Full wwPDB EM Validation Report (i)

Sep 10, 2026 – 04:15 pm BST

PDB ID	:	7BLX / pdb_00007blx
EMDB ID	:	EMD-12227
Title	:	Photosystem I of a temperature sensitive mutant Chlamydomonas reinhardtii
Authors	:	Caspy, I.; Nelson, N.
Deposited on	:	2021-01-19
Resolution	:	3.15 Å(reported)
Based on initial model	:	6JO5

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 (i) 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 (i)) were used in the production of this report:

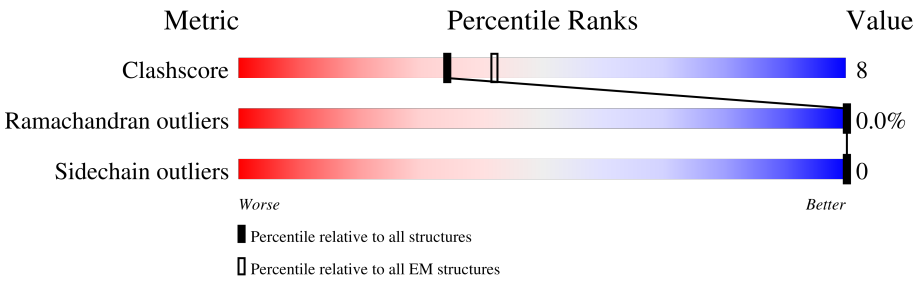
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

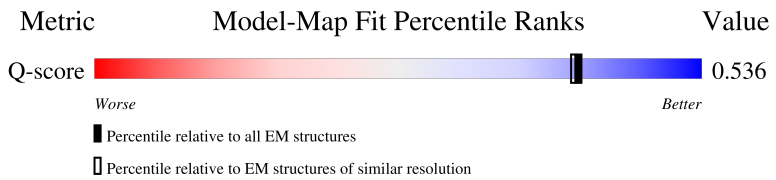
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	14486 (2.65 - 3.65)

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	A	741	17% 86% 14%
2	B	733	21% 86% 14%
3	C	80	21% 92% 8%
4	D	144	47% 95% 5%

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Mol	Chain	Length	Quality of chain
5	E	63	38% 97%
6	F	165	38% 91% 9%
7	G	91	77% 71% 10% 19%
8	I	37	70% 86% 14%
9	J	39	28% 82% 18%
10	K	84	88% 88% 12%
11	L	126	86% 88% 12%
12	1	194	59% 88% 12%
12	Z	194	86% 94% 6%
13	3	219	52% 82% 18%
14	7	213	37% 90% 10%
15	8	217	42% 87% 13%
16	4	210	85% 85% 15%
17	5	227	77% 87% 13%
18	6	229	79% 85% 15%

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
33	RRX	F	4001	X	-	-	-
34	C7Z	1	503	X	-	-	-
34	C7Z	5	505	X	-	-	-
34	C7Z	J	4002	X	-	-	-
37	CHL	1	609	X	-	-	-
37	CHL	3	611	X	-	-	-
37	CHL	4	610	X	-	-	-
37	CHL	4	613	X	-	-	-
37	CHL	5	610	X	-	-	-
37	CHL	6	610	X	-	-	-
37	CHL	6	613	X	-	-	-
37	CHL	8	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	8	613	X	-	-	-
37	CHL	Z	609	X	-	-	-
37	CHL	Z	610	X	-	-	-
39	QTB	Z	504	X	-	-	-

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 47524 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5820	3805	993	1000	22	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5825	3825	977	1005	18	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	601	369	103	117	12	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1135	725	201	202	7	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	497	316	87	94	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1266	817	213	233	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	74	550	354	94	102	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	37	282	195	39	47	1	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	39	321	219	45	56	1	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	84	571	362	98	109	2	0	0

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	126	914	595	148	168	3	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	PRO	deletion	UNP A8IL32
L	?	-	SER	deletion	UNP A8IL32
L	?	-	ILE	deletion	UNP A8IL32
L	?	-	GLY	deletion	UNP A8IL32
L	?	-	VAL	deletion	UNP A8IL32
L	?	-	LYS	deletion	UNP A8IL32
L	?	-	THR	deletion	UNP A8IL32
L	?	-	LEU	deletion	UNP A8IL32
L	?	-	SER	deletion	UNP A8IL32
L	?	-	GLY	deletion	UNP A8IL32
L	?	-	ARG	deletion	UNP A8IL32

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	SER	deletion	UNP A8IL32

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1	194	1445	941	240	261	3	0	0
12	Z	194	1445	941	240	261	3	0	0

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	3	219	1674	1092	270	304	8	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	7	213	1650	1072	274	298	6	0	0

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	8	217	1650	1073	280	293	4	0	0

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	4	210	1628	1068	262	293	5	0	0

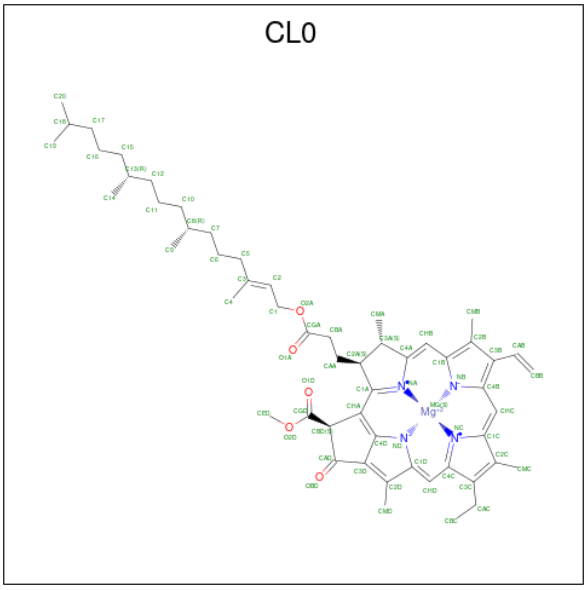
- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5	227	1775	1154	297	316	8	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

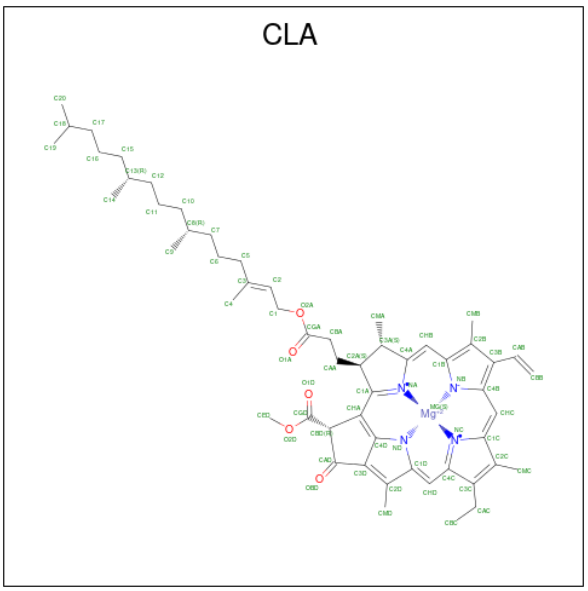
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	6	229	1766	1164	292	304	6	0	0

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	A	1	65	55	1	4	5	0

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
20	A	1	55	45	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	60	50	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	61	51	1	4	5	0
20	A	1	60	50	1	4	5	0
20	A	1	60	50	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	60	50	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	55	45	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	56	46	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
20	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
20	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	G	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
20	K	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	K	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
20	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	Z	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	3	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
20	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
20	7	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
20	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	4	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	4	1	60	50	1	4	5	0
20	5	1	60	50	1	4	5	0
20	5	1	61	51	1	4	5	0
20	5	1	56	46	1	4	5	0
20	5	1	65	55	1	4	5	0
20	5	1	55	45	1	4	5	0
20	5	1	50	40	1	4	5	0
20	5	1	61	51	1	4	5	0
20	5	1	45	35	1	4	5	0
20	5	1	65	55	1	4	5	0
20	5	1	65	55	1	4	5	0
20	5	1	55	45	1	4	5	0
20	5	1	50	40	1	4	5	0
20	5	1	65	55	1	4	5	0
20	5	1	46	36	1	4	5	0
20	6	1	55	45	1	4	5	0
20	6	1	65	55	1	4	5	0
20	6	1	60	50	1	4	5	0
20	6	1	52	42	1	4	5	0
20	6	1	65	55	1	4	5	0
20	6	1	65	55	1	4	5	0

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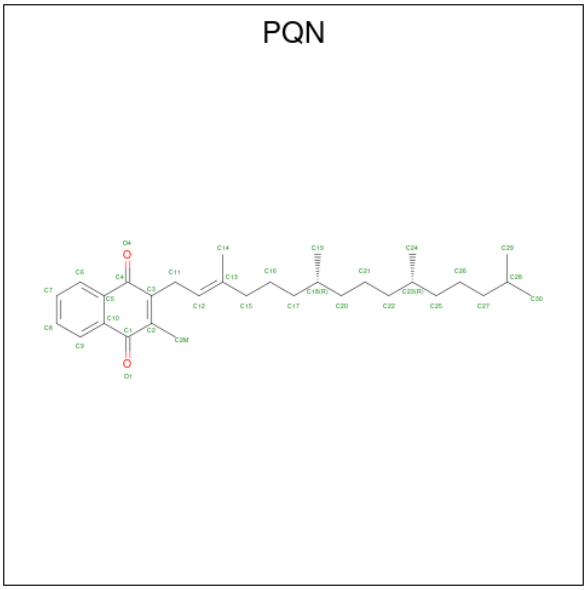
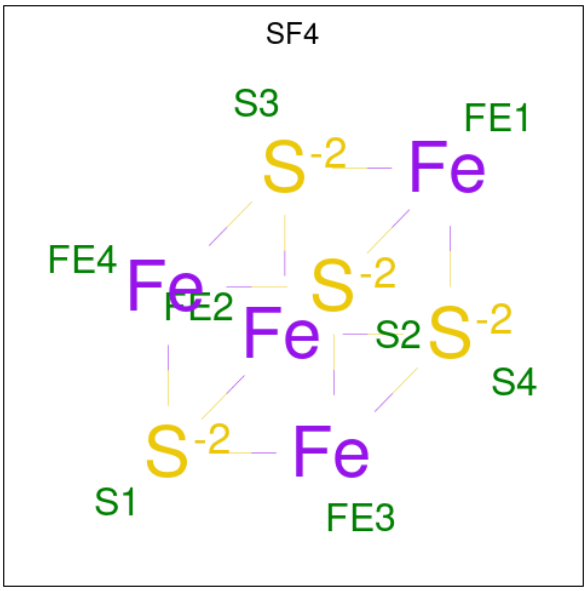
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
20	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
20	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
20	6	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
20	6	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
20	6	1	65	55	1	4	5	0

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



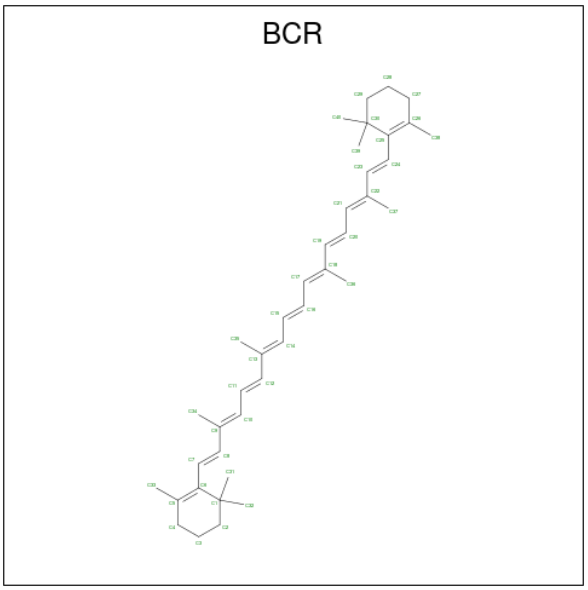
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	A	1	33	31	2	0
			Total	C	O	
21	B	1	33	31	2	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	A	1	8	4	4	0
22	C	1	8	4	4	0
22	C	1	8	4	4	0

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
23	A	1	40	40	0
			Total	C	
23	A	1	40	40	0
			Total	C	
23	A	1	40	40	0
			Total	C	
23	A	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	B	1	40	40	0
			Total	C	
23	G	1	40	40	0
			Total	C	
23	I	1	40	40	0
			Total	C	
23	J	1	40	40	0
			Total	C	
23	K	1	40	40	0
			Total	C	
23	K	1	40	40	0
			Total	C	
23	L	1	40	40	0
			Total	C	
23	L	1	40	40	0
			Total	C	
23	3	1	40	40	0
			Total	C	
23	3	1	40	40	0
			Total	C	
23	3	1	40	40	0

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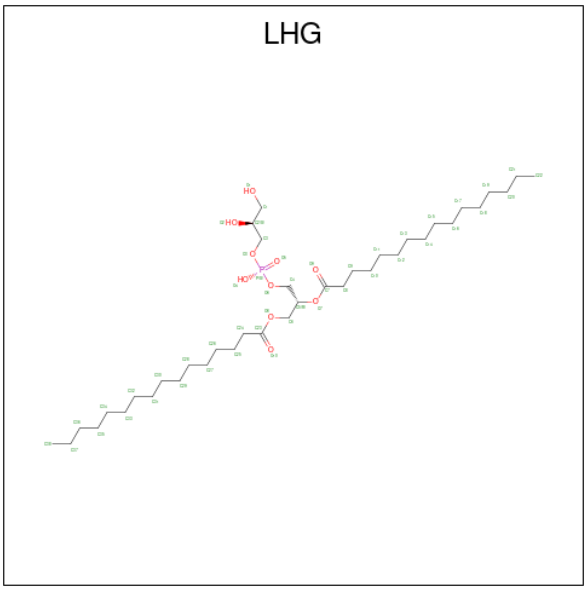
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
23	3	1	40	40	0
			Total	C	
23	7	1	40	40	0
			Total	C	
23	7	1	40	40	0
			Total	C	
23	8	1	40	40	0
			Total	C	
23	4	1	40	40	0
			Total	C	
23	5	1	40	40	0
			Total	C	
23	5	1	40	40	0
			Total	C	
23	6	1	40	40	0
			Total	C	
23	6	1	40	40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
24	A	1	35	24	10	1	0
			Total	C	O	P	
24	A	1	49	38	10	1	0

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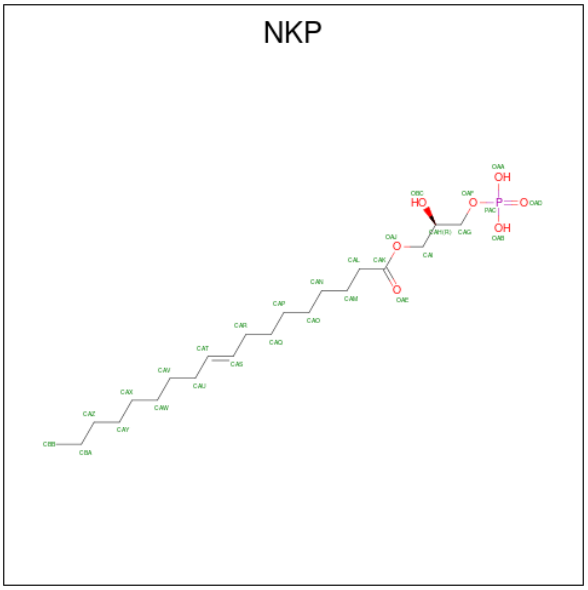
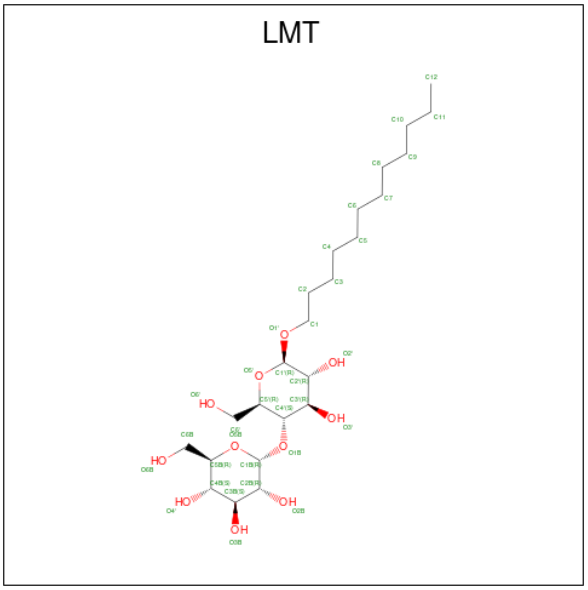
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
24	B	1	23	12	10	1	0
			Total	C	O	P	
24	B	1	20	9	10	1	0
			Total	C	O	P	
24	B	1	33	22	10	1	0
			Total	C	O	P	
24	1	1	43	32	10	1	0
			Total	C	O	P	
24	Z	1	43	32	10	1	0
			Total	C	O	P	
24	3	1	20	9	10	1	0
			Total	C	O	P	
24	7	1	37	26	10	1	0
			Total	C	O	P	
24	8	1	38	27	10	1	0
			Total	C	O	P	
24	4	1	49	38	10	1	0
			Total	C	O	P	
24	4	1	32	21	10	1	0
			Total	C	O	P	
24	5	1	37	26	10	1	0
			Total	C	O	P	
24	6	1	49	38	10	1	0

- Molecule 25 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: $C_{21}H_{41}O_7P$).



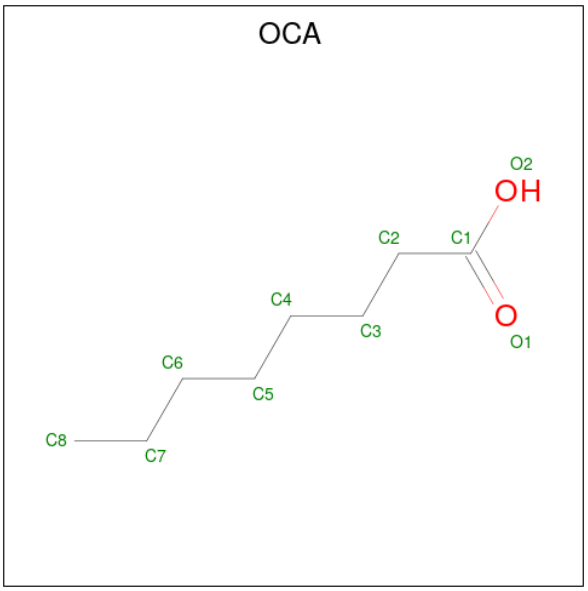
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			29	21	7	1	
25	3	1	Total	C	O	P	0
			16	8	7	1	
25	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



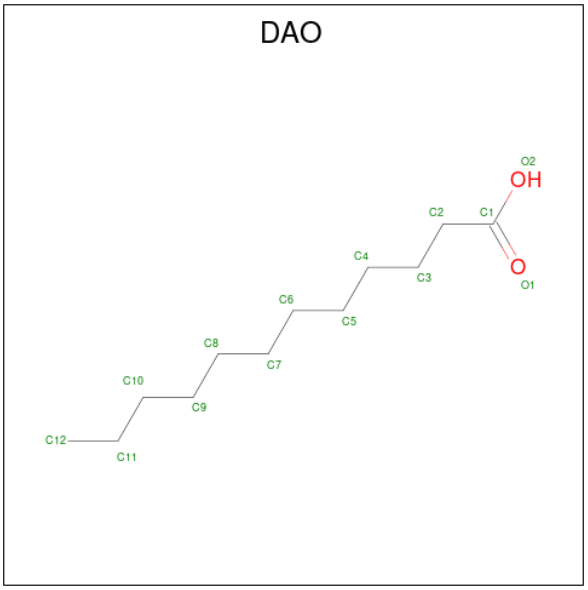
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	
26	B	1	Total	C	O	0
			35	24	11	
26	B	1	Total	C	O	0
			35	24	11	
26	F	1	Total	C	O	0
			35	24	11	
26	1	1	Total	C	O	0
			35	24	11	
26	8	1	Total	C	O	0
			35	24	11	
26	4	1	Total	C	O	0
			35	24	11	

- Molecule 27 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



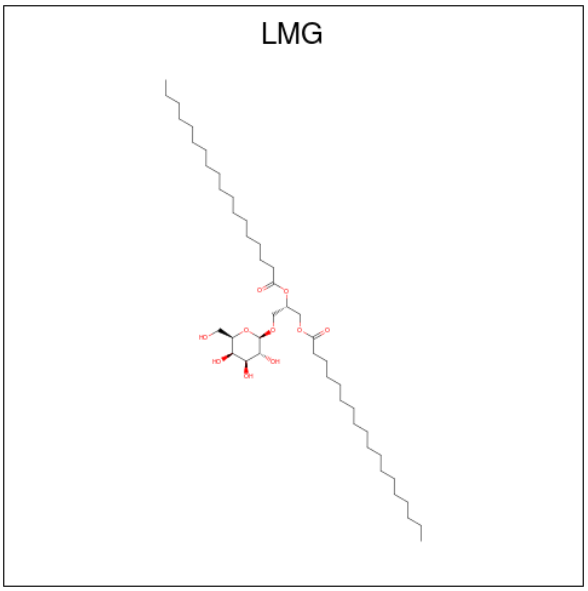
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	A	1	10	8	2	0

- Molecule 28 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



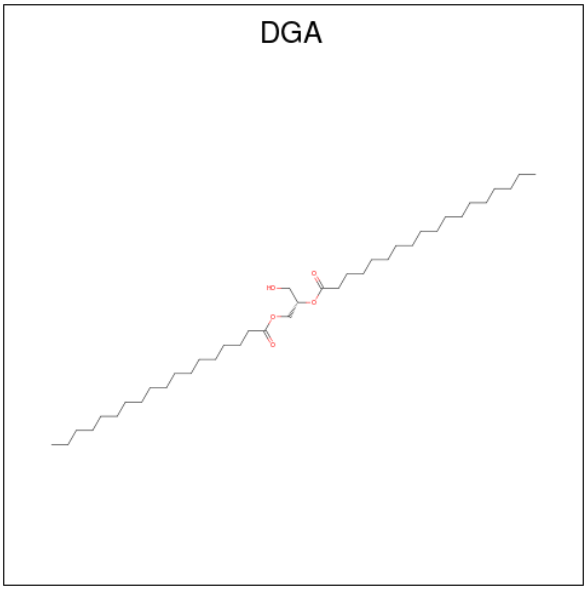
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	A	1	14	12	2	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	29	19	10	0
			Total	C	O	
29	J	1	35	25	10	0

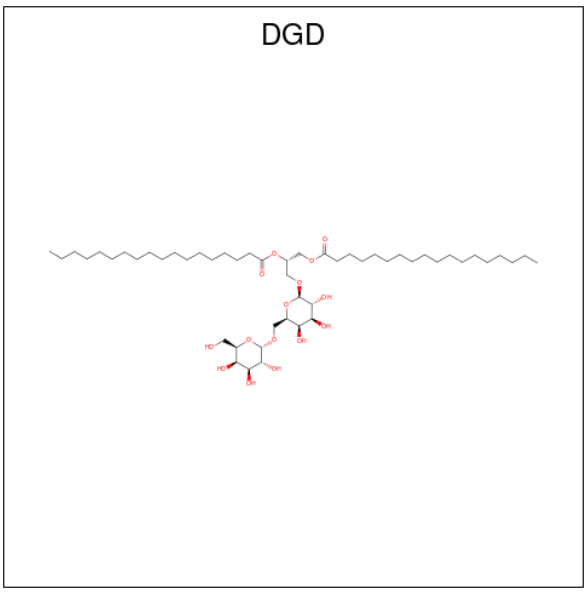
- Molecule 30 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	A	1	44	39	5	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

$C_{51}H_{96}O_{15}$).

