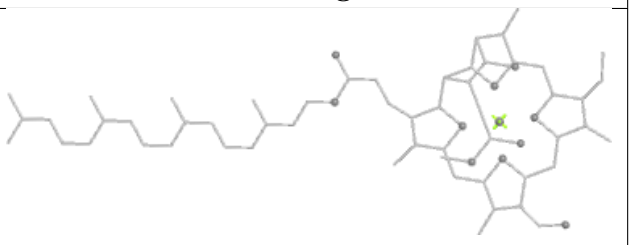
Bond lengths



Bond angles

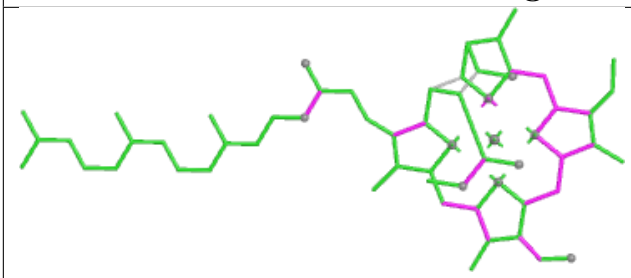


Torsions

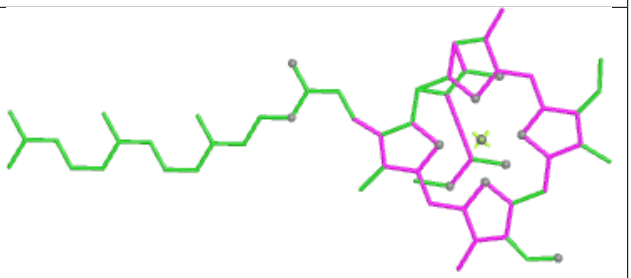


Rings

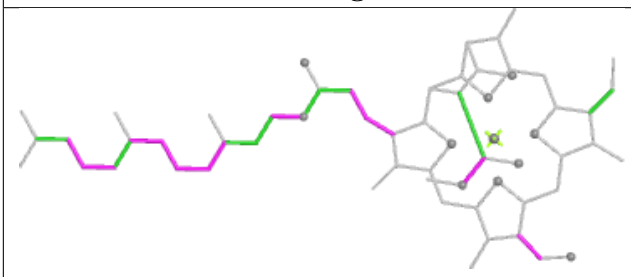
Ligand CL7 11 402



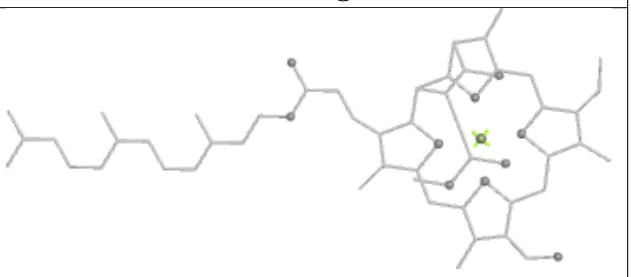
Bond lengths



Bond angles

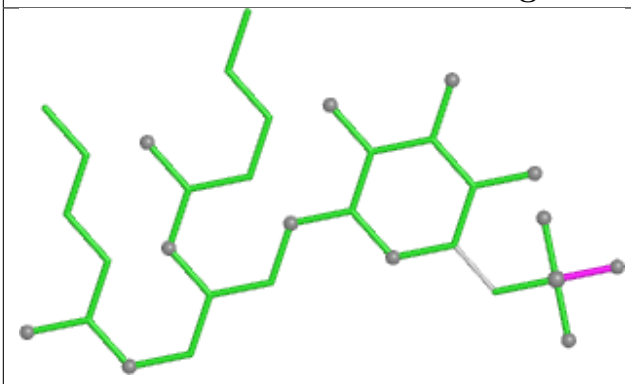


Torsions

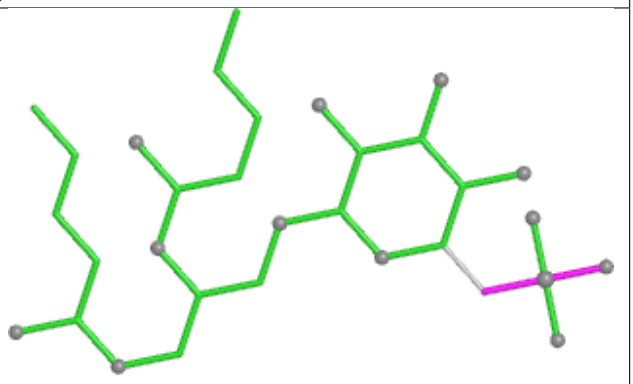


Rings

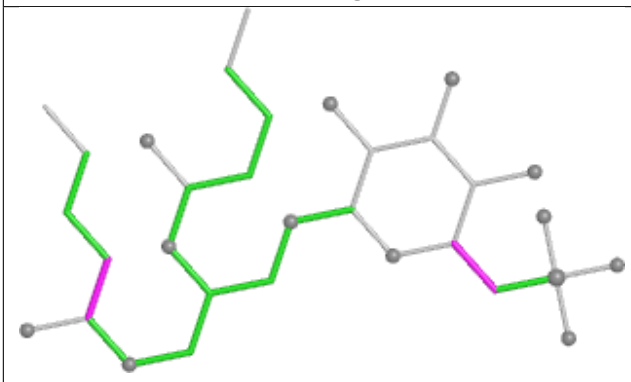
Ligand SQD 11 423



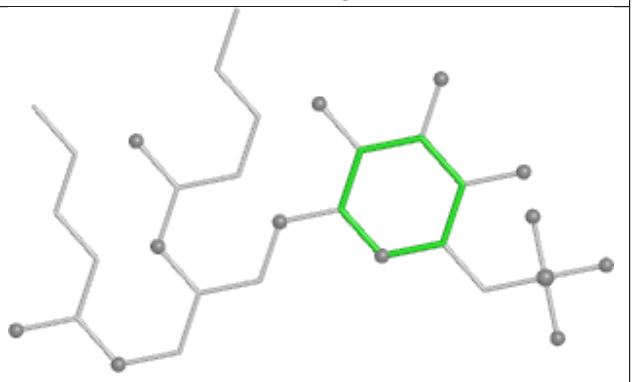
Bond lengths



Bond angles

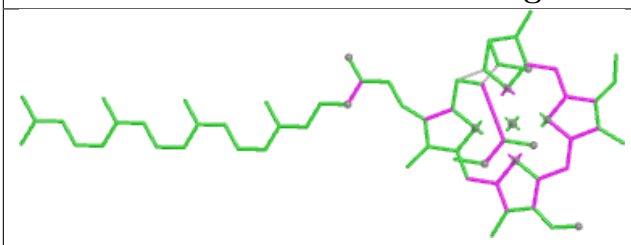


Torsions

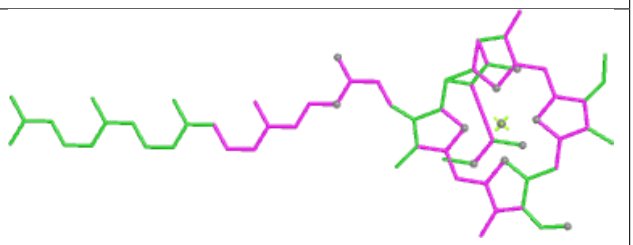


Rings

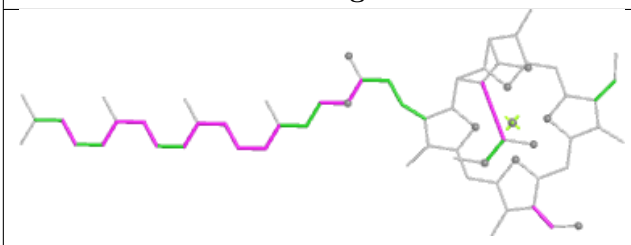
Ligand CL7 33 511



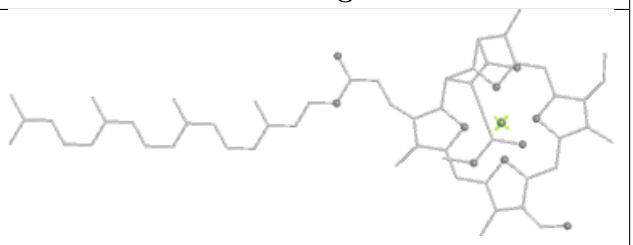
Bond lengths



Bond angles

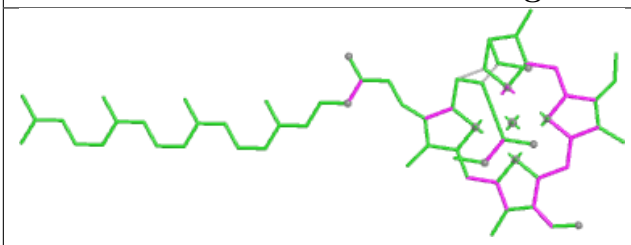


Torsions

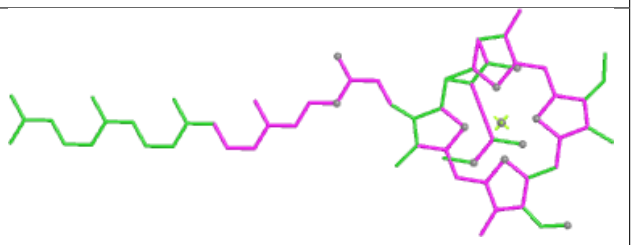


Rings

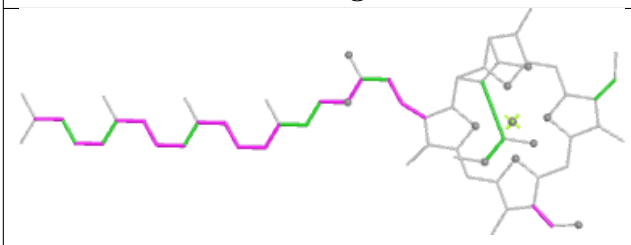
Ligand CL7 44 405



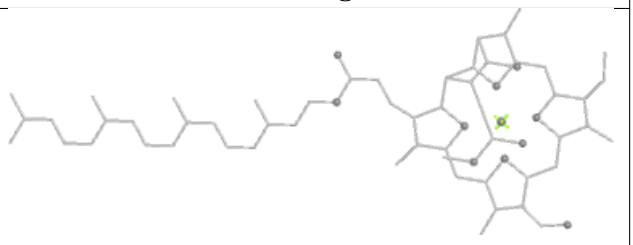
Bond lengths



Bond angles

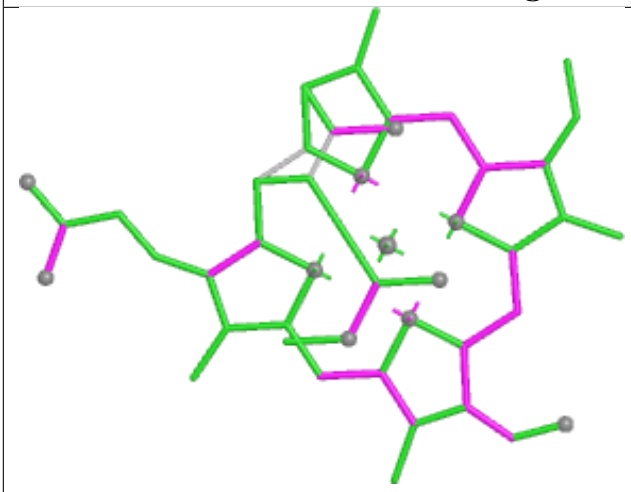


Torsions

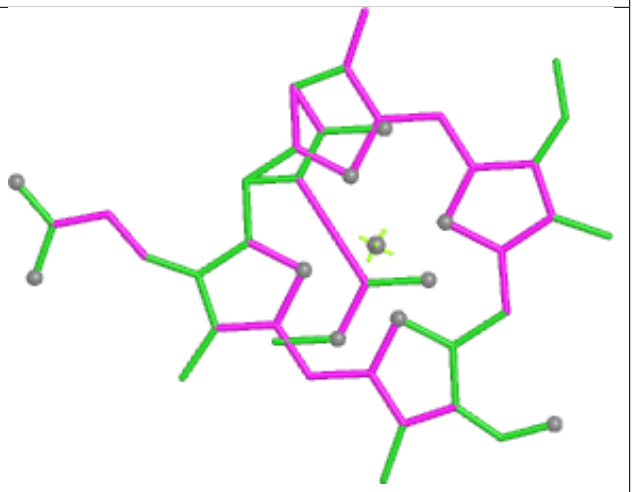


Rings

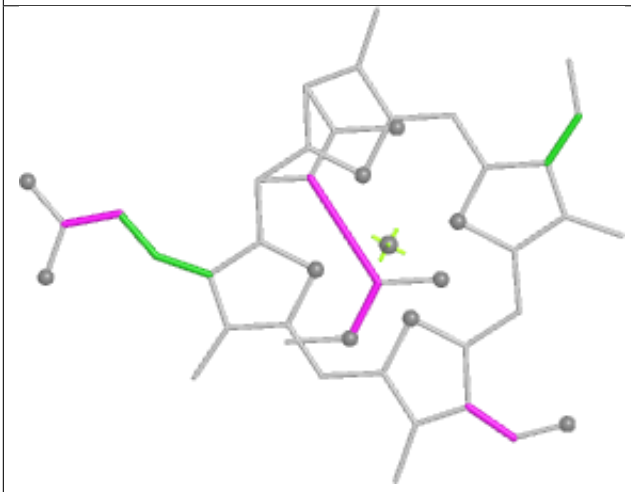
Ligand CL7 11 411



Bond lengths



Bond angles

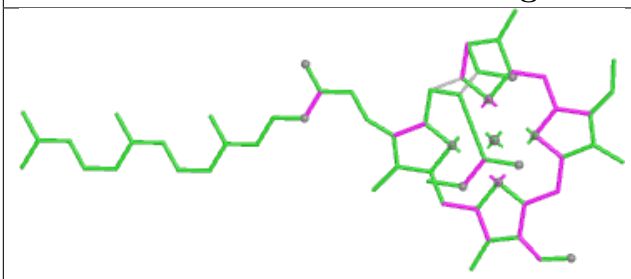


Torsions

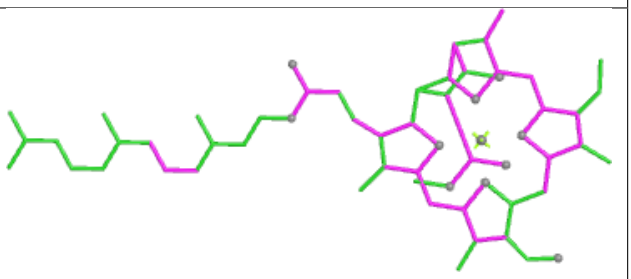


Rings

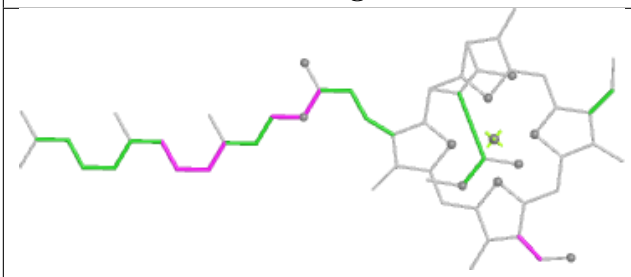
Ligand CL7 2B 603



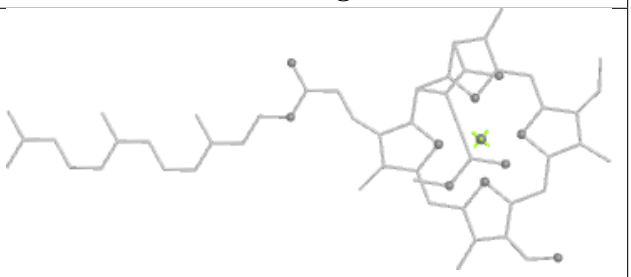
Bond lengths



Bond angles



Torsions

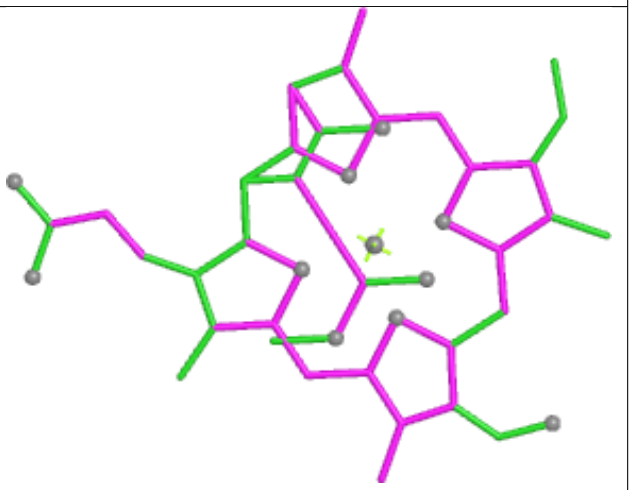


Rings

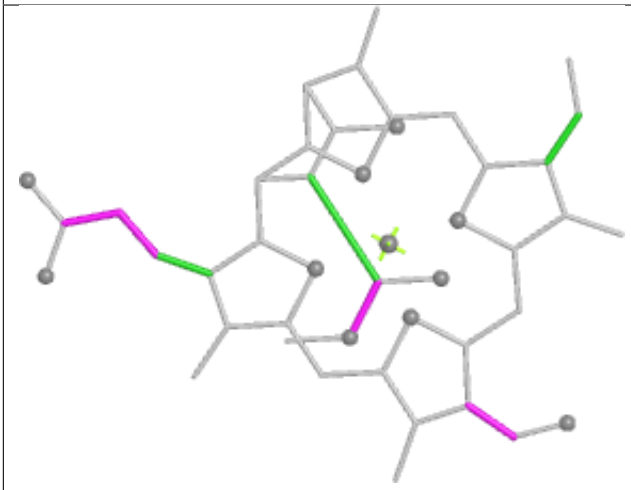
Ligand CL7 43 419



Bond lengths



Bond angles

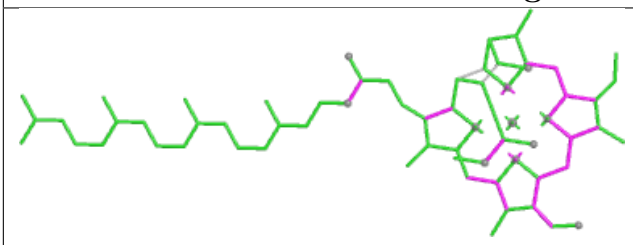


Torsions

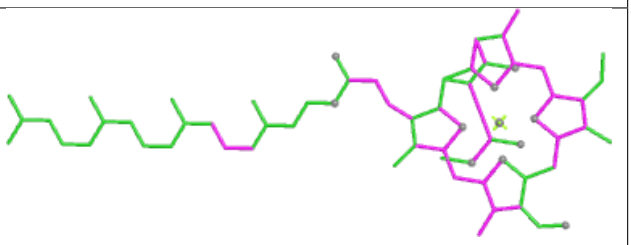