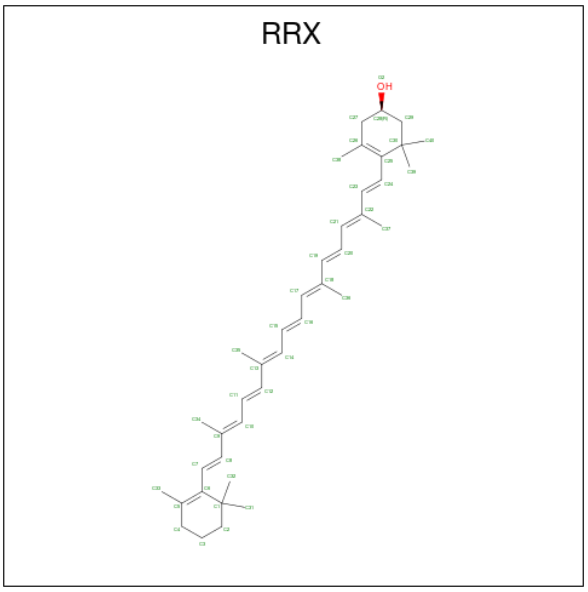


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	B	1	66	51	15	0

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

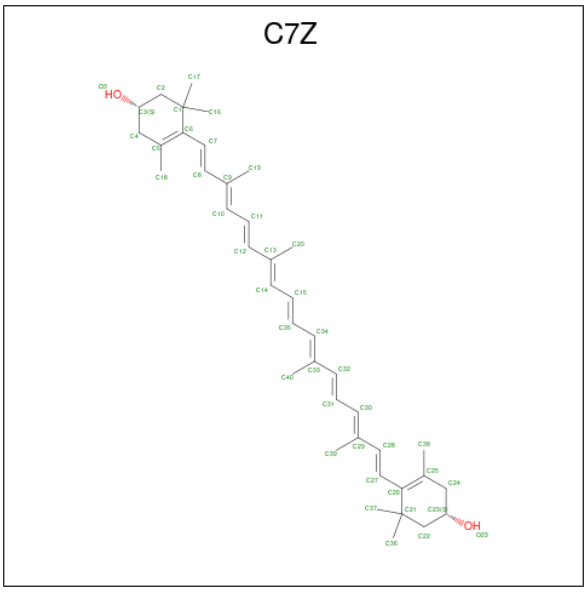
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
32	B	1	1	1	0

- Molecule 33 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



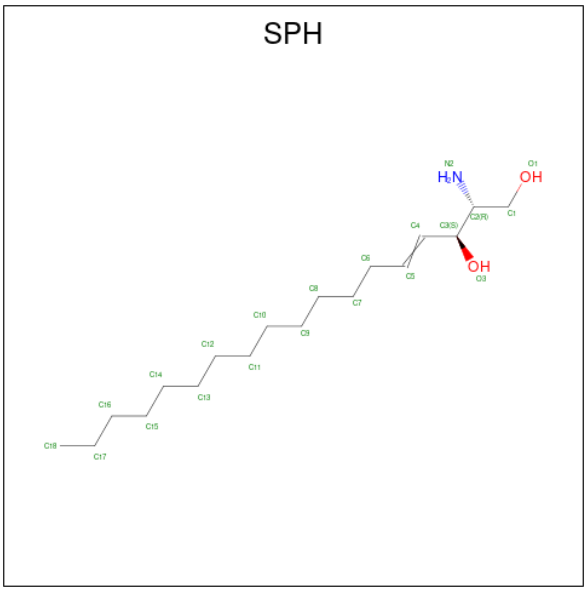
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	F	1	41	40	1	0

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



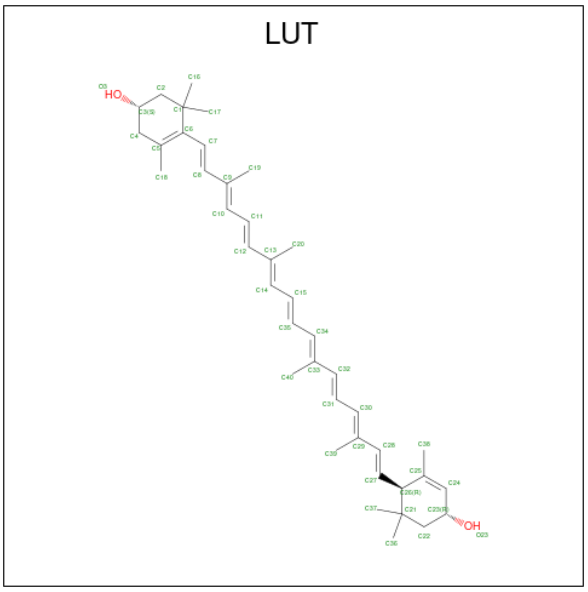
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	J	1	42	40	2	0
			Total	C	O	
34	1	1	42	40	2	0
			Total	C	O	
34	5	1	42	40	2	0

- Molecule 35 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



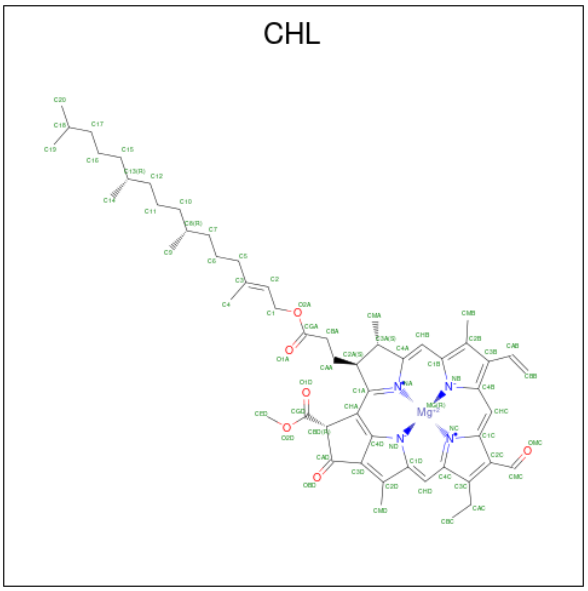
Mol	Chain	Residues	Atoms				AltConf
35	K	1	Total	C	N	O	0
			21	18	1	2	
35	7	1	Total	C	N	O	0
			21	18	1	2	
35	7	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	1	1	42	40	2	0
			Total	C	O	
36	1	1	42	40	2	0
			Total	C	O	
36	Z	1	42	40	2	0
			Total	C	O	
36	Z	1	42	40	2	0
			Total	C	O	
36	Z	1	42	40	2	0
			Total	C	O	
36	3	1	42	40	2	0
			Total	C	O	
36	3	1	42	40	2	0
			Total	C	O	
36	7	1	42	40	2	0
			Total	C	O	
36	7	1	42	40	2	0
			Total	C	O	
36	8	1	42	40	2	0
			Total	C	O	
36	8	1	42	40	2	0
			Total	C	O	
36	4	1	42	40	2	0
			Total	C	O	
36	4	1	42	40	2	0
			Total	C	O	
36	5	1	42	40	2	0
			Total	C	O	
36	5	1	42	40	2	0
			Total	C	O	
36	6	1	42	40	2	0
			Total	C	O	
36	6	1	42	40	2	0

- Molecule 37 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	1	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
37	1	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
37	Z	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
37	Z	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
37	Z	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
37	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
37	7	1	54	43	1	4	6	0
			Total	C	Mg	N	O	
37	8	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
37	8	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
37	4	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
37	4	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
37	4	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
37	4	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
37	5	1	66	55	1	4	6	0

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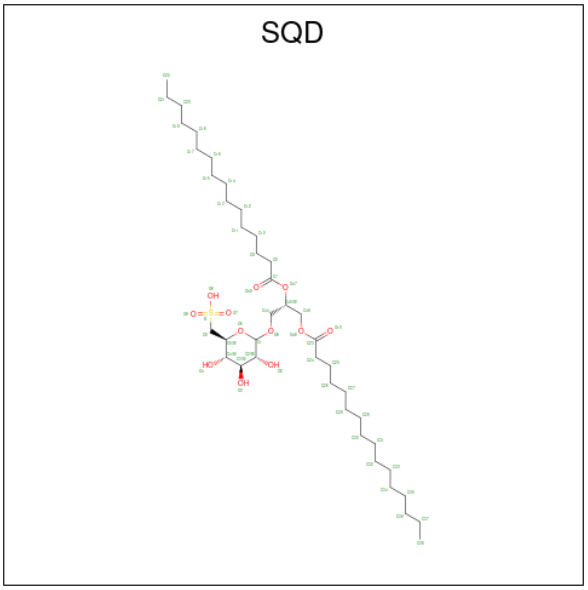
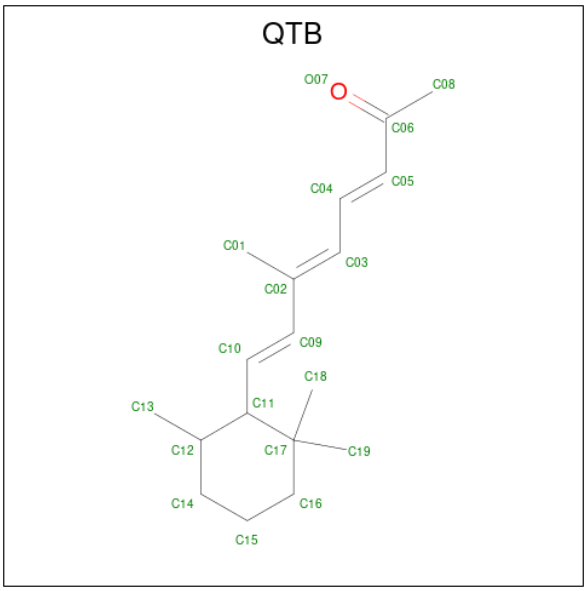
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
37	5	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
37	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
37	6	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
37	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
37	6	1	43	34	1	4	4	0

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



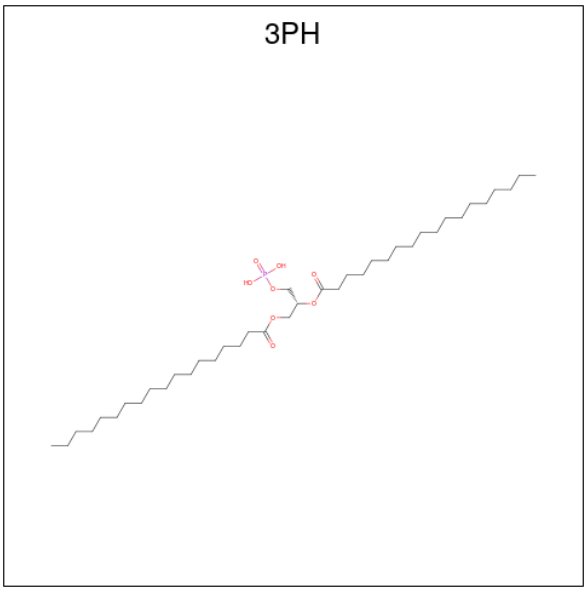
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	1	1	48	35	12	1	0

- Molecule 39 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: $C_{18}H_{28}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	Z	1	19	18	1	0

- Molecule 40 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	7	1	39	30	8	1	0
			Total	C	O	P	
40	8	1	30	21	8	1	0

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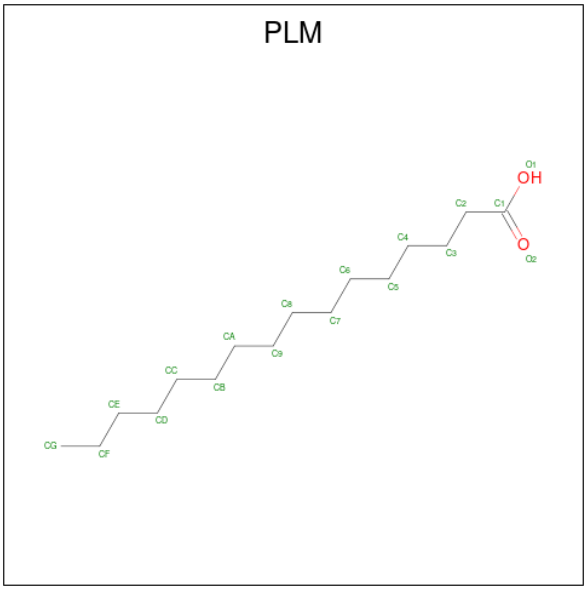
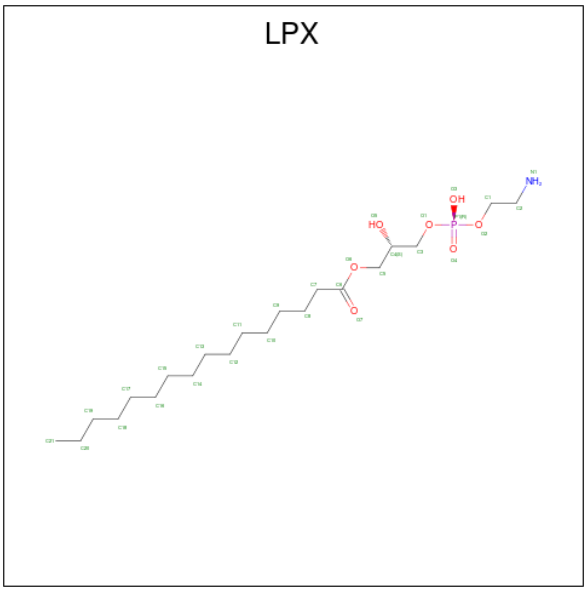
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	5	1	23	14	8	1	0
			Total	C	O	P	
40	6	1	29	20	8	1	0

- Molecule 41 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	7	1	18	16	2	0

- Molecule 42 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
42	8	1	Total 30	C 21	N 1	O 7	P 1	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	A	3	Total 3	O 3	0
43	A	10	Total 10	O 10	0
43	A	17	Total 17	O 17	0
43	A	7	Total 7	O 7	0
43	A	6	Total 6	O 6	0
43	A	3	Total 3	O 3	0
43	A	5	Total 5	O 5	0
43	A	14	Total 14	O 14	0
43	A	3	Total 3	O 3	0
43	A	16	Total 16	O 16	0
43	A	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	A	1	1	1	0
43	A	1	1	1	0
43	A	1	1	1	0
43	A	1	1	1	0
43	A	1	1	1	0
43	A	1	1	1	0
43	B	2	2	2	0
43	B	1	1	1	0
43	B	1	1	1	0
43	B	1	1	1	0
43	B	5	5	5	0
43	B	15	15	15	0
43	B	4	4	4	0
43	B	12	12	12	0
43	B	18	18	18	0
43	B	2	2	2	0
43	B	15	15	15	0
43	B	3	3	3	0
43	C	1	1	1	0
43	C	1	1	1	0
43	C	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	C	1	1	1	0
43	C	2	2	2	0
43	C	8	8	8	0
43	C	1	1	1	0
43	C	1	1	1	0
43	C	1	1	1	0
43	C	1	1	1	0
43	C	1	1	1	0
43	D	1	1	1	0
43	D	1	1	1	0
43	D	1	1	1	0
43	D	1	1	1	0
43	D	1	1	1	0
43	D	1	1	1	0
43	D	1	1	1	0
43	D	2	2	2	0
43	D	2	2	2	0
43	D	1	1	1	0
43	E	1	1	1	0
43	E	1	1	1	0
43	E	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	E	4	4	4	0
			Total	O	
43	F	1	1	1	0
			Total	O	
43	F	1	1	1	0
			Total	O	
43	F	1	1	1	0
			Total	O	
43	F	3	3	3	0
			Total	O	
43	F	6	6	6	0
			Total	O	
43	F	1	1	1	0
			Total	O	
43	F	1	1	1	0
			Total	O	
43	J	1	1	1	0
			Total	O	
43	J	2	2	2	0
			Total	O	
43	K	1	1	1	0
			Total	O	
43	K	1	1	1	0
			Total	O	
43	L	1	1	1	0
			Total	O	
43	L	4	4	4	0
			Total	O	
43	1	15	15	15	0
			Total	O	
43	1	1	1	1	0
			Total	O	
43	Z	8	8	8	0
			Total	O	
43	3	16	16	16	0
			Total	O	
43	3	1	1	1	0
			Total	O	
43	7	18	18	18	0
			Total	O	
43	8	1	1	1	0

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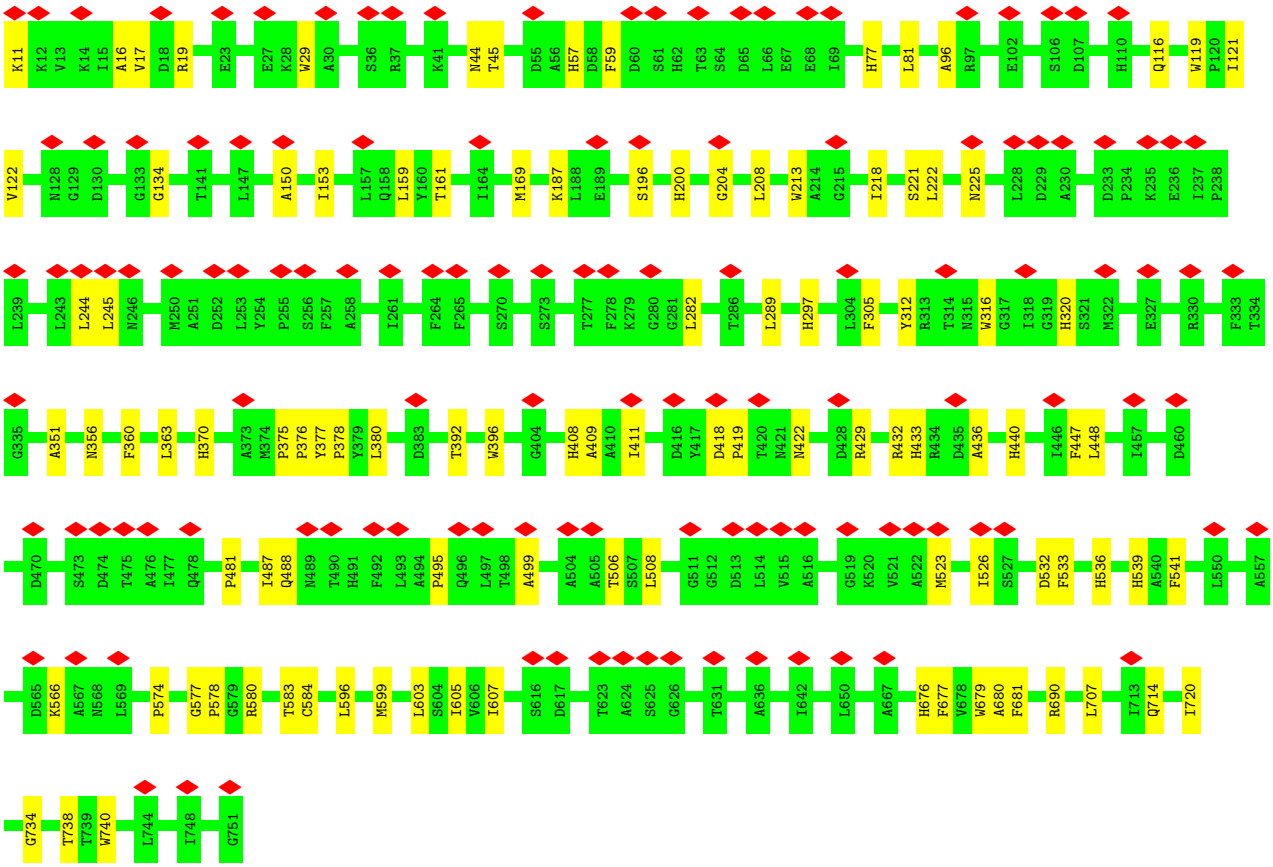
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
43	8	15	15	15	0
			Total	O	
43	4	7	7	7	0
			Total	O	
43	5	9	9	9	0
			Total	O	
43	6	8	8	8	0

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.

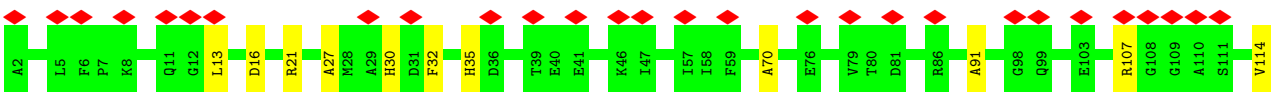
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

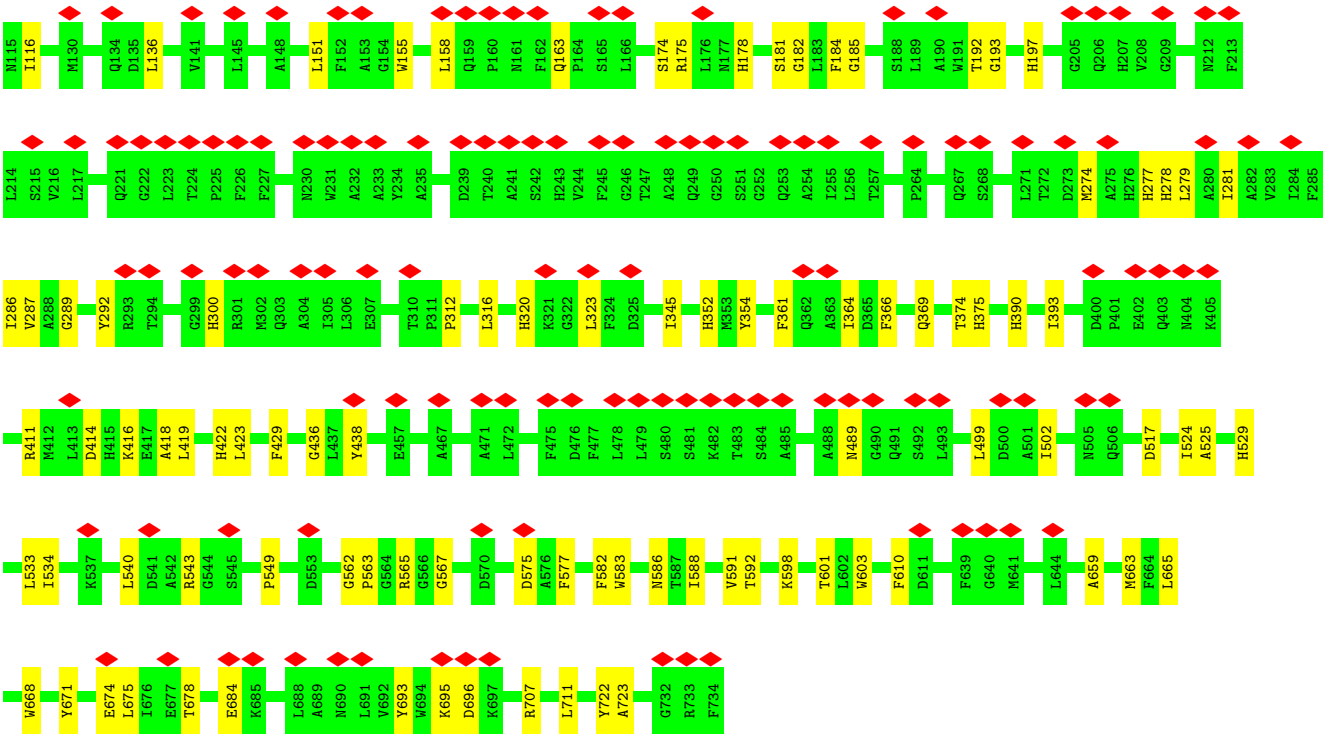
Chain A: 17% 86% 14%



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

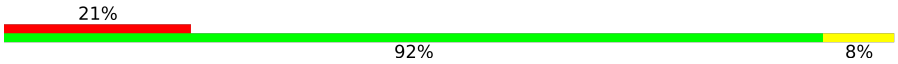
Chain B: 21% 86% 14%

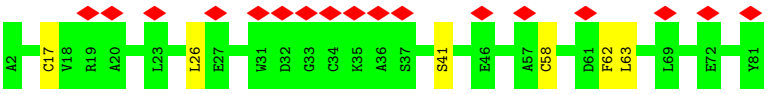




- Molecule 3: Photosystem I iron-sulfur center

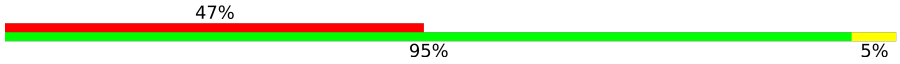
Chain C:

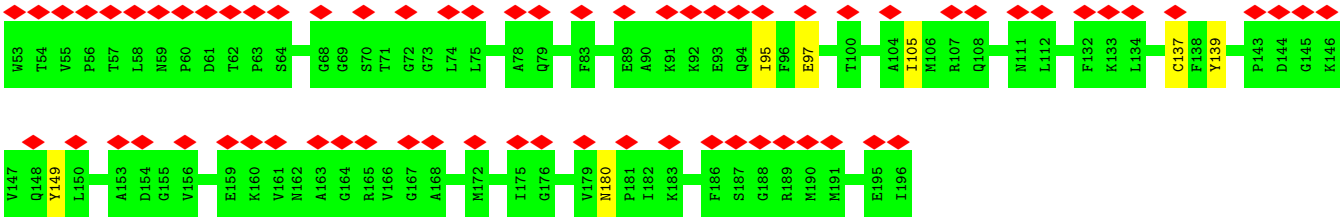




- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

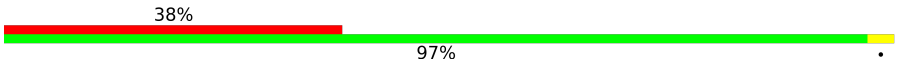
Chain D:

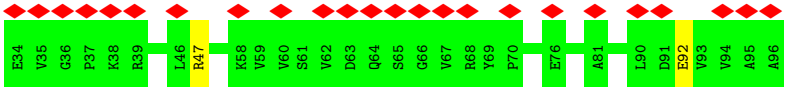




- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

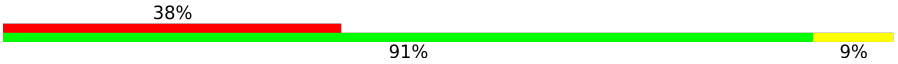
Chain E:

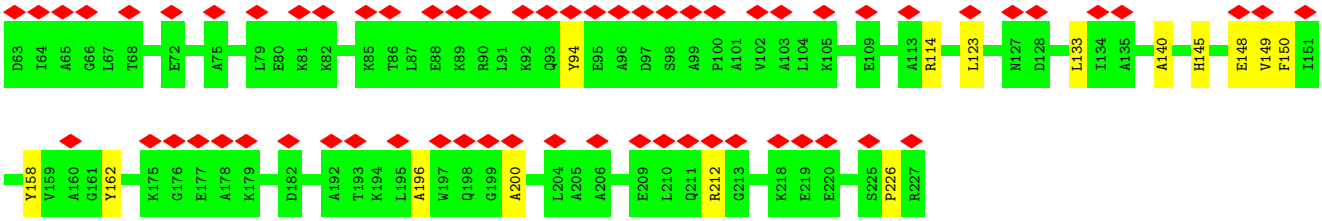




- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

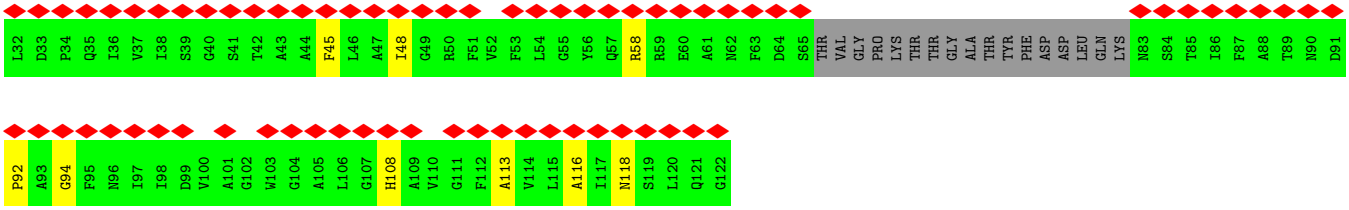
Chain F:





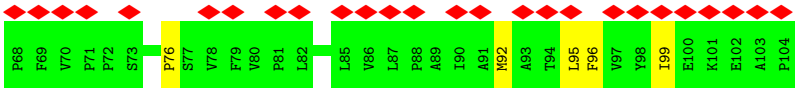
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



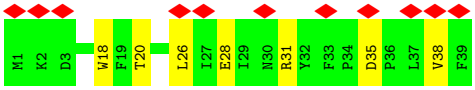
- Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



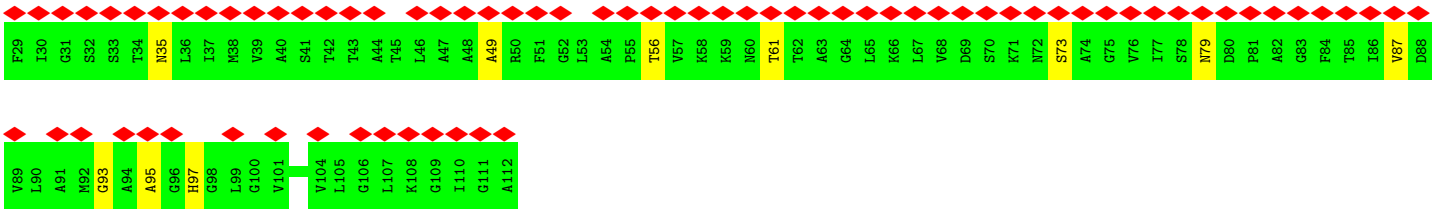
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:



- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



- Molecule 11: PSI subunit V

Chain L:

G53 M54 L55 E56 T57 P58 V59 T60 S61 A62 P63 I64 V65 A66 T67 Y68 L69 S70 N71 L72 P73 A74 Y75 R76 T77 G78 V79 A80 P81 V82 L83 R84 G85 V86 E87 I88 G89 L90 A91 H92 G93 F94 L95 L96 A97 F100 I101 K102 L103 G104 P105 L106 R107 N108 V109 P110 E111 T112 A113

E114 I115 A116 G117 S118 L119 S120 A121 A122 G123 L124 V125 L126 I127 L128 A129 L130 C131 L132 S133 I134 Y135 G136 S137 A138 Q139 F140 Q141 S142 T143 V156 A157 R158 D159 P160 L161 F162 S163 A164 D165 S168 E169 F170 A171 A172 G173 F174 L175 V176 G177 G178 E179 A180 G181 V182 A183 W184 A185 Y186

V187 C188 T189 Q190

- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

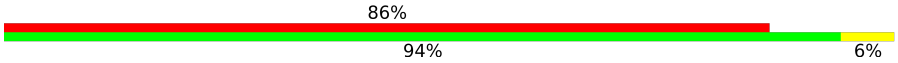
K31 A32 L36 S39 D40 A41 L45 P46 D47 D48 L49 P50 G51 N52 F55 L58 S59 E63 P64 A65 S66 L67 T71 E72 I76 H77 G78 R79 W80 A81 M82 V85 L89 A90 V91 E92 L93 L94 G95 Y96 G97 N98 D101 A102 P103 L104 W105 A106 V107

N108 G109 G110 K111 A112 T113 W114 F115 G116 I117 E118 V119 P120 F121 D122 L123 N124 A125 L126 L127 A128 F129 E130 F131 V132 A133 M134 A135 A136 A137 E138 G139 Q140 R141 G142 D143 A144 G145 G146 V147 V148 Y149 P150 A153 F154 D155 P156 L157 G158 F159 A160 K161 D162 S163 S164 K165 S166 G167 E168

L169 K170 L171 K172 E173 R178 L179 A180 M181 V182 A183 G186 A189 A193 K196 G197 P198 I199 A200 A201 L202 G203 E204 H205 L206 A207 N208 P209 W210 G211 A212 T216 N217 G218 I219 P222 F223 F224

- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:



K31 A32 G33 N34 W35 L36 P37 G38 S39 D40 A41 P42 A43 W44 L45 P46 D47 D48 L49 P50 G51 N52 Y53 G54 F55 S59 L60 G61 K62 E63 P64 A65 S66 L67 K68 R69 F70 T71 E72 I76 R79 W80 A81 M82 L83 G84 V85 A86 G87 S88 L89 A90 V91 E92 L93 L94 G95

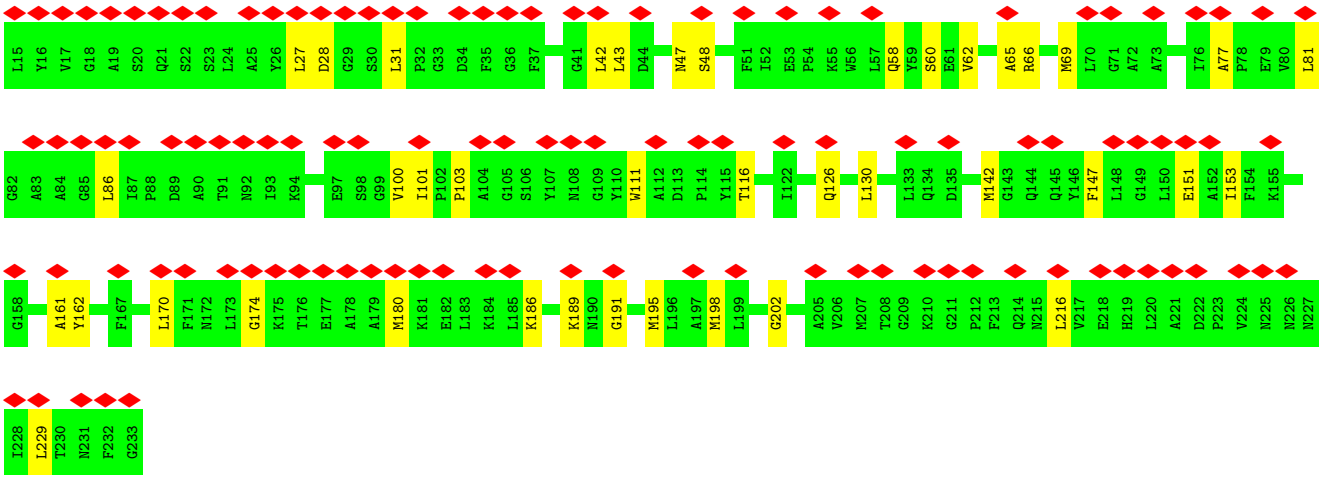
Y96 G97 N98 W99 Y100 D101 A102 P103 L104 W105 A106 V107 N108 G109 G110 K111 A112 T113 W114 F115 G116 I117 E118 V119 P120 F121 D122 L123 N124 A125 L126 L127 A128 F129 E130 F131 V132 A133 M134 A135 A136 A137 E138 G139 Q140 R141 G142 D143 A144 G145 G146 V147 V148 Y149 P150 G151 G152 A153 F154 D155

P156 L157 G158 F159 A160 K161 D162 S163 S164 K165 S166 G167 E168 L169 K170 L171 K172 E173 I174 K175 N176 G177 R178 L179 A180 M181 V182 L185 G186 F187 V188 A189 Q190 H191 A192 A193 T194 G195 K196 G197 P198 I199 A200 A201 L202 G203 E204 H205 L206 A207 N208 P209 W210 G211 A212 N213 F214 A215 T216

N217 G218 I219 P222 F223 F224

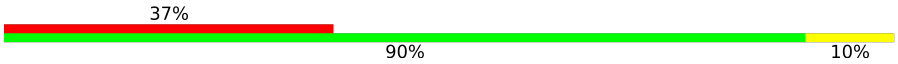
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

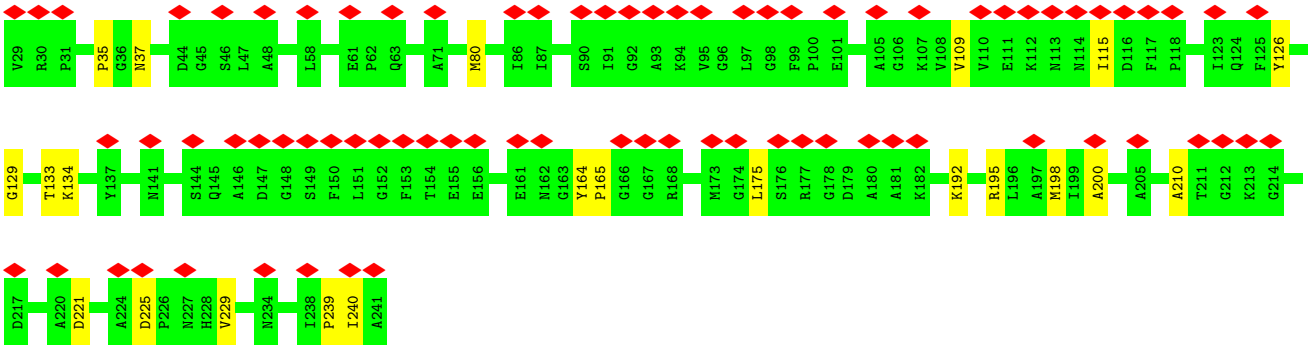
Chain 3:



• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

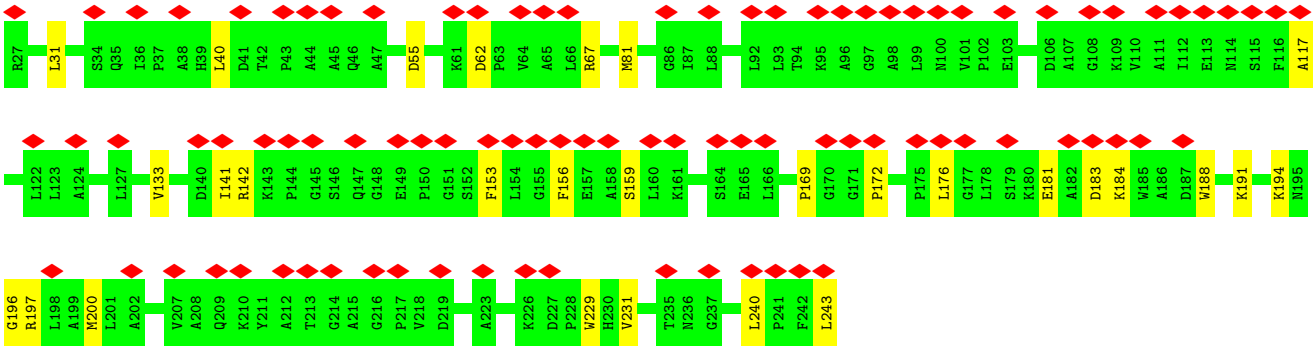
Chain 7:





• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:

D55 A56 A57 L58 P59 S60 P63 G64 A65 D66 L67 P68 G69 Y70 L71 N72 G73 T74 L75 P76 G77 D78 F79 G80 F81 D82 P83 L84 Y85 L86 G87 Q88 D89 P90 V91 K92 L93 K94 W95 Y96 A97 Q98 A99 A104 R105 F106 A107 M108 L109 A110 V111 A112 G113 I114 L115 V116 P117 E118

L119 L120 S121 N122 I123 G124 F125 S126 W127 P128 G129 A130 G131 V132 A133 W134 Y135 D136 A137 G138 K139 F140 E141 Y142 F143 A144 P145 A146 S147 S148 L149 F150 G151 V152 Q153 M154 L155 L156 F157 A158 W159 I162 Q166 D167 F168 V169 K170 P171 G172 S173 A174 N175 Q176 D177 P178 I179 F180 T181

N182 N183 K184 L185 P186 D187 G188 N189 E190 P191 G192 Y193 P194 G195 G196 I197 F198 D199 P200 F201 G202 W203 S204 K205 G206 D207 I208 K209 S210 L211 K212 L213 K214 E215 I216 K217 N218 G219 R220 L221 A222 M223 L224 A225 F226 A227 G228 F229 I230 A233 Y234 T235 T236 G237 T238 T239 P240 L241 K242

N243 L244 S245 T246 H247 L248 A249 D250 P251 W252 S253 T254 T255 V256 W257 Q258 N259 D260 L261 A262 R263 L264

- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5:

D31 R32 K33 L34 W35 A36 P37 G38 V39 V40 A41 P42 E43 Y44 L45 K46 G47 D48 L49 A50 G51 G54 W55 D56 P57 L58 G59 L60 G61 A62 D63 K68 R71 L75 Q76 H77 A78 R79 M82 L83 G84 V85 A86 G87 V88 L89 V90 Q91 E92 I93 V94 K95 P96 D97 V98

Y99 F100 Y101 E102 A103 G104 L105 P106 Q107 N108 L109 P110 E111 P112 F113 T114 N115 I116 N117 M118 G119 G120 L121 L122 A123 W124 E125 F126 I127 L128 M129 H130 W131 R135 R136 W137 Q138 D139 Y140 K141 N142 F143 G144 S145 V146 N147 E148 D149 P150 I151 F152 K153 G154 N155 K156 V157 P158 N159 P160

E161 M162 G163 Y164 P165 G166 G167 I168 F169 D170 P171 F172 G173 F174 S175 K176 G177 N178 L179 K180 E181 L182 Q183 T184 K185 E186 I187 K188 N189 G190 R191 L192 A193 M194 I195 A196 Y197 M198 A199 F200 I201 L202 Q203 A204 Q205 A206 T207 G208 K209 G210 P211 L212 A213 A214 L215 S216 A217 H218 L219 S220

N221 P222 F223 G224 N225 N226 I227 L228 K229 N230 I231 G232 T233 C234 T235 V236 P237 H238 S239 V240 D241 V242 Q243 G244 L245 T246 I247 P248 L249 T250 C251 P254 G255 S256 Q257

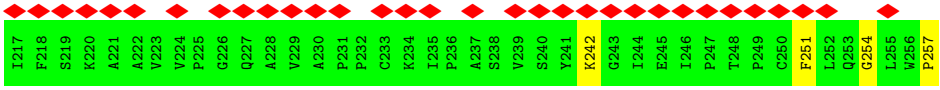
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

R29 P30 L31 W32 L33 P34 G35 S36 T37 P38 P39 A40 H41 L42 K43 G44 D45 L46 P47 G48 D49 F50 G51 F52 D53 P54 L55 G56 L57 G58 A59 N60 A61 E62 S63 L64 K65 K68 E69 S70 E71 L72 S75 R76 M79 A80 A81 V82 A83 G84 I85 L86 V87 Q88 E89 I90 V91

R92 P93 D94 V95 F96 W97 A100 G101 K102 E103 V104 E105 S106 P107 L108 G109 P110 L111 G112 L113 L114 A115 V116 E117 F118 F119 L120 M121 H122 W123 V124 E125 V126 R127 R128 W129 Q130 D131 L132 R133 K134 P135 G136 S137 V138 D139 Q140 D141 P142 I143 F144 S145 Q146 Y147 K148 L149 P150 P151 H152

E153 V154 G155 Y156 P157 G158 G159 V160 F161 A162 P163 F164 I165 P166 G167 D168 L169 A170 E171 L172 K173 V174 K175 E176 I177 K178 N179 G180 R181 L182 A183 M184 L185 A186 F187 V188 A193 A194 Q195 V196 T197 G198 K199 G200 P201 I202 A203 A204 L205 Q206 E207 H208 L209 A210 D211 P212 W213 T216


I217
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G243
I244
E245
I246
P247
T248
P249
C250
F251
L252
Q253
G254
L255
W256
P257

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17311	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	264.64, 264.64, 264.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	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: OCA, DGD, LPX, QTB, 3PH, LMG, CL0, SNC, CHL, SPH, CA, SF4, LHG, C7Z, RRX, BCR, PQN, DAO, CLA, PLM, NKP, LMT, LUT, SQD, DGA

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	A	0.24	0/6016	0.50	1/8201 (0.0%)
2	B	0.24	0/6037	0.50	0/8242
3	C	0.21	0/611	0.48	0/826
4	D	0.21	0/1154	0.51	0/1556
5	E	0.18	0/507	0.39	0/689
6	F	0.23	0/1292	0.50	0/1747
7	G	0.17	0/561	0.44	0/760
8	I	0.27	0/294	0.56	0/406
9	J	0.27	0/332	0.47	0/454
10	K	0.20	0/576	0.47	0/779
11	L	0.19	0/935	0.43	0/1277
12	1	0.20	0/1491	0.44	0/2028
12	Z	0.18	0/1491	0.42	0/2028
13	3	0.23	0/1722	0.48	0/2336
14	7	0.21	0/1702	0.44	0/2310
15	8	0.22	0/1701	0.46	0/2315
16	4	0.22	0/1683	0.46	0/2296
17	5	0.20	0/1830	0.45	0/2492
18	6	0.21	0/1828	0.44	0/2497
All	All	0.22	0/31763	0.47	1/43239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	ASN	N-CA-C	-6.43	107.29	114.62

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	A	5820	0	5670	81	0
2	B	5825	0	5579	78	0
3	C	601	0	581	4	0
4	D	1135	0	1148	4	0
5	E	497	0	491	1	0
6	F	1266	0	1301	13	0
7	G	550	0	532	7	0
8	I	282	0	292	5	0
9	J	321	0	322	6	0
10	K	571	0	606	10	0
11	L	914	0	921	10	0
12	1	1445	0	1396	19	0
12	Z	1445	0	1396	10	0
13	3	1674	0	1633	36	0
14	7	1650	0	1589	20	0
15	8	1650	0	1629	22	0
16	4	1628	0	1576	24	0
17	5	1775	0	1746	29	0
18	6	1766	0	1765	29	0
19	A	65	0	72	3	0
20	1	712	0	712	26	0
20	3	748	0	720	24	0
20	4	613	0	566	20	0
20	5	799	0	757	24	0
20	6	759	0	741	34	0
20	7	790	0	751	29	0
20	8	694	0	672	24	0
20	A	2699	0	2866	129	0
20	B	2680	0	2834	111	0
20	F	110	0	105	9	0
20	G	96	0	72	2	0
20	J	42	0	30	0	0
20	K	205	0	168	8	0
20	L	115	0	110	3	0
20	Z	622	0	584	20	0
21	A	33	0	46	0	0
21	B	33	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	8	0	0	0	0
22	C	16	0	0	1	0
23	3	160	0	212	9	0
23	4	40	0	53	1	0
23	5	80	0	105	3	0
23	6	80	0	106	6	0
23	7	80	0	106	5	0
23	8	40	0	53	2	0
23	A	200	0	264	18	0
23	B	280	0	370	19	0
23	G	40	0	53	3	0
23	I	40	0	52	2	0
23	J	40	0	53	3	0
23	K	80	0	106	5	0
23	L	80	0	106	6	0
24	1	43	0	56	2	0
24	3	20	0	12	0	0
24	4	81	0	108	4	0
24	5	37	0	44	1	0
24	6	49	0	74	4	0
24	7	37	0	44	2	0
24	8	38	0	46	2	0
24	A	84	0	114	4	0
24	B	76	0	64	3	0
24	Z	43	0	56	0	0
25	3	16	0	12	1	0
25	8	29	0	39	0	0
25	A	29	0	39	0	0
26	1	35	0	45	1	0
26	4	35	0	43	2	0
26	8	35	0	45	2	0
26	A	35	0	42	2	0
26	B	70	0	89	2	0
26	F	35	0	45	0	0
27	A	10	0	15	0	0
28	A	14	0	23	0	0
29	A	29	0	28	0	0
29	J	35	0	40	0	0
30	A	44	0	76	5	0
31	B	66	0	96	5	0
32	B	1	0	0	0	0
33	F	41	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	1	42	0	0	0	0
34	5	42	0	0	0	0
34	J	42	0	0	0	0
35	7	42	0	74	3	0
35	K	21	0	37	2	0
36	1	84	0	110	4	0
36	3	84	0	110	11	0
36	4	84	0	110	9	0
36	5	84	0	110	11	0
36	6	84	0	110	5	0
36	7	84	0	110	1	0
36	8	84	0	110	5	0
36	Z	126	0	165	4	0
37	1	106	0	82	4	0
37	3	66	0	69	4	0
37	4	201	0	146	3	0
37	5	160	0	133	7	0
37	6	206	0	157	5	0
37	7	54	0	42	2	0
37	8	122	0	115	5	0
37	Z	178	0	168	8	0
38	1	48	0	62	1	0
39	Z	19	0	0	0	0
40	5	23	0	19	0	0
40	6	29	0	31	0	0
40	7	39	0	51	5	0
40	8	30	0	33	0	0
41	7	18	0	31	0	0
42	8	30	0	43	0	0
43	1	16	0	0	0	0
43	3	17	0	0	0	0
43	4	7	0	0	0	0
43	5	9	0	0	1	0
43	6	8	0	0	0	0
43	7	18	0	0	0	0
43	8	16	0	0	0	0
43	A	91	0	0	2	0
43	B	79	0	0	0	0
43	C	19	0	0	1	0
43	D	12	0	0	0	0
43	E	7	0	0	0	0
43	F	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	J	3	0	0	0	0
43	K	2	0	0	0	0
43	L	5	0	0	0	0
43	Z	8	0	0	0	0
All	All	47524	0	47243	762	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 8.