Rings

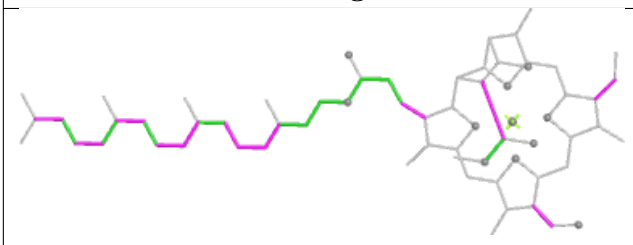
Ligand CL7 43 405



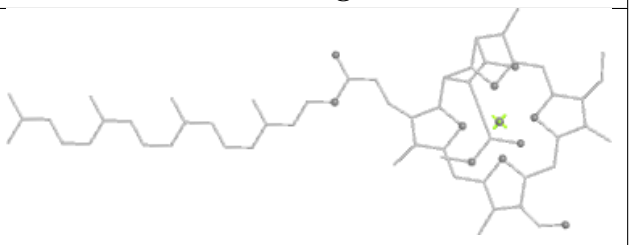
Bond lengths



Bond angles

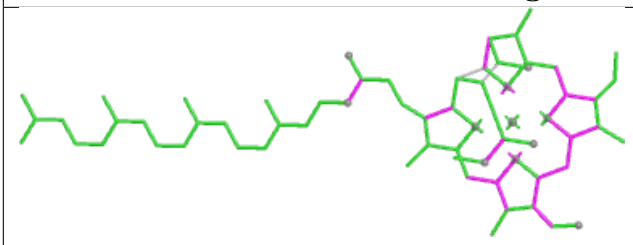


Torsions

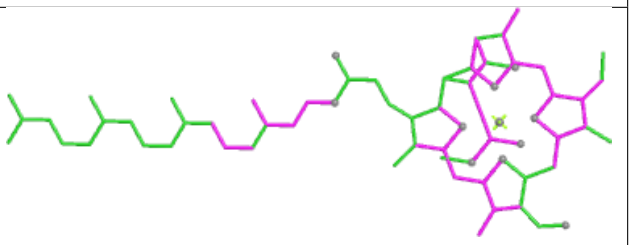


Rings

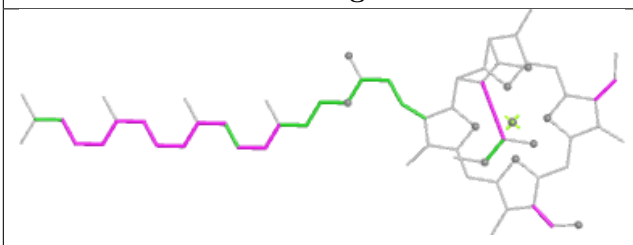
Ligand CL7 42 505



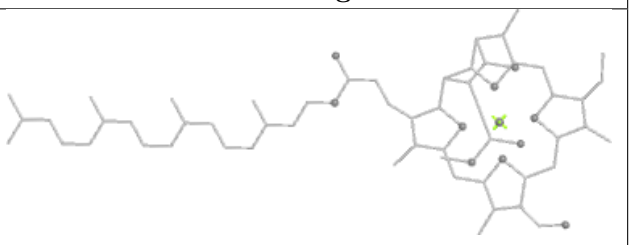
Bond lengths



Bond angles

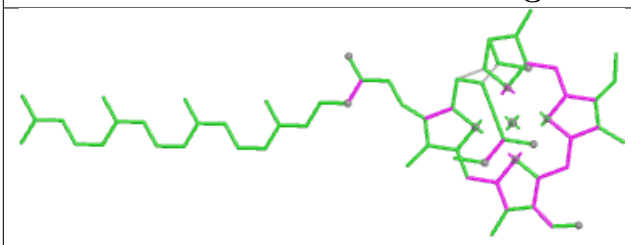


Torsions

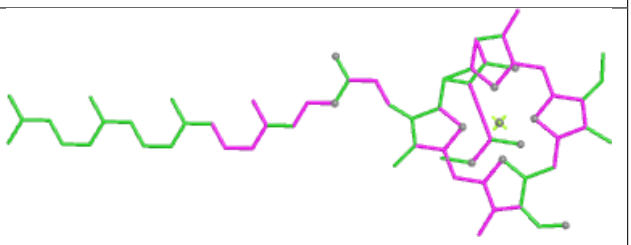


Rings

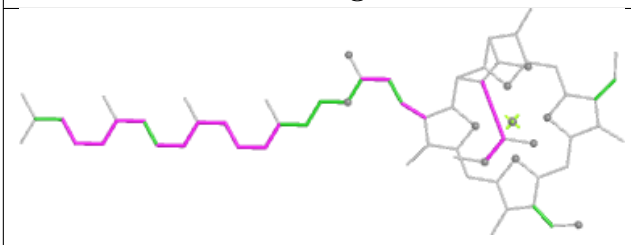
Ligand CL7 42 510



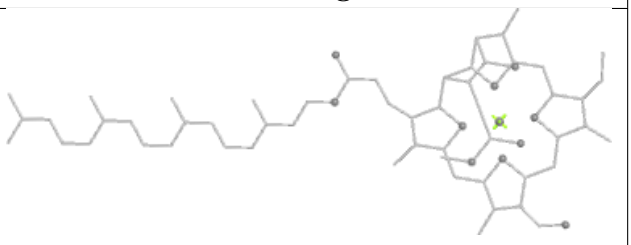
Bond lengths



Bond angles

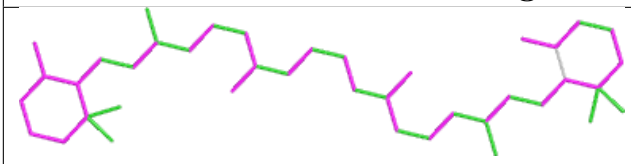


Torsions

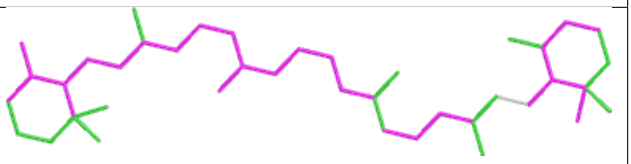


Rings

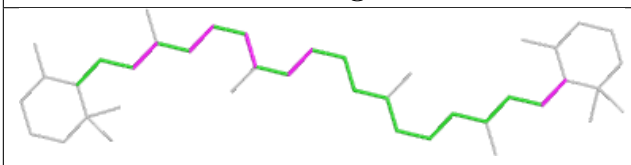
Ligand 8CT 2B 618



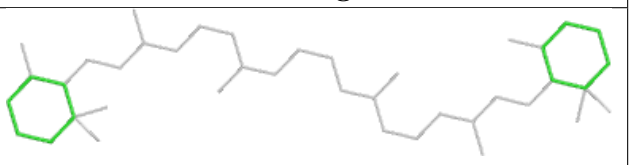
Bond lengths



Bond angles

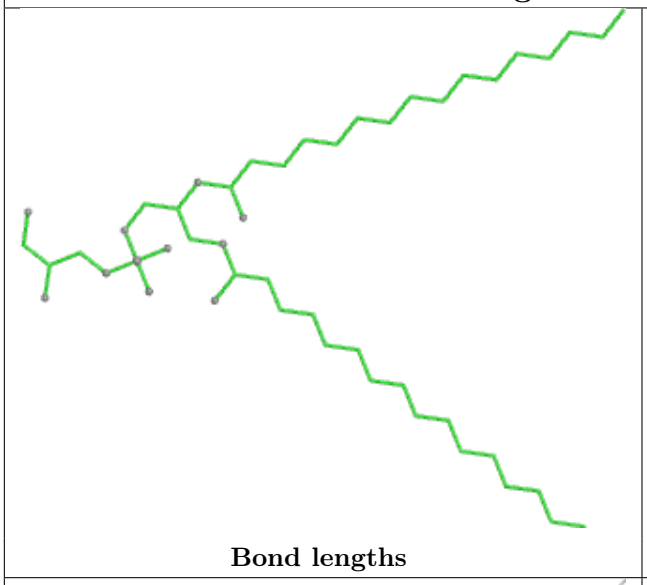


Torsions

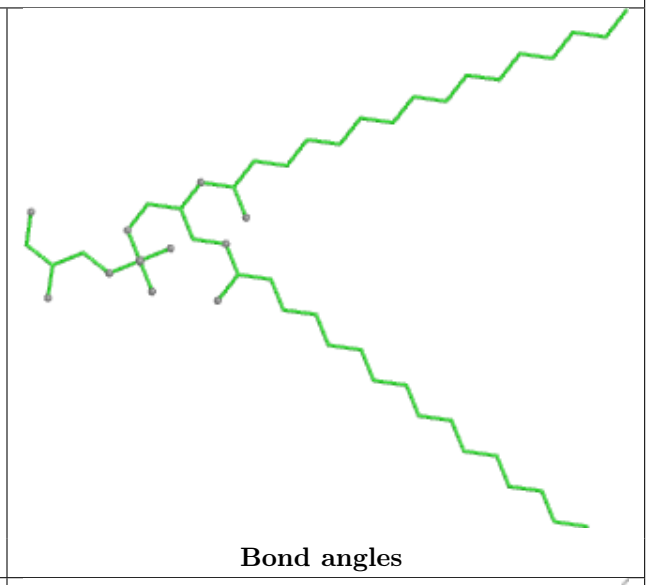


Rings

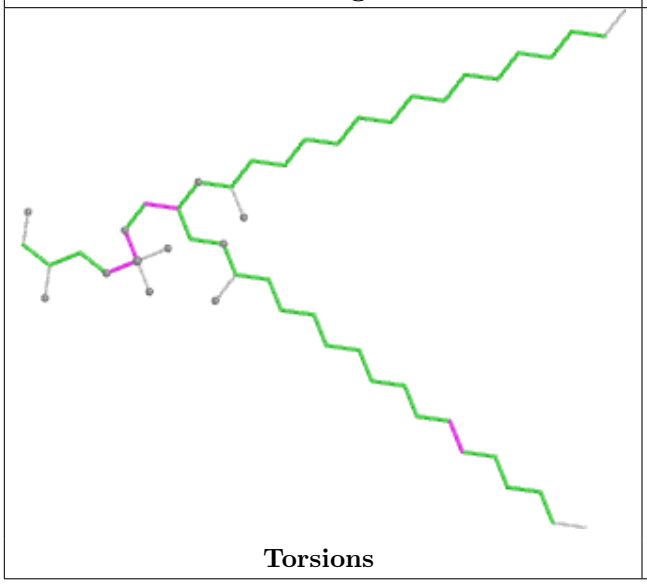
Ligand LHG 4D 409



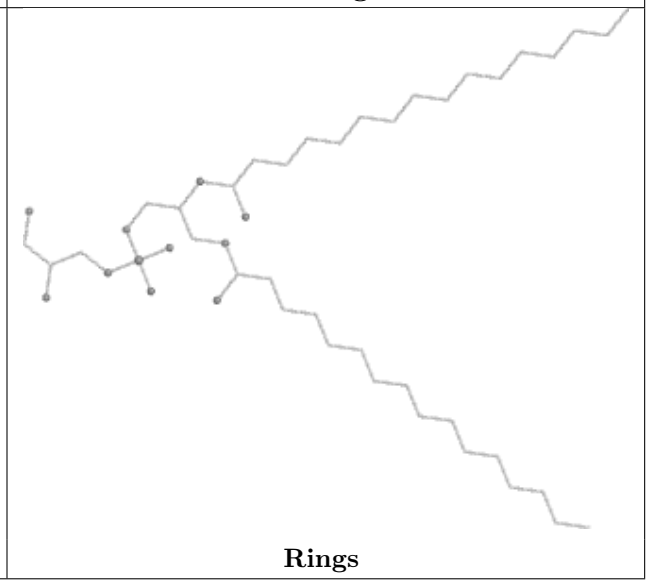
Bond lengths



Bond angles

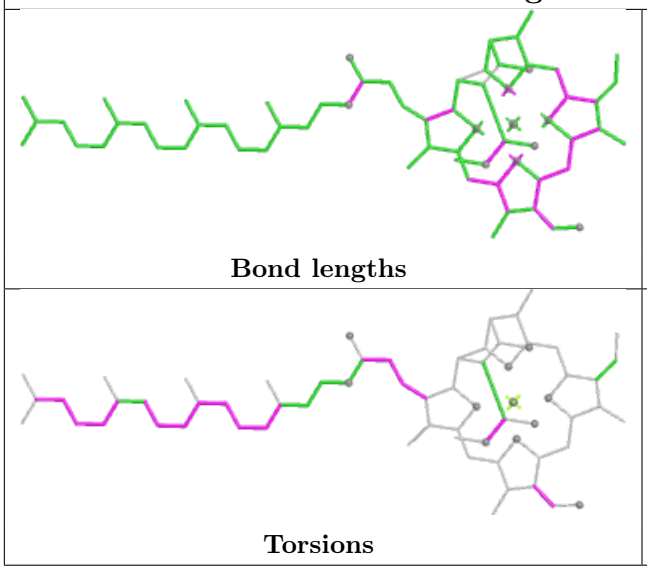


Torsions

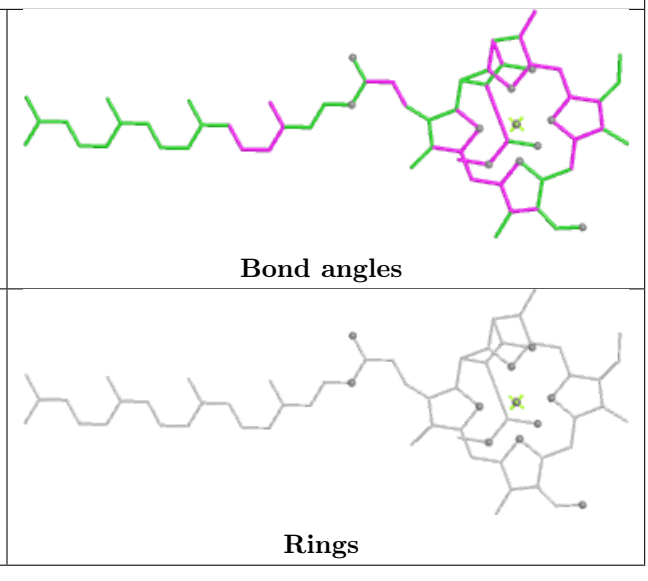


Rings

Ligand CL7 24 406



Bond lengths

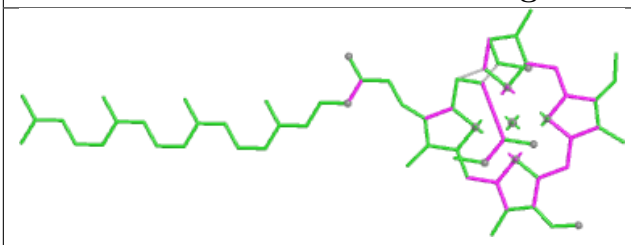


Bond angles

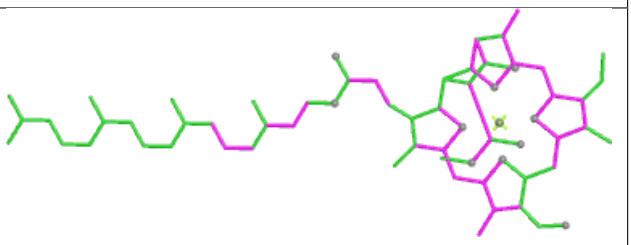
Torsions

Rings

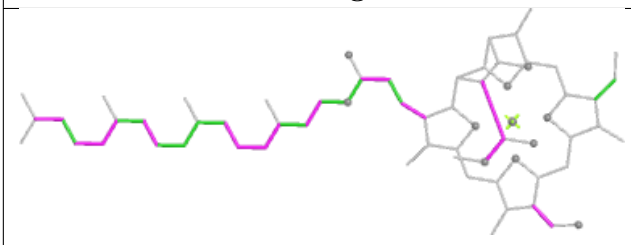
Ligand CL7 2C 509



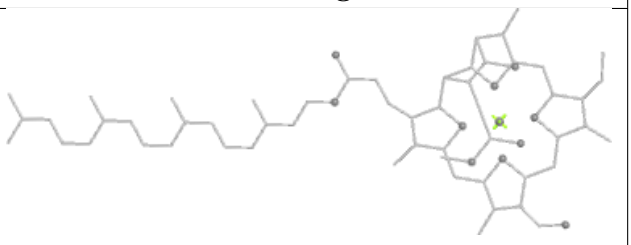
Bond lengths



Bond angles

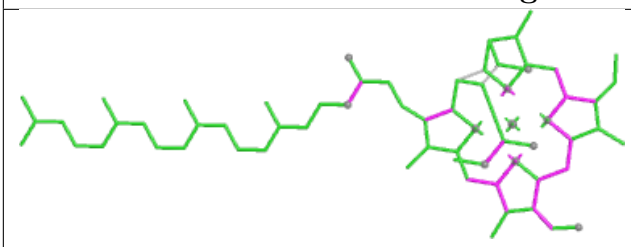


Torsions

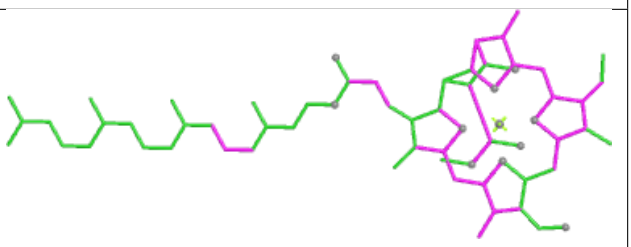


Rings

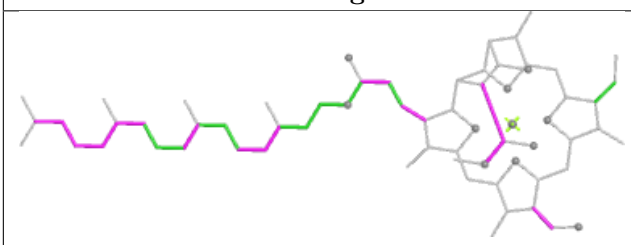
Ligand CL7 1C 501



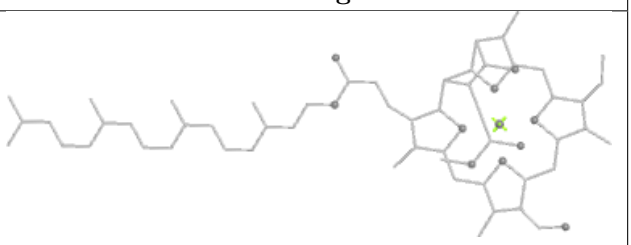
Bond lengths