All (762) 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)
36:4:502:LUT:H32	20:4:604:CLA:HAB	1.44	0.98
20:5:605:CLA:H52	20:5:622:CLA:HAB	1.66	0.77
20:B:1218:CLA:HMD2	23:B:4001:BCR:HC7	1.67	0.76
1:A:396:TRP:CD1	20:A:1126:CLA:HAB	2.23	0.74
20:F:1301:CLA:HBB1	33:F:4001:RRX:H11	1.70	0.73
18:6:82:VAL:HG11	36:6:501:LUT:H12	1.70	0.73
20:A:1012:CLA:H2	23:A:4005:BCR:H362	1.70	0.73
1:A:204:GLY:O	1:A:208:LEU:HB2	1.89	0.72
36:4:502:LUT:H30	20:4:604:CLA:H72	1.76	0.68
20:B:1023:CLA:H152	23:B:4007:BCR:H16C	1.74	0.68
20:A:1117:CLA:HAB	20:A:1117:CLA:H8	1.76	0.67
20:B:1217:CLA:H71	20:B:1217:CLA:HBB1	1.77	0.67
23:3:504:BCR:H362	20:3:601:CLA:H142	1.76	0.67
2:B:345:ILE:HG13	20:B:1221:CLA:H41	1.76	0.67
2:B:722:TYR:HB2	20:B:1021:CLA:HED3	1.76	0.67
2:B:352:HIS:ND1	20:B:1214:CLA:OBD	2.27	0.66
20:A:1112:CLA:H122	30:A:5005:DGA:HBW1	1.78	0.66
2:B:174:SER:O	2:B:178:HIS:ND1	2.27	0.66
20:A:1104:CLA:H2	20:A:1104:CLA:HED2	1.76	0.65
8:I:92:MET:HG2	23:L:4001:BCR:H10C	1.77	0.65
20:6:609:CLA:HBB2	20:6:604:CLA:HHD	1.79	0.64
23:3:503:BCR:H383	20:3:606:CLA:HAB	1.79	0.64
20:A:1139:CLA:HBA2	24:A:5002:LHG:H161	1.80	0.64
12:1:149:TYR:HB3	20:1:601:CLA:HED3	1.80	0.64
6:F:162:TYR:HE2	20:F:1302:CLA:HBD	1.63	0.63
14:7:210:ALA:HB2	20:7:615:CLA:HED3	1.79	0.63
20:B:1222:CLA:HBA1	20:B:1223:CLA:HED2	1.81	0.63
18:6:79:MET:SD	20:6:601:CLA:HAB	2.39	0.63
6:F:123:LEU:HD21	9:J:38:VAL:HG11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:109:VAL:HG21	20:7:606:CLA:HAA2	1.81	0.63
14:7:115:ILE:HG12	23:7:504:BCR:H281	1.81	0.63
12:1:46:PRO:HG2	12:1:49:LEU:HB2	1.81	0.63
1:A:305:PHE:HE1	20:A:1119:CLA:HAB	1.64	0.62
20:B:1240:CLA:HBB1	20:1:605:CLA:H12	1.82	0.62
20:A:1138:CLA:H172	20:A:1140:CLA:H52	1.81	0.62
16:4:153:GLN:NE2	37:4:610:CHL:OMC	2.26	0.62
1:A:370:HIS:ND1	20:A:1116:CLA:OBD	2.33	0.62
20:B:1211:CLA:H2	23:B:4003:BCR:H362	1.82	0.62
20:A:1012:CLA:HAB	2:B:583:TRP:CH2	2.35	0.61
13:3:142:MET:HE1	14:7:35:PRO:HB2	1.82	0.61
12:Z:82:MET:SD	20:Z:601:CLA:HAB	2.40	0.61
12:1:210:TRP:HB3	15:8:117:ALA:HB2	1.82	0.61
20:A:1116:CLA:HAC1	20:A:1133:CLA:H42	1.82	0.61
38:1:802:SQD:O9	15:8:142:ARG:NH2	2.33	0.60
20:5:612:CLA:H43	20:6:619:CLA:H92	1.82	0.60
17:5:82:MET:SD	20:5:601:CLA:HAB	2.40	0.60
16:4:104:ALA:HB1	16:4:219:GLY:HA3	1.83	0.60
15:8:81:MET:SD	20:8:601:CLA:HAB	2.41	0.60
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.83	0.60
2:B:181:SER:HB3	2:B:289:GLY:HA3	1.84	0.60
23:3:505:BCR:H343	20:3:603:CLA:HBC1	1.84	0.60
17:5:85:VAL:HG11	36:5:501:LUT:H12	1.84	0.60
1:A:363:LEU:HD11	20:A:1117:CLA:H72	1.83	0.60
36:5:502:LUT:H371	20:5:604:CLA:H142	1.84	0.60
17:5:109:LEU:HD21	20:5:613:CLA:HAC1	1.84	0.59
17:5:164:TYR:HB3	20:5:601:CLA:HED3	1.84	0.59
20:B:1220:CLA:HAB	20:B:1227:CLA:HMD2	1.83	0.59
13:3:198:MET:HE2	36:3:502:LUT:H10	1.84	0.59
16:4:108:MET:SD	20:4:601:CLA:HAB	2.41	0.59
20:A:1113:CLA:H122	13:3:202:GLY:HA3	1.84	0.59
13:3:31:LEU:HD22	13:3:58:GLN:HG3	1.84	0.59
1:A:169:MET:HE2	30:A:5005:DGA:HAG1	1.85	0.59
12:1:72:GLU:HB3	12:1:148:VAL:HG22	1.84	0.59
36:6:501:LUT:H30	20:6:601:CLA:H72	1.85	0.59
4:D:95:ILE:HG12	4:D:105:ILE:HG12	1.85	0.58
2:B:107:ARG:NH1	2:B:114:VAL:O	2.36	0.58
20:Z:605:CLA:H162	37:8:613:CHL:H11	1.84	0.58
13:3:65:ALA:HB1	13:3:191:GLY:HA3	1.85	0.58
20:6:609:CLA:H62	24:6:801:LHG:H152	1.85	0.58
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1127:CLA:H2	23:A:4002:BCR:HC7	1.86	0.58
20:7:616:CLA:H11	18:6:251:PHE:HA	1.86	0.58
23:A:4005:BCR:H24C	20:B:1230:CLA:HMC2	1.85	0.58
1:A:436:ALA:O	1:A:440:HIS:ND1	2.27	0.58
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.86	0.58
16:4:127:TRP:NE1	16:4:129:GLY:O	2.36	0.58
18:6:205:LEU:HD12	36:6:501:LUT:H163	1.86	0.58
23:B:4002:BCR:H333	26:B:6101:LMT:H102	1.85	0.58
20:A:1106:CLA:HBB2	20:A:1126:CLA:H202	1.86	0.58
20:A:1112:CLA:C1B	23:A:4001:BCR:H10C	2.34	0.58
2:B:695:LYS:HB2	20:B:1238:CLA:HED3	1.85	0.58
12:Z:149:TYR:HB3	20:Z:601:CLA:HED3	1.86	0.58
20:5:618:CLA:HED1	24:6:801:LHG:H301	1.86	0.58
12:1:46:PRO:O	12:1:52:ASN:ND2	2.37	0.57
12:1:138:GLU:OE1	12:1:141:ARG:NH2	2.36	0.57
13:3:77:ALA:HB2	23:3:504:BCR:H383	1.86	0.57
20:Z:608:CLA:H2	37:Z:609:CHL:H151	1.86	0.57
2:B:711:LEU:HD23	31:B:5003:DGD:HBT1	1.86	0.57
13:3:100:VAL:HG21	36:3:502:LUT:H22	1.86	0.57
15:8:176:LEU:HD12	36:8:501:LUT:H222	1.86	0.57
20:A:1133:CLA:H172	20:A:1137:CLA:H112	1.87	0.57
24:B:5001:LHG:O3	24:B:5001:LHG:O1	2.22	0.57
20:B:1240:CLA:HBC1	26:B:5005:LMT:H6E	1.87	0.57
12:Z:193:ALA:HB2	20:Z:615:CLA:HED3	1.87	0.57
2:B:565:ARG:NH1	43:C:6010:HOH:O	2.38	0.56
13:3:174:GLY:HA3	13:3:180:MET:HE2	1.88	0.56
17:5:78:ALA:HB1	17:5:190:GLY:HA3	1.86	0.56
17:5:142:ASN:ND2	18:6:35:GLY:O	2.36	0.56
13:3:69:MET:SD	20:3:601:CLA:HAB	2.45	0.56
1:A:81:LEU:HD12	20:A:1111:CLA:HED1	1.88	0.56
13:3:189:LYS:HG2	23:3:506:BCR:H291	1.86	0.56
20:B:1203:CLA:H151	20:B:1225:CLA:HBB2	1.87	0.55
7:G:58:ARG:NH2	7:G:94:GLY:O	2.39	0.55
15:8:67:ARG:NH2	15:8:141:ILE:O	2.38	0.55
16:4:260:ASP:OD1	16:4:263:ARG:NH2	2.40	0.55
20:A:1107:CLA:H42	23:J:4001:BCR:H10C	1.88	0.55
3:C:17:CYS:HB3	22:C:3003:SF4:S4	2.46	0.55
13:3:147:PHE:CE2	37:3:611:CHL:HBB2	2.41	0.55
17:5:131:TRP:HB2	20:6:609:CLA:H11	1.87	0.55
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.86	0.55
2:B:429:PHE:CE2	20:B:1235:CLA:HAB	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:223:PHE:HE1	20:1:615:CLA:HAB	1.70	0.55
20:B:1205:CLA:H121	20:B:1224:CLA:H193	1.88	0.55
13:3:101:ILE:HG22	13:3:103:PRO:HD2	1.89	0.55
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.87	0.55
23:4:503:BCR:H24C	37:4:613:CHL:HAA1	1.89	0.55
2:B:21:ARG:NH2	2:B:696:ASP:OD2	2.39	0.55
18:6:257:PRO:HB2	20:6:619:CLA:HAB	1.89	0.55
20:A:1104:CLA:H191	24:A:5002:LHG:H212	1.88	0.55
20:4:609:CLA:H52	23:6:503:BCR:H332	1.89	0.54
6:F:162:TYR:CE2	20:F:1302:CLA:HBD	2.43	0.54
20:A:1118:CLA:H102	20:3:603:CLA:H172	1.89	0.54
1:A:161:THR:HG23	30:A:5005:DGA:HAE2	1.90	0.54
1:A:244:LEU:O	26:A:5006:LMT:O2'	2.26	0.54
36:3:501:LUT:H30	20:3:601:CLA:H72	1.90	0.54
14:7:129:GLY:O	14:7:133:THR:OG1	2.23	0.54
14:7:164:TYR:HB3	20:7:601:CLA:HED3	1.89	0.54
1:A:580:ARG:NH1	43:A:6042:HOH:O	2.41	0.54
20:A:1012:CLA:HMB2	20:B:1021:CLA:H191	1.90	0.54
30:A:5005:DGA:HA51	14:7:239:PRO:HB2	1.90	0.54
20:B:1238:CLA:H2	20:B:1239:CLA:H142	1.90	0.54
12:1:171:LEU:HD23	20:1:607:CLA:HED3	1.90	0.54
1:A:218:ILE:HA	1:A:222:LEU:HD12	1.89	0.53
12:1:193:ALA:HB2	20:1:615:CLA:HED3	1.89	0.53
2:B:175:ARG:HB2	20:B:1210:CLA:HBC2	1.88	0.53
13:3:153:ILE:HD13	17:5:58:LEU:HA	1.91	0.53
20:3:613:CLA:H93	20:5:609:CLA:H93	1.90	0.53
1:A:680:ALA:HB3	20:A:1013:CLA:HBB2	1.91	0.53
1:A:245:LEU:HD22	25:3:802:NKP:HAGA	1.90	0.53
2:B:525:ALA:O	2:B:529:HIS:ND1	2.34	0.53
20:Z:615:CLA:H3A	20:8:606:CLA:H101	1.90	0.53
20:A:1012:CLA:H192	20:A:1126:CLA:H122	1.91	0.53
20:B:1207:CLA:H12	11:L:106:LEU:HD11	1.91	0.53
17:5:135:ARG:NH2	17:5:146:VAL:O	2.42	0.53
2:B:438:TYR:HD2	20:B:1021:CLA:H203	1.73	0.52
14:7:80:MET:SD	20:7:601:CLA:HAB	2.50	0.52
17:5:90:VAL:HG11	20:5:606:CLA:HAC2	1.91	0.52
2:B:287:VAL:HG22	23:B:4001:BCR:H14C	1.90	0.52
36:4:501:LUT:H30	20:4:601:CLA:H52	1.92	0.52
20:B:1234:CLA:HMB2	20:B:1236:CLA:HED1	1.91	0.52
16:4:175:ASN:HA	16:4:185:LEU:HD12	1.91	0.52
16:4:204:SER:HB3	20:4:601:CLA:HAA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:6:608:CLA:H62	20:6:609:CLA:H8	1.91	0.52
36:6:502:LUT:H181	20:6:606:CLA:HBB1	1.90	0.52
20:A:1117:CLA:H2	20:A:1127:CLA:H92	1.91	0.52
24:1:801:LHG:H331	37:1:609:CHL:H93	1.92	0.52
23:5:504:BCR:H383	37:5:610:CHL:H12	1.92	0.52
20:K:1401:CLA:HBB1	23:K:4002:BCR:C10	2.40	0.52
20:1:603:CLA:H192	24:1:801:LHG:H121	1.91	0.52
2:B:91:ALA:HA	2:B:114:VAL:HG12	1.92	0.52
1:A:429:ARG:O	1:A:433:HIS:ND1	2.43	0.52
37:Z:609:CHL:HHC	37:Z:609:CHL:HBB1	1.92	0.52
1:A:495:PRO:HA	1:A:499:ALA:HB3	1.92	0.52
26:A:5006:LMT:H5B	26:A:5006:LMT:H6E	1.92	0.52
20:B:1218:CLA:H2	23:B:4001:BCR:HC32	1.92	0.52
2:B:27:ALA:HA	20:B:1226:CLA:H42	1.90	0.51
20:6:609:CLA:H2	24:6:801:LHG:H141	1.91	0.51
10:K:79:ASN:H	20:K:1404:CLA:HED1	1.74	0.51
37:1:609:CHL:HHC	37:1:609:CHL:HBB1	1.92	0.51
1:A:161:THR:HG21	20:A:1114:CLA:HBA1	1.92	0.51
1:A:418:ASP:O	1:A:422:ASN:ND2	2.42	0.51
2:B:659:ALA:C	20:B:1023:CLA:HAB	2.35	0.51
20:B:1235:CLA:H202	33:F:4001:RRX:H33	1.91	0.51
20:A:1106:CLA:HHC	20:A:1106:CLA:HBB1	1.93	0.51
10:K:93:GLY:O	10:K:97:HIS:ND1	2.43	0.51
37:5:610:CHL:H62	20:6:619:CLA:HED3	1.91	0.51
18:6:162:ALA:HB2	20:6:601:CLA:HBD	1.93	0.51
20:A:1103:CLA:H52	23:A:4002:BCR:HC8	1.91	0.51
12:1:82:MET:SD	20:1:601:CLA:HAB	2.51	0.51
20:B:1204:CLA:HED2	8:I:76:PRO:HB3	1.93	0.51
18:6:197:THR:HG21	20:6:603:CLA:HED3	1.93	0.51
1:A:11:LYS:O	10:K:73:SER:OG	2.25	0.51
2:B:277:HIS:HB2	20:B:1214:CLA:C1B	2.41	0.51
23:B:4001:BCR:H372	23:G:4001:BCR:HC42	1.93	0.51
12:1:150:PRO:HB3	20:1:611:CLA:HBC2	1.93	0.51
20:8:607:CLA:HMA2	26:8:805:LMT:H5'	1.93	0.51
16:4:252:TRP:HB3	18:6:109:GLY:H	1.75	0.51
17:5:202:LEU:HD12	20:5:603:CLA:HAC2	1.93	0.51
20:B:1022:CLA:H191	20:B:1206:CLA:H2	1.93	0.50
20:7:603:CLA:HBA1	20:7:603:CLA:HBD	1.93	0.50
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.94	0.50
20:A:1106:CLA:H71	23:J:4001:BCR:H343	1.93	0.50
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:PRO:HB3	6:F:226:PRO:HG2	1.93	0.50
20:B:1236:CLA:H193	20:B:1236:CLA:H102	1.93	0.50
6:F:212:ARG:NH1	15:8:62:ASP:OD2	2.42	0.50
13:3:216:LEU:HB2	36:3:501:LUT:H22	1.93	0.50
17:5:79:ARG:NH1	37:5:611:CHL:OBD	2.42	0.50
13:3:116:THR:HG23	20:7:608:CLA:HED1	1.93	0.50
16:4:123:ILE:HG13	16:4:125:PHE:H	1.75	0.50
1:A:297:HIS:HB2	20:A:1116:CLA:C1B	2.42	0.50
20:B:1222:CLA:H41	20:B:1234:CLA:H42	1.94	0.50
17:5:191:ARG:HA	17:5:194:MET:HE3	1.92	0.50
18:6:216:THR:HG22	20:6:603:CLA:HBA1	1.93	0.50
18:6:127:ARG:NH2	18:6:138:VAL:O	2.44	0.50
1:A:577:GLY:HA2	2:B:563:PRO:HD3	1.93	0.50
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.93	0.50
2:B:436:GLY:HA3	20:B:1230:CLA:HAB	1.93	0.50
11:L:79:VAL:O	11:L:84:ARG:NH2	2.44	0.50
15:8:188:TRP:HB3	20:8:601:CLA:HMA2	1.94	0.50
35:K:5001:SPH:H161	23:3:505:BCR:H311	1.94	0.50
1:A:57:HIS:HB2	20:A:1128:CLA:HBA1	1.93	0.50
20:1:606:CLA:H52	20:1:613:CLA:HBA1	1.93	0.50
20:A:1109:CLA:H72	20:A:1101:CLA:HBB2	1.93	0.49
20:A:1124:CLA:HBA1	20:A:1125:CLA:HED2	1.94	0.49
1:A:408:HIS:HA	1:A:411:ILE:HD12	1.94	0.49
20:A:1110:CLA:HHC	20:A:1110:CLA:HBB1	1.94	0.49
2:B:517:ASP:OD2	2:B:598:LYS:NZ	2.43	0.49
23:7:503:BCR:H10C	20:8:608:CLA:H41	1.94	0.49
20:5:612:CLA:H193	20:5:615:CLA:HBB1	1.92	0.49
13:3:81:LEU:HD22	13:3:86:LEU:HD12	1.94	0.49
14:7:37:ASN:HD21	40:7:802:3PH:H11	1.77	0.49
2:B:588:ILE:HA	2:B:591:VAL:HG22	1.95	0.49
6:F:149:VAL:O	43:F:6003:HOH:O	2.20	0.49
12:Z:119:VAL:HG11	37:Z:613:CHL:HMD1	1.92	0.49
14:7:192:LYS:HE3	24:7:801:LHG:HC42	1.94	0.49
20:6:608:CLA:H71	20:6:609:CLA:H52	1.94	0.49
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.95	0.49
1:A:221:SER:O	1:A:225:ASN:HB2	2.13	0.49
2:B:182:GLY:HA3	20:B:1210:CLA:HBB1	1.94	0.49
2:B:390:HIS:HA	2:B:393:ILE:HD12	1.95	0.49
2:B:489:ASN:ND2	20:B:1232:CLA:OBD	2.42	0.49
20:B:1203:CLA:H201	31:B:5003:DGD:HAG1	1.95	0.49
15:8:194:LYS:HE3	24:8:801:LHG:HC41	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:603:CLA:H71	24:4:801:LHG:H171	1.94	0.49
20:A:1123:CLA:HBA2	20:A:1127:CLA:H192	1.94	0.49
20:1:615:CLA:H2	20:1:615:CLA:H61	1.60	0.49
15:8:181:GLU:OE1	15:8:184:LYS:NZ	2.41	0.49
12:1:91:VAL:HG23	12:1:96:TYR:HB2	1.93	0.49
20:1:604:CLA:HHD	37:1:609:CHL:HBB2	1.95	0.49
14:7:165:PRO:HB3	20:7:611:CLA:HBC2	1.94	0.49
16:4:60:SER:HB2	16:4:67:LEU:HD11	1.95	0.49
2:B:320:HIS:HB3	2:B:323:LEU:HD12	1.94	0.49
23:B:4004:BCR:H24C	23:B:4005:BCR:H371	1.94	0.49
12:Z:34:ASN:ND2	12:Z:39:SER:O	2.37	0.49
37:3:611:CHL:HHC	37:3:611:CHL:HBB1	1.95	0.49
36:3:502:LUT:H32	20:3:604:CLA:CAB	2.42	0.49
20:A:1124:CLA:HBA2	20:A:1124:CLA:H3A	1.71	0.48
20:B:1235:CLA:H152	33:F:4001:RRX:H25	1.95	0.48
8:I:95:LEU:O	8:I:99:ILE:HG12	2.13	0.48
23:5:503:BCR:H10C	20:6:608:CLA:H52	1.95	0.48
12:Z:114:TRP:HD1	20:Z:606:CLA:HBA2	1.78	0.48
1:A:59:PHE:CD2	20:A:1103:CLA:HMC2	2.49	0.48
1:A:419:PRO:HG3	4:D:97:GLU:HB2	1.94	0.48
20:A:1105:CLA:H93	9:J:20:THR:HG21	1.95	0.48
20:B:1229:CLA:HBB2	23:B:4006:BCR:HC41	1.95	0.48
20:B:1240:CLA:H62	20:B:1240:CLA:H41	1.51	0.48
14:7:195:ARG:NH2	20:7:604:CLA:O1D	2.46	0.48
20:8:605:CLA:HAC1	37:8:610:CHL:HBB2	1.96	0.48
2:B:13:LEU:HG	31:B:5003:DGD:HE62	1.95	0.48
16:4:105:ARG:HA	16:4:108:MET:HE3	1.96	0.48
7:G:45:PHE:HA	7:G:48:ILE:HG12	1.95	0.48
20:7:616:CLA:HED1	18:6:254:GLY:HA3	1.96	0.48
18:6:156:TYR:HB3	20:6:601:CLA:HED3	1.96	0.48
2:B:375:HIS:HB2	20:B:1224:CLA:C1B	2.44	0.48
2:B:151:LEU:HD23	24:B:5006:LHG:H292	1.95	0.48
36:1:501:LUT:H30	20:1:601:CLA:H52	1.95	0.48
20:7:606:CLA:H42	35:7:804:SPH:H61	1.96	0.48
17:5:200:PHE:HE1	36:5:501:LUT:H41	1.79	0.48
37:5:617:CHL:HHC	37:5:617:CHL:HBB1	1.95	0.48
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.95	0.48
9:J:28:GLU:OE1	9:J:31:ARG:NH2	2.46	0.48
20:8:612:CLA:H3A	20:8:612:CLA:HBA2	1.53	0.48
37:4:617:CHL:HHC	37:4:617:CHL:HBB1	1.95	0.48
20:A:1103:CLA:HBA1	20:A:1103:CLA:H3A	1.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1229:CLA:H8	20:B:1229:CLA:H2	1.96	0.48
13:3:100:VAL:HG22	20:3:613:CLA:HMC2	1.96	0.48
20:F:1302:CLA:HMB1	9:J:26:LEU:HD11	1.96	0.47
13:3:126:GLN:O	13:3:130:LEU:HB2	2.13	0.47
13:3:195:MET:SD	20:3:604:CLA:HAB	2.53	0.47
16:4:111:VAL:HG11	36:4:501:LUT:H10	1.96	0.47
20:4:601:CLA:HBA2	20:4:601:CLA:H3A	1.57	0.47
18:6:152:HIS:ND1	18:6:153:GLU:O	2.44	0.47
20:B:1207:CLA:H192	20:B:1238:CLA:H201	1.96	0.47
16:4:213:LEU:HD23	20:4:607:CLA:HED3	1.96	0.47
20:A:1118:CLA:HAA2	10:K:87:VAL:HG13	1.97	0.47
20:B:1205:CLA:H122	20:B:1224:CLA:H121	1.96	0.47
20:B:1224:CLA:H3A	20:B:1224:CLA:HBA2	1.56	0.47
17:5:50:ALA:O	17:5:71:ARG:NH2	2.43	0.47
18:6:46:LEU:HD11	18:6:64:LEU:HD21	1.97	0.47
18:6:242:LYS:HD2	23:6:504:BCR:H343	1.95	0.47
20:6:605:CLA:H2	20:6:605:CLA:H61	1.65	0.47
20:6:612:CLA:H3A	20:6:612:CLA:HBA2	1.52	0.47
1:A:19:ARG:NE	13:3:48:SER:O	2.47	0.47
2:B:184:PHE:HZ	20:B:1221:CLA:H12	1.78	0.47
40:7:802:3PH:H3E1	40:7:802:3PH:H3B2	1.72	0.47
20:A:1120:CLA:H3A	20:A:1120:CLA:HBA2	1.45	0.47
20:B:1209:CLA:HHC	20:B:1209:CLA:HBB1	1.97	0.47
20:B:1224:CLA:H151	20:B:1226:CLA:H162	1.97	0.47
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.96	0.47
11:L:62:ALA:HB3	11:L:65:VAL:HG22	1.96	0.47
12:1:205:HIS:CG	20:1:603:CLA:HAA2	2.50	0.47
20:1:608:CLA:H3A	20:1:608:CLA:HBA2	1.39	0.47
20:5:601:CLA:H3A	20:5:601:CLA:HBA2	1.57	0.47
37:6:617:CHL:HHC	37:6:617:CHL:HBB1	1.96	0.47
20:A:1012:CLA:HBC2	2:B:586:ASN:HB2	1.97	0.47
20:A:1129:CLA:HBA1	20:A:1129:CLA:H3A	1.78	0.47
20:6:601:CLA:H71	20:6:602:CLA:HMA3	1.96	0.47
1:A:213:TRP:NE1	20:A:1117:CLA:O1D	2.41	0.47
1:A:447:PHE:HE2	20:A:1136:CLA:HAB	1.80	0.47
1:A:508:LEU:HB2	1:A:523:MET:HG3	1.95	0.47
23:A:4005:BCR:H21C	20:A:1013:CLA:H122	1.97	0.47
2:B:575:ASP:OD1	2:B:707:ARG:NH1	2.47	0.47
2:B:684:GLU:OE2	2:B:693:TYR:OH	2.29	0.47
20:Z:611:CLA:H51	20:Z:611:CLA:H11	1.68	0.47
17:5:32:ARG:NH2	17:5:45:LEU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1220:CLA:H3A	20:B:1220:CLA:HBA2	1.58	0.47
20:1:604:CLA:HBA2	20:1:604:CLA:H3A	1.57	0.47
37:1:610:CHL:HMC	20:1:613:CLA:HAB	1.97	0.47
20:Z:604:CLA:H142	20:Z:604:CLA:H112	1.75	0.47
20:A:1111:CLA:H61	20:A:1111:CLA:H41	1.60	0.46
20:B:1216:CLA:H13	20:B:1221:CLA:H172	1.97	0.46
23:3:506:BCR:H351	23:3:506:BCR:H15C	1.67	0.46
20:6:609:CLA:H3A	20:6:609:CLA:HBA2	1.72	0.46
1:A:508:LEU:HD12	1:A:523:MET:HB3	1.98	0.46
20:A:1103:CLA:H2	20:A:1103:CLA:H62	1.57	0.46
17:5:185:LYS:HG3	20:5:607:CLA:HED2	1.98	0.46
36:5:502:LUT:H373	20:5:604:CLA:H8	1.97	0.46
20:A:1126:CLA:H92	20:A:1126:CLA:H41	1.97	0.46
20:7:612:CLA:H3A	20:7:612:CLA:HBA2	1.49	0.46
20:4:609:CLA:H11	18:6:123:TRP:HB2	1.97	0.46
1:A:487:ILE:HD11	20:A:1135:CLA:H2	1.97	0.46
23:B:4006:BCR:C11	20:F:1302:CLA:HAB	2.45	0.46
6:F:196:ALA:HB1	20:F:1302:CLA:HED2	1.98	0.46
7:G:118:ASN:OD1	12:1:124:ASN:ND2	2.48	0.46
20:1:601:CLA:H3A	20:1:601:CLA:HBA2	1.58	0.46
20:7:602:CLA:HBB1	20:7:607:CLA:H143	1.97	0.46
1:A:16:ALA:HB1	1:A:187:LYS:HD3	1.96	0.46
1:A:196:SER:O	1:A:200:HIS:ND1	2.29	0.46
1:A:204:GLY:HA3	20:A:1111:CLA:HBB1	1.98	0.46
20:A:1012:CLA:H162	20:A:1013:CLA:H162	1.96	0.46
20:A:1106:CLA:HBA2	20:A:1106:CLA:H3A	1.40	0.46
20:A:1013:CLA:H143	20:A:1013:CLA:H111	1.80	0.46
36:Z:503:LUT:H11	36:Z:503:LUT:H191	1.79	0.46
16:4:204:SER:HB2	16:4:208:ILE:HD13	1.98	0.46
20:B:1216:CLA:HBA2	20:B:1216:CLA:H3A	1.48	0.46
12:Z:40:ASP:OD1	12:Z:40:ASP:N	2.41	0.46
37:8:613:CHL:HHC	37:8:613:CHL:HBB1	1.97	0.46
18:6:69:GLU:HG2	18:6:132:LEU:HD12	1.98	0.46
20:A:1105:CLA:H3A	20:A:1105:CLA:HBA2	1.68	0.46
15:8:191:LYS:NZ	26:4:803:LMT:O4'	2.48	0.46
20:4:609:CLA:OBD	18:6:127:ARG:NH1	2.49	0.46
1:A:679:TRP:CD2	19:A:1011:CL0:H5	2.51	0.46
20:A:1129:CLA:CHA	24:A:5001:LHG:HC92	2.45	0.46
12:1:45:LEU:HD21	20:1:604:CLA:HAA2	1.98	0.46
15:8:81:MET:HG3	15:8:196:GLY:HA2	1.98	0.46
20:B:1235:CLA:HBA2	20:B:1235:CLA:H3A	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1238:CLA:H193	23:I:4001:BCR:H362	1.98	0.46
20:8:604:CLA:HBC1	24:8:801:LHG:H132	1.97	0.46
20:4:602:CLA:H52	20:4:602:CLA:H11	1.77	0.46
1:A:116:GLN:NE2	20:A:1107:CLA:OBD	2.47	0.45
1:A:409:ALA:HB1	23:A:4003:BCR:H271	1.98	0.45
1:A:740:TRP:NE1	20:A:1126:CLA:O1A	2.48	0.45
2:B:316:LEU:HD22	20:B:1227:CLA:HMD2	1.98	0.45
36:Z:503:LUT:H15	36:Z:503:LUT:H201	1.79	0.45
20:3:612:CLA:H92	20:3:612:CLA:H61	1.77	0.45
20:8:601:CLA:H41	20:8:601:CLA:H62	1.71	0.45
20:A:1106:CLA:H203	20:A:1101:CLA:HMA3	1.96	0.45
20:A:1116:CLA:HBA2	20:A:1116:CLA:H3A	1.60	0.45
20:A:1120:CLA:HED1	10:K:61:THR:H	1.81	0.45
20:B:1220:CLA:HAB	20:B:1227:CLA:CMD	2.46	0.45
10:K:49:ALA:HB1	10:K:56:THR:HG22	1.98	0.45
40:7:802:3PH:H262	40:7:802:3PH:H382	1.98	0.45
36:4:501:LUT:H35	36:4:501:LUT:H401	1.80	0.45
1:A:289:LEU:HB2	1:A:376:PRO:HA	1.98	0.45
20:A:1115:CLA:H62	20:A:1115:CLA:H41	1.47	0.45
2:B:158:LEU:O	2:B:163:GLN:NE2	2.47	0.45
20:B:1226:CLA:H141	20:B:1226:CLA:H161	1.75	0.45
20:K:1402:CLA:H3A	20:K:1402:CLA:HBA2	1.61	0.45
20:Z:604:CLA:HBA2	20:Z:604:CLA:H3A	1.57	0.45
20:3:605:CLA:HED3	20:3:605:CLA:H62	1.98	0.45
17:5:60:LEU:HD13	20:5:604:CLA:H42	1.99	0.45
20:6:608:CLA:HBB1	20:6:609:CLA:H192	1.97	0.45
20:B:1225:CLA:HHC	20:B:1225:CLA:HBB1	1.98	0.45
20:B:1227:CLA:HAB	20:B:1236:CLA:CBB	2.46	0.45
20:K:1401:CLA:HBB1	23:K:4002:BCR:H10C	1.98	0.45
20:1:611:CLA:H93	20:1:611:CLA:H62	1.77	0.45
20:8:607:CLA:H3A	20:8:607:CLA:HBA2	1.66	0.45
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.97	0.45