Bond angles

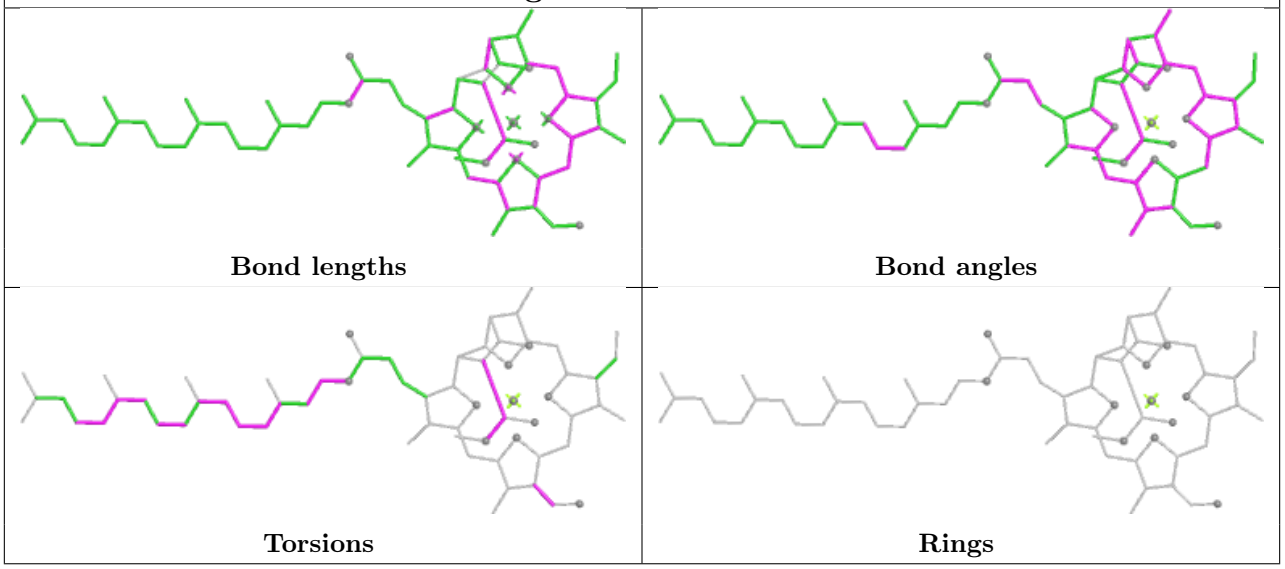


Torsions

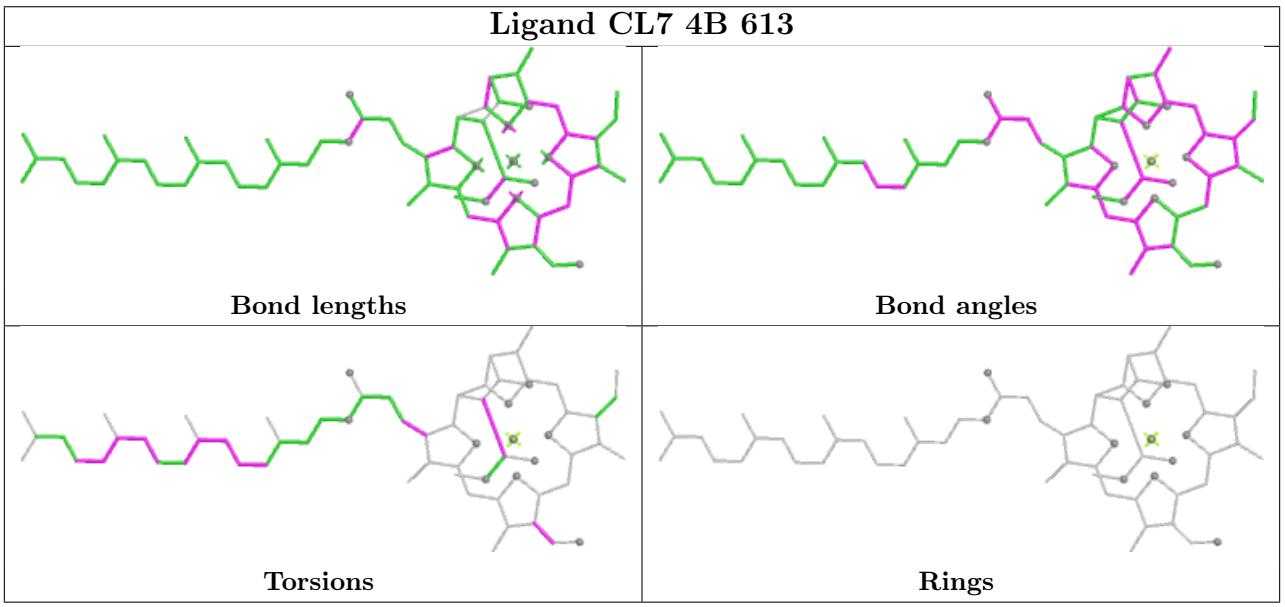


Rings

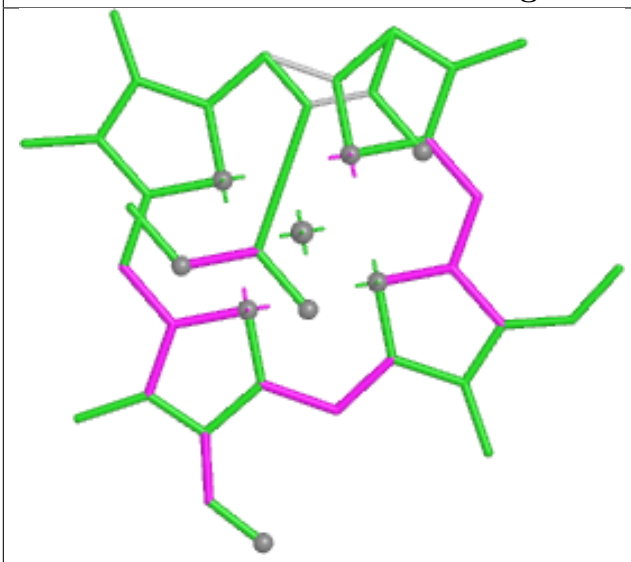
Ligand CL7 32 509



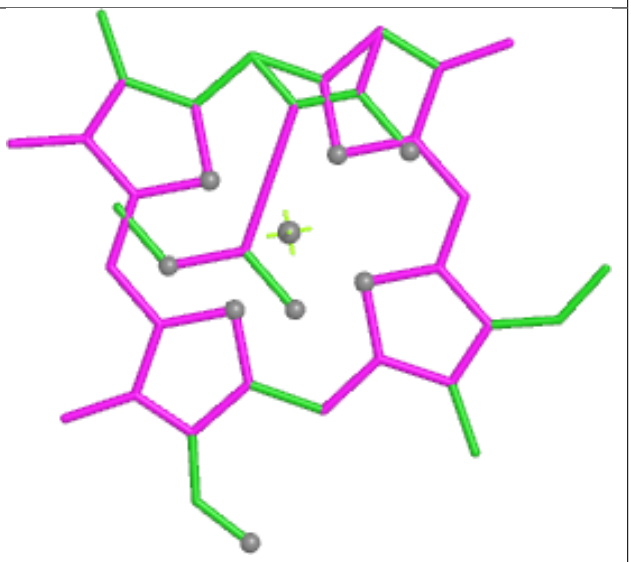
Ligand CL7 4B 613



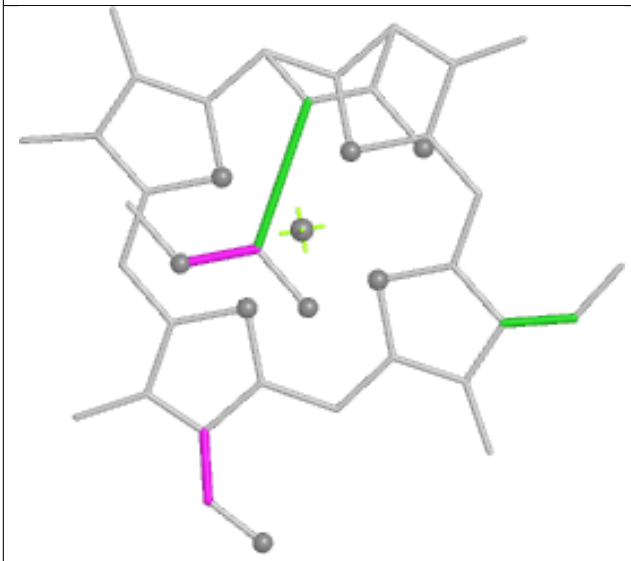
Ligand CL7 2C 512



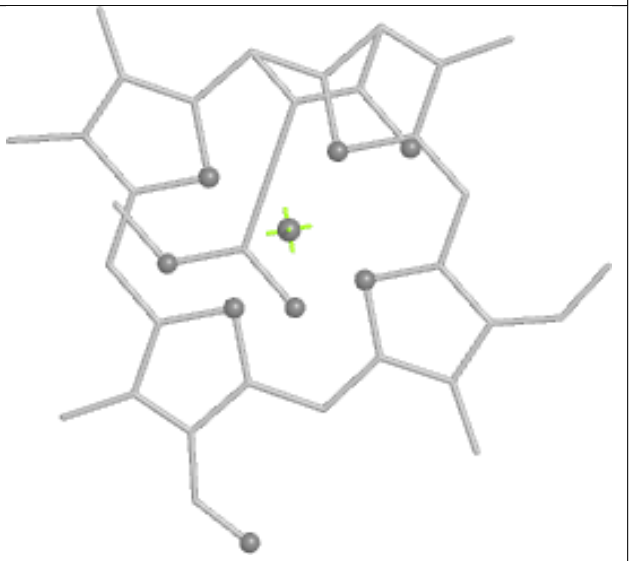
Bond lengths



Bond angles

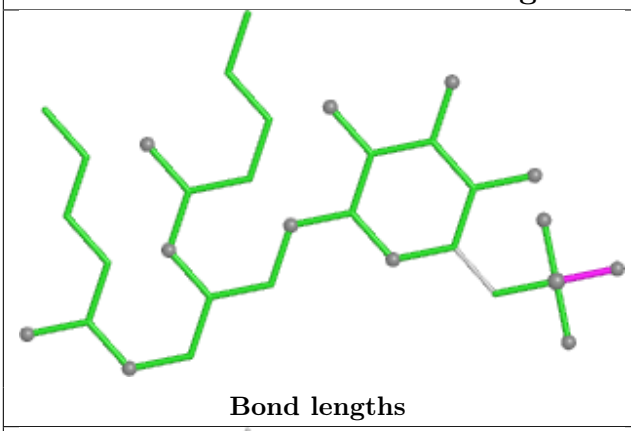


Torsions

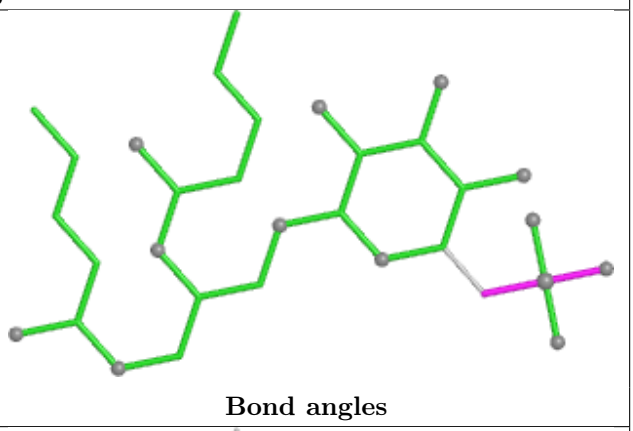


Rings

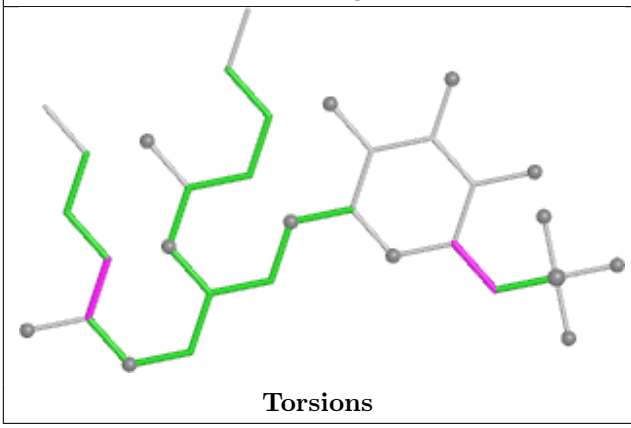
Ligand SQD 31 423



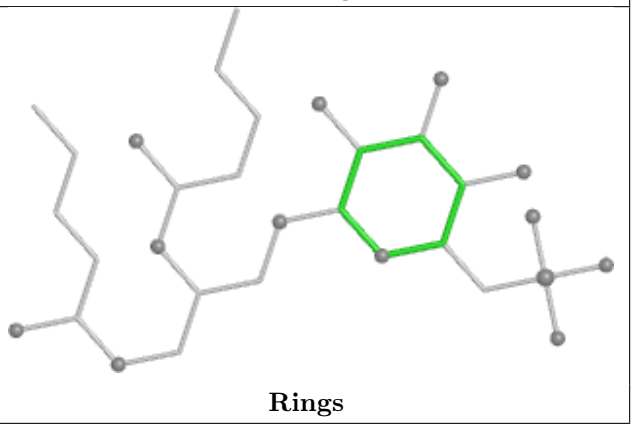
Bond lengths



Bond angles

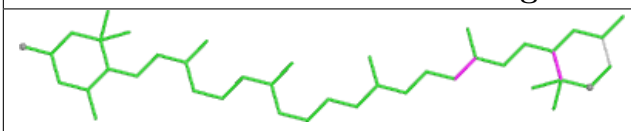


Torsions

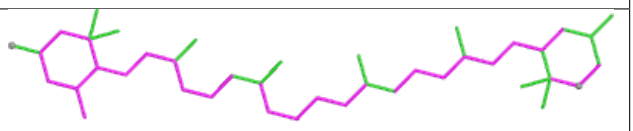


Rings

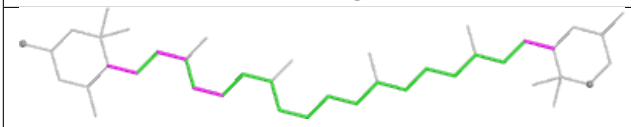
Ligand ZEX 11 422



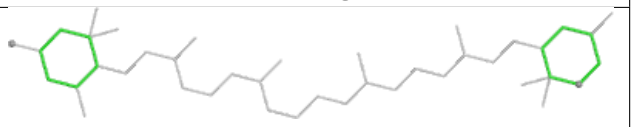
Bond lengths



Bond angles

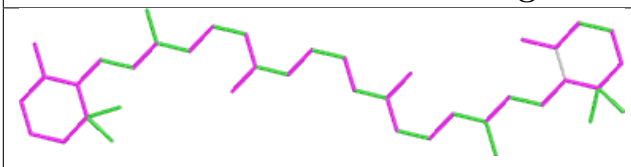


Torsions

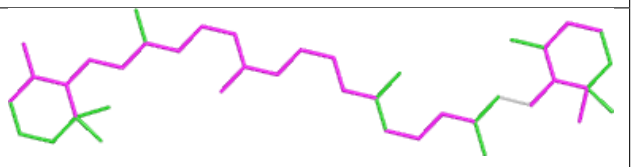


Rings

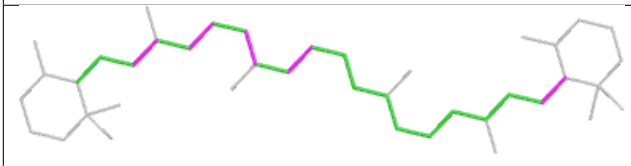
Ligand 8CT 1B 617



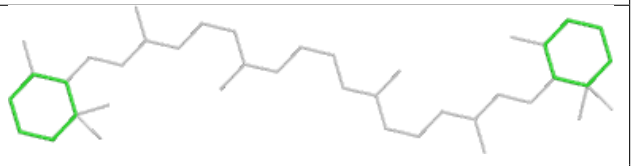
Bond lengths



Bond angles

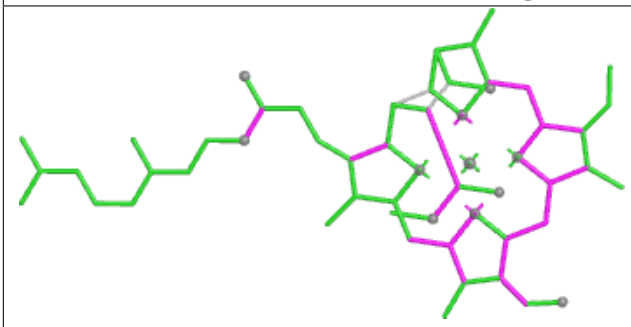


Torsions

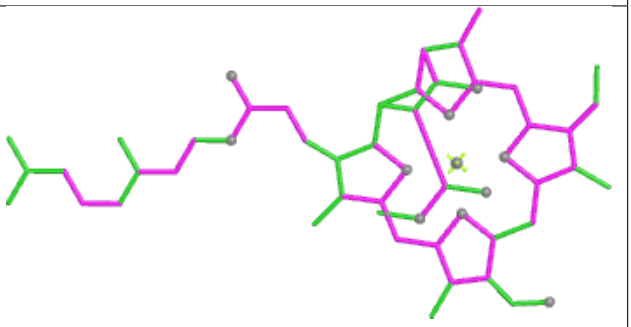


Rings

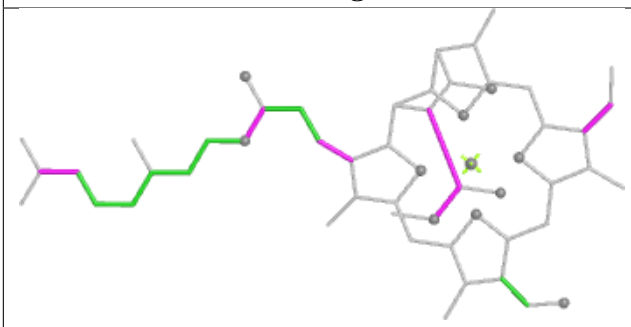
Ligand CL7 1A 403



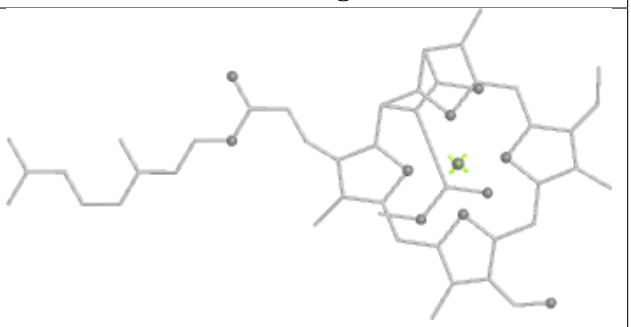
Bond lengths



Bond angles

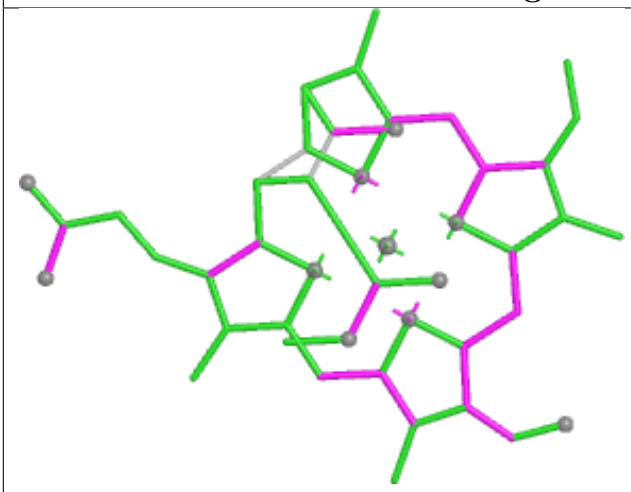


Torsions

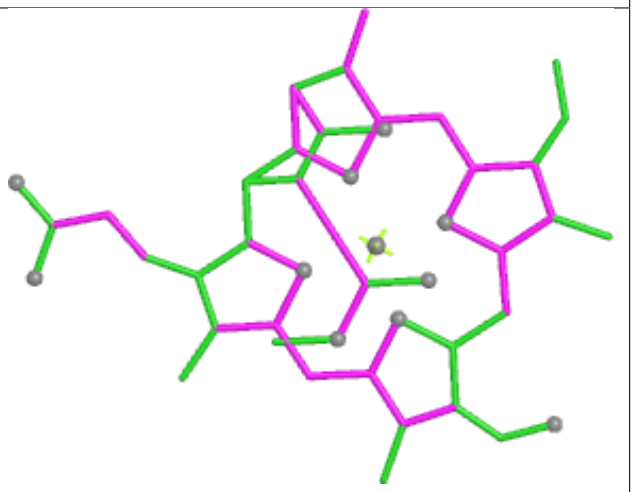


Rings

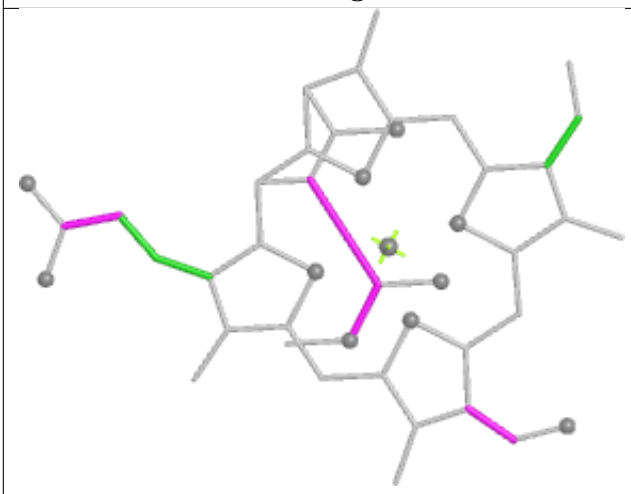
Ligand CL7 41 411



Bond lengths



Bond angles

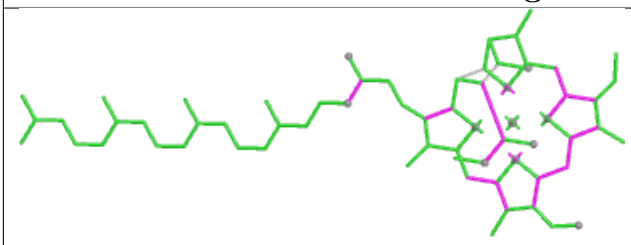


Torsions

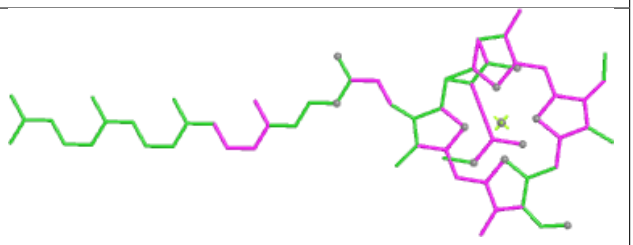


Rings

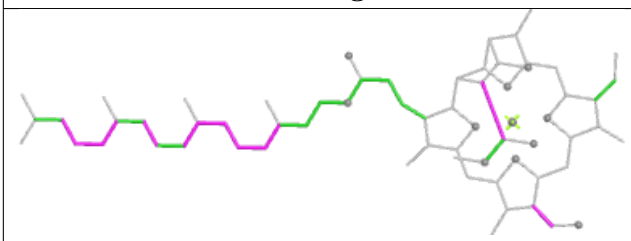
Ligand CL7 33 507



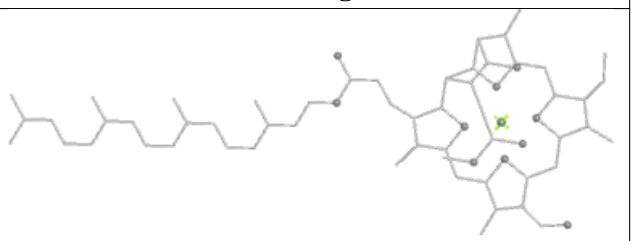
Bond lengths



Bond angles

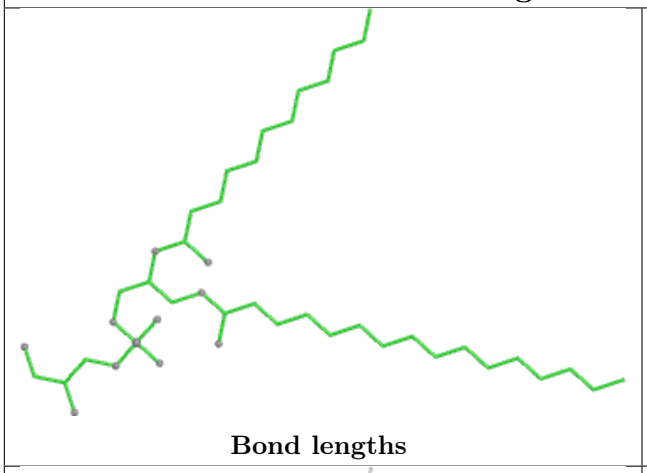


Torsions

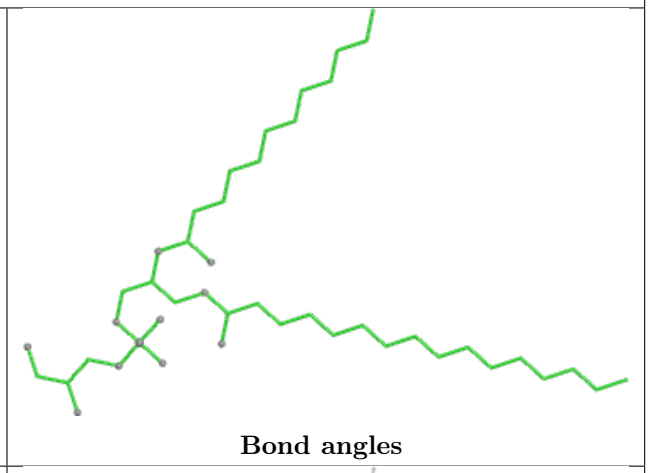


Rings

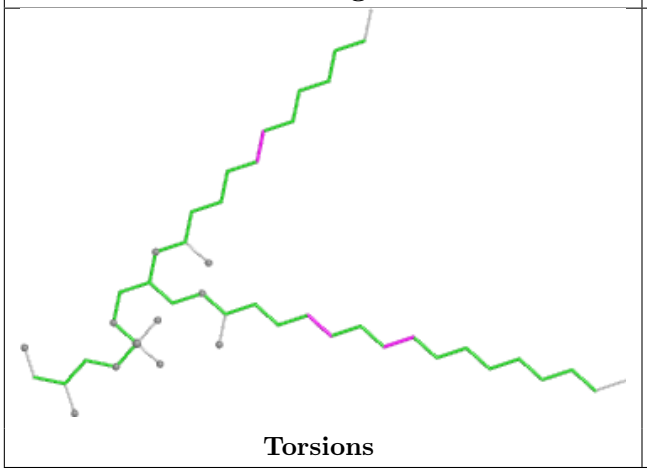
Ligand LHG 4B 624



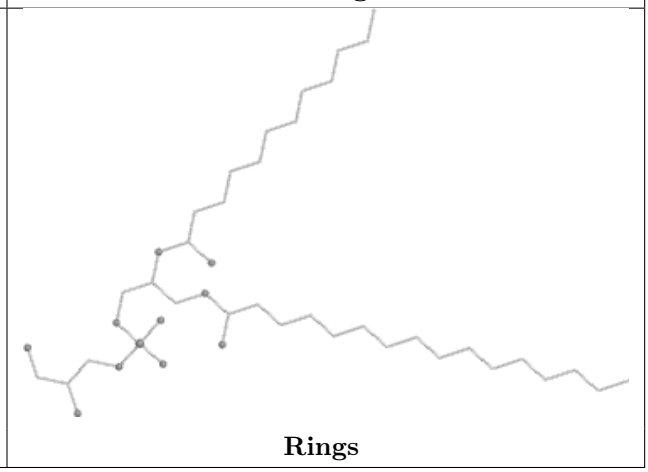
Bond lengths



Bond angles

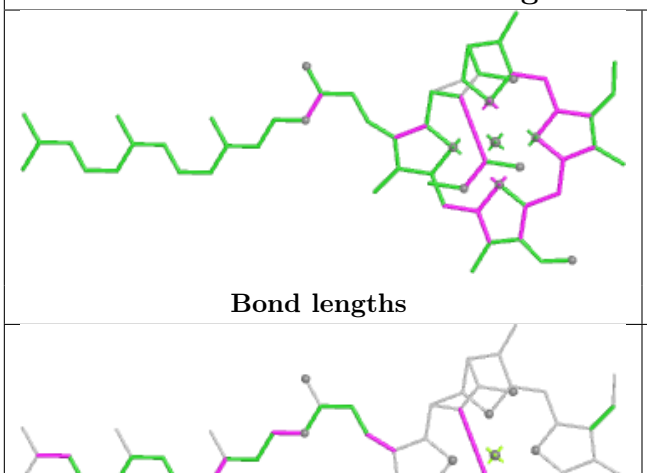


Torsions

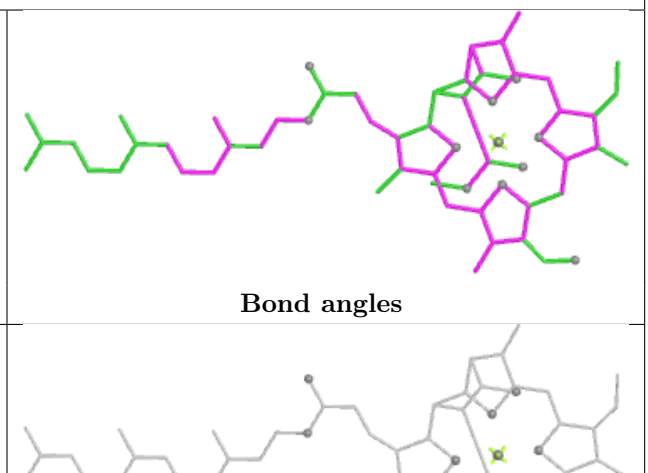


Rings

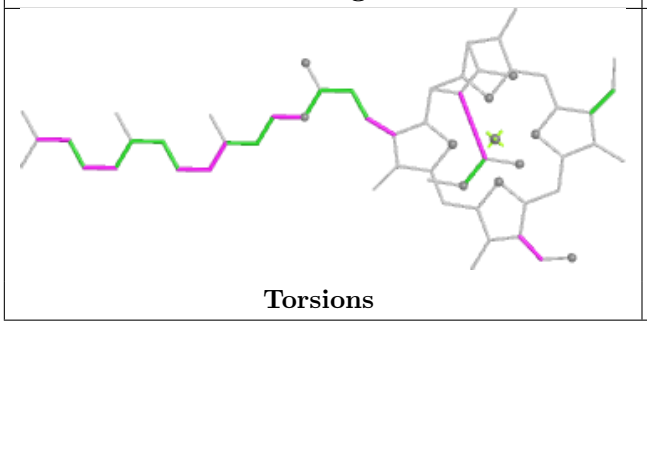
Ligand CL7 4B 615



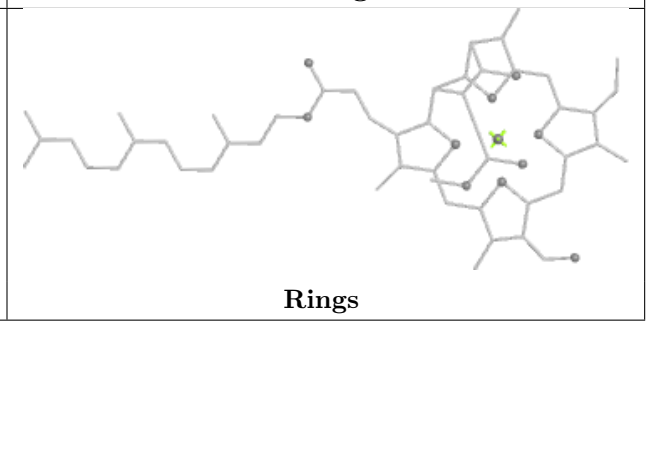
Bond lengths



Bond angles

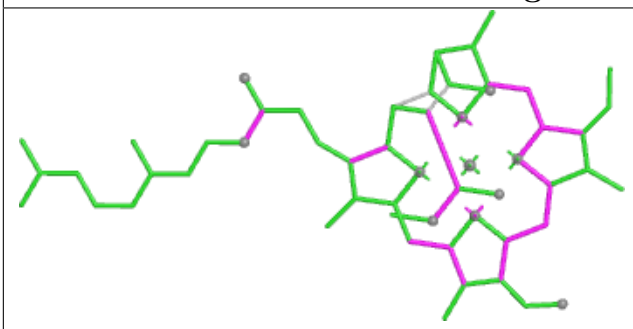


Torsions

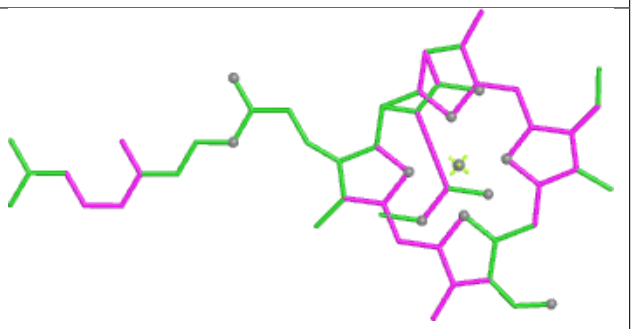


Rings

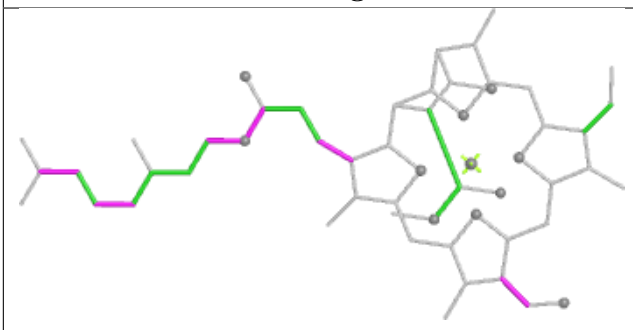
Ligand CL7 41 417



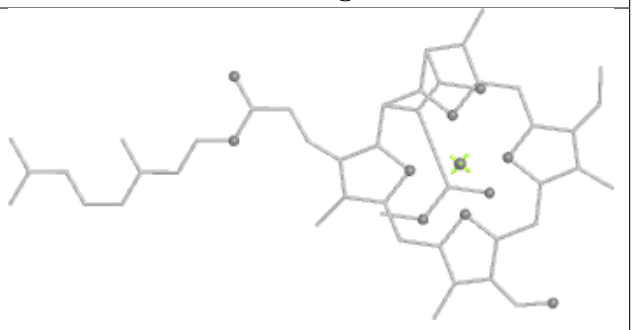
Bond lengths



Bond angles

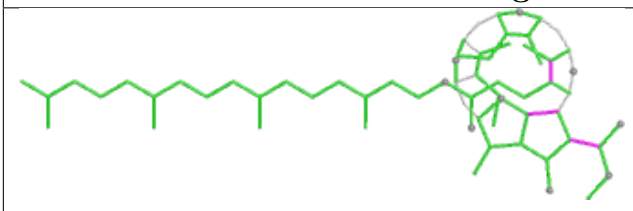


Torsions

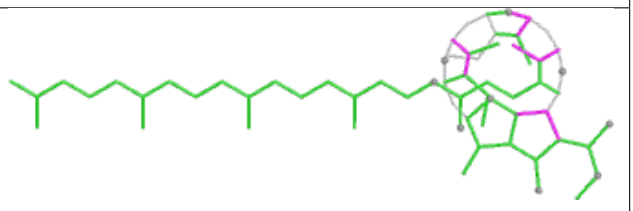


Rings

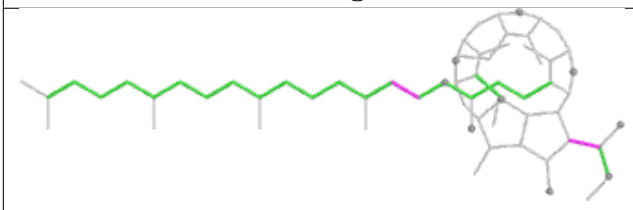
Ligand PHO 2A 402



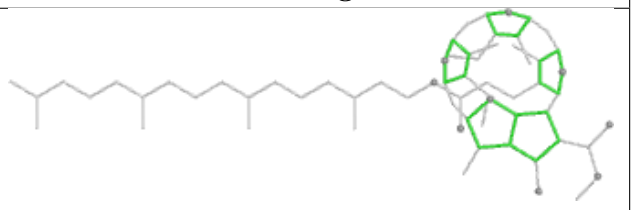
Bond lengths



Bond angles

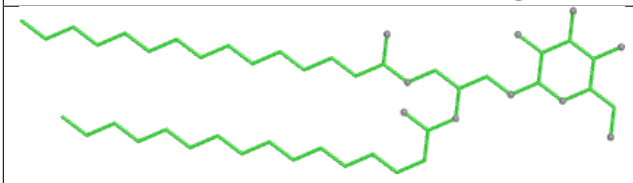


Torsions

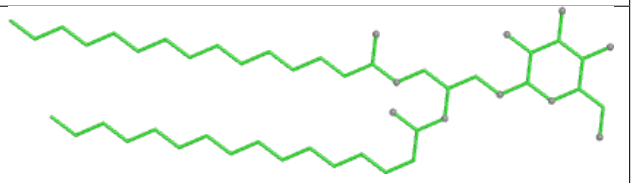


Rings

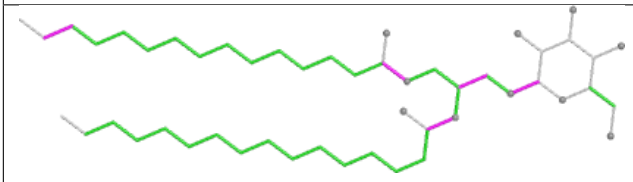
Ligand LMG 4A 405



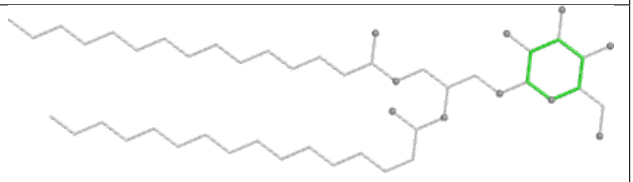
Bond lengths



Bond angles

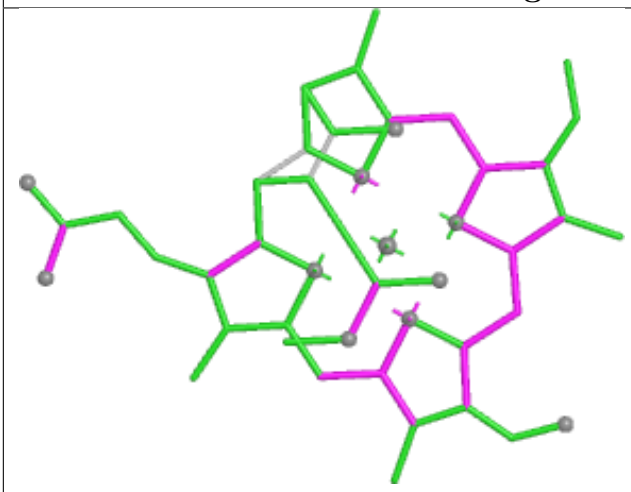


Torsions

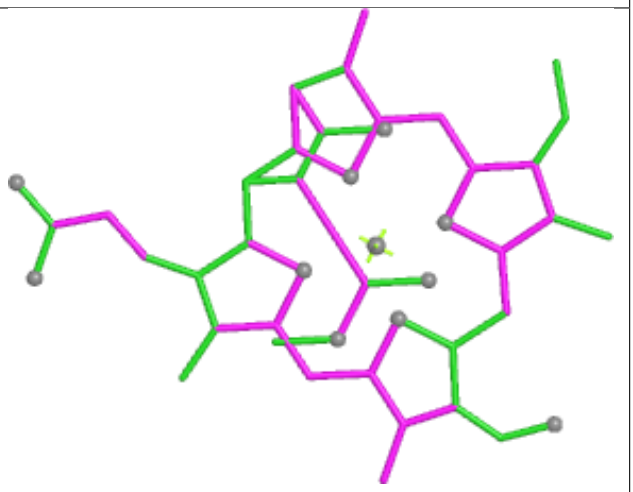


Rings

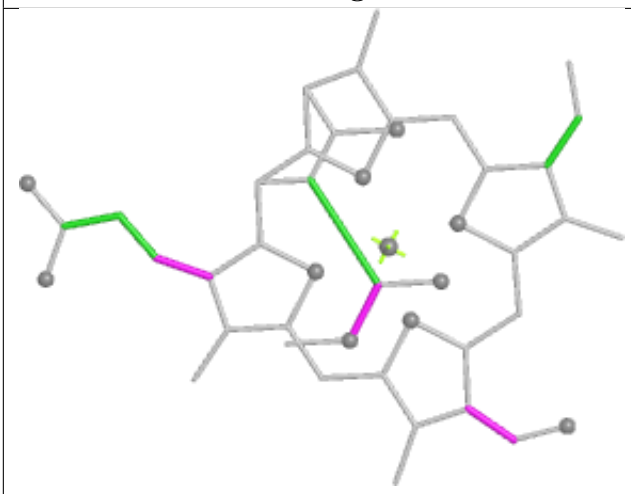
Ligand CL7 22 504



Bond lengths



Bond angles

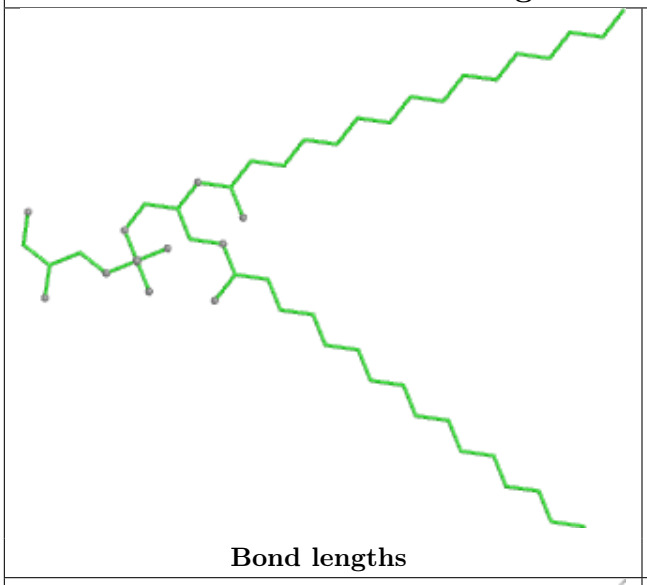


Torsions

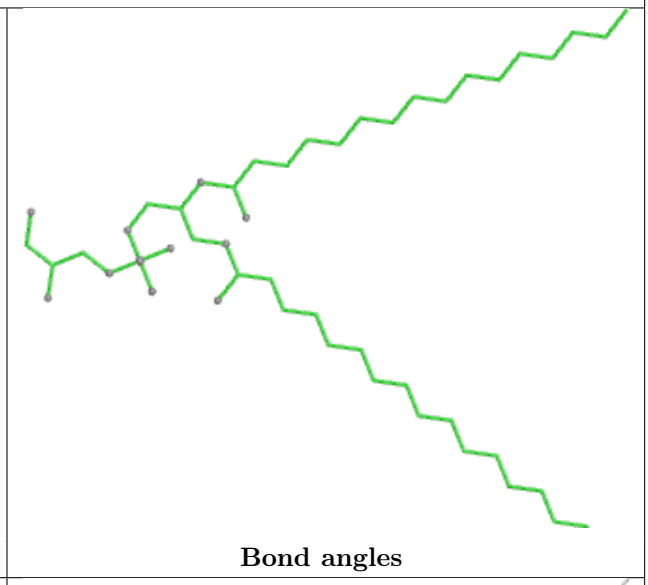


Rings

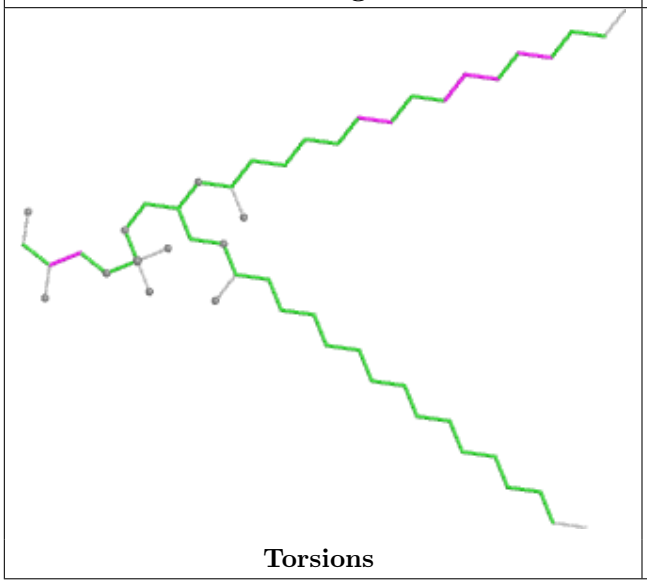
Ligand LHG 3B 625



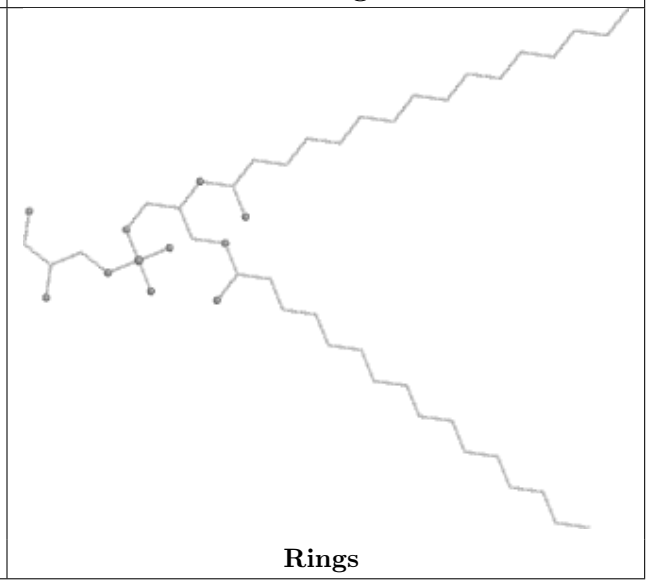
Bond lengths



Bond angles