20:A:1124:CLA:H193	20:A:1124:CLA:H162	1.84	0.45
20:B:1207:CLA:H93	20:B:1207:CLA:H61	1.83	0.45
20:B:1208:CLA:H3A	20:B:1208:CLA:HBA2	1.50	0.45
20:B:1209:CLA:H3A	20:B:1209:CLA:HBA2	1.60	0.45
12:Z:48:ASP:OD1	12:Z:48:ASP:N	2.49	0.45
16:4:226:PHE:CZ	36:4:502:LUT:H10	2.51	0.45
1:A:740:TRP:HB2	20:A:1126:CLA:HBB1	1.97	0.45
2:B:361:PHE:HB3	2:B:364:ILE:HD11	1.99	0.45
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:ARG:NE	5:E:92:GLU:OE2	2.47	0.45
37:7:610:CHL:CMC	20:7:613:CLA:HAB	2.46	0.45
15:8:153:PHE:HD2	15:8:156:PHE:HB3	1.80	0.45
16:4:175:ASN:HB3	16:4:185:LEU:HB2	1.98	0.45
1:A:707:LEU:HD22	33:F:4001:RRX:H48	1.98	0.45
20:A:1130:CLA:H193	20:A:1130:CLA:H162	1.84	0.45
2:B:418:ALA:O	2:B:422:HIS:ND1	2.30	0.45
36:7:502:LUT:H15	36:7:502:LUT:H201	1.85	0.45
20:8:602:CLA:H193	20:8:602:CLA:H161	1.74	0.45
20:4:603:CLA:H41	20:4:603:CLA:H62	1.76	0.45
1:A:29:TRP:HE1	20:A:1109:CLA:CHB	2.30	0.45
6:F:133:LEU:HD22	6:F:148:GLU:HB3	1.98	0.45
1:A:580:ARG:HH11	1:A:583:THR:HG21	1.81	0.45
1:A:596:LEU:HD21	20:A:1128:CLA:HBC1	1.98	0.45
20:A:1111:CLA:H93	20:A:1111:CLA:H111	1.85	0.45
2:B:723:ALA:HB2	20:B:1224:CLA:HBB1	1.99	0.45
20:B:1209:CLA:HMC3	23:B:4002:BCR:H10C	1.99	0.45
23:B:4006:BCR:H333	20:B:1230:CLA:H2	1.99	0.45
8:I:96:PHE:HB2	23:L:4001:BCR:H14C	1.99	0.45
11:L:96:LEU:HD21	11:L:124:LEU:HB3	1.97	0.45
18:6:75:SER:HB3	18:6:180:GLY:HA3	1.99	0.45
1:A:153:ILE:HA	20:A:1112:CLA:HED1	1.99	0.44
7:G:108:HIS:CE1	23:G:4001:BCR:H14C	2.52	0.44
10:K:35:ASN:HD21	20:K:1401:CLA:HED2	1.82	0.44
17:5:197:TYR:CZ	36:5:502:LUT:H8	2.52	0.44
18:6:168:ASP:HB3	18:6:171:GLU:HB3	1.98	0.44
1:A:17:VAL:H	13:3:47:ASN:HB3	1.82	0.44
20:B:1203:CLA:H93	20:B:1203:CLA:H61	1.82	0.44
6:F:162:TYR:HE1	6:F:200:ALA:HA	1.81	0.44
20:G:1602:CLA:ND	23:G:4001:BCR:H272	2.33	0.44
36:3:502:LUT:H35	36:3:502:LUT:H401	1.82	0.44
20:7:607:CLA:H13	20:6:615:CLA:HBB2	1.99	0.44
17:5:57:PRO:HD2	36:5:502:LUT:H23	1.99	0.44
20:F:1301:CLA:H143	20:F:1301:CLA:H112	1.78	0.44
20:1:605:CLA:HBC1	20:1:612:CLA:HAC1	1.99	0.44
37:Z:610:CHL:HBB2	37:Z:613:CHL:HBB2	2.00	0.44
20:8:601:CLA:HBA2	20:8:601:CLA:H3A	1.56	0.44
23:5:503:BCR:H15C	23:5:503:BCR:H351	1.74	0.44
1:A:356:ASN:O	1:A:360:PHE:HB2	2.18	0.44
20:A:1126:CLA:O1D	20:A:1127:CLA:HHB	2.16	0.44
14:7:134:LYS:NZ	20:8:609:CLA:OBD	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:167:ASP:HB2	16:4:174:ALA:HB3	1.99	0.44
20:5:618:CLA:HED3	24:6:801:LHG:H142	2.00	0.44
1:A:605:ILE:HD12	19:A:1011:CL0:H53	2.00	0.44
20:A:1121:CLA:H91	20:A:1121:CLA:H112	1.83	0.44
20:B:1225:CLA:H3A	20:B:1225:CLA:HBA2	1.50	0.44
20:F:1301:CLA:H141	20:F:1301:CLA:H161	1.84	0.44
20:A:1126:CLA:H191	23:J:4001:BCR:H19C	2.00	0.44
20:A:1132:CLA:H203	20:A:1132:CLA:H161	1.82	0.44
20:A:1136:CLA:H3A	20:A:1136:CLA:HBA2	1.64	0.44
2:B:374:THR:HG23	2:B:592:THR:HG21	2.00	0.44
20:B:1218:CLA:H143	20:B:1218:CLA:H111	1.88	0.44
40:7:802:3PH:H232	40:7:802:3PH:H362	2.00	0.44
17:5:197:TYR:CD2	36:5:502:LUT:H12	2.53	0.44
18:6:166:PRO:HD2	20:6:601:CLA:H11	1.98	0.44
20:A:1106:CLA:H62	20:A:1106:CLA:H41	1.78	0.44
20:A:1013:CLA:H41	20:A:1013:CLA:H62	1.71	0.44
2:B:277:HIS:CE1	2:B:281:ILE:HD13	2.53	0.44
16:4:244:LEU:HD13	36:4:501:LUT:H163	1.98	0.44
20:B:1203:CLA:H51	31:B:5003:DGD:HB71	1.99	0.44
23:B:4002:BCR:H351	23:B:4002:BCR:H15C	1.68	0.44
12:Z:105:TRP:CE2	12:Z:112:ALA:HB2	2.53	0.44
37:7:610:CHL:HHC	37:7:610:CHL:HBB1	2.00	0.44
15:8:240:LEU:HD13	15:8:243:LEU:HD12	1.99	0.44
16:4:217:LYS:NZ	24:4:801:LHG:O5	2.44	0.44
20:A:1112:CLA:H142	20:A:1114:CLA:HAB	1.99	0.44
20:4:604:CLA:HBA2	20:4:604:CLA:H3A	1.59	0.44
20:4:609:CLA:H92	20:4:609:CLA:H62	1.85	0.44
18:6:181:ARG:HA	18:6:184:MET:HE3	1.99	0.44
1:A:506:THR:HG22	20:A:1116:CLA:H42	2.00	0.43
1:A:690:ARG:HD3	2:B:567:GLY:HA3	2.00	0.43
20:A:1132:CLA:HMA2	11:L:103:LEU:HD13	2.00	0.43
20:A:1138:CLA:H3A	20:A:1138:CLA:HBA2	1.69	0.43
2:B:663:MET:HB2	20:B:1023:CLA:C1C	2.48	0.43
36:4:501:LUT:H34	20:4:601:CLA:HBB2	1.99	0.43
23:A:4005:BCR:H291	23:B:4006:BCR:H14C	2.00	0.43
20:B:1225:CLA:H8	23:B:4002:BCR:H21C	1.99	0.43
20:B:1240:CLA:H92	20:B:1240:CLA:H61	1.82	0.43
13:3:111:TRP:HB3	17:5:254:PRO:HB3	1.99	0.43
20:7:609:CLA:H143	20:7:615:CLA:H71	1.99	0.43
40:7:802:3PH:H3A1	40:7:802:3PH:H372	1.65	0.43
15:8:169:PRO:HB3	20:8:611:CLA:HBC2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:801:LHG:H223	24:4:801:LHG:H192	1.88	0.43
20:6:605:CLA:HBA1	20:6:605:CLA:H3A	1.80	0.43
20:A:1112:CLA:C2B	23:A:4001:BCR:H10C	2.49	0.43
2:B:193:GLY:O	2:B:197:HIS:HB2	2.18	0.43
20:B:1202:CLA:H61	20:B:1202:CLA:H102	1.58	0.43
8:I:92:MET:HG2	23:L:4001:BCR:C10	2.46	0.43
12:1:178:ARG:HA	12:1:181:MET:HE3	2.01	0.43
23:3:503:BCR:HC22	24:7:801:LHG:HC81	2.00	0.43
15:8:31:LEU:HD12	15:8:31:LEU:HA	1.88	0.43
36:6:501:LUT:H401	36:6:501:LUT:H35	1.76	0.43
20:A:1119:CLA:H42	20:A:1125:CLA:H93	1.99	0.43
20:A:1139:CLA:H101	20:A:1139:CLA:H62	1.87	0.43
2:B:292:TYR:HA	2:B:300:HIS:H	1.84	0.43
2:B:366:PHE:HB3	2:B:603:TRP:CZ3	2.53	0.43
20:B:1215:CLA:HBA2	20:B:1215:CLA:H3A	1.56	0.43
20:B:1215:CLA:HBC2	20:B:1225:CLA:H91	2.00	0.43
37:Z:610:CHL:H143	37:Z:610:CHL:H112	1.90	0.43
13:3:62:VAL:HG11	13:3:161:ALA:HB1	2.01	0.43
20:8:602:CLA:H52	20:4:612:CLA:H42	1.99	0.43
20:A:1110:CLA:H13	23:A:4002:BCR:H401	2.00	0.43
20:A:1113:CLA:H62	20:A:1113:CLA:H41	1.77	0.43
23:B:4004:BCR:H351	23:B:4004:BCR:H15C	1.85	0.43
36:1:502:LUT:H35	36:1:502:LUT:H401	1.86	0.43
17:5:127:ILE:HG13	20:6:608:CLA:HBA2	1.99	0.43
1:A:599:MET:HG2	1:A:603:LEU:HD13	2.00	0.43
19:A:1011:CL0:H8	19:A:1011:CL0:CGD	2.48	0.43
20:B:1210:CLA:H143	20:B:1210:CLA:H112	1.77	0.43
20:B:1225:CLA:H61	20:B:1225:CLA:H41	1.68	0.43
20:7:615:CLA:HBA2	20:7:615:CLA:H3A	1.51	0.43
35:7:803:SPH:H82	35:7:803:SPH:H5	1.74	0.43
20:8:603:CLA:H143	20:8:603:CLA:H161	1.86	0.43
20:6:604:CLA:H193	20:6:615:CLA:HBA2	2.01	0.43
37:6:613:CHL:H41	37:6:613:CHL:H61	1.85	0.43
1:A:312:TYR:HA	1:A:320:HIS:H	1.83	0.43
20:A:1124:CLA:HAB	23:A:4004:BCR:C8	2.49	0.43
20:B:1213:CLA:H8	7:G:113:ALA:HB2	2.01	0.43
14:7:221:ASP:HB3	14:7:229:VAL:HG11	1.99	0.43
16:4:226:PHE:CD2	36:4:502:LUT:H12	2.54	0.43
17:5:188:LYS:HE3	24:5:801:LHG:HC61	2.00	0.43
18:6:251:PHE:HB2	23:6:504:BCR:H282	2.01	0.43
20:A:1114:CLA:HHD	13:3:103:PRO:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:LEU:HA	3:C:41:SER:O	2.19	0.43
23:K:4001:BCR:H351	23:K:4001:BCR:H15C	1.75	0.43
36:8:501:LUT:H35	36:8:501:LUT:H401	1.86	0.43
20:A:1137:CLA:H141	23:A:4004:BCR:H383	2.01	0.43
20:A:1139:CLA:H61	20:A:1139:CLA:H41	1.74	0.43
2:B:499:LEU:HA	2:B:502:ILE:HG22	2.01	0.43
4:D:139:TYR:HD1	4:D:149:TYR:HA	1.84	0.43
6:F:114:ARG:NH1	9:J:35:ASP:OD2	2.48	0.43
20:Z:608:CLA:H62	37:Z:609:CHL:H122	2.00	0.43
13:3:147:PHE:N	13:3:151:GLU:OE1	2.48	0.43
23:8:503:BCR:H17C	37:8:613:CHL:H43	2.00	0.43
36:5:502:LUT:H32	20:5:604:CLA:CBB	2.49	0.43
20:A:1102:CLA:HBA2	20:A:1109:CLA:H62	2.00	0.43
2:B:274:MET:O	2:B:278:HIS:ND1	2.51	0.43
2:B:671:TYR:OH	20:B:1023:CLA:OBD	2.28	0.43
20:B:1239:CLA:HBC1	21:B:2002:PQN:H2M2	2.01	0.43
11:L:128:LEU:HD13	23:L:4001:BCR:H401	2.00	0.43
14:7:195:ARG:HA	14:7:198:MET:HE3	2.01	0.43
23:7:503:BCR:H351	23:7:503:BCR:H15C	1.81	0.43
17:5:202:LEU:HD23	17:5:202:LEU:HA	1.85	0.43
20:5:607:CLA:H61	20:5:607:CLA:H41	1.85	0.43
23:6:503:BCR:H382	20:6:606:CLA:H13	2.00	0.43
1:A:121:ILE:HG13	1:A:122:VAL:HG13	2.01	0.42
20:A:1107:CLA:H162	20:A:1107:CLA:H193	1.75	0.42
20:A:1013:CLA:H161	20:A:1013:CLA:H121	1.70	0.42
20:A:1130:CLA:H143	20:A:1130:CLA:H111	1.87	0.42
2:B:354:TYR:HA	2:B:369:GLN:HE22	1.84	0.42
20:B:1234:CLA:H41	20:B:1234:CLA:H61	1.50	0.42
20:B:1239:CLA:H201	11:L:130:LEU:HD23	2.01	0.42
11:L:101:ILE:HG12	11:L:114:GLU:HA	2.00	0.42
23:3:504:BCR:HC32	17:5:58:LEU:HD21	2.00	0.42
20:3:606:CLA:H3A	20:3:606:CLA:HBA2	1.62	0.42
15:8:159:SER:HB3	15:8:172:PRO:HD3	2.00	0.42
16:4:176:GLN:NE2	16:4:181:THR:O	2.52	0.42
20:5:601:CLA:H142	20:5:601:CLA:H111	1.85	0.42
20:6:615:CLA:HBA1	20:6:615:CLA:H3A	1.61	0.42
1:A:432:ARG:NH1	43:A:6069:HOH:O	2.52	0.42
20:A:1113:CLA:H141	20:A:1113:CLA:H161	1.75	0.42
20:B:1238:CLA:H13	23:I:4001:BCR:H372	2.00	0.42
20:1:608:CLA:H62	20:1:608:CLA:H41	1.79	0.42
20:Z:605:CLA:H192	37:8:613:CHL:H11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:200:ALA:HA	20:7:603:CLA:HBB1	2.01	0.42
15:8:197:ARG:HA	15:8:200:MET:HE3	2.00	0.42
16:4:220:ARG:HA	16:4:223:MET:HE3	2.01	0.42
20:4:603:CLA:H12	20:4:608:CLA:CAD	2.49	0.42
1:A:77:HIS:ND1	20:A:1111:CLA:OBD	2.46	0.42
20:A:1104:CLA:H71	20:A:1104:CLA:H111	1.76	0.42
20:A:1110:CLA:H62	20:A:1110:CLA:H41	1.71	0.42
12:Z:205:HIS:CG	20:Z:603:CLA:HAA2	2.54	0.42
37:5:610:CHL:HHC	37:5:610:CHL:HBB1	2.00	0.42
20:6:603:CLA:HBC1	20:6:615:CLA:HAA1	2.01	0.42
1:A:488:GLN:NE2	1:A:526:ILE:O	2.51	0.42
1:A:677:PHE:CG	23:A:4005:BCR:H363	2.54	0.42
2:B:411:ARG:HA	2:B:414:ASP:HB2	2.00	0.42
2:B:438:TYR:CD2	20:B:1021:CLA:H203	2.54	0.42
20:B:1220:CLA:H91	20:B:1220:CLA:H111	1.81	0.42
20:B:1226:CLA:H91	20:B:1226:CLA:H111	1.89	0.42
20:L:1502:CLA:H141	20:L:1502:CLA:H161	1.85	0.42
20:L:1502:CLA:H51	23:L:4002:BCR:HC21	2.00	0.42
36:1:502:LUT:H15	36:1:502:LUT:H201	1.87	0.42
20:3:607:CLA:H51	20:3:607:CLA:H11	1.84	0.42
20:7:605:CLA:H12	20:7:605:CLA:HBA1	1.80	0.42
20:8:604:CLA:H91	20:8:605:CLA:H152	2.00	0.42
37:5:610:CHL:H142	20:6:619:CLA:H112	2.00	0.42
20:A:1126:CLA:H3A	20:A:1126:CLA:HBA2	1.71	0.42
2:B:107:ARG:HG3	2:B:116:ILE:HD11	2.00	0.42
2:B:416:LYS:HD2	2:B:540:LEU:HB3	2.01	0.42
20:B:1218:CLA:H203	20:B:1218:CLA:H162	1.88	0.42
20:B:1225:CLA:H171	23:B:4002:BCR:H352	2.01	0.42
1:A:351:ALA:HB1	23:A:4003:BCR:H391	2.01	0.42
1:A:377:TYR:CE2	20:A:1127:CLA:HED2	2.54	0.42
20:A:1103:CLA:H93	20:A:1103:CLA:H111	1.83	0.42
20:A:1113:CLA:H201	36:3:502:LUT:H173	2.01	0.42
20:B:1213:CLA:O1A	7:G:116:ALA:HB1	2.20	0.42
20:3:612:CLA:H3A	20:3:612:CLA:HBA2	1.51	0.42
20:7:613:CLA:HED2	23:7:504:BCR:H21C	2.01	0.42
36:5:501:LUT:H11	36:5:501:LUT:H191	1.92	0.42
1:A:245:LEU:HD11	13:3:103:PRO:HB3	2.02	0.42
20:A:1120:CLA:HMD1	23:K:4001:BCR:H24C	2.00	0.42
20:B:1205:CLA:H3A	20:B:1205:CLA:HBA2	1.64	0.42
20:B:1212:CLA:H51	20:B:1212:CLA:H11	1.88	0.42
12:1:90:ALA:HB2	20:1:601:CLA:H192	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:66:ARG:NH1	37:3:611:CHL:OBD	2.48	0.42
13:3:162:TYR:HB3	20:3:601:CLA:HED3	2.02	0.42
20:7:616:CLA:H93	20:7:616:CLA:H111	1.88	0.42
36:5:502:LUT:H15	36:5:502:LUT:H201	1.84	0.42
23:6:503:BCR:H351	23:6:503:BCR:H15C	1.73	0.42
1:A:566:LYS:NZ	2:B:674:GLU:OE2	2.41	0.42
1:A:574:PRO:HB3	1:A:720:ILE:HB	2.02	0.42
20:B:1214:CLA:HBA2	20:B:1214:CLA:H3A	1.44	0.42
6:F:140:ALA:HA	6:F:145:HIS:HB2	2.01	0.42
13:3:28:ASP:OD1	13:3:28:ASP:N	2.48	0.42
20:7:615:CLA:H102	20:7:615:CLA:H62	1.89	0.42
15:8:133:VAL:HG21	23:8:503:BCR:H362	2.02	0.42
17:5:125:GLU:OE1	43:5:6001:HOH:O	2.22	0.42
20:A:1121:CLA:H191	10:K:95:ALA:HA	2.02	0.42
20:A:1125:CLA:H61	20:A:1125:CLA:H102	1.85	0.42
36:3:501:LUT:H401	36:3:501:LUT:H35	1.82	0.42
14:7:175:LEU:HD21	18:6:57:LEU:HA	2.02	0.42
14:7:225:ASP:HB3	14:7:229:VAL:HG23	2.02	0.42
1:A:377:TYR:HD2	1:A:380:LEU:HD22	1.84	0.42
1:A:532:ASP:O	1:A:536:HIS:ND1	2.31	0.42
23:A:4003:BCR:H381	23:A:4004:BCR:HC42	2.02	0.42
2:B:185:GLY:HA3	2:B:286:ILE:HG13	2.02	0.42
2:B:582:PHE:HZ	2:B:665:LEU:HD21	1.85	0.42
20:B:1207:CLA:H91	23:L:4002:BCR:H281	2.02	0.42
20:B:1207:CLA:H71	11:L:119:LEU:HB3	2.01	0.42
20:1:611:CLA:H51	20:1:611:CLA:H11	1.69	0.42
20:7:616:CLA:H41	20:7:616:CLA:H61	1.70	0.42
20:4:603:CLA:H122	20:4:603:CLA:H162	1.87	0.42
1:A:96:ALA:HB2	1:A:159:LEU:HB2	2.01	0.41
20:A:1122:CLA:HMD3	20:A:1123:CLA:HAB	2.02	0.41
20:B:1240:CLA:H91	20:B:1240:CLA:H112	1.80	0.41
23:B:4001:BCR:H351	23:B:4001:BCR:H15C	1.91	0.41
10:K:35:ASN:ND2	20:K:1401:CLA:OBD	2.43	0.41
20:K:1402:CLA:H11	20:K:1402:CLA:H51	1.71	0.41
20:1:606:CLA:HBA1	20:1:613:CLA:C1D	2.50	0.41
13:3:27:LEU:HD21	13:3:43:LEU:HD12	2.02	0.41
20:A:1119:CLA:H92	20:A:1119:CLA:H62	1.89	0.41
20:A:1123:CLA:H193	20:A:1123:CLA:H161	1.84	0.41
20:A:1013:CLA:HMD3	2:B:534:ILE:HG12	2.03	0.41
20:B:1021:CLA:H112	20:B:1021:CLA:H152	1.78	0.41
20:1:612:CLA:HMA2	26:1:803:LMT:H4'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:186:LYS:HD3	20:3:602:CLA:HAA2	2.01	0.41
14:7:126:TYR:HB3	20:8:609:CLA:H43	2.02	0.41
15:8:183:ASP:OD1	15:8:183:ASP:N	2.54	0.41
36:5:502:LUT:H372	20:5:609:CLA:H62	2.02	0.41
37:5:610:CHL:H111	37:5:610:CHL:H152	1.87	0.41
18:6:116:VAL:HG11	37:6:613:CHL:HED3	2.02	0.41
20:A:1124:CLA:H111	20:A:1124:CLA:H71	1.80	0.41
20:A:1140:CLA:H203	20:A:1140:CLA:H162	1.87	0.41
2:B:543:ARG:NH2	4:D:180:ASN:OD1	2.49	0.41
2:B:577:PHE:CE1	20:B:1226:CLA:HAC2	2.54	0.41
20:B:1237:CLA:H111	20:B:1237:CLA:H142	1.81	0.41
20:B:1222:CLA:H3A	20:B:1222:CLA:HBA2	1.64	0.41
36:Z:501:LUT:H35	36:Z:501:LUT:H401	1.85	0.41
36:Z:502:LUT:H11	36:Z:502:LUT:H191	1.90	0.41
16:4:146:ALA:HA	16:4:149:LEU:HD12	2.02	0.41
16:4:214:LYS:HD3	20:4:602:CLA:HAA2	2.01	0.41
20:5:609:CLA:H111	20:5:609:CLA:H91	1.79	0.41
23:6:503:BCR:H17C	37:6:613:CHL:H43	2.03	0.41
20:A:1124:CLA:HAA2	20:A:1125:CLA:OBD	2.19	0.41
2:B:601:THR:HG21	2:B:610:PHE:HB2	2.02	0.41
20:B:1214:CLA:H111	20:B:1214:CLA:H72	1.77	0.41
20:B:1221:CLA:H2	20:B:1221:CLA:H61	1.76	0.41
23:B:4004:BCR:H24C	23:B:4005:BCR:H24C	2.01	0.41
13:3:42:LEU:HD13	20:3:604:CLA:H42	2.02	0.41
13:3:170:LEU:N	36:3:501:LUT:O23	2.54	0.41
36:8:501:LUT:H32	20:8:601:CLA:CAB	2.51	0.41
20:A:1122:CLA:H51	20:A:1122:CLA:H11	1.78	0.41
23:A:4002:BCR:H351	23:A:4002:BCR:H15C	1.77	0.41
24:A:5002:LHG:H312	24:A:5002:LHG:H281	1.77	0.41
2:B:675:LEU:O	2:B:678:THR:OG1	2.35	0.41
20:B:1226:CLA:HBC2	31:B:5003:DGD:HB72	2.02	0.41
20:7:615:CLA:H91	20:7:615:CLA:H111	1.86	0.41
20:6:604:CLA:H162	20:6:604:CLA:H192	1.81	0.41
20:A:1111:CLA:H202	20:A:1111:CLA:H162	1.85	0.41
20:A:1119:CLA:H2	20:A:1119:CLA:H61	1.75	0.41
20:A:1126:CLA:H8	23:A:4005:BCR:H343	2.01	0.41
35:7:804:SPH:H112	20:7:616:CLA:HAC2	2.01	0.41
36:8:501:LUT:H15	36:8:501:LUT:H201	1.86	0.41
1:A:134:GLY:HA2	6:F:94:TYR:HE1	1.85	0.41
1:A:734:GLY:O	1:A:738:THR:OG1	2.33	0.41
20:A:1114:CLA:HBA2	30:A:5005:DGA:HB31	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1206:CLA:HBA1	20:B:1206:CLA:H3A	1.67	0.41
20:1:612:CLA:HBA2	20:1:612:CLA:H3A	1.52	0.41
13:3:147:PHE:HE2	37:3:611:CHL:HBB2	1.85	0.41
20:8:602:CLA:H12	26:4:803:LMT:H6'2	2.01	0.41
24:4:802:LHG:O1	18:6:133:ARG:NH1	2.52	0.41
20:A:1106:CLA:H151	20:A:1101:CLA:H111	2.03	0.41
20:A:1115:CLA:H3A	20:A:1115:CLA:HBA2	1.74	0.41
2:B:32:PHE:HA	2:B:35:HIS:CD2	2.56	0.41
20:B:1210:CLA:H93	20:B:1210:CLA:H61	1.87	0.41
7:G:92:PRO:HG3	20:G:1602:CLA:HBC2	2.01	0.41
20:Z:605:CLA:H111	20:Z:605:CLA:H91	1.88	0.41
36:3:501:LUT:H15	36:3:501:LUT:H201	1.86	0.41
20:3:610:CLA:OBD	20:3:613:CLA:HAB	2.20	0.41
20:A:1122:CLA:HAC1	23:A:4003:BCR:H24C	2.02	0.41
20:A:1138:CLA:H112	20:A:1138:CLA:HAB	2.03	0.41
2:B:312:PRO:HB2	12:1:63:GLU:HG3	2.02	0.41
2:B:345:ILE:HD12	20:B:1215:CLA:H71	2.03	0.41
2:B:549:PRO:HD2	3:C:62:PHE:CZ	2.55	0.41
20:B:1203:CLA:H3A	20:B:1203:CLA:HBA1	1.88	0.41
6:F:158:TYR:O	6:F:162:TYR:HB2	2.21	0.41
20:F:1301:CLA:H93	20:F:1301:CLA:H111	1.89	0.41
20:Z:604:CLA:HHD	37:Z:609:CHL:HBB2	2.03	0.41
20:Z:606:CLA:H11	20:Z:606:CLA:H52	1.87	0.41
20:3:607:CLA:H41	20:3:607:CLA:H61	1.77	0.41
20:7:601:CLA:H62	20:7:601:CLA:H41	1.81	0.41
20:8:603:CLA:H141	20:8:607:CLA:HMC1	2.02	0.41
20:8:607:CLA:HBA2	26:8:805:LMT:H22	2.02	0.41
17:5:137:TRP:CG	20:5:618:CLA:HBC1	2.55	0.41
1:A:681:PHE:HZ	20:A:1139:CLA:HBC2	1.86	0.41
20:A:1126:CLA:H13	20:A:1126:CLA:H72	2.03	0.41
20:L:1502:CLA:H92	20:L:1502:CLA:H61	1.81	0.41
36:1:501:LUT:H15	36:1:501:LUT:H201	1.92	0.41
20:Z:605:CLA:H51	20:Z:605:CLA:H11	1.75	0.41
20:7:606:CLA:HMA2	20:7:613:CLA:HAC2	2.03	0.41
18:6:125:GLU:HG3	20:6:612:CLA:C4B	2.51	0.41
20:A:1114:CLA:C4C	20:3:610:CLA:HBB2	2.50	0.40
20:A:1126:CLA:H143	20:A:1126:CLA:H161	1.93	0.40
35:K:5001:SPH:N2	13:3:229:LEU:O	2.54	0.40
20:Z:605:CLA:H112	20:Z:605:CLA:H151	1.81	0.40
20:3:610:CLA:H12	14:7:240:ILE:HD11	2.02	0.40
23:7:504:BCR:H402	15:8:229:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:618:CLA:H41	20:5:618:CLA:H61	1.61	0.40
20:6:608:CLA:H92	20:6:609:CLA:H102	2.02	0.40
20:B:1235:CLA:H91	20:B:1235:CLA:H111	1.91	0.40
20:B:1241:CLA:H193	20:B:1241:CLA:H161	1.87	0.40
11:L:160:PRO:O	11:L:163:SER:OG	2.36	0.40
20:Z:601:CLA:H111	20:Z:601:CLA:H142	1.85	0.40
37:Z:610:CHL:CBB	37:Z:613:CHL:HBB2	2.51	0.40
36:3:501:LUT:H371	20:3:601:CLA:H61	2.02	0.40
1:A:119:TRP:CD2	20:A:1107:CLA:HED3	2.56	0.40
1:A:539:HIS:HE1	1:A:605:ILE:HG22	1.86	0.40
1:A:584:CYS:HB3	2:B:668:TRP:HE3	1.86	0.40
20:A:1128:CLA:H41	20:A:1128:CLA:H62	1.88	0.40
2:B:155:TRP:CD2	24:B:5006:LHG:H242	2.56	0.40
20:K:1401:CLA:HBB1	23:K:4002:BCR:C11	2.51	0.40
13:3:60:SER:HA	20:3:612:CLA:HED2	2.03	0.40
20:7:601:CLA:H91	20:7:601:CLA:H111	1.83	0.40
36:8:502:LUT:H11	36:8:502:LUT:H191	1.97	0.40
37:6:610:CHL:H8	37:6:610:CHL:H51	1.97	0.40
1:A:316:TRP:CD1	10:K:87:VAL:HG21	2.57	0.40
20:A:1105:CLA:H62	20:A:1105:CLA:H41	1.87	0.40
20:B:1203:CLA:H193	20:B:1203:CLA:H161	1.88	0.40
20:B:1216:CLA:H41	20:B:1216:CLA:H61	1.83	0.40
20:B:1235:CLA:HMA3	20:B:1236:CLA:HED2	2.03	0.40
20:B:1241:CLA:H93	20:B:1241:CLA:H61	1.81	0.40
20:Z:604:CLA:H112	20:Z:604:CLA:H91	1.89	0.40
15:8:40:LEU:HD11	15:8:55:ASP:HB2	2.03	0.40
15:8:231:VAL:HG12	20:8:603:CLA:HED1	2.03	0.40
17:5:194:MET:SD	20:5:604:CLA:HBB1	2.61	0.40
18:6:44:GLY:HA2	18:6:49:ASP:HB3	2.02	0.40
1:A:578:PRO:HD3	2:B:562:GLY:HA2	2.04	0.40
1:A:676:HIS:HB3	20:A:1012:CLA:HBD	2.03	0.40
20:A:1140:CLA:H152	9:J:18:TRP:HE3	1.85	0.40
2:B:30:HIS:HB2	20:B:1226:CLA:CGA	2.51	0.40
20:B:1218:CLA:H18	12:1:127:LEU:HB3	2.03	0.40
20:7:607:CLA:H141	20:7:607:CLA:H161	1.74	0.40
20:8:607:CLA:H93	20:8:607:CLA:H62	1.93	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	A	739/741 (100%)	716 (97%)	23 (3%)	0	100	100
2	B	731/733 (100%)	705 (96%)	26 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	157 (96%)	5 (3%)	1 (1%)	21	52
7	G	70/91 (77%)	70 (100%)	0	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
11	L	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
12	1	192/194 (99%)	182 (95%)	10 (5%)	0	100	100
12	Z	192/194 (99%)	189 (98%)	3 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
15	8	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
16	4	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	5	225/227 (99%)	221 (98%)	4 (2%)	0	100	100
18	6	227/229 (99%)	222 (98%)	5 (2%)	0	100	100
All	All	3946/4006 (98%)	3820 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE