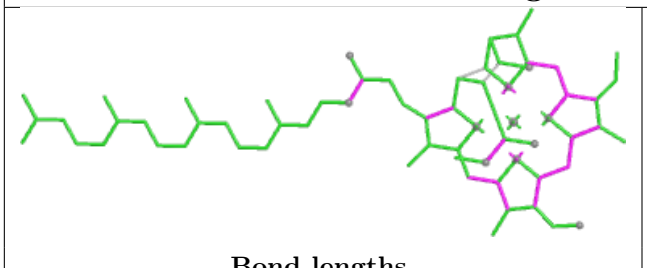


Torsions

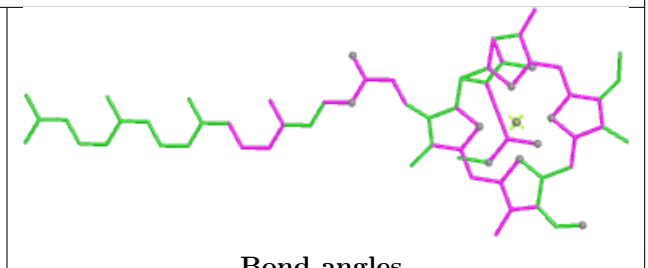


Rings

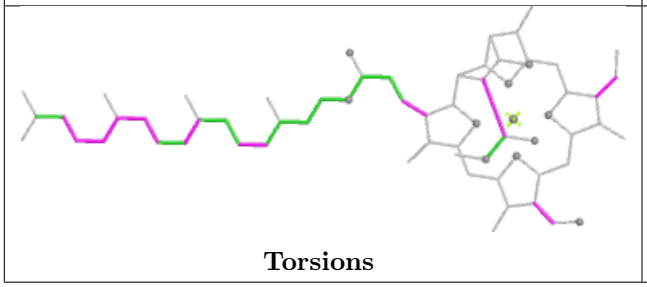
Ligand CL7 11 408



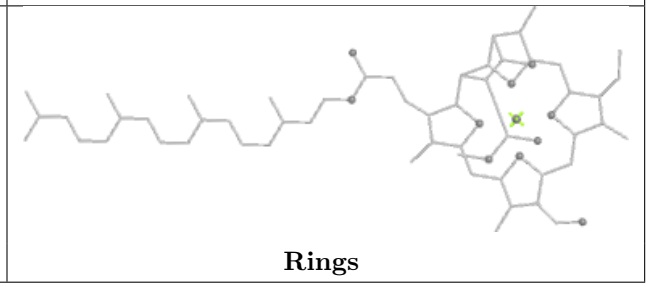
Bond lengths



Bond angles

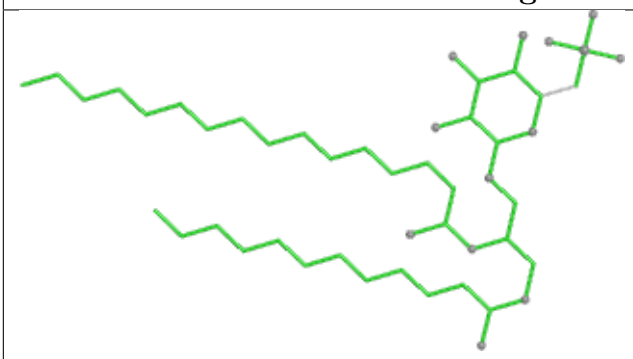


Torsions

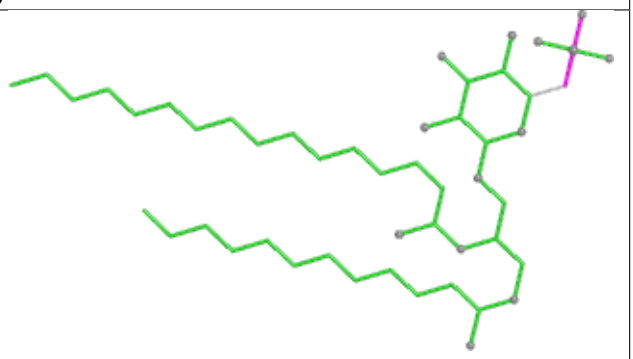


Rings

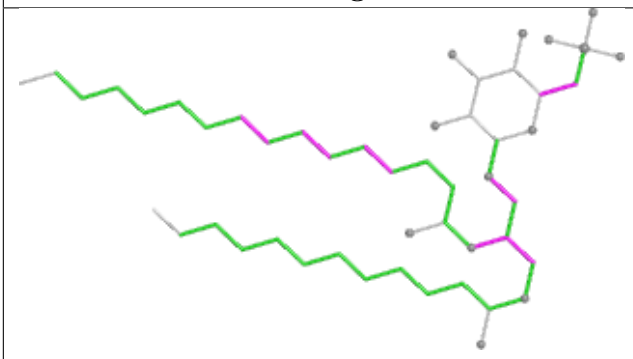
Ligand SQD 13 523



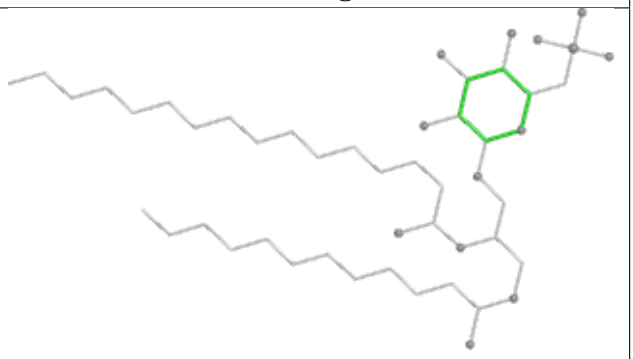
Bond lengths



Bond angles

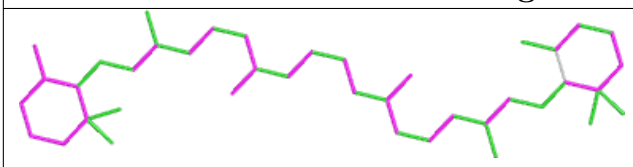


Torsions

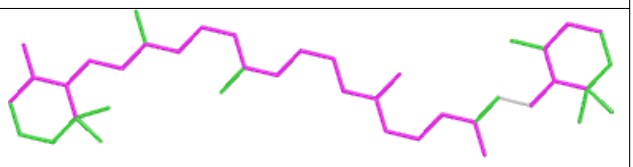


Rings

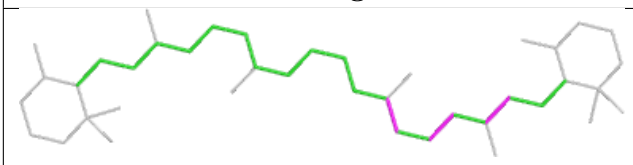
Ligand 8CT 1A 404



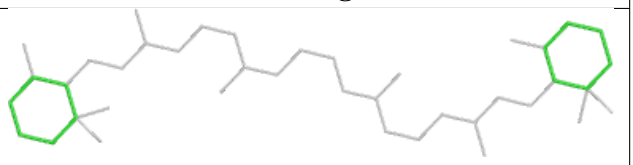
Bond lengths



Bond angles

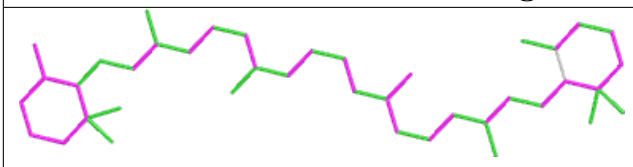


Torsions

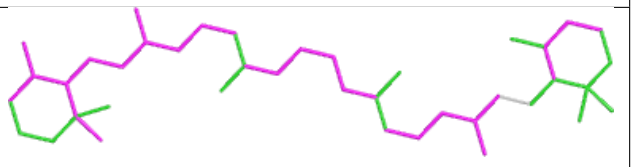


Rings

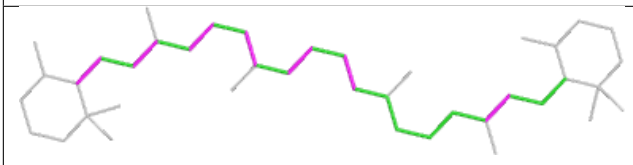
Ligand 8CT 3B 618



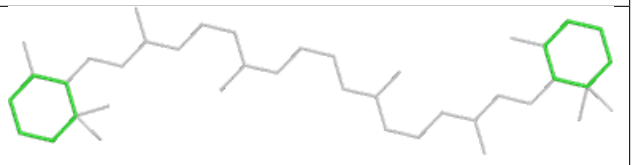
Bond lengths



Bond angles

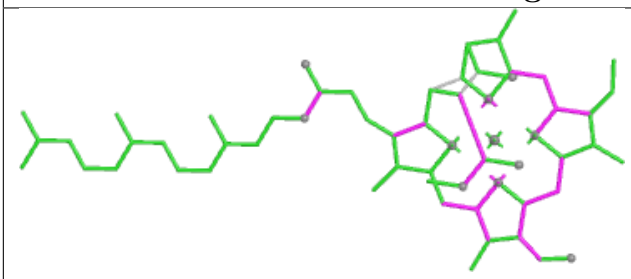


Torsions

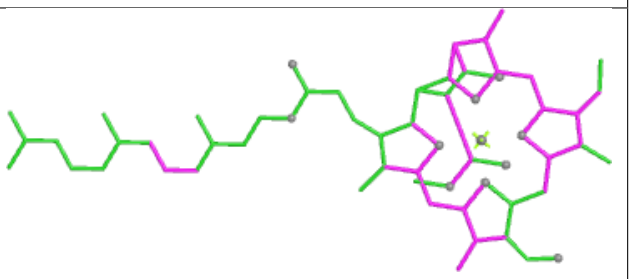


Rings

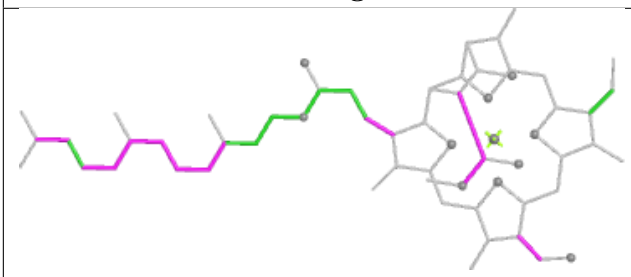
Ligand CL7 32 511



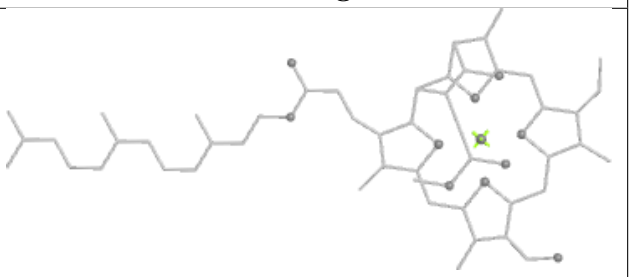
Bond lengths



Bond angles

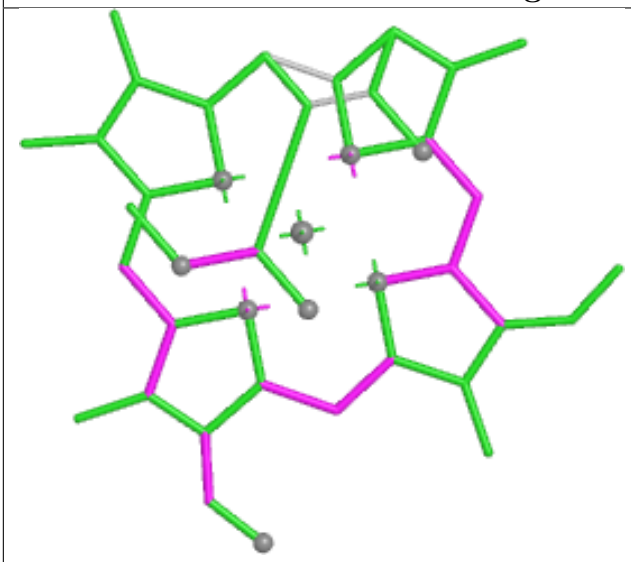


Torsions

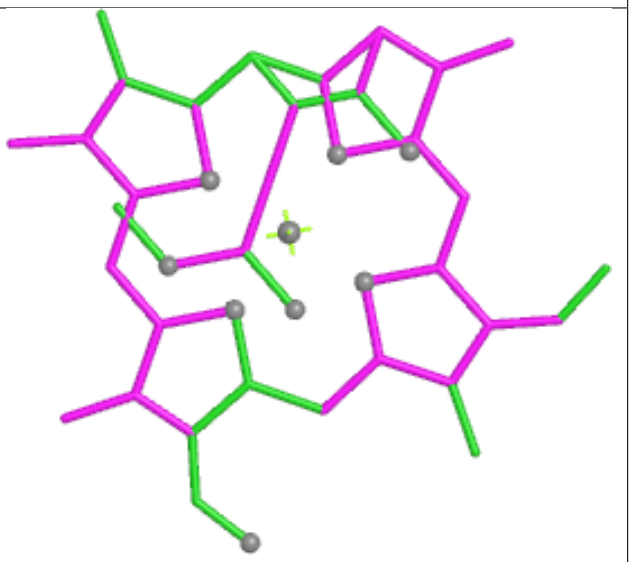


Rings

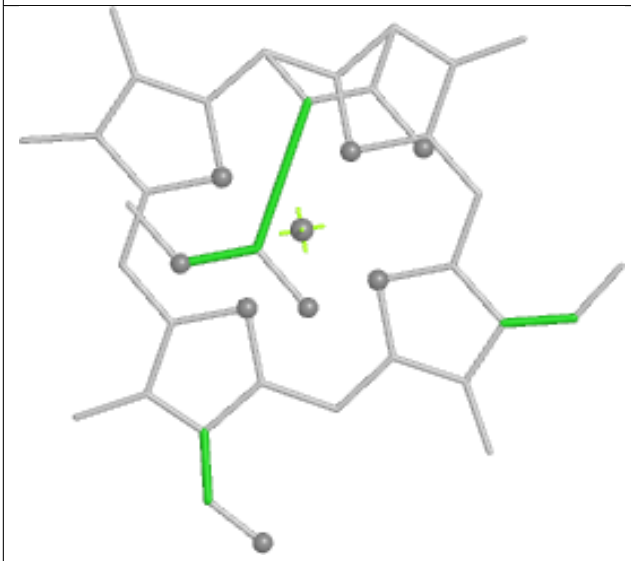
Ligand CL7 43 416



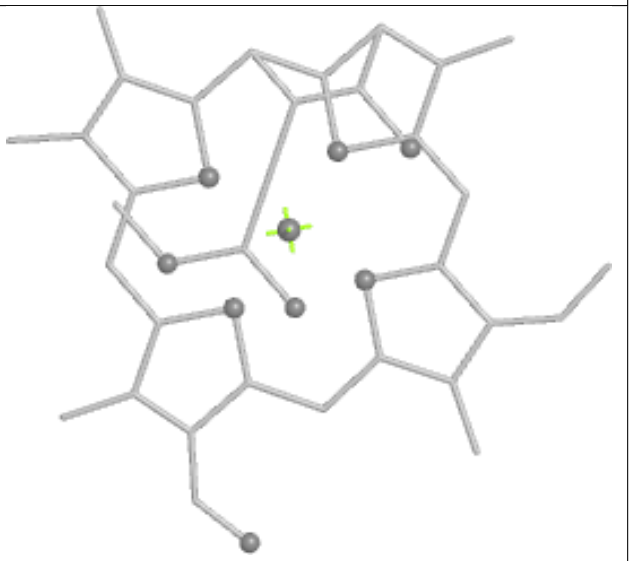
Bond lengths



Bond angles

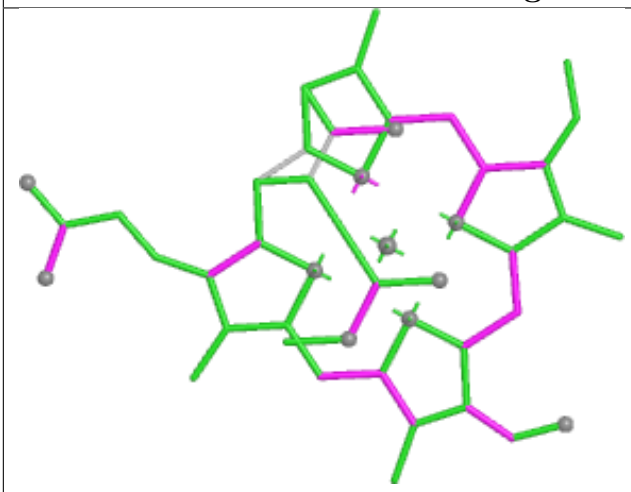


Torsions

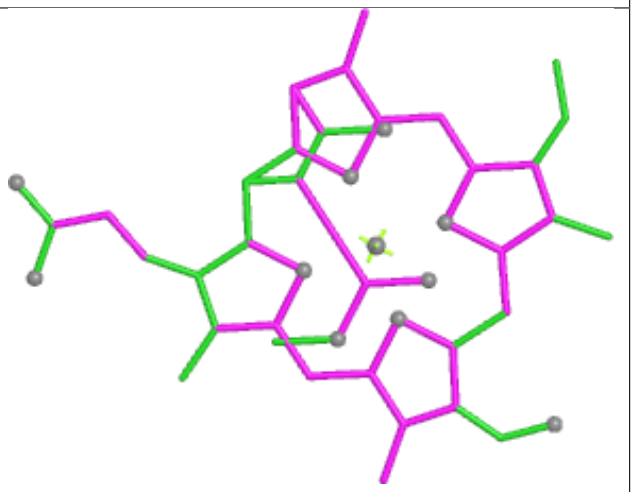


Rings

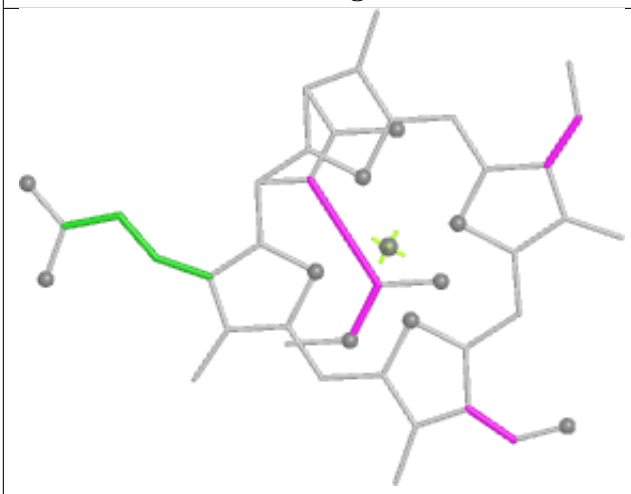
Ligand CL7 11 420



Bond lengths



Bond angles

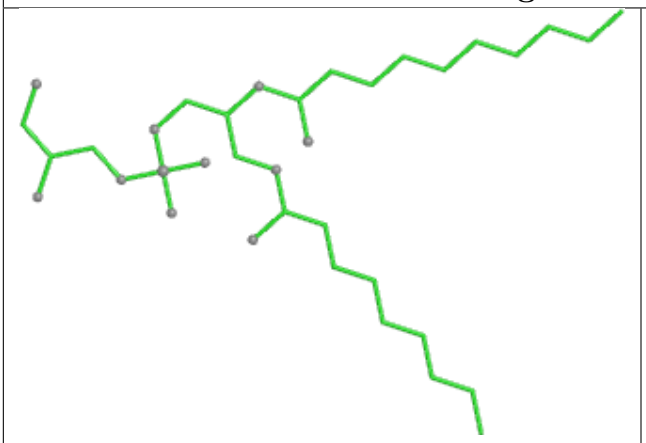


Torsions

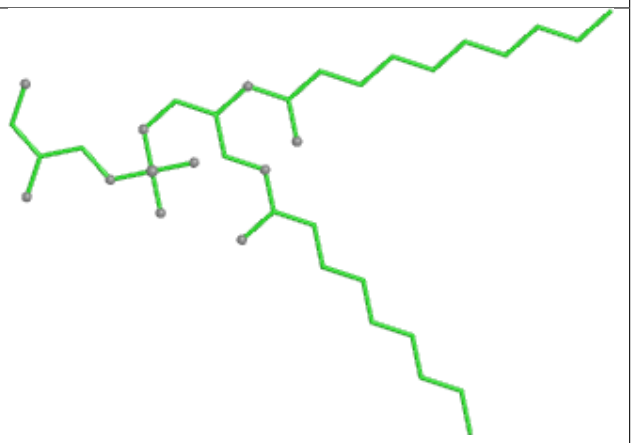