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	A	601/601 (100%)	601 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	120/120 (100%)	120 (100%)	0	100	100
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	54/68 (79%)	54 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	58/58 (100%)	58 (100%)	0	100	100
11	L	92/92 (100%)	92 (100%)	0	100	100
12	1	137/137 (100%)	137 (100%)	0	100	100
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	167/167 (100%)	167 (100%)	0	100	100
14	7	164/164 (100%)	164 (100%)	0	100	100
15	8	163/163 (100%)	163 (100%)	0	100	100
16	4	164/165 (99%)	164 (100%)	0	100	100
17	5	184/184 (100%)	184 (100%)	0	100	100
18	6	183/183 (100%)	183 (100%)	0	100	100
All	All	3136/3151 (100%)	3136 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	241	HIS

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Mol	Chain	Res	Type
1	A	296	HIS
1	A	442	ASN
1	A	637	GLN
2	B	133	ASN
2	B	159	GLN
2	B	491	GLN
2	B	504	ASN
4	D	108	GLN
4	D	162	ASN
5	E	64	GLN
5	E	87	ASN
7	G	108	HIS
9	J	30	ASN
10	K	35	ASN
12	1	52	ASN
12	Z	52	ASN
13	3	190	ASN
13	3	225	ASN
14	7	162	ASN
17	5	76	GLN
17	5	108	ASN
17	5	230	ASN
18	6	140	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SNC	D	137	4	4,7,8	1.00	0	1,7,9	3.26	1 (100%)

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
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	137	SNC	CA-CB-SG	-3.26	105.99	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 317 ligands modelled in this entry, 1 is monoatomic - leaving 316 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	$\#\|Z\| > 2$
20	CLA	7	609	14	69,73,73	1.35	7 (10%)	83,113,113	1.99	21 (25%)
23	BCR	6	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.10	17 (30%)
24	LHG	7	801	-	36,36,48	0.46	0	39,42,54	1.17	3 (7%)
20	CLA	6	609	18	69,73,73	1.37	7 (10%)	83,113,113	1.91	17 (20%)
36	LUT	5	501	-	42,43,43	2.42	1 (2%)	51,60,60	1.94	11 (21%)
28	DAO	A	5007	-	13,13,13	0.81	1 (7%)	13,13,13	0.92	0
20	CLA	8	606	-	64,68,73	1.42	7 (10%)	77,107,113	1.93	16 (20%)
36	LUT	6	502	-	42,43,43	2.38	1 (2%)	51,60,60	1.88	16 (31%)
20	CLA	1	605	-	59,63,73	1.47	7 (11%)	71,101,113	2.05	19 (26%)
26	LMT	A	5006	-	36,36,36	1.22	6 (16%)	47,47,47	1.04	1 (2%)
23	BCR	B	4003	-	41,41,41	1.84	4 (9%)	56,56,56	4.30	18 (32%)
20	CLA	B	1229	-	69,73,73	1.35	9 (13%)	83,113,113	1.97	22 (26%)
30	DGA	A	5005	-	43,43,43	1.14	3 (6%)	45,45,45	1.48	3 (6%)
23	BCR	3	506	-	41,41,41	1.87	4 (9%)	56,56,56	4.48	15 (26%)
20	CLA	3	607	-	64,68,73	1.41	7 (10%)	77,107,113	2.06	19 (24%)
23	BCR	5	504	-	41,41,41	1.83	5 (12%)	56,56,56	4.57	21 (37%)
20	CLA	A	1106	-	69,73,73	1.37	8 (11%)	83,113,113	2.02	17 (20%)
20	CLA	A	1128	-	69,73,73	1.42	8 (11%)	83,113,113	1.90	15 (18%)
23	BCR	3	503	-	41,41,41	1.83	5 (12%)	56,56,56	4.19	16 (28%)
24	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
41	PLM	7	805	-	17,17,17	0.58	0	17,17,17	1.04	0
20	CLA	A	1116	-	64,68,73	1.43	7 (10%)	77,107,113	2.01	22 (28%)
20	CLA	5	613	-	59,63,73	1.49	7 (11%)	71,101,113	2.02	19 (26%)
20	CLA	A	1118	-	64,68,73	1.41	8 (12%)	77,107,113	2.02	19 (24%)
20	CLA	A	1122	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
20	CLA	A	1012	-	69,73,73	1.36	7 (10%)	83,113,113	2.02	19 (22%)
20	CLA	B	1222	-	69,73,73	1.39	7 (10%)	83,113,113	1.90	22 (26%)
20	CLA	A	1141	24	56,60,73	1.54	6 (10%)	67,97,113	2.13	18 (26%)
20	CLA	Z	612	-	69,73,73	1.37	6 (8%)	83,113,113	1.93	17 (20%)
37	CHL	7	610	-	58,62,74	0.93	2 (3%)	65,99,114	1.35	12 (18%)
20	CLA	1	601	-	69,73,73	1.37	6 (8%)	83,113,113	1.96	20 (24%)
20	CLA	A	1113	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	15 (18%)
34	C7Z	J	4002	-	43,43,43	5.36	27 (62%)	58,60,60	2.29	20 (34%)
20	CLA	1	613	-	50,54,73	1.60	8 (16%)	60,90,113	2.08	15 (25%)
20	CLA	7	601	-	64,68,73	1.44	8 (12%)	77,107,113	2.06	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	A	1136	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	16 (19%)
20	CLA	A	1107	1	69,73,73	1.38	8 (11%)	83,113,113	1.93	20 (24%)
23	BCR	B	4001	-	41,41,41	1.84	5 (12%)	56,56,56	4.19	13 (23%)
26	LMT	B	6101	-	36,36,36	1.18	5 (13%)	47,47,47	1.11	5 (10%)
20	CLA	B	1240	-	69,73,73	1.37	9 (13%)	83,113,113	1.89	20 (24%)
20	CLA	5	606	-	54,58,73	1.54	7 (12%)	65,95,113	2.16	18 (27%)
20	CLA	5	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	20 (25%)
20	CLA	7	613	-	46,50,73	1.68	7 (15%)	55,85,113	2.12	15 (27%)
20	CLA	A	1131	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	17 (20%)
20	CLA	6	605	-	59,63,73	1.50	8 (13%)	71,101,113	2.07	18 (25%)
20	CLA	B	1221	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	18 (21%)
20	CLA	1	608	-	64,68,73	1.39	6 (9%)	77,107,113	1.99	17 (22%)
20	CLA	1	611	-	69,73,73	1.35	7 (10%)	83,113,113	1.94	21 (25%)
36	LUT	3	501	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
20	CLA	4	608	-	59,63,73	1.49	8 (13%)	71,101,113	2.02	18 (25%)
36	LUT	Z	503	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	11 (21%)
20	CLA	B	1206	-	69,73,73	1.38	6 (8%)	83,113,113	1.91	17 (20%)
20	CLA	6	608	-	59,63,73	1.48	7 (11%)	71,101,113	2.11	18 (25%)
20	CLA	8	608	-	59,63,73	1.49	7 (11%)	71,101,113	1.99	17 (23%)
20	CLA	B	1212	-	61,65,73	1.45	6 (9%)	73,103,113	2.07	19 (26%)
20	CLA	1	615	12	69,73,73	1.39	7 (10%)	83,113,113	1.82	16 (19%)
20	CLA	Z	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)
20	CLA	7	611	-	54,58,73	1.53	7 (12%)	65,95,113	2.21	19 (29%)
24	LHG	B	5002	-	19,19,48	0.84	1 (5%)	20,24,54	1.34	1 (5%)
20	CLA	B	1223	-	69,73,73	1.38	6 (8%)	83,113,113	1.95	20 (24%)
20	CLA	6	607	-	59,63,73	1.47	7 (11%)	71,101,113	1.99	19 (26%)
20	CLA	A	1127	-	69,73,73	1.38	6 (8%)	83,113,113	1.82	18 (21%)
20	CLA	3	604	-	64,68,73	1.44	7 (10%)	77,107,113	2.09	21 (27%)
24	LHG	8	801	-	37,37,48	0.43	0	40,43,54	1.14	4 (10%)
20	CLA	A	1114	-	65,69,73	1.44	7 (10%)	78,108,113	1.97	15 (19%)
37	CHL	1	609	12	62,66,74	0.90	3 (4%)	70,104,114	1.31	12 (17%)
23	BCR	4	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	16 (28%)
29	LMG	J	5001	-	35,35,55	0.46	0	43,43,63	1.13	2 (4%)
20	CLA	3	602	-	50,54,73	1.60	7 (14%)	60,90,113	1.98	13 (21%)
20	CLA	8	607	-	59,63,73	1.50	6 (10%)	71,101,113	2.03	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	A	1111	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	18 (21%)
20	CLA	B	1023	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	18 (21%)
23	BCR	8	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.24	14 (25%)
20	CLA	A	1115	-	64,68,73	1.40	7 (10%)	77,107,113	2.01	19 (24%)
20	CLA	K	1404	-	59,63,73	1.48	7 (11%)	71,101,113	2.15	18 (25%)
19	CL0	A	1011	-	69,73,73	2.34	20 (28%)	83,113,113	2.58	26 (31%)
37	CHL	Z	609	12	70,74,74	0.88	3 (4%)	80,114,114	1.27	11 (13%)
35	SPH	7	803	-	19,20,20	0.66	0	18,21,21	0.90	0
20	CLA	7	602	-	54,58,73	1.53	7 (12%)	65,95,113	2.11	17 (26%)
23	BCR	G	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	15 (26%)
20	CLA	4	602	-	56,60,73	1.52	6 (10%)	67,97,113	2.13	17 (25%)
20	CLA	B	1218	-	69,73,73	1.38	7 (10%)	83,113,113	2.00	21 (25%)
20	CLA	3	601	-	69,73,73	1.38	8 (11%)	83,113,113	1.99	18 (21%)
23	BCR	7	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.28	14 (25%)
20	CLA	6	619	18	69,73,73	1.38	6 (8%)	83,113,113	1.91	17 (20%)
20	CLA	8	602	-	69,73,73	1.36	7 (10%)	83,113,113	2.00	21 (25%)
20	CLA	A	1125	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	20 (24%)
20	CLA	B	1241	-	69,73,73	1.39	9 (13%)	83,113,113	1.94	18 (21%)
29	LMG	A	5003	-	29,29,55	0.55	0	37,37,63	1.26	4 (10%)
22	SF4	C	3002	3	0,12,12	-	-	-		
37	CHL	5	617	-	47,51,74	1.01	2 (4%)	52,86,114	1.40	9 (17%)
23	BCR	5	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.30	19 (33%)
20	CLA	B	1205	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	17 (20%)
20	CLA	L	1503	-	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
20	CLA	8	611	-	54,58,73	1.53	7 (12%)	65,95,113	2.23	18 (27%)
20	CLA	4	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
20	CLA	A	1102	-	59,63,73	1.46	8 (13%)	71,101,113	2.15	20 (28%)
23	BCR	B	4005	-	41,41,41	1.89	4 (9%)	56,56,56	4.48	17 (30%)
20	CLA	1	603	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
24	LHG	A	5001	20	34,34,48	0.45	0	37,40,54	1.16	3 (8%)
20	CLA	6	604	-	69,73,73	1.36	6 (8%)	83,113,113	1.95	22 (26%)
20	CLA	6	603	-	69,73,73	1.36	6 (8%)	83,113,113	2.00	19 (22%)
20	CLA	7	603	-	69,73,73	1.36	8 (11%)	83,113,113	2.12	22 (26%)
25	NKP	A	5004	-	28,28,28	1.56	3 (10%)	31,32,32	1.23	3 (9%)
20	CLA	8	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.13	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	B	1213	2	69,73,73	1.37	8 (11%)	83,113,113	2.07	23 (27%)
22	SF4	C	3003	3	0,12,12	-	-	-		
26	LMT	B	5005	-	36,36,36	1.24	5 (13%)	47,47,47	1.15	4 (8%)
20	CLA	B	1224	-	69,73,73	1.39	7 (10%)	83,113,113	1.96	18 (21%)
20	CLA	B	1232	-	49,53,73	1.63	7 (14%)	59,89,113	2.06	13 (22%)
20	CLA	7	604	-	69,73,73	1.37	6 (8%)	83,113,113	1.91	20 (24%)
20	CLA	Z	607	-	61,65,73	1.45	7 (11%)	73,103,113	2.01	17 (23%)
20	CLA	B	1217	2	60,64,73	1.47	7 (11%)	72,102,113	2.01	17 (23%)
36	LUT	6	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.85	11 (21%)
26	LMT	4	803	-	36,36,36	1.21	6 (16%)	47,47,47	1.05	3 (6%)
20	CLA	3	612	-	64,68,73	1.42	8 (12%)	77,107,113	1.97	17 (22%)
20	CLA	8	605	-	69,73,73	1.39	7 (10%)	83,113,113	1.92	18 (21%)
20	CLA	A	1138	-	69,73,73	1.35	7 (10%)	83,113,113	2.05	17 (20%)
20	CLA	Z	602	-	50,54,73	1.60	6 (12%)	60,90,113	2.00	13 (21%)
36	LUT	Z	501	-	42,43,43	2.29	1 (2%)	51,60,60	1.91	11 (21%)
20	CLA	A	1126	-	69,73,73	1.39	8 (11%)	83,113,113	1.93	17 (20%)
20	CLA	4	609	16	64,68,73	1.41	7 (10%)	77,107,113	1.99	19 (24%)
20	CLA	A	1101	-	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
20	CLA	5	604	-	69,73,73	1.37	8 (11%)	83,113,113	1.96	20 (24%)
20	CLA	B	1225	-	69,73,73	1.39	8 (11%)	83,113,113	1.80	16 (19%)
22	SF4	A	3001	2,1	0,12,12	-	-	-		
40	3PH	5	802	-	22,22,47	1.24	4 (18%)	26,27,52	1.35	2 (7%)
20	CLA	B	1226	-	69,73,73	1.41	7 (10%)	83,113,113	2.05	21 (25%)
20	CLA	B	1228	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)
20	CLA	A	1120	-	59,63,73	1.46	7 (11%)	71,101,113	2.19	21 (29%)
20	CLA	4	604	-	64,68,73	1.42	7 (10%)	77,107,113	1.93	17 (22%)
20	CLA	5	609	-	69,73,73	1.37	9 (13%)	83,113,113	1.88	17 (20%)
20	CLA	J	1901	-	46,50,73	1.66	7 (15%)	55,85,113	2.17	16 (29%)
20	CLA	B	1022	43	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
25	NKP	3	802	-	15,15,28	2.07	3 (20%)	18,19,32	1.52	2 (11%)
24	LHG	Z	801	-	42,42,48	0.41	0	45,48,54	1.16	4 (8%)
31	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.07	6 (7%)
37	CHL	8	610	-	60,64,74	0.93	2 (3%)	68,102,114	1.35	12 (17%)
20	CLA	B	1215	-	64,68,73	1.42	7 (10%)	77,107,113	1.95	18 (23%)
25	NKP	8	802	-	28,28,28	1.51	2 (7%)	31,32,32	1.25	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	BCR	A	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.11	14 (25%)
26	LMT	F	5001	-	36,36,36	1.21	6 (16%)	47,47,47	0.92	1 (2%)
33	RRX	F	4001	-	42,42,42	4.79	24 (57%)	57,58,58	2.53	23 (40%)
20	CLA	F	1302	-	49,53,73	1.62	8 (16%)	59,89,113	2.02	15 (25%)
26	LMT	1	803	-	36,36,36	1.17	5 (13%)	47,47,47	0.99	1 (2%)
36	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	2.00	16 (31%)
20	CLA	6	601	-	64,68,73	1.43	7 (10%)	77,107,113	2.02	22 (28%)
36	LUT	4	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.83	14 (27%)
20	CLA	8	609	15	69,73,73	1.37	7 (10%)	83,113,113	1.96	20 (24%)
24	LHG	5	801	-	36,36,48	0.44	0	39,42,54	1.18	3 (7%)
38	SQD	1	802	-	47,48,54	0.83	0	56,59,65	0.94	2 (3%)
37	CHL	4	613	-	60,64,74	0.93	2 (3%)	68,102,114	1.32	10 (14%)
37	CHL	5	610	-	70,74,74	0.84	2 (2%)	80,114,114	1.19	10 (12%)
36	LUT	7	502	-	42,43,43	2.30	1 (2%)	51,60,60	1.96	12 (23%)
20	CLA	A	1135	-	55,59,73	1.54	8 (14%)	66,96,113	2.22	20 (30%)
37	CHL	4	610	-	55,59,74	0.93	2 (3%)	62,96,114	1.48	12 (19%)
20	CLA	A	1108	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	17 (20%)
20	CLA	1	607	-	64,68,73	1.43	6 (9%)	77,107,113	1.98	18 (23%)
23	BCR	B	4007	-	41,41,41	1.83	4 (9%)	56,56,56	4.18	16 (28%)
20	CLA	Z	606	-	61,65,73	1.48	9 (14%)	73,103,113	2.02	20 (27%)
26	LMT	8	805	-	36,36,36	1.20	5 (13%)	47,47,47	1.01	1 (2%)
20	CLA	8	615	15	50,54,73	1.59	7 (14%)	60,90,113	2.12	17 (28%)
23	BCR	B	4004	-	41,41,41	1.82	4 (9%)	56,56,56	4.25	14 (25%)
21	PQN	A	2001	-	34,34,34	0.39	0	42,45,45	1.15	2 (4%)
20	CLA	7	607	-	69,73,73	1.37	6 (8%)	83,113,113	1.98	18 (21%)
34	C7Z	1	503	-	43,43,43	5.38	26 (60%)	58,60,60	2.36	20 (34%)
20	CLA	A	1121	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	20 (24%)
20	CLA	3	616	-	60,64,73	1.45	6 (10%)	72,102,113	2.11	18 (25%)
23	BCR	K	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	14 (25%)
20	CLA	G	1601	-	54,58,73	1.52	6 (11%)	65,95,113	2.17	18 (27%)
20	CLA	Z	601	-	64,68,73	1.41	7 (10%)	77,107,113	2.00	19 (24%)
24	LHG	B	5006	-	32,32,48	0.45	0	35,38,54	1.16	2 (5%)
20	CLA	A	1130	-	69,73,73	1.37	7 (10%)	83,113,113	1.88	18 (21%)
21	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.09	2 (4%)
23	BCR	L	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	BCR	6	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	15 (26%)
20	CLA	B	1207	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
20	CLA	7	612	-	54,58,73	1.55	7 (12%)	65,95,113	2.08	17 (26%)
20	CLA	5	618	-	69,73,73	1.35	7 (10%)	83,113,113	2.06	19 (22%)
20	CLA	B	1227	-	54,58,73	1.57	7 (12%)	65,95,113	2.14	18 (27%)
20	CLA	5	615	17	54,58,73	1.54	6 (11%)	65,95,113	2.15	18 (27%)
20	CLA	7	615	14	62,66,73	1.44	8 (12%)	74,104,113	2.00	17 (22%)
20	CLA	B	1230	-	62,66,73	1.45	6 (9%)	74,104,113	2.07	19 (25%)
37	CHL	4	611	-	55,59,74	0.95	2 (3%)	62,96,114	1.37	10 (16%)
23	BCR	L	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.27	13 (23%)
20	CLA	Z	608	-	60,64,73	1.47	9 (15%)	72,102,113	2.04	19 (26%)
20	CLA	Z	611	-	59,63,73	1.47	8 (13%)	71,101,113	2.08	19 (26%)
20	CLA	6	602	-	56,60,73	1.53	6 (10%)	67,97,113	2.08	18 (26%)
20	CLA	B	1201	-	49,53,73	1.61	8 (16%)	59,89,113	2.10	20 (33%)
36	LUT	8	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.92	14 (27%)
24	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
36	LUT	8	501	-	42,43,43	2.30	1 (2%)	51,60,60	1.95	14 (27%)
20	CLA	3	608	-	49,53,73	1.62	7 (14%)	59,89,113	2.10	15 (25%)
20	CLA	A	1134	1	59,63,73	1.47	6 (10%)	71,101,113	2.12	17 (23%)
20	CLA	Z	615	-	50,54,73	1.58	6 (12%)	60,90,113	2.04	17 (28%)
20	CLA	K	1401	-	50,54,73	1.61	7 (14%)	60,90,113	2.00	15 (25%)
23	BCR	I	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.27	15 (26%)
20	CLA	B	1235	-	69,73,73	1.36	8 (11%)	83,113,113	1.97	17 (20%)
20	CLA	B	1239	-	69,73,73	1.34	7 (10%)	83,113,113	2.04	17 (20%)
36	LUT	3	502	-	42,43,43	2.43	1 (2%)	51,60,60	2.02	16 (31%)
20	CLA	4	603	-	69,73,73	1.35	6 (8%)	83,113,113	2.08	21 (25%)
20	CLA	5	602	-	65,69,73	1.40	8 (12%)	78,108,113	1.92	16 (20%)
20	CLA	G	1602	-	50,54,73	1.58	8 (16%)	60,90,113	2.18	17 (28%)
40	3PH	8	806	-	29,29,47	1.09	4 (13%)	33,34,52	1.11	2 (6%)
20	CLA	B	1208	-	60,64,73	1.46	7 (11%)	72,102,113	2.09	17 (23%)
23	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	14 (25%)
24	LHG	B	5001	-	22,22,48	0.55	0	25,28,54	1.30	2 (8%)
27	OCA	A	5008	-	9,9,9	0.65	0	9,9,9	0.97	0
24	LHG	4	802	-	31,31,48	0.46	0	34,37,54	1.13	2 (5%)
39	QTB	Z	504	-	19,19,19	2.50	5 (26%)	20,26,26	2.80	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	K	1403	-	53,57,73	1.53	6 (11%)	62,93,113	2.13	18 (29%)
20	CLA	A	1119	-	69,73,73	1.38	6 (8%)	83,113,113	1.82	17 (20%)
20	CLA	1	606	-	65,69,73	1.42	7 (10%)	78,108,113	1.97	16 (20%)
20	CLA	3	618	-	50,54,73	1.62	7 (14%)	60,90,113	2.07	15 (25%)
20	CLA	A	1112	-	64,68,73	1.41	7 (10%)	77,107,113	1.99	20 (25%)
20	CLA	B	1238	-	69,73,73	1.36	8 (11%)	83,113,113	1.98	18 (21%)
20	CLA	7	606	-	60,64,73	1.47	6 (10%)	72,102,113	2.00	17 (23%)
20	CLA	4	605	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	18 (21%)
20	CLA	1	604	-	64,68,73	1.42	6 (9%)	77,107,113	1.98	19 (24%)
20	CLA	6	606	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
20	CLA	4	607	-	59,63,73	1.48	7 (11%)	71,101,113	2.02	17 (23%)
20	CLA	6	615	-	65,69,73	1.40	6 (9%)	78,108,113	2.09	20 (25%)
20	CLA	7	605	14	65,69,73	1.38	7 (10%)	78,108,113	2.02	21 (26%)
20	CLA	3	605	-	69,73,73	1.37	8 (11%)	83,113,113	1.85	18 (21%)
20	CLA	5	603	-	60,64,73	1.44	6 (10%)	72,102,113	2.17	17 (23%)
37	CHL	1	610	-	52,56,74	0.93	2 (3%)	58,92,114	1.28	10 (17%)
35	SPH	7	804	-	19,20,20	0.69	0	18,21,21	1.06	1 (5%)
20	CLA	8	604	-	66,70,73	1.39	6 (9%)	79,109,113	2.03	22 (27%)
20	CLA	B	1209	-	69,73,73	1.36	7 (10%)	83,113,113	1.89	18 (21%)
36	LUT	5	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.77	12 (23%)
20	CLA	B	1231	-	69,73,73	1.36	6 (8%)	83,113,113	1.98	18 (21%)
23	BCR	A	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.14	12 (21%)
20	CLA	Z	603	-	54,58,73	1.55	7 (12%)	65,95,113	2.16	19 (29%)
20	CLA	7	608	-	47,51,73	1.67	9 (19%)	56,86,113	2.16	15 (26%)
20	CLA	4	612	-	54,58,73	1.56	6 (11%)	65,95,113	2.21	19 (29%)
23	BCR	A	4004	-	41,41,41	1.81	4 (9%)	56,56,56	4.37	16 (28%)
20	CLA	A	1123	-	69,73,73	1.38	8 (11%)	83,113,113	1.92	15 (18%)
20	CLA	A	1104	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	21 (25%)
37	CHL	6	610	-	60,64,74	0.89	2 (3%)	68,102,114	1.31	11 (16%)
20	CLA	B	1216	-	69,73,73	1.36	8 (11%)	83,113,113	1.87	16 (19%)
20	CLA	A	1109	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	17 (20%)
37	CHL	6	611	-	55,59,74	0.96	2 (3%)	62,96,114	1.29	7 (11%)
20	CLA	A	1140	-	69,73,73	1.37	7 (10%)	83,113,113	1.87	17 (20%)
20	CLA	8	612	-	50,54,73	1.61	8 (16%)	60,90,113	1.95	13 (21%)
20	CLA	8	601	15	64,68,73	1.43	7 (10%)	77,107,113	2.02	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	CHL	3	611	-	70,74,74	0.87	2 (2%)	80,114,114	1.30	12 (15%)
20	CLA	B	1214	-	63,67,73	1.45	8 (12%)	75,105,113	2.12	23 (30%)
20	CLA	B	1219	-	63,67,73	1.44	7 (11%)	75,105,113	2.09	21 (28%)
20	CLA	B	1236	-	69,73,73	1.38	8 (11%)	83,113,113	1.97	17 (20%)
20	CLA	A	1139	1	69,73,73	1.37	7 (10%)	83,113,113	1.98	23 (27%)
20	CLA	5	605	-	59,63,73	1.49	7 (11%)	71,101,113	2.17	21 (29%)
20	CLA	A	1129	-	54,58,73	1.55	7 (12%)	65,95,113	2.10	16 (24%)
23	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.21	17 (30%)
20	CLA	Z	605	-	69,73,73	1.37	6 (8%)	83,113,113	1.92	20 (24%)
35	SPH	K	5001	-	19,20,20	0.66	0	18,21,21	1.00	0
42	LPX	8	803	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
40	3PH	7	802	-	38,38,47	0.98	3 (7%)	42,43,52	1.16	2 (4%)
23	BCR	3	505	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	11 (19%)
20	CLA	B	1203	-	69,73,73	1.35	8 (11%)	83,113,113	1.90	20 (24%)
20	CLA	A	1103	1	69,73,73	1.33	6 (8%)	83,113,113	1.98	17 (20%)
23	BCR	A	4003	-	41,41,41	1.80	4 (9%)	56,56,56	4.35	20 (35%)
20	CLA	L	1502	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	19 (22%)
23	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.36	12 (21%)
37	CHL	4	617	-	47,51,74	1.01	2 (4%)	52,86,114	1.41	8 (15%)
20	CLA	A	1110	1	69,73,73	1.37	7 (10%)	83,113,113	2.05	17 (20%)
37	CHL	Z	610	-	70,74,74	0.80	2 (2%)	80,114,114	1.17	10 (12%)
20	CLA	A	1132	-	69,73,73	1.36	8 (11%)	83,113,113	1.94	18 (21%)
24	LHG	3	801	-	19,19,48	0.91	1 (5%)	20,24,54	1.44	1 (5%)
20	CLA	B	1234	-	64,68,73	1.44	7 (10%)	77,107,113	1.98	17 (22%)
20	CLA	B	1204	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	17 (20%)
20	CLA	F	1301	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	22 (26%)
24	LHG	4	801	-	48,48,48	0.40	0	51,54,54	1.13	4 (7%)
20	CLA	5	608	-	49,53,73	1.62	7 (14%)	59,89,113	2.16	15 (25%)
20	CLA	A	1117	-	69,73,73	1.37	7 (10%)	83,113,113	1.99	17 (20%)
37	CHL	5	611	-	55,59,74	0.89	2 (3%)	62,96,114	1.35	9 (14%)
20	CLA	3	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.06	19 (22%)
20	CLA	1	612	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
23	BCR	7	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	17 (30%)
20	CLA	B	1237	-	69,73,73	1.36	7 (10%)	83,113,113	1.86	17 (20%)
20	CLA	7	616	-	64,68,73	1.38	7 (10%)	77,107,113	2.14	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	A	1105	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)
20	CLA	3	606	-	69,73,73	1.34	7 (10%)	83,113,113	2.01	19 (22%)
20	CLA	A	1013	-	69,73,73	1.39	8 (11%)	83,113,113	1.88	20 (24%)
37	CHL	6	617	-	47,51,74	0.96	2 (4%)	52,86,114	1.33	8 (15%)
20	CLA	B	1210	-	69,73,73	1.38	6 (8%)	83,113,113	1.95	18 (21%)
20	CLA	K	1402	-	59,63,73	1.48	9 (15%)	71,101,113	2.07	19 (26%)
20	CLA	B	1202	-	69,73,73	1.37	6 (8%)	83,113,113	1.99	20 (24%)
34	C7Z	5	505	-	43,43,43	5.43	26 (60%)	58,60,60	2.17	17 (29%)
20	CLA	B	1021	-	69,73,73	1.37	6 (8%)	83,113,113	1.95	19 (22%)
36	LUT	Z	502	-	42,43,43	2.29	1 (2%)	51,60,60	1.98	13 (25%)
37	CHL	Z	613	-	50,54,74	0.98	2 (4%)	56,90,114	1.30	8 (14%)
36	LUT	1	501	-	42,43,43	2.31	1 (2%)	51,60,60	1.80	10 (19%)
36	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.94	13 (25%)
20	CLA	5	622	-	50,54,73	1.63	7 (14%)	60,90,113	2.11	14 (23%)
20	CLA	6	612	-	54,58,73	1.55	7 (12%)	65,95,113	2.16	18 (27%)
20	CLA	A	1124	-	69,73,73	1.37	6 (8%)	83,113,113	1.88	19 (22%)
20	CLA	6	618	-	50,54,73	1.58	6 (12%)	60,90,113	2.13	16 (26%)
20	CLA	3	613	-	59,63,73	1.48	7 (11%)	71,101,113	2.06	17 (23%)
20	CLA	4	606	-	54,58,73	1.53	8 (14%)	65,95,113	2.20	19 (29%)
20	CLA	4	615	-	45,49,73	1.68	6 (13%)	54,84,113	2.19	16 (29%)
20	CLA	A	1137	-	69,73,73	1.37	8 (11%)	83,113,113	2.01	21 (25%)
20	CLA	3	610	13	64,68,73	1.42	7 (10%)	77,107,113	1.98	20 (25%)
36	LUT	7	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.90	12 (23%)
37	CHL	6	613	-	60,64,74	0.90	2 (3%)	68,102,114	1.20	9 (13%)
37	CHL	8	613	-	70,74,74	0.91	3 (4%)	80,114,114	1.22	11 (13%)
24	LHG	1	801	-	42,42,48	0.45	0	45,48,54	1.11	2 (4%)
20	CLA	A	1133	1	69,73,73	1.38	7 (10%)	83,113,113	1.84	16 (19%)
20	CLA	B	1211	-	64,68,73	1.45	7 (10%)	77,107,113	1.86	14 (18%)
23	BCR	A	4005	-	41,41,41	1.83	5 (12%)	56,56,56	4.17	11 (19%)
23	BCR	J	4001	-	41,41,41	1.81	4 (9%)	56,56,56	4.27	17 (30%)
20	CLA	5	612	-	69,73,73	1.35	6 (8%)	83,113,113	1.86	17 (20%)
20	CLA	B	1220	-	69,73,73	1.37	6 (8%)	83,113,113	1.87	16 (19%)
23	BCR	3	504	-	41,41,41	1.83	5 (12%)	56,56,56	4.28	15 (26%)
20	CLA	5	607	-	65,69,73	1.41	7 (10%)	78,108,113	1.97	19 (24%)
20	CLA	1	602	-	49,53,73	1.64	9 (18%)	59,89,113	2.04	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
40	3PH	6	802	-	28,28,47	1.11	4 (14%)	32,33,52	1.29	2 (6%)

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
20	CLA	7	609	14	-	21/39/115/115	-
23	BCR	6	504	-	-	11/29/63/63	0/2/2/2
24	LHG	7	801	-	-	26/41/41/53	-
20	CLA	6	609	18	-	13/39/115/115	-
36	LUT	5	501	-	-	3/29/67/67	0/2/2/2
28	DAO	A	5007	-	-	1/11/11/11	-
20	CLA	8	606	-	-	13/33/109/115	-
36	LUT	6	502	-	-	2/29/67/67	0/2/2/2
20	CLA	1	605	-	-	11/27/103/115	-
26	LMT	A	5006	-	-	12/21/61/61	0/2/2/2
23	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
20	CLA	B	1229	-	-	13/39/115/115	-
30	DGA	A	5005	-	-	21/45/45/45	-
23	BCR	3	506	-	-	15/29/63/63	0/2/2/2
20	CLA	3	607	-	-	23/33/109/115	-
23	BCR	5	504	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1106	-	-	18/39/115/115	-
20	CLA	A	1128	-	-	19/39/115/115	-
23	BCR	3	503	-	-	10/29/63/63	0/2/2/2
24	LHG	6	801	-	-	33/53/53/53	-
41	PLM	7	805	-	-	7/15/15/15	-
20	CLA	A	1116	-	-	14/33/109/115	-
20	CLA	5	613	-	-	14/27/103/115	-
20	CLA	A	1118	-	-	16/33/109/115	-
20	CLA	A	1122	-	-	21/39/115/115	-
20	CLA	A	1012	-	-	19/39/115/115	-
20	CLA	B	1222	-	-	15/39/115/115	-
20	CLA	A	1141	24	-	11/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	Z	612	-	-	18/39/115/115	-
37	CHL	7	610	-	-	5/27/103/117	-
20	CLA	1	601	-	-	17/39/115/115	-
20	CLA	A	1113	-	-	12/39/115/115	-
34	C7Z	J	4002	-	1/1/12/26	11/29/67/67	0/2/2/2
20	CLA	1	613	-	-	10/17/93/115	-
20	CLA	7	601	-	-	14/33/109/115	-
20	CLA	A	1136	-	-	16/39/115/115	-
20	CLA	A	1107	1	-	17/39/115/115	-
23	BCR	B	4001	-	-	13/29/63/63	0/2/2/2
26	LMT	B	6101	-	-	10/21/61/61	0/2/2/2
20	CLA	B	1240	-	-	21/39/115/115	-
20	CLA	5	606	-	-	14/21/97/115	-
20	CLA	5	601	-	-	17/33/109/115	-
20	CLA	7	613	-	-	6/12/88/115	-
20	CLA	A	1131	-	-	17/39/115/115	-
20	CLA	6	605	-	-	16/27/103/115	-
20	CLA	B	1221	-	-	16/39/115/115	-
20	CLA	1	608	-	-	14/33/109/115	-
20	CLA	1	611	-	-	16/39/115/115	-
36	LUT	3	501	-	-	1/29/67/67	0/2/2/2
20	CLA	4	608	-	-	10/27/103/115	-
36	LUT	Z	503	-	-	6/29/67/67	0/2/2/2
20	CLA	B	1206	-	-	18/39/115/115	-
20	CLA	6	608	-	-	14/27/103/115	-
20	CLA	8	608	-	-	13/27/103/115	-
20	CLA	B	1212	-	-	9/30/106/115	-
20	CLA	1	615	12	-	17/39/115/115	-
20	CLA	Z	604	-	-	19/39/115/115	-
20	CLA	7	611	-	-	4/21/97/115	-
24	LHG	B	5002	-	-	11/22/22/53	-
20	CLA	B	1223	-	-	18/39/115/115	-
20	CLA	6	607	-	-	8/27/103/115	-
20	CLA	A	1127	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	604	-	-	9/33/109/115	-
24	LHG	8	801	-	-	20/42/42/53	-
37	CHL	1	609	12	1/1/13/21	5/32/108/117	-
20	CLA	A	1114	-	-	9/35/111/115	-
23	BCR	4	503	-	-	16/29/63/63	0/2/2/2
29	LMG	J	5001	-	-	10/30/50/70	0/1/1/1
20	CLA	3	602	-	-	6/17/93/115	-
20	CLA	8	607	-	-	16/27/103/115	-
20	CLA	A	1111	-	-	17/39/115/115	-
20	CLA	B	1023	-	-	17/39/115/115	-
23	BCR	8	503	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1115	-	-	15/33/109/115	-
20	CLA	K	1404	-	-	13/27/103/115	-
19	CL0	A	1011	-	-	11/39/115/115	-
37	CHL	Z	609	12	1/1/15/21	12/41/117/117	-
35	SPH	7	803	-	-	7/21/21/21	-
20	CLA	7	602	-	-	7/21/97/115	-
23	BCR	G	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	4	602	-	-	8/24/100/115	-
20	CLA	B	1218	-	-	16/39/115/115	-
20	CLA	3	601	-	-	12/39/115/115	-
23	BCR	7	503	-	-	10/29/63/63	0/2/2/2
20	CLA	6	619	18	-	18/39/115/115	-
20	CLA	8	602	-	-	17/39/115/115	-
20	CLA	A	1125	-	-	22/39/115/115	-
20	CLA	B	1241	-	-	23/39/115/115	-
29	LMG	A	5003	-	-	8/24/44/70	0/1/1/1
22	SF4	C	3002	3	-	-	0/6/5/5
37	CHL	5	617	-	-	3/14/90/117	-
23	BCR	5	503	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1205	-	-	18/39/115/115	-
20	CLA	L	1503	-	-	10/21/97/115	-
20	CLA	8	611	-	-	7/21/97/115	-
20	CLA	4	601	-	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1102	-	-	15/27/103/115	-
23	BCR	B	4005	-	-	13/29/63/63	0/2/2/2
20	CLA	1	603	-	-	17/39/115/115	-
24	LHG	A	5001	20	-	22/39/39/53	-
20	CLA	6	604	-	-	12/39/115/115	-
20	CLA	6	603	-	-	21/39/115/115	-
20	CLA	7	603	-	-	15/39/115/115	-
25	NKP	A	5004	-	-	14/28/28/28	-
20	CLA	8	603	-	-	8/39/115/115	-
20	CLA	B	1213	2	-	21/39/115/115	-
26	LMT	B	5005	-	-	14/21/61/61	0/2/2/2
22	SF4	C	3003	3	-	-	0/6/5/5
20	CLA	B	1224	-	-	17/39/115/115	-
20	CLA	B	1232	-	-	4/15/91/115	-
20	CLA	7	604	-	-	15/39/115/115	-
20	CLA	Z	607	-	-	15/30/106/115	-
20	CLA	B	1217	2	-	17/29/105/115	-
36	LUT	6	501	-	-	4/29/67/67	0/2/2/2
26	LMT	4	803	-	-	11/21/61/61	0/2/2/2
20	CLA	3	612	-	-	11/33/109/115	-
20	CLA	8	605	-	-	19/39/115/115	-
20	CLA	A	1138	-	-	16/39/115/115	-
20	CLA	Z	602	-	-	4/17/93/115	-
36	LUT	Z	501	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1126	-	-	22/39/115/115	-
20	CLA	4	609	16	-	15/33/109/115	-
20	CLA	A	1101	-	-	16/39/115/115	-
20	CLA	5	604	-	-	13/39/115/115	-
20	CLA	B	1225	-	-	11/39/115/115	-
22	SF4	A	3001	2,1	-	-	0/6/5/5
40	3PH	5	802	-	-	9/24/24/49	-
20	CLA	B	1226	-	-	17/39/115/115	-
20	CLA	B	1228	-	-	18/39/115/115	-
20	CLA	A	1120	-	-	15/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	604	-	-	9/33/109/115	-
20	CLA	5	609	-	-	13/39/115/115	-
20	CLA	J	1901	-	-	4/12/88/115	-
20	CLA	B	1022	43	-	9/39/115/115	-
25	NKP	3	802	-	-	2/15/15/28	-
24	LHG	Z	801	-	-	29/47/47/53	-
31	DGD	B	5003	-	-	17/55/95/95	0/2/2/2
37	CHL	8	610	-	1/1/13/21	6/29/105/117	-
20	CLA	B	1215	-	-	17/33/109/115	-
25	NKP	8	802	-	-	15/28/28/28	-
23	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
26	LMT	F	5001	-	-	8/21/61/61	0/2/2/2
33	RRX	F	4001	-	1/1/11/25	9/29/65/65	0/2/2/2
20	CLA	F	1302	-	-	6/15/91/115	-
26	LMT	1	803	-	-	6/21/61/61	0/2/2/2
36	LUT	1	502	-	-	1/29/67/67	0/2/2/2
20	CLA	6	601	-	-	15/33/109/115	-
36	LUT	4	502	-	-	4/29/67/67	0/2/2/2
20	CLA	8	609	15	-	19/39/115/115	-
24	LHG	5	801	-	-	27/41/41/53	-
38	SQD	1	802	-	-	21/43/63/69	0/1/1/1
37	CHL	4	613	-	1/1/13/21	3/29/105/117	-
37	CHL	5	610	-	1/1/15/21	9/41/117/117	-
36	LUT	7	502	-	-	2/29/67/67	0/2/2/2
37	CHL	4	610	-	1/1/12/21	5/23/99/117	-
20	CLA	A	1135	-	-	11/23/99/115	-
20	CLA	A	1108	-	-	25/39/115/115	-
20	CLA	1	607	-	-	14/33/109/115	-
23	BCR	B	4007	-	-	12/29/63/63	0/2/2/2
20	CLA	Z	606	-	-	9/30/106/115	-
26	LMT	8	805	-	-	5/21/61/61	0/2/2/2
20	CLA	8	615	15	-	9/17/93/115	-
23	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
21	PQN	A	2001	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	607	-	-	23/39/115/115	-
34	C7Z	1	503	-	1/1/12/26	6/29/67/67	0/2/2/2
20	CLA	A	1121	-	-	23/39/115/115	-
20	CLA	3	616	-	-	10/29/105/115	-
23	BCR	K	4002	-	-	8/29/63/63	0/2/2/2
20	CLA	G	1601	-	-	10/21/97/115	-
20	CLA	Z	601	-	-	12/33/109/115	-
24	LHG	B	5006	-	-	24/37/37/53	-
20	CLA	A	1130	-	-	17/39/115/115	-
21	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
23	BCR	L	4002	-	-	11/29/63/63	0/2/2/2
23	BCR	6	503	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1207	-	-	16/39/115/115	-
20	CLA	7	612	-	-	10/21/97/115	-
20	CLA	5	618	-	-	18/39/115/115	-
20	CLA	B	1227	-	-	11/21/97/115	-
20	CLA	5	615	17	-	7/21/97/115	-
20	CLA	7	615	14	-	17/31/107/115	-
20	CLA	B	1230	-	-	13/31/107/115	-
37	CHL	4	611	-	-	6/23/99/117	-
23	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	Z	608	-	-	13/29/105/115	-
20	CLA	Z	611	-	-	10/27/103/115	-
20	CLA	6	602	-	-	7/24/100/115	-
20	CLA	B	1201	-	-	4/15/91/115	-
36	LUT	8	502	-	-	2/29/67/67	0/2/2/2
24	LHG	A	5002	-	-	29/53/53/53	-
36	LUT	8	501	-	-	2/29/67/67	0/2/2/2
20	CLA	3	608	-	-	8/15/91/115	-
20	CLA	A	1134	1	-	12/27/103/115	-
20	CLA	Z	615	-	-	9/17/93/115	-
20	CLA	K	1401	-	-	7/17/93/115	-
23	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1235	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1239	-	-	16/39/115/115	-
36	LUT	3	502	-	-	1/29/67/67	0/2/2/2
20	CLA	4	603	-	-	16/39/115/115	-
20	CLA	5	602	-	-	16/35/111/115	-
20	CLA	G	1602	-	-	8/17/93/115	-
40	3PH	8	806	-	-	13/31/31/49	-
20	CLA	B	1208	-	-	11/29/105/115	-
23	BCR	B	4002	-	-	12/29/63/63	0/2/2/2
24	LHG	B	5001	-	-	15/26/26/53	-
27	OCA	A	5008	-	-	2/7/7/7	-
24	LHG	4	802	-	-	20/36/36/53	-
39	QTB	Z	504	-	1/1/5/10	6/11/28/28	0/1/1/1
20	CLA	K	1403	-	-	12/20/96/115	-
20	CLA	A	1119	-	-	19/39/115/115	-
20	CLA	1	606	-	-	15/35/111/115	-
20	CLA	3	618	-	-	11/17/93/115	-
20	CLA	A	1112	-	-	15/33/109/115	-
20	CLA	B	1238	-	-	15/39/115/115	-
20	CLA	7	606	-	-	15/29/105/115	-
20	CLA	4	605	-	-	14/39/115/115	-
20	CLA	1	604	-	-	13/33/109/115	-
20	CLA	6	606	-	-	18/39/115/115	-
20	CLA	4	607	-	-	10/27/103/115	-
20	CLA	6	615	-	-	14/35/111/115	-
20	CLA	7	605	14	-	19/35/111/115	-
20	CLA	3	605	-	-	11/39/115/115	-
20	CLA	5	603	-	-	10/29/105/115	-
37	CHL	1	610	-	-	4/20/96/117	-
35	SPH	7	804	-	-	11/21/21/21	-
20	CLA	8	604	-	-	13/36/112/115	-
20	CLA	B	1209	-	-	25/39/115/115	-
36	LUT	5	502	-	-	2/29/67/67	0/2/2/2
20	CLA	B	1231	-	-	12/39/115/115	-
23	BCR	A	4001	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	Z	603	-	-	12/21/97/115	-
20	CLA	7	608	-	-	8/13/89/115	-
20	CLA	4	612	-	-	9/21/97/115	-
23	BCR	A	4004	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1123	-	-	13/39/115/115	-
20	CLA	A	1104	-	-	21/39/115/115	-
37	CHL	6	610	-	1/1/13/21	9/29/105/117	-
20	CLA	B	1216	-	-	22/39/115/115	-
20	CLA	A	1109	-	-	13/39/115/115	-
37	CHL	6	611	-	-	7/23/99/117	-
20	CLA	A	1140	-	-	19/39/115/115	-
20	CLA	8	612	-	-	9/17/93/115	-
20	CLA	8	601	15	-	13/33/109/115	-
37	CHL	3	611	-	1/1/15/21	7/41/117/117	-
20	CLA	B	1214	-	-	15/32/108/115	-
20	CLA	B	1219	-	-	17/32/108/115	-
20	CLA	B	1236	-	-	24/39/115/115	-
20	CLA	A	1139	1	-	15/39/115/115	-
20	CLA	5	605	-	-	14/27/103/115	-
20	CLA	A	1129	-	-	9/21/97/115	-
23	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
20	CLA	Z	605	-	-	12/39/115/115	-
35	SPH	K	5001	-	-	14/21/21/21	-
42	LPX	8	803	-	-	11/31/31/31	-
40	3PH	7	802	-	-	21/40/40/49	-
23	BCR	3	505	-	-	10/29/63/63	0/2/2/2
20	CLA	B	1203	-	-	19/39/115/115	-
20	CLA	A	1103	1	-	17/39/115/115	-
23	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
20	CLA	L	1502	-	-	26/39/115/115	-
23	BCR	K	4001	-	-	14/29/63/63	0/2/2/2
37	CHL	4	617	-	-	1/14/90/117	-
20	CLA	A	1110	1	-	20/39/115/115	-
37	CHL	Z	610	-	1/1/15/21	5/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1132	-	-	20/39/115/115	-
24	LHG	3	801	-	-	12/22/22/53	-
20	CLA	B	1234	-	-	21/33/109/115	-
20	CLA	B	1204	-	-	15/39/115/115	-
20	CLA	F	1301	-	-	15/39/115/115	-
24	LHG	4	801	-	-	33/53/53/53	-
20	CLA	5	608	-	-	7/15/91/115	-
20	CLA	A	1117	-	-	19/39/115/115	-
37	CHL	5	611	-	-	3/23/99/117	-
20	CLA	3	603	-	-	18/39/115/115	-
20	CLA	1	612	-	-	24/39/115/115	-
23	BCR	7	504	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1237	-	-	20/39/115/115	-
20	CLA	7	616	-	-	13/33/109/115	-
20	CLA	A	1105	-	-	14/39/115/115	-
20	CLA	3	606	-	-	20/39/115/115	-
20	CLA	A	1013	-	-	18/39/115/115	-
37	CHL	6	617	-	-	2/14/90/117	-
20	CLA	B	1210	-	-	20/39/115/115	-
20	CLA	K	1402	-	-	16/27/103/115	-
20	CLA	B	1202	-	-	17/39/115/115	-
34	C7Z	5	505	-	1/1/12/26	12/29/67/67	0/2/2/2
20	CLA	B	1021	-	-	15/39/115/115	-
36	LUT	Z	502	-	-	1/29/67/67	0/2/2/2
37	CHL	Z	613	-	-	3/17/93/117	-
36	LUT	1	501	-	-	5/29/67/67	0/2/2/2
36	LUT	4	501	-	-	5/29/67/67	0/2/2/2
20	CLA	5	622	-	-	7/17/93/115	-
20	CLA	6	612	-	-	9/21/97/115	-
20	CLA	A	1124	-	-	16/39/115/115	-
20	CLA	6	618	-	-	10/17/93/115	-
20	CLA	3	613	-	-	7/27/103/115	-
20	CLA	4	606	-	-	11/21/97/115	-
20	CLA	4	615	-	-	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1137	-	-	13/39/115/115	-
20	CLA	3	610	13	-	14/33/109/115	-
36	LUT	7	501	-	-	3/29/67/67	0/2/2/2
37	CHL	6	613	-	1/1/13/21	3/29/105/117	-
37	CHL	8	613	-	2/2/15/21	10/41/117/117	-
24	LHG	1	801	-	-	24/47/47/53	-
20	CLA	A	1133	1	-	16/39/115/115	-
20	CLA	B	1211	-	-	16/33/109/115	-
23	BCR	A	4005	-	-	15/29/63/63	0/2/2/2
23	BCR	J	4001	-	-	17/29/63/63	0/2/2/2
20	CLA	5	612	-	-	10/39/115/115	-
20	CLA	B	1220	-	-	21/39/115/115	-
23	BCR	3	504	-	-	11/29/63/63	0/2/2/2
20	CLA	5	607	-	-	15/35/111/115	-
20	CLA	1	602	-	-	5/15/91/115	-
40	3PH	6	802	-	-	15/30/30/49	-