Rings

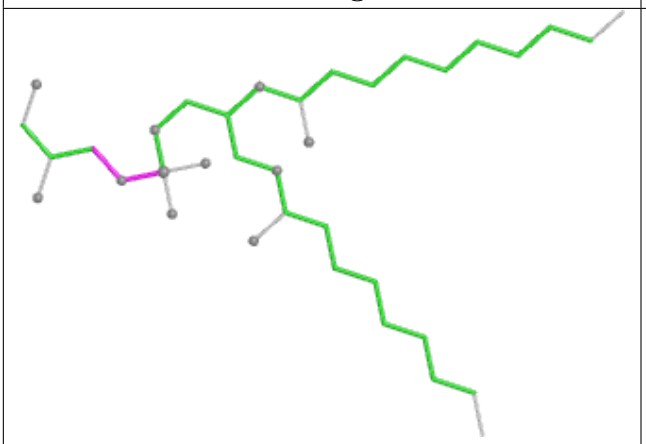
Ligand LHG 33 524



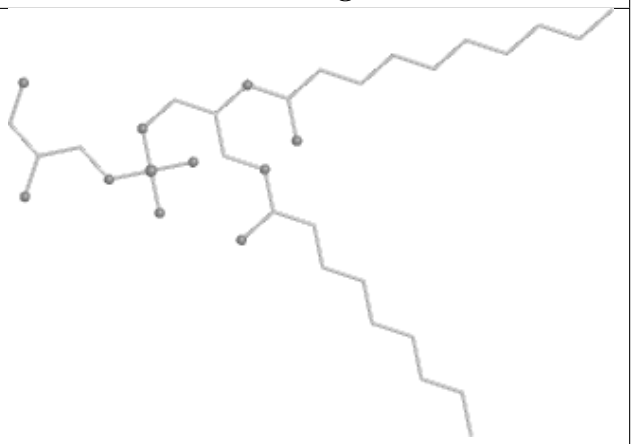
Bond lengths



Bond angles

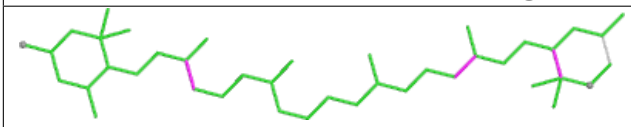


Torsions

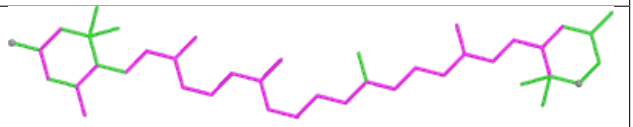


Rings

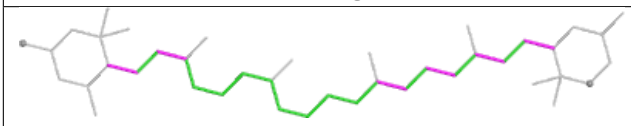
Ligand ZEX 13 519



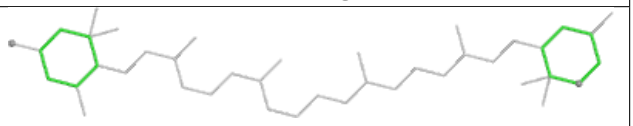
Bond lengths



Bond angles

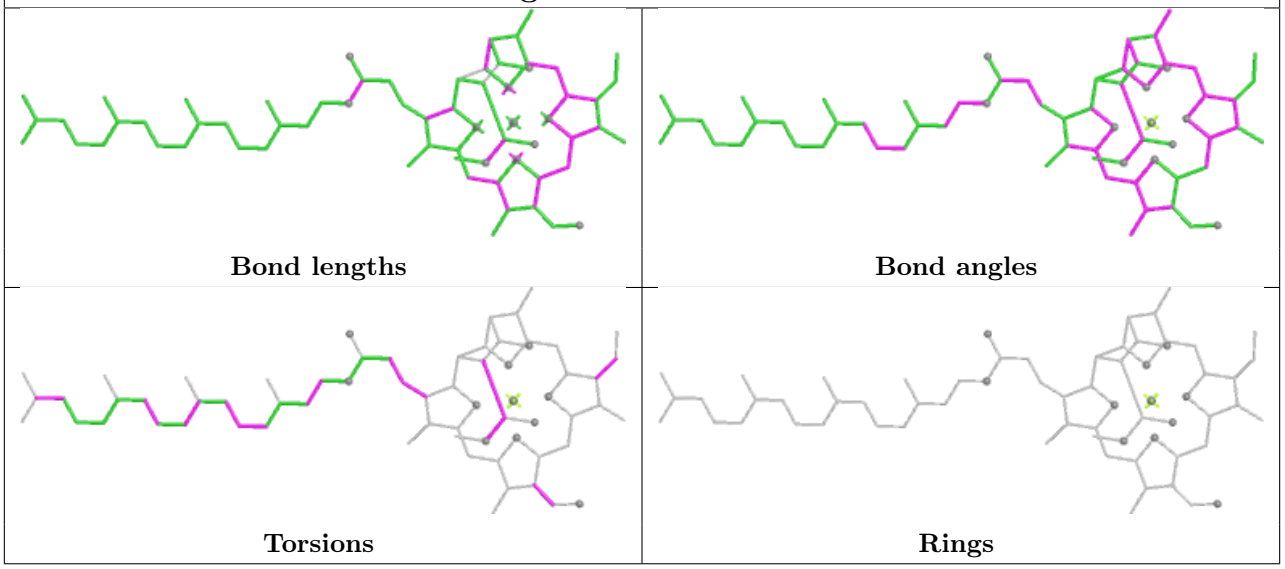


Torsions

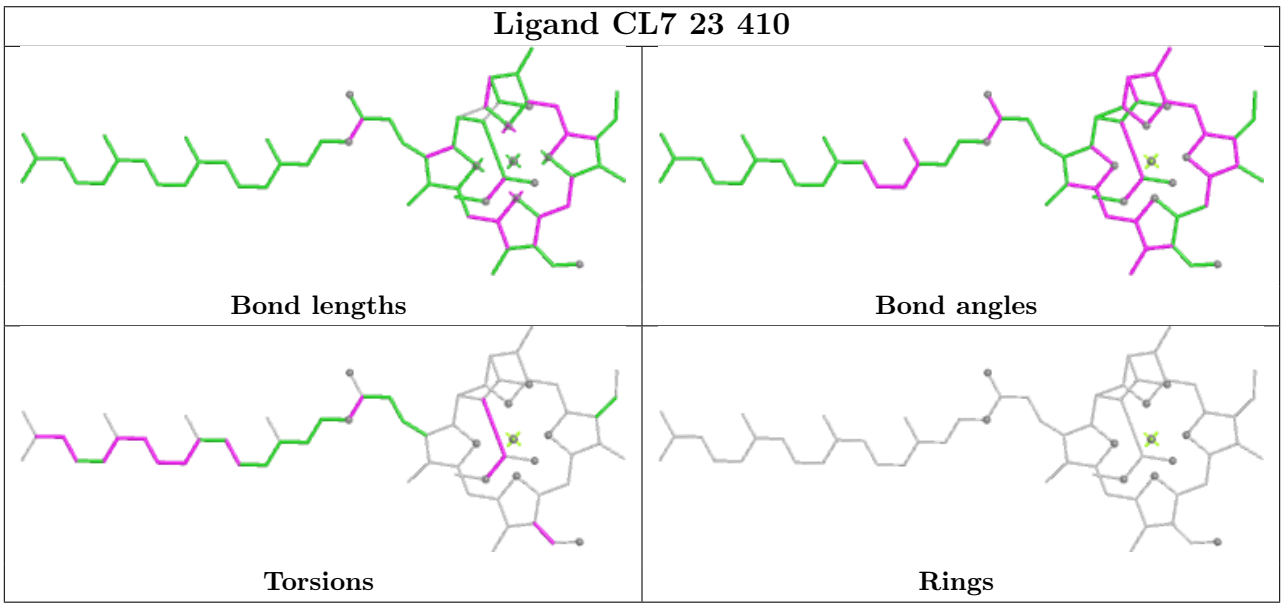


Rings

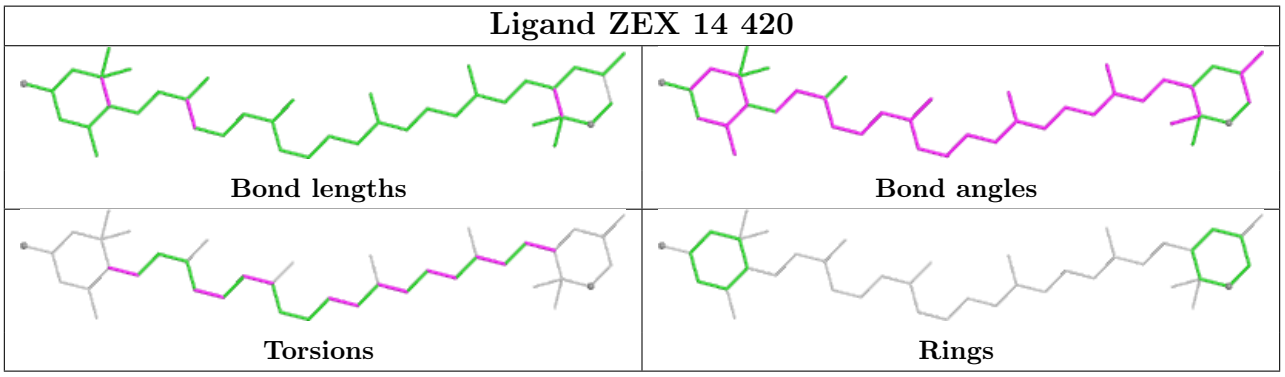
Ligand CL7 2A 407



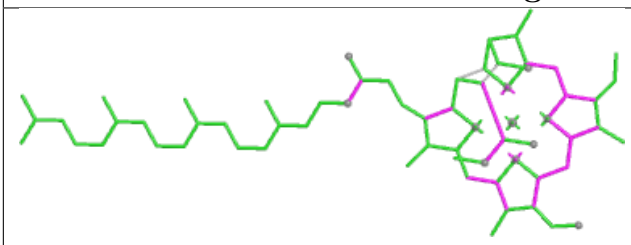
Ligand CL7 23 410



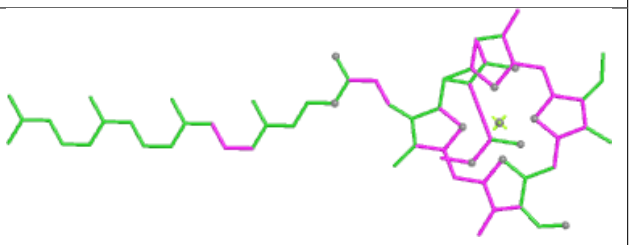
Ligand ZEX 14 420



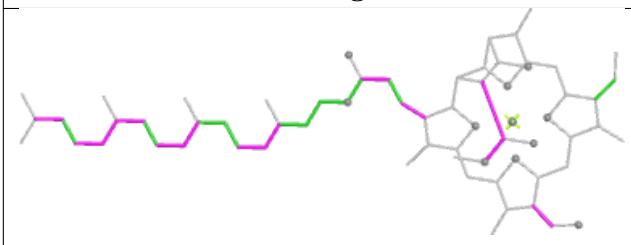
Ligand CL7 12 507



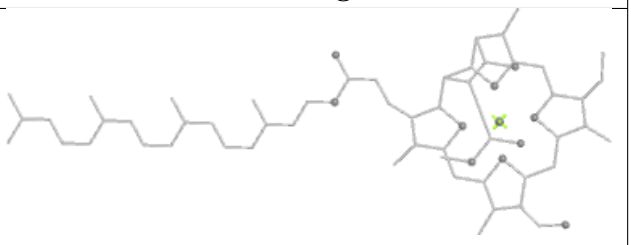
Bond lengths



Bond angles

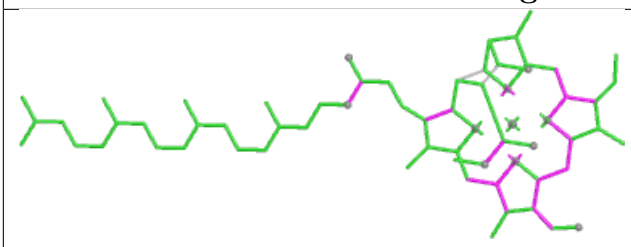


Torsions

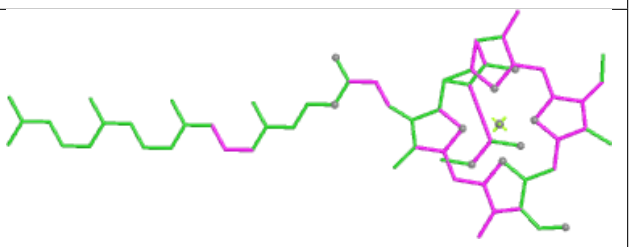


Rings

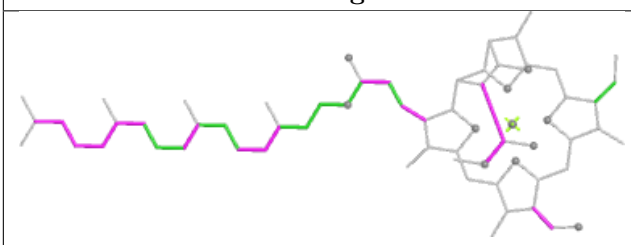
Ligand CL7 2C 501



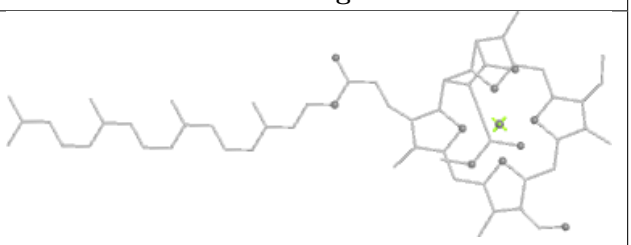
Bond lengths



Bond angles

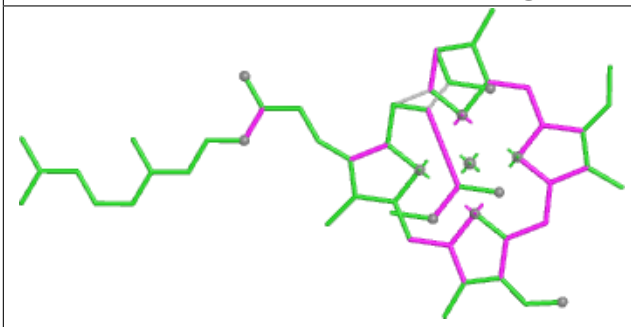


Torsions

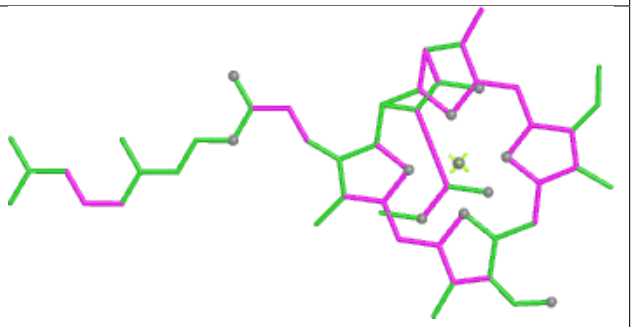


Rings

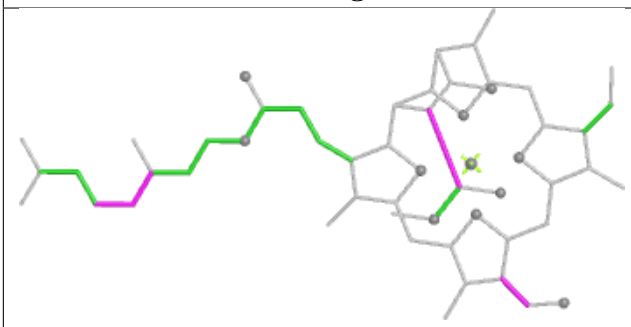
Ligand CL7 1B 613



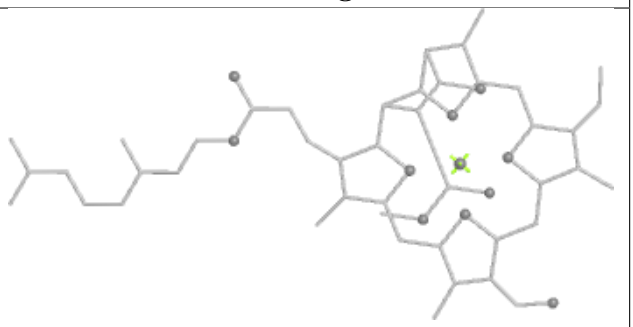
Bond lengths



Bond angles

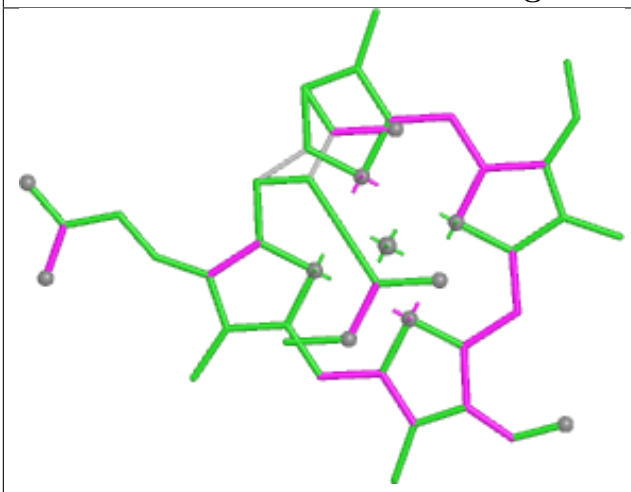


Torsions

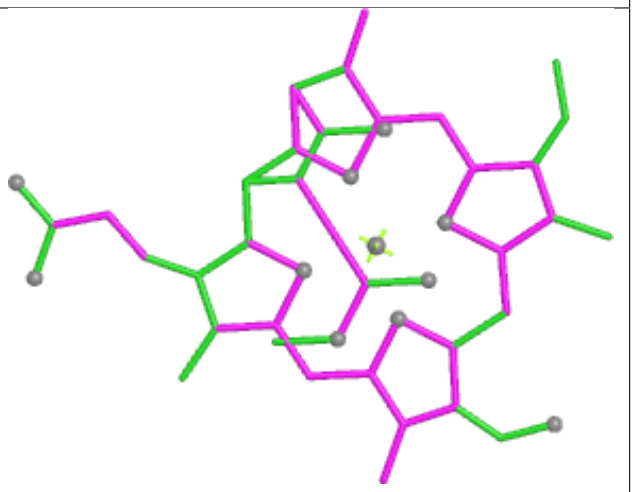


Rings

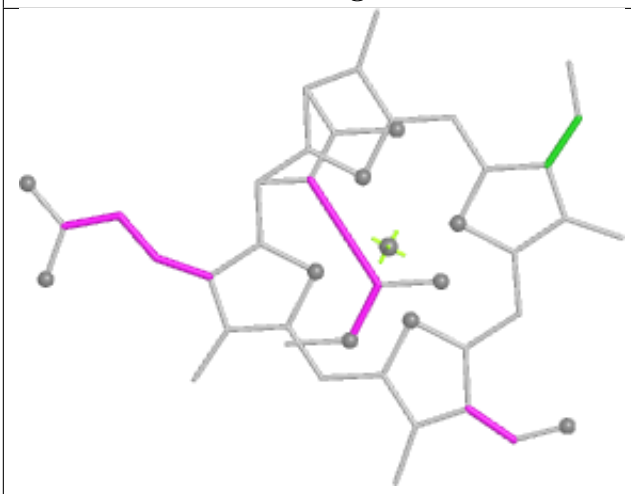
Ligand CL7 21 412



Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

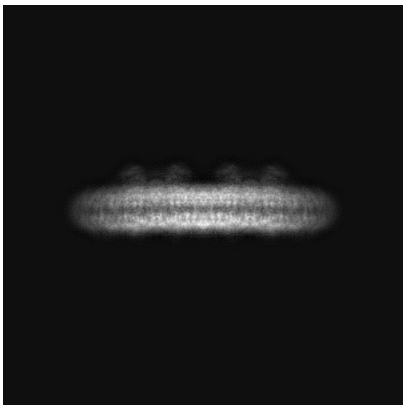
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33933. These allow visual inspection of the internal detail of the map and identification of artifacts.

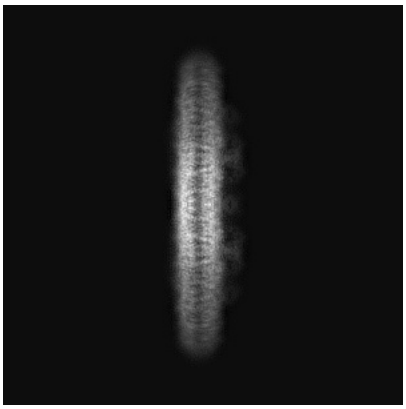
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

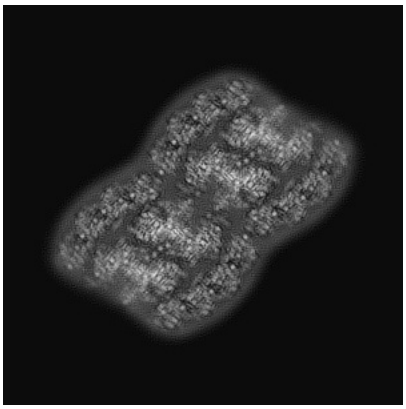
6.1.1 Primary map



X

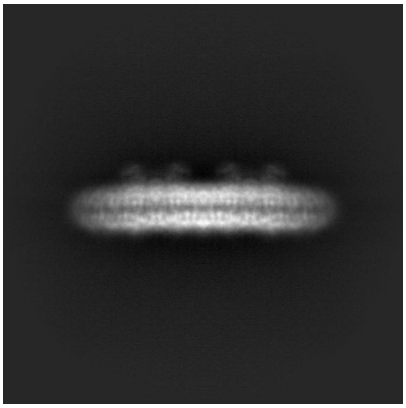


Y

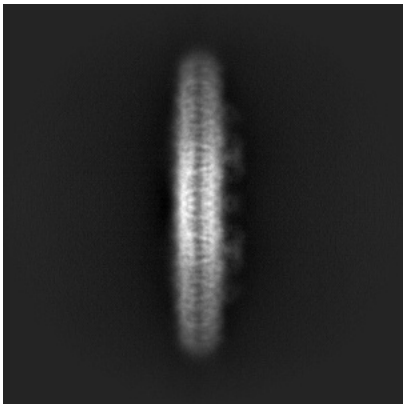


Z

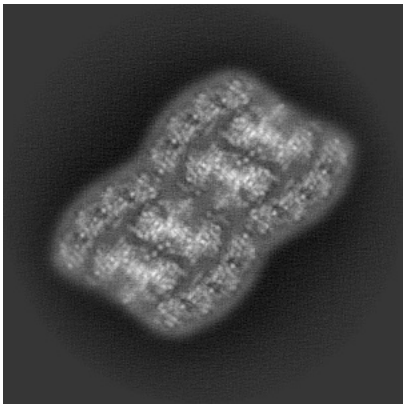
6.1.2 Raw map



X



Y

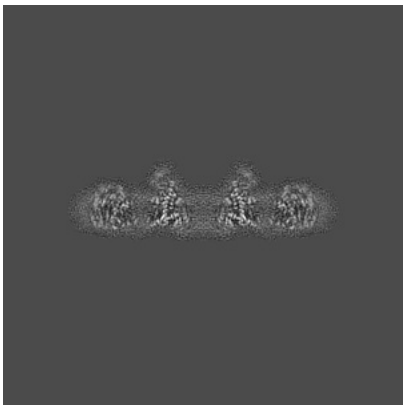


Z

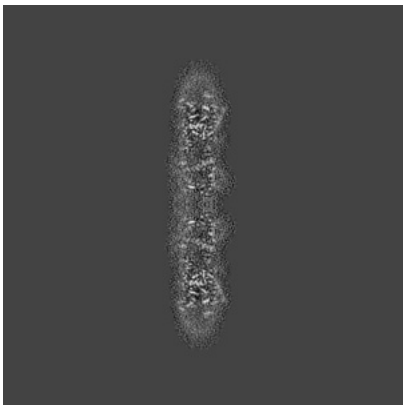
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

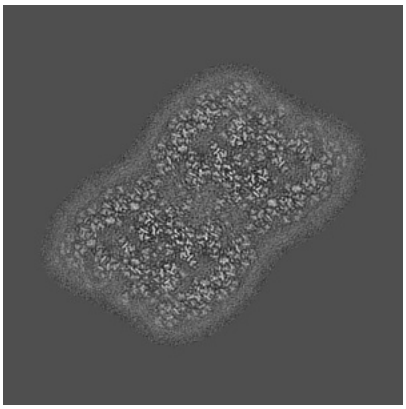
6.2.1 Primary map



X Index: 240

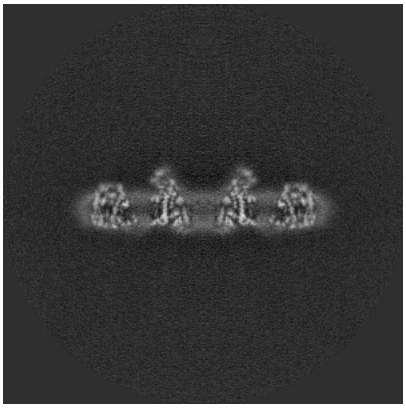


Y Index: 240

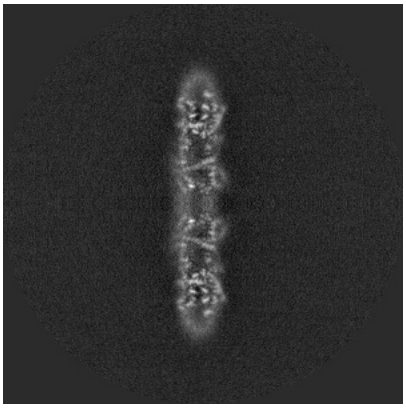


Z Index: 240

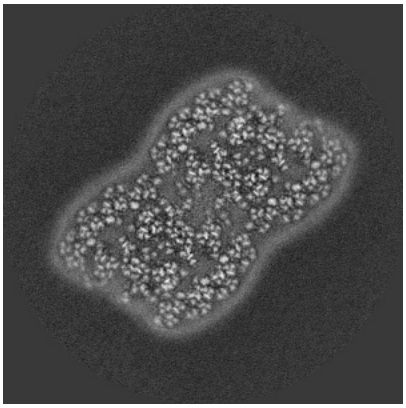
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

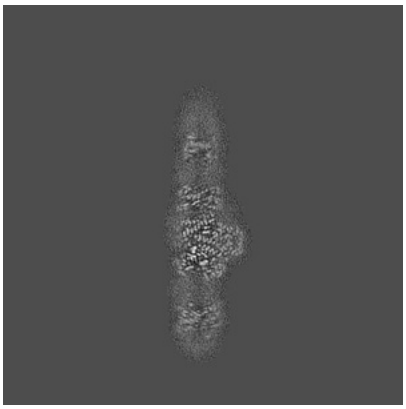
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

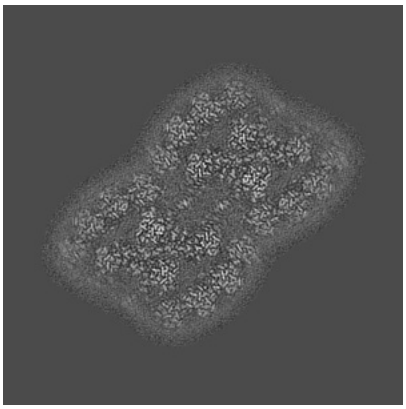
6.3.1 Primary map



X Index: 204

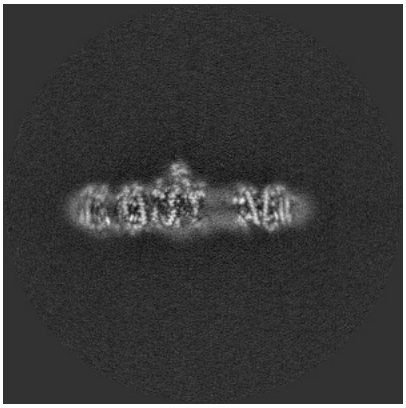


Y Index: 208

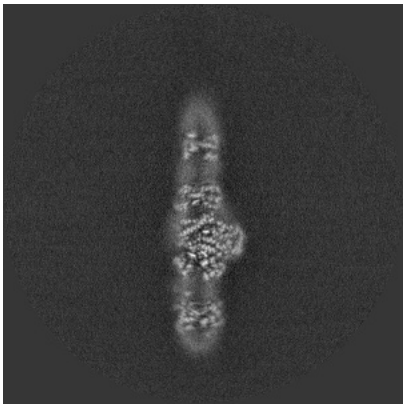


Z Index: 225

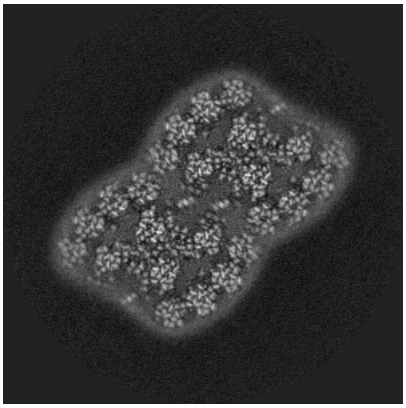
6.3.2 Raw map



X Index: 204



Y Index: 209

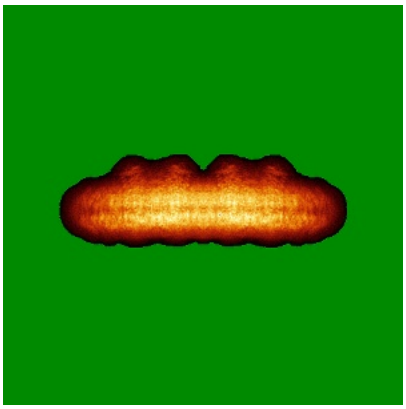


Z Index: 224

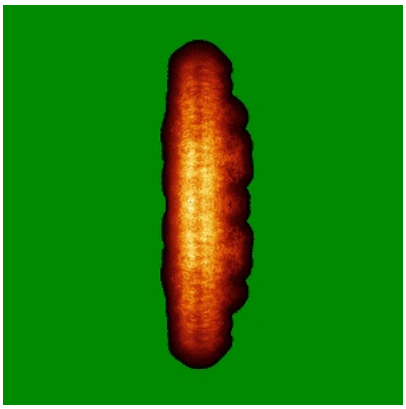
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

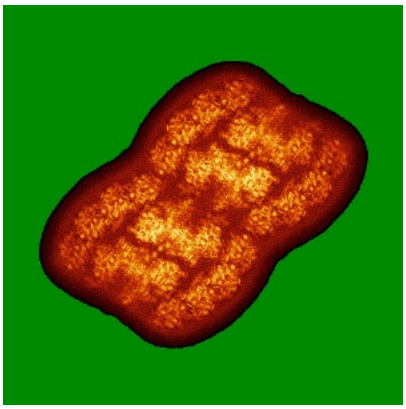
6.4.1 Primary map



X

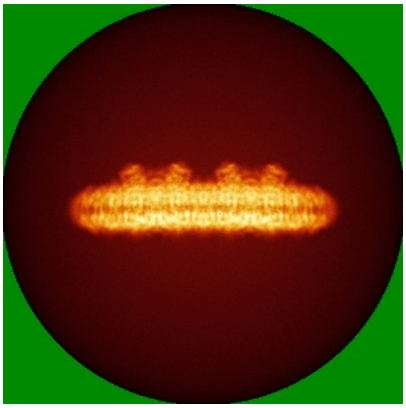


Y

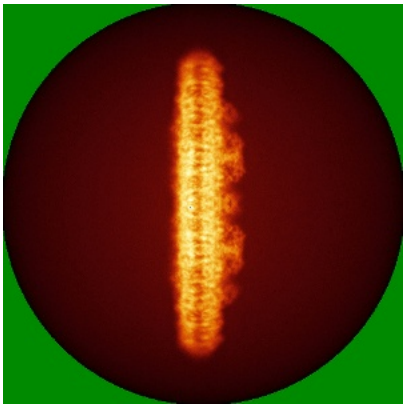


Z

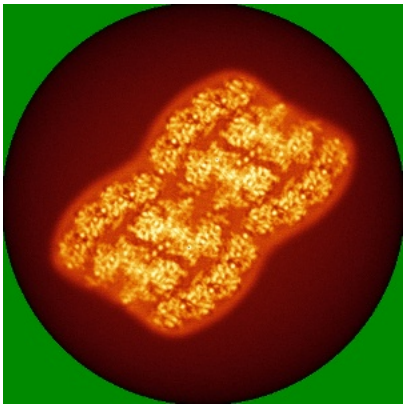
6.4.2 Raw map



X



Y

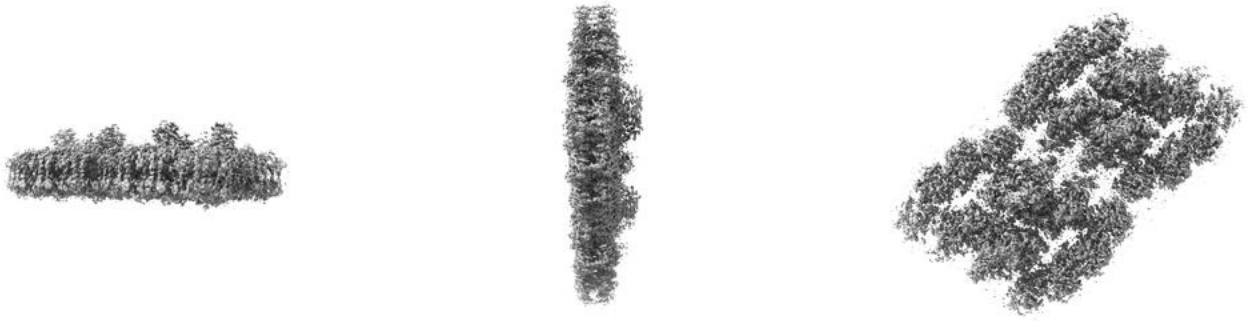


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

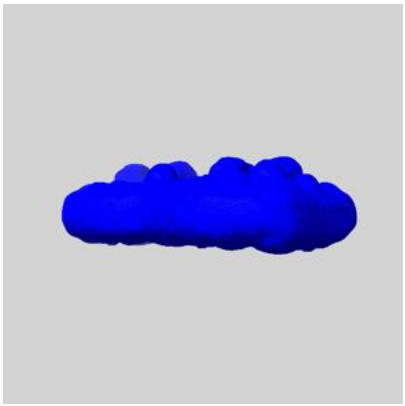
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

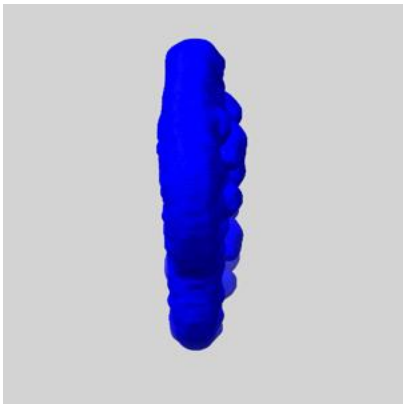
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

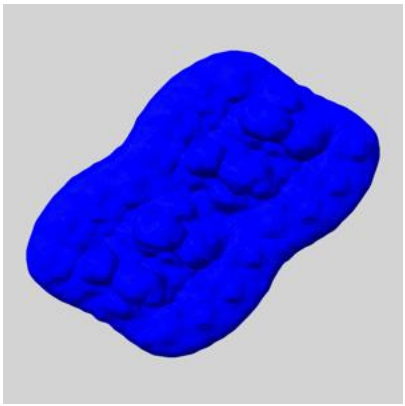
6.6.1 emd_33933_msk_1.map



X



Y

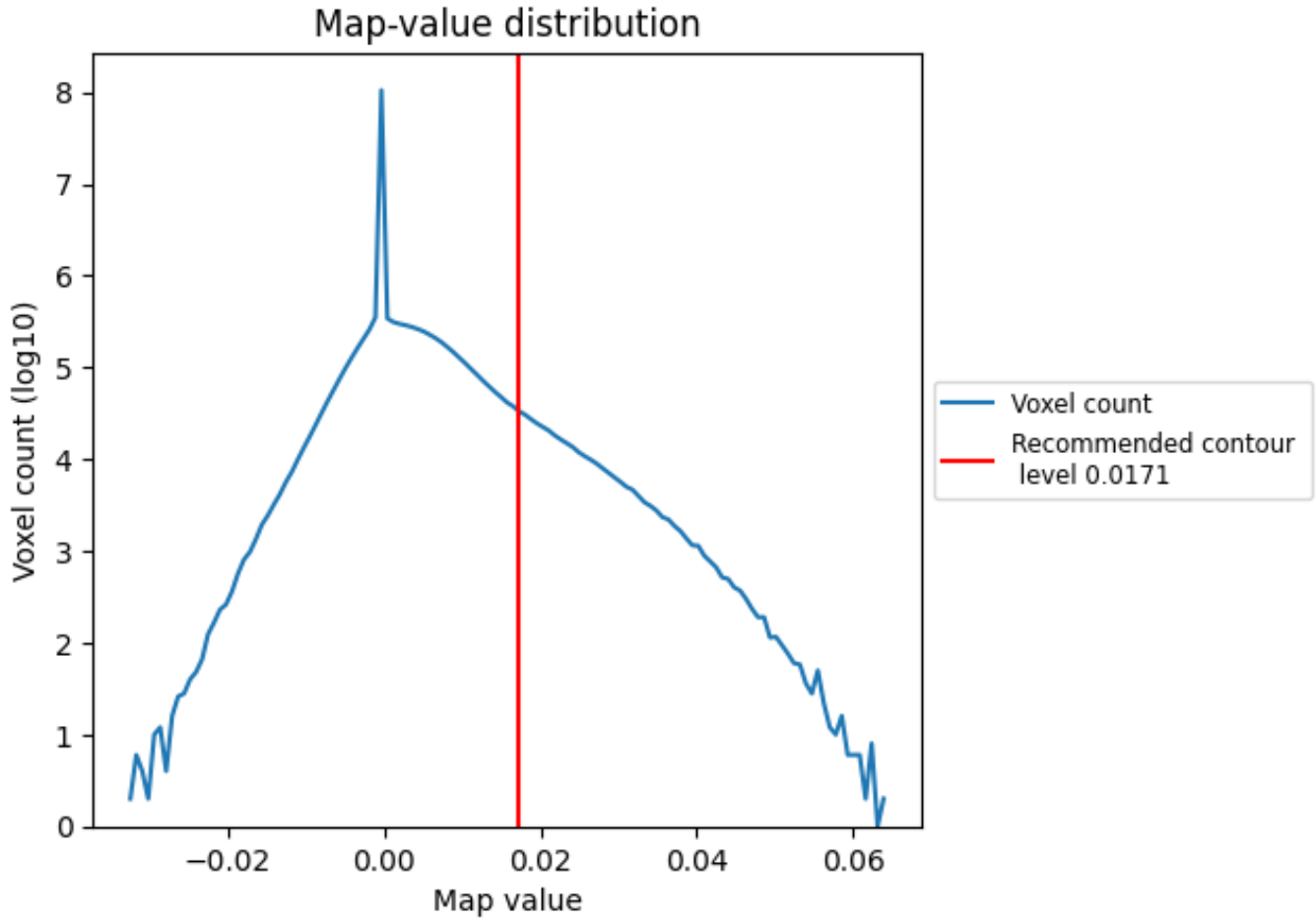


Z

7 Map analysis

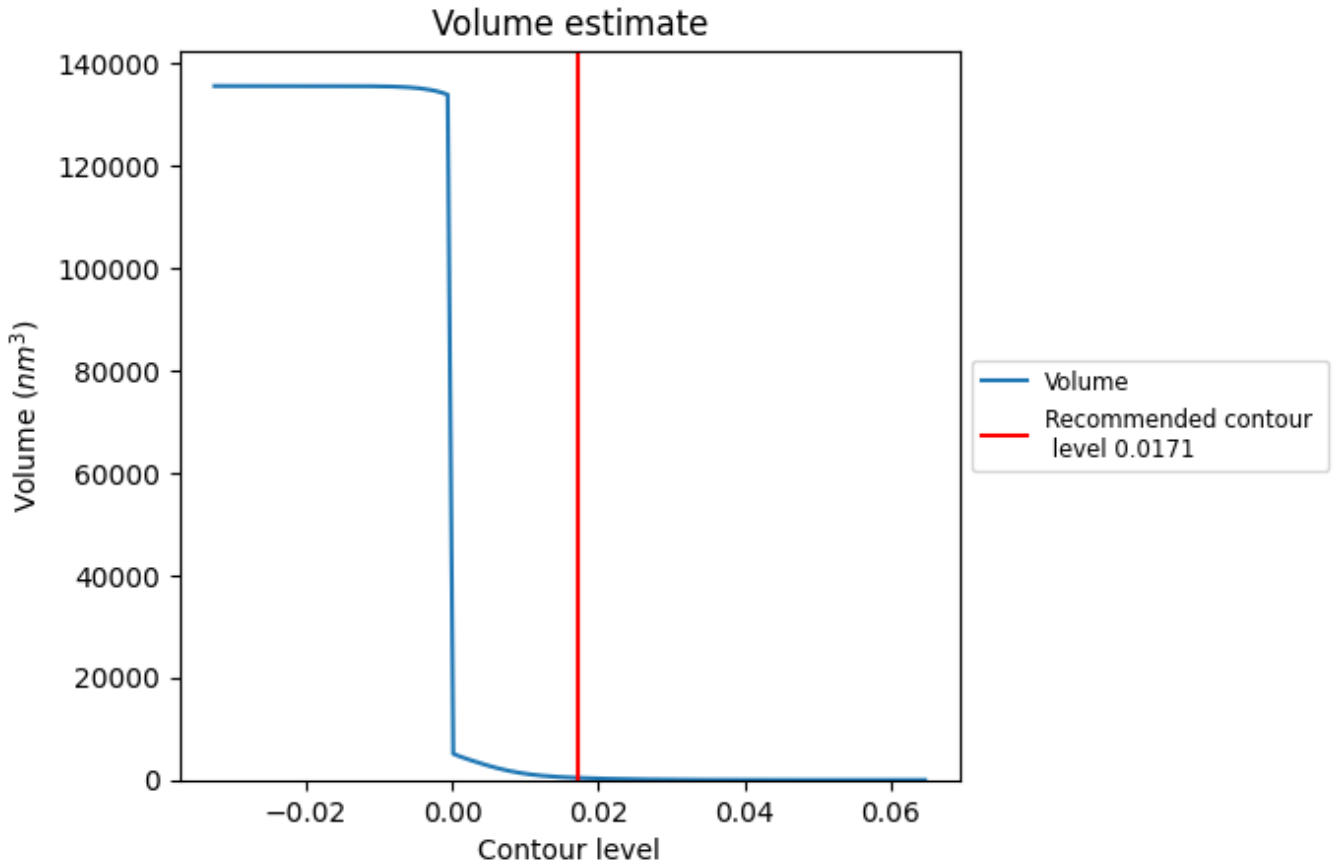
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

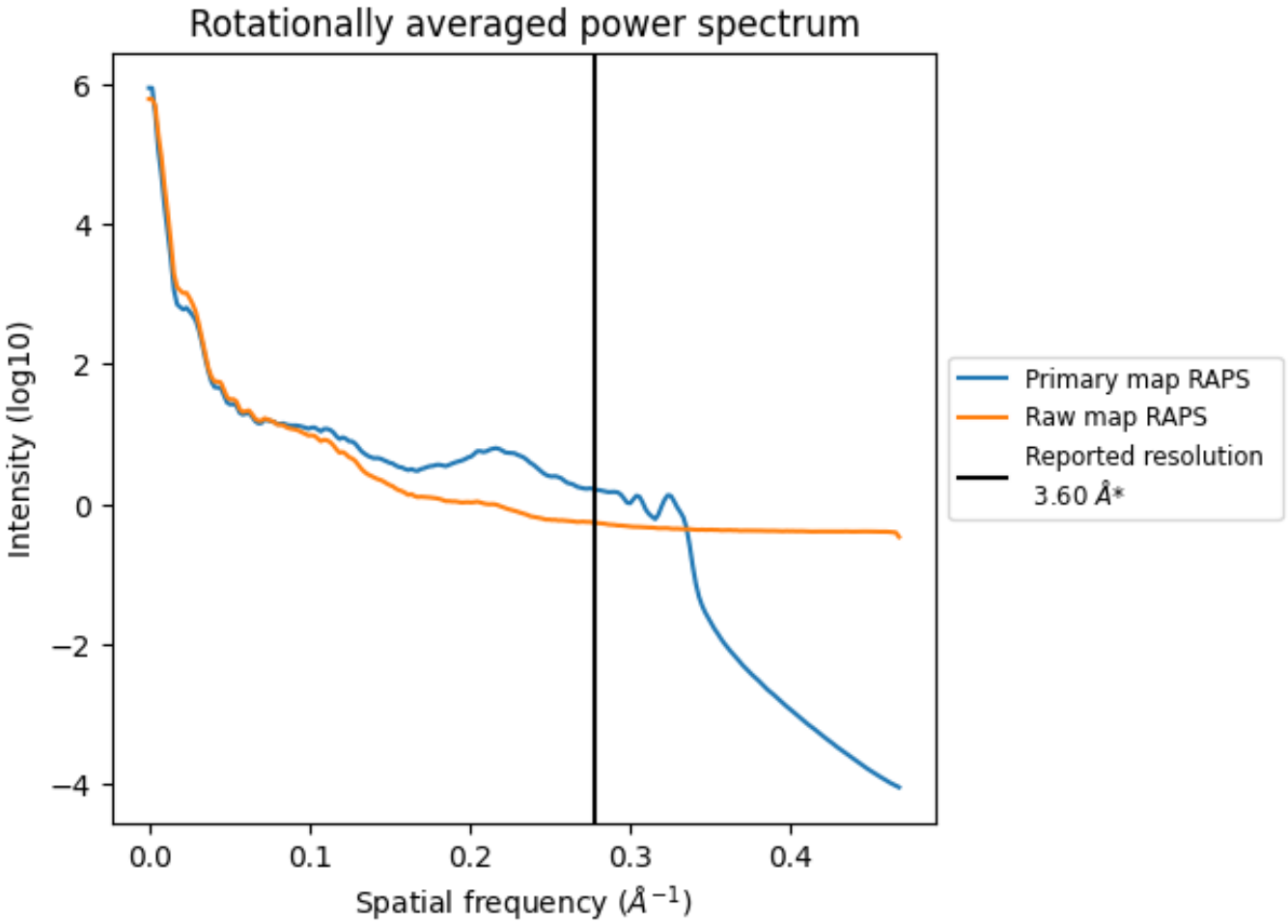
7.2 Volume estimate



The volume at the recommended contour level is 416 nm^3; this corresponds to an approximate mass of 376 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

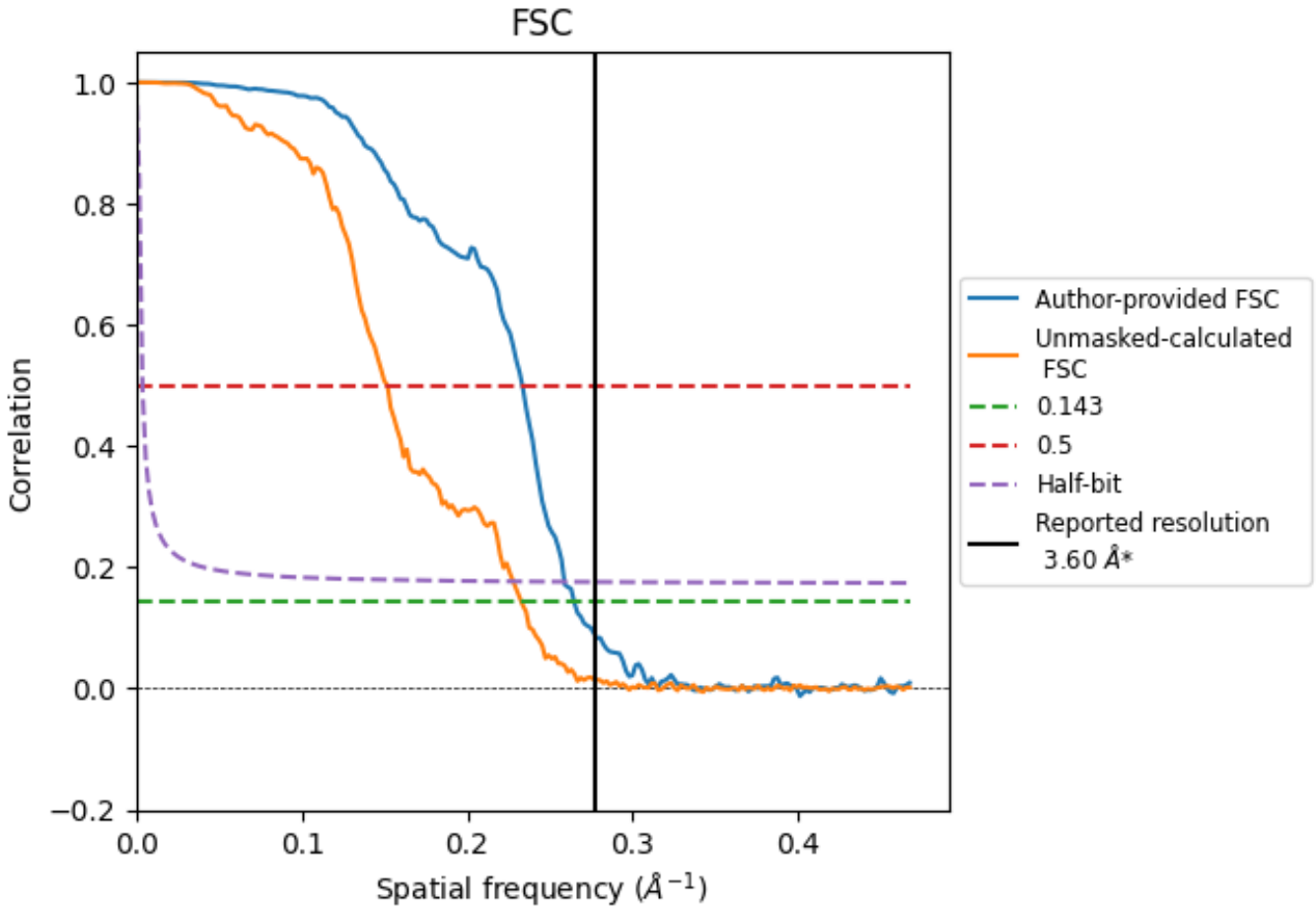


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

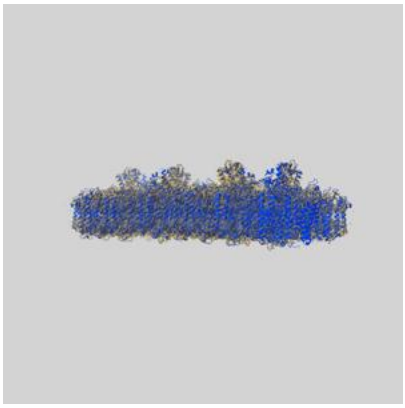
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.78	4.28	3.87
Unmasked-calculated*	4.30	6.59	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.6 by more than 10 %

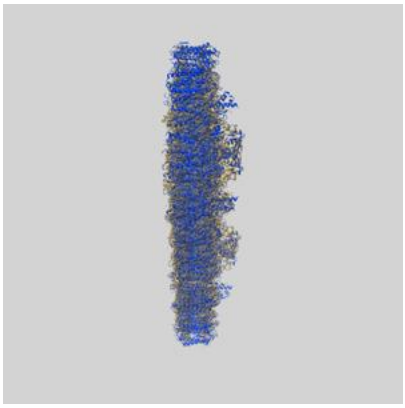
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33933 and PDB model 7YMM. Per-residue inclusion information can be found in section 3 on page 59.

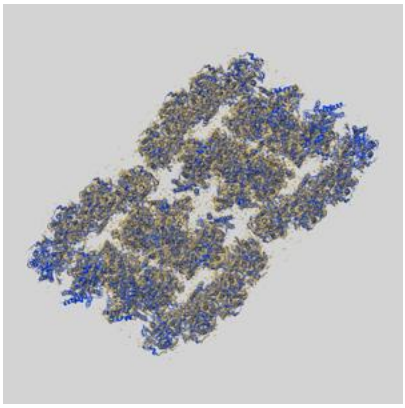
9.1 Map-model overlay



X



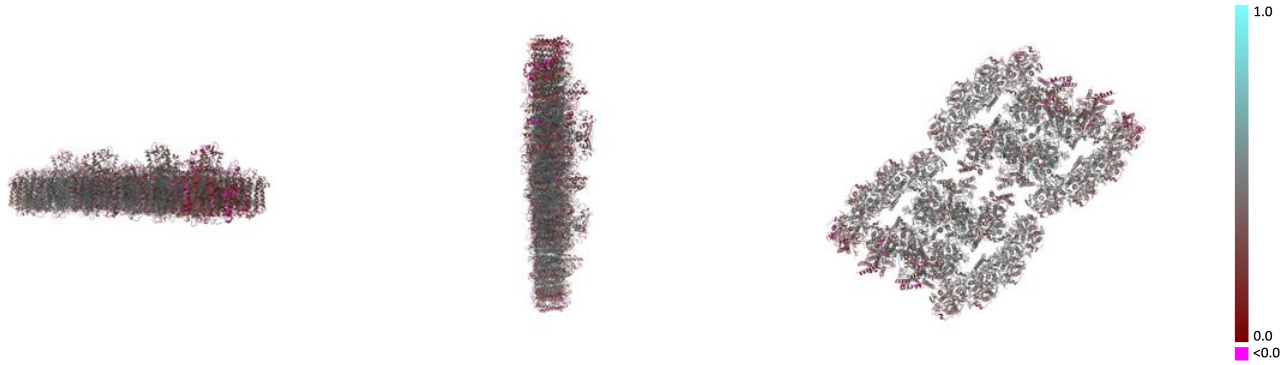
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

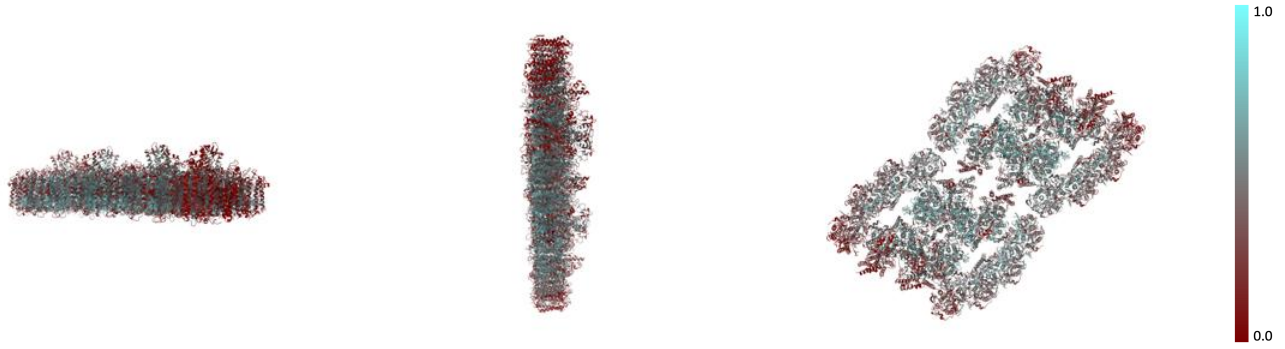
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

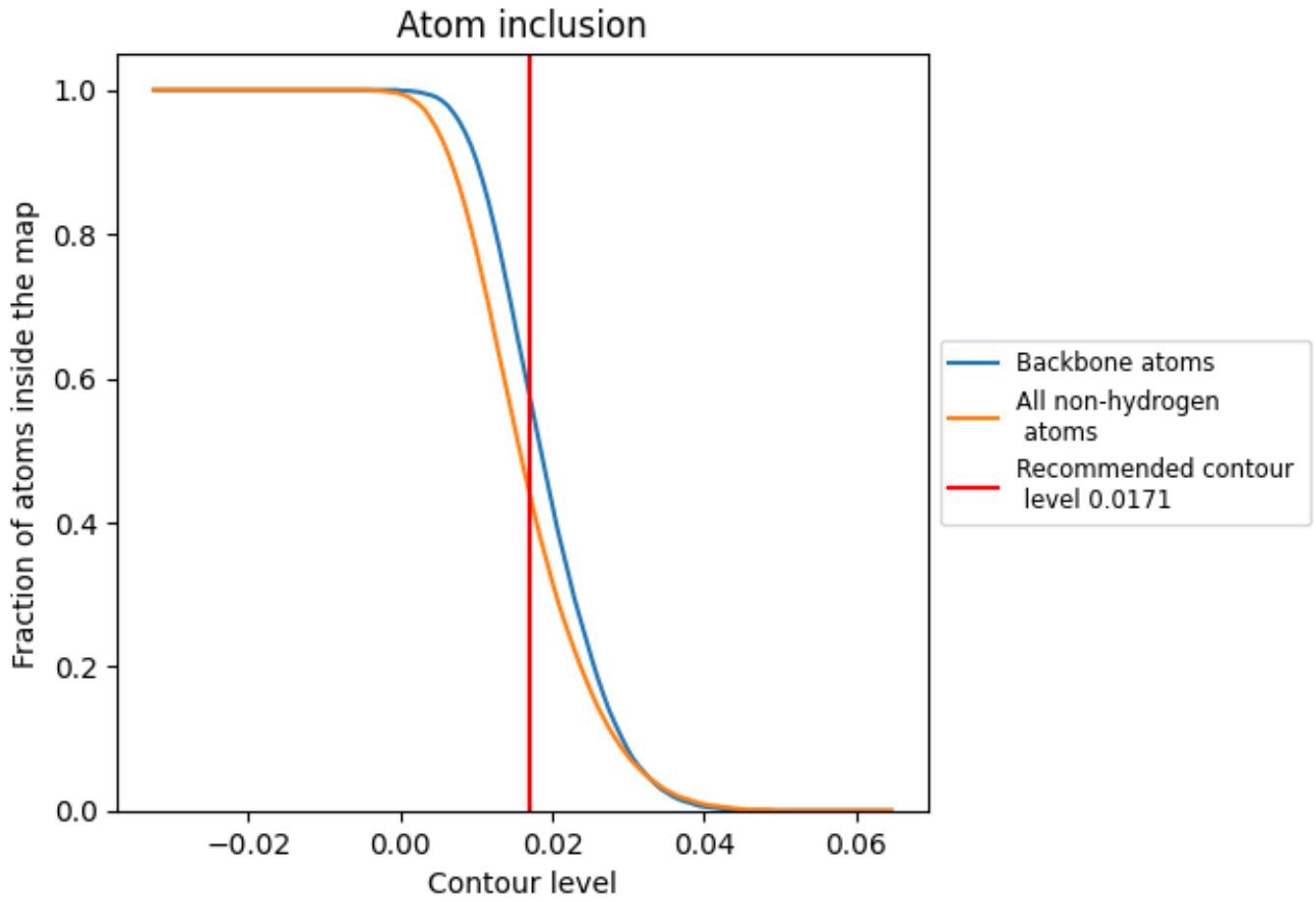
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0171).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4360	0.4150
11	0.1630	0.2740
12	0.3730	0.4020
13	0.4540	0.4310
14	0.2890	0.3650
1A	0.4920	0.4560
1B	0.4770	0.4460
1C	0.3450	0.3770
1D	0.4680	0.4410
1E	0.1260	0.1690
1F	0.1880	0.2640
1G	0.3900	0.3740
1H	0.3600	0.3920
1I	0.4510	0.4530
1K	0.0670	0.2420
1L	0.5750	0.4890
1M	0.4540	0.4280
1T	0.4120	0.4430
1X	0.1080	0.2590
1Y	0.0000	0.1200
1Z	0.0140	0.1310
21	0.4480	0.4060
22	0.4910	0.4500
23	0.4660	0.4370
24	0.4680	0.4210
2A	0.5940	0.4900
2B	0.5820	0.4800
2C	0.5220	0.4400
2D	0.6000	0.4840
2E	0.2790	0.2920
2F	0.4420	0.3740
2G	0.4240	0.4160
2H	0.5190	0.4680
2I	0.5920	0.4840
2K	0.2630	0.3470



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
2L	0.6180	0.5070
2M	0.5020	0.4500
2T	0.4870	0.4680
2X	0.2610	0.3470
2Y	0.1480	0.2450
2Z	0.1690	0.2230
31	0.4470	0.4050
32	0.4920	0.4480
33	0.4660	0.4380
34	0.4680	0.4210
3A	0.5950	0.4900
3B	0.5810	0.4800
3C	0.5230	0.4420
3D	0.5980	0.4840
3E	0.2770	0.2940
3F	0.4420	0.3720
3G	0.4240	0.4120
3H	0.5170	0.4680
3I	0.5960	0.4850
3K	0.2660	0.3490
3L	0.6140	0.5100
3M	0.5020	0.4520
3T	0.4870	0.4660
3X	0.2610	0.3460
3Y	0.1480	0.2410
3Z	0.1690	0.2290
41	0.1630	0.2750
42	0.3730	0.4020
43	0.4550	0.4300
44	0.2900	0.3640
4A	0.4930	0.4570
4B	0.4770	0.4450
4C	0.3460	0.3780
4D	0.4660	0.4410
4E	0.1240	0.1710
4F	0.1880	0.2690
4G	0.3760	0.3820
4H	0.3620	0.3910
4I	0.4440	0.4520
4K	0.0700	0.2420
4L	0.5750	0.4870
4M	0.4540	0.4300

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
4T	0.4120	0.4440
4X	0.1080	0.2570
4Y	0.0000	0.1250
4Z	0.0160	0.1280