All (1775) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	4002	C7Z	C25-C26	15.76	1.61	1.34
34	5	505	C7Z	C5-C6	15.72	1.61	1.34
34	1	503	C7Z	C25-C26	15.70	1.61	1.34
34	5	505	C7Z	C25-C26	15.69	1.61	1.34
34	1	503	C7Z	C5-C6	15.12	1.60	1.34
36	5	501	LUT	C24-C25	14.92	1.51	1.33
36	3	502	LUT	C24-C25	14.91	1.51	1.33
34	J	4002	C7Z	C5-C6	14.90	1.60	1.34
33	F	4001	RRX	C26-C25	14.89	1.60	1.34
36	Z	503	LUT	C24-C25	14.70	1.51	1.33
36	4	501	LUT	C24-C25	14.56	1.51	1.33
36	6	502	LUT	C24-C25	14.51	1.51	1.33
36	6	501	LUT	C24-C25	14.50	1.51	1.33
36	7	501	LUT	C24-C25	14.40	1.51	1.33
33	F	4001	RRX	C5-C6	14.39	1.59	1.34
36	3	501	LUT	C24-C25	14.26	1.50	1.33
36	1	501	LUT	C24-C25	14.17	1.50	1.33
36	1	502	LUT	C24-C25	14.15	1.50	1.33
36	8	501	LUT	C24-C25	14.08	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	502	LUT	C24-C25	14.07	1.50	1.33
36	Z	501	LUT	C24-C25	14.06	1.50	1.33
36	Z	502	LUT	C24-C25	14.01	1.50	1.33
36	7	502	LUT	C24-C25	14.01	1.50	1.33
36	5	502	LUT	C24-C25	13.87	1.50	1.33
36	8	502	LUT	C24-C25	13.72	1.50	1.33
34	1	503	C7Z	C24-C23	12.02	1.73	1.52
34	5	505	C7Z	C24-C23	12.00	1.73	1.52
34	J	4002	C7Z	C24-C23	11.51	1.72	1.52
34	5	505	C7Z	C2-C3	-10.90	1.36	1.52
34	J	4002	C7Z	C2-C3	-10.67	1.37	1.52
34	J	4002	C7Z	C22-C23	-10.54	1.37	1.52
34	1	503	C7Z	C2-C3	-10.40	1.37	1.52
34	5	505	C7Z	C22-C23	-10.40	1.37	1.52
34	1	503	C7Z	C22-C23	-10.35	1.37	1.52
33	F	4001	RRX	C29-C28	-9.49	1.38	1.52
19	A	1011	CL0	MG-NA	8.93	2.27	2.06
34	1	503	C7Z	C4-C3	8.87	1.67	1.52
34	J	4002	C7Z	C4-C3	8.57	1.67	1.52
33	F	4001	RRX	C27-C28	8.29	1.66	1.52
34	5	505	C7Z	C4-C3	8.13	1.66	1.52
39	Z	504	QTB	C11-C12	-7.88	1.36	1.54
23	3	506	BCR	C10-C9	7.49	1.45	1.35
23	7	504	BCR	C10-C9	7.41	1.45	1.35
23	6	503	BCR	C10-C9	7.26	1.45	1.35
23	3	505	BCR	C10-C9	7.20	1.45	1.35
23	K	4002	BCR	C10-C9	7.17	1.45	1.35
23	8	503	BCR	C10-C9	7.16	1.45	1.35
23	I	4001	BCR	C10-C9	7.13	1.45	1.35
23	A	4001	BCR	C10-C9	7.12	1.45	1.35
23	A	4002	BCR	C10-C9	7.10	1.45	1.35
25	A	5004	NKP	PAC-OAF	7.10	1.83	1.60
23	K	4001	BCR	C10-C9	7.09	1.45	1.35
23	B	4002	BCR	C10-C9	7.08	1.45	1.35
23	6	504	BCR	C10-C9	7.07	1.45	1.35
23	A	4003	BCR	C10-C9	7.03	1.45	1.35
23	L	4001	BCR	C10-C9	7.02	1.45	1.35
23	B	4003	BCR	C10-C9	7.01	1.45	1.35
23	B	4005	BCR	C10-C9	6.98	1.45	1.35
23	L	4002	BCR	C10-C9	6.96	1.45	1.35
25	3	802	NKP	PAC-OAF	6.96	1.82	1.60
23	4	503	BCR	C10-C9	6.92	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	802	NKP	PAC-OAF	6.91	1.82	1.60
23	B	4006	BCR	C10-C9	6.85	1.44	1.35
23	5	503	BCR	C10-C9	6.79	1.44	1.35
23	7	503	BCR	C10-C9	6.78	1.44	1.35
23	G	4001	BCR	C10-C9	6.76	1.44	1.35
23	J	4001	BCR	C10-C9	6.76	1.44	1.35
23	B	4007	BCR	C10-C9	6.68	1.44	1.35
20	B	1240	CLA	MG-NA	6.54	2.21	2.06
23	B	4001	BCR	C10-C9	6.53	1.44	1.35
23	A	4005	BCR	C10-C9	6.53	1.44	1.35
23	3	504	BCR	C10-C9	6.52	1.44	1.35
20	K	1402	CLA	MG-NA	6.49	2.21	2.06
20	F	1302	CLA	MG-NA	6.49	2.21	2.06
33	F	4001	RRX	C2-C3	-6.47	1.36	1.52
20	B	1241	CLA	MG-NA	6.47	2.21	2.06
23	B	4004	BCR	C10-C9	6.46	1.44	1.35
20	B	1232	CLA	MG-NA	6.46	2.21	2.06
20	B	1218	CLA	MG-NA	6.46	2.21	2.06
20	4	608	CLA	MG-NA	6.45	2.21	2.06
20	A	1116	CLA	MG-NA	6.45	2.21	2.06
20	B	1234	CLA	MG-NA	6.45	2.21	2.06
20	1	615	CLA	MG-NA	6.44	2.21	2.06
20	7	608	CLA	MG-NA	6.44	2.21	2.06
20	A	1110	CLA	MG-NA	6.43	2.21	2.06
20	K	1401	CLA	MG-NA	6.43	2.21	2.06
20	5	622	CLA	MG-NA	6.43	2.21	2.06
23	A	4004	BCR	C10-C9	6.43	1.44	1.35
20	7	603	CLA	MG-NA	6.42	2.21	2.06
20	5	604	CLA	MG-NA	6.41	2.21	2.06
20	6	605	CLA	MG-NA	6.41	2.21	2.06
20	1	613	CLA	MG-NA	6.41	2.21	2.06
20	1	607	CLA	MG-NA	6.41	2.21	2.06
20	3	602	CLA	MG-NA	6.41	2.21	2.06
20	A	1130	CLA	MG-NA	6.41	2.21	2.06
20	B	1214	CLA	MG-NA	6.41	2.21	2.06
20	3	618	CLA	MG-NA	6.40	2.21	2.06
20	Z	607	CLA	MG-NA	6.40	2.21	2.06
20	5	607	CLA	MG-NA	6.40	2.21	2.06
20	A	1123	CLA	MG-NA	6.39	2.21	2.06
20	3	608	CLA	MG-NA	6.39	2.21	2.06
20	5	609	CLA	MG-NA	6.39	2.21	2.06
20	3	607	CLA	MG-NA	6.38	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	602	CLA	MG-NA	6.38	2.21	2.06
20	A	1139	CLA	MG-NA	6.38	2.21	2.06
20	B	1219	CLA	MG-NA	6.37	2.21	2.06
20	Z	605	CLA	MG-NA	6.37	2.21	2.06
20	4	602	CLA	MG-NA	6.37	2.21	2.06
20	Z	611	CLA	MG-NA	6.37	2.21	2.06
20	5	613	CLA	MG-NA	6.36	2.21	2.06
20	3	603	CLA	MG-NA	6.36	2.21	2.06
20	Z	602	CLA	MG-NA	6.36	2.21	2.06
20	A	1141	CLA	MG-NA	6.35	2.21	2.06
20	8	609	CLA	MG-NA	6.35	2.21	2.06
23	3	503	BCR	C10-C9	6.35	1.44	1.35
20	7	605	CLA	MG-NA	6.35	2.21	2.06
23	5	504	BCR	C10-C9	6.35	1.44	1.35
20	A	1114	CLA	MG-NA	6.35	2.21	2.06
20	3	605	CLA	MG-NA	6.34	2.21	2.06
20	6	608	CLA	MG-NA	6.34	2.21	2.06
20	B	1236	CLA	MG-NA	6.34	2.21	2.06
20	G	1602	CLA	MG-NA	6.34	2.21	2.06
20	7	607	CLA	MG-NA	6.34	2.21	2.06
20	B	1221	CLA	MG-NA	6.34	2.21	2.06
20	B	1238	CLA	MG-NA	6.34	2.21	2.06
20	1	602	CLA	MG-NA	6.34	2.21	2.06
20	8	604	CLA	MG-NA	6.34	2.21	2.06
20	B	1217	CLA	MG-NA	6.33	2.21	2.06
20	Z	612	CLA	MG-NA	6.33	2.21	2.06
20	A	1140	CLA	MG-NA	6.33	2.21	2.06
20	G	1601	CLA	MG-NA	6.33	2.21	2.06
20	Z	604	CLA	MG-NA	6.33	2.21	2.06
20	4	604	CLA	MG-NA	6.33	2.21	2.06
20	6	604	CLA	MG-NA	6.33	2.21	2.06
20	A	1122	CLA	MG-NA	6.33	2.21	2.06
20	B	1213	CLA	MG-NA	6.33	2.21	2.06
20	A	1135	CLA	MG-NA	6.33	2.21	2.06
20	Z	606	CLA	MG-NA	6.32	2.21	2.06
20	4	607	CLA	MG-NA	6.32	2.21	2.06
20	4	615	CLA	MG-NA	6.32	2.21	2.06
20	K	1404	CLA	MG-NA	6.32	2.21	2.06
20	1	612	CLA	MG-NA	6.32	2.21	2.06
20	A	1134	CLA	MG-NA	6.31	2.21	2.06
20	A	1121	CLA	MG-NA	6.31	2.21	2.06
20	B	1209	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	603	CLA	MG-NA	6.30	2.21	2.06
20	3	616	CLA	MG-NA	6.30	2.21	2.06
20	L	1503	CLA	MG-NA	6.30	2.21	2.06
20	4	609	CLA	MG-NA	6.30	2.21	2.06
20	6	601	CLA	MG-NA	6.30	2.21	2.06
20	Z	603	CLA	MG-NA	6.30	2.21	2.06
20	K	1403	CLA	MG-NA	6.29	2.21	2.06
20	B	1223	CLA	MG-NA	6.29	2.21	2.06
20	1	605	CLA	MG-NA	6.29	2.21	2.06
20	B	1229	CLA	MG-NA	6.29	2.21	2.06
20	7	613	CLA	MG-NA	6.29	2.21	2.06
20	8	605	CLA	MG-NA	6.29	2.21	2.06
20	6	603	CLA	MG-NA	6.28	2.21	2.06
20	6	607	CLA	MG-NA	6.28	2.21	2.06
20	J	1901	CLA	MG-NA	6.28	2.21	2.06
20	1	604	CLA	MG-NA	6.28	2.21	2.06
20	6	615	CLA	MG-NA	6.28	2.21	2.06
20	A	1107	CLA	MG-NA	6.28	2.21	2.06
20	B	1210	CLA	MG-NA	6.27	2.21	2.06
20	3	613	CLA	MG-NA	6.27	2.21	2.06
20	8	607	CLA	MG-NA	6.27	2.21	2.06
20	A	1115	CLA	MG-NA	6.27	2.21	2.06
20	4	605	CLA	MG-NA	6.27	2.21	2.06
20	B	1206	CLA	MG-NA	6.27	2.21	2.06
20	8	615	CLA	MG-NA	6.27	2.21	2.06
20	6	606	CLA	MG-NA	6.27	2.21	2.06
20	5	602	CLA	MG-NA	6.27	2.21	2.06
20	8	602	CLA	MG-NA	6.27	2.21	2.06
20	B	1227	CLA	MG-NA	6.27	2.21	2.06
20	B	1224	CLA	MG-NA	6.27	2.21	2.06
20	7	615	CLA	MG-NA	6.26	2.21	2.06
20	5	608	CLA	MG-NA	6.26	2.21	2.06
20	A	1111	CLA	MG-NA	6.26	2.21	2.06
20	B	1225	CLA	MG-NA	6.26	2.21	2.06
20	7	602	CLA	MG-NA	6.25	2.21	2.06
20	7	606	CLA	MG-NA	6.25	2.21	2.06
20	Z	615	CLA	MG-NA	6.25	2.21	2.06
20	B	1230	CLA	MG-NA	6.24	2.21	2.06
20	A	1126	CLA	MG-NA	6.24	2.21	2.06
20	7	601	CLA	MG-NA	6.24	2.21	2.06
20	Z	608	CLA	MG-NA	6.24	2.21	2.06
20	5	605	CLA	MG-NA	6.24	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1105	CLA	MG-NA	6.23	2.21	2.06
20	8	606	CLA	MG-NA	6.23	2.21	2.06
20	B	1228	CLA	MG-NA	6.22	2.21	2.06
20	B	1226	CLA	MG-NA	6.22	2.21	2.06
20	3	610	CLA	MG-NA	6.22	2.21	2.06
20	4	612	CLA	MG-NA	6.22	2.21	2.06
20	A	1137	CLA	MG-NA	6.21	2.21	2.06
20	A	1113	CLA	MG-NA	6.21	2.21	2.06
20	5	615	CLA	MG-NA	6.21	2.21	2.06
20	5	606	CLA	MG-NA	6.21	2.21	2.06
20	7	604	CLA	MG-NA	6.21	2.21	2.06
20	B	1212	CLA	MG-NA	6.21	2.21	2.06
20	A	1101	CLA	MG-NA	6.20	2.21	2.06
20	A	1129	CLA	MG-NA	6.20	2.21	2.06
20	B	1204	CLA	MG-NA	6.20	2.21	2.06
20	B	1237	CLA	MG-NA	6.20	2.21	2.06
20	A	1104	CLA	MG-NA	6.19	2.21	2.06
20	4	603	CLA	MG-NA	6.19	2.21	2.06
20	5	618	CLA	MG-NA	6.19	2.21	2.06
20	A	1112	CLA	MG-NA	6.19	2.21	2.06
20	8	608	CLA	MG-NA	6.19	2.21	2.06
20	A	1127	CLA	MG-NA	6.19	2.21	2.06
20	B	1211	CLA	MG-NA	6.19	2.21	2.06
20	6	618	CLA	MG-NA	6.18	2.21	2.06
20	B	1203	CLA	MG-NA	6.18	2.21	2.06
20	5	603	CLA	MG-NA	6.18	2.21	2.06
20	B	1215	CLA	MG-NA	6.18	2.20	2.06
20	B	1207	CLA	MG-NA	6.18	2.20	2.06
20	B	1220	CLA	MG-NA	6.18	2.20	2.06
20	A	1132	CLA	MG-NA	6.17	2.20	2.06
20	A	1109	CLA	MG-NA	6.17	2.20	2.06
20	3	612	CLA	MG-NA	6.17	2.20	2.06
20	6	612	CLA	MG-NA	6.17	2.20	2.06
20	1	611	CLA	MG-NA	6.17	2.20	2.06
20	A	1120	CLA	MG-NA	6.17	2.20	2.06
20	8	611	CLA	MG-NA	6.17	2.20	2.06
20	3	601	CLA	MG-NA	6.16	2.20	2.06
20	5	601	CLA	MG-NA	6.16	2.20	2.06
20	8	612	CLA	MG-NA	6.15	2.20	2.06
20	B	1022	CLA	MG-NA	6.15	2.20	2.06
20	1	603	CLA	MG-NA	6.15	2.20	2.06
20	A	1133	CLA	MG-NA	6.15	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1136	CLA	MG-NA	6.14	2.20	2.06
20	A	1131	CLA	MG-NA	6.14	2.20	2.06
20	4	606	CLA	MG-NA	6.14	2.20	2.06
20	1	601	CLA	MG-NA	6.13	2.20	2.06
20	1	606	CLA	MG-NA	6.13	2.20	2.06
20	6	609	CLA	MG-NA	6.13	2.20	2.06
20	B	1208	CLA	MG-NA	6.13	2.20	2.06
20	6	619	CLA	MG-NA	6.13	2.20	2.06
34	J	4002	C7Z	C1-C6	-6.13	1.45	1.53
20	B	1235	CLA	MG-NA	6.12	2.20	2.06
20	A	1117	CLA	MG-NA	6.11	2.20	2.06
20	A	1125	CLA	MG-NA	6.11	2.20	2.06
20	8	601	CLA	MG-NA	6.10	2.20	2.06
20	L	1502	CLA	MG-NA	6.10	2.20	2.06
20	1	608	CLA	MG-NA	6.09	2.20	2.06
20	A	1118	CLA	MG-NA	6.09	2.20	2.06
20	A	1124	CLA	MG-NA	6.08	2.20	2.06
20	B	1202	CLA	MG-NA	6.08	2.20	2.06
20	A	1119	CLA	MG-NA	6.07	2.20	2.06
20	A	1106	CLA	MG-NA	6.07	2.20	2.06
20	A	1128	CLA	MG-NA	6.07	2.20	2.06
20	7	609	CLA	MG-NA	6.07	2.20	2.06
20	B	1239	CLA	MG-NA	6.06	2.20	2.06
20	Z	601	CLA	MG-NA	6.06	2.20	2.06
20	B	1231	CLA	MG-NA	6.06	2.20	2.06
20	B	1216	CLA	MG-NA	6.05	2.20	2.06
20	3	604	CLA	MG-NA	6.05	2.20	2.06
20	F	1301	CLA	MG-NA	6.05	2.20	2.06
20	7	611	CLA	MG-NA	6.05	2.20	2.06
20	7	616	CLA	MG-NA	6.04	2.20	2.06
20	A	1012	CLA	MG-NA	6.03	2.20	2.06
20	A	1108	CLA	MG-NA	6.01	2.20	2.06
20	A	1013	CLA	MG-NA	6.01	2.20	2.06
20	3	606	CLA	MG-NA	6.00	2.20	2.06
20	5	612	CLA	MG-NA	6.00	2.20	2.06
20	B	1205	CLA	MG-NA	5.99	2.20	2.06
20	A	1138	CLA	MG-NA	5.98	2.20	2.06
20	B	1222	CLA	MG-NA	5.97	2.20	2.06
20	4	601	CLA	MG-NA	5.97	2.20	2.06
20	A	1103	CLA	MG-NA	5.93	2.20	2.06
20	7	612	CLA	MG-NA	5.93	2.20	2.06
20	A	1102	CLA	MG-NA	5.91	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1023	CLA	MG-NA	5.91	2.20	2.06
20	B	1021	CLA	MG-NA	5.88	2.20	2.06
23	B	4003	BCR	C24-C23	5.88	1.50	1.33
34	5	505	C7Z	C12-C13	5.86	1.58	1.45
23	5	504	BCR	C24-C23	5.85	1.50	1.33
23	3	506	BCR	C24-C23	5.83	1.50	1.33
23	G	4001	BCR	C24-C23	5.83	1.50	1.33
23	6	504	BCR	C24-C23	5.76	1.50	1.33
23	7	504	BCR	C24-C23	5.73	1.50	1.33
23	L	4001	BCR	C24-C23	5.72	1.50	1.33
23	7	503	BCR	C24-C23	5.72	1.50	1.33
23	3	505	BCR	C24-C23	5.71	1.50	1.33
20	B	1201	CLA	MG-NA	5.71	2.19	2.06
23	A	4004	BCR	C24-C23	5.71	1.50	1.33
23	K	4002	BCR	C24-C23	5.69	1.50	1.33
33	F	4001	RRX	C1-C6	-5.67	1.46	1.53
34	1	503	C7Z	C1-C6	-5.66	1.46	1.53
23	4	503	BCR	C24-C23	5.65	1.50	1.33
23	L	4002	BCR	C24-C23	5.64	1.50	1.33
23	B	4002	BCR	C24-C23	5.64	1.50	1.33
23	6	503	BCR	C24-C23	5.63	1.50	1.33
23	B	4005	BCR	C24-C23	5.63	1.50	1.33
23	J	4001	BCR	C24-C23	5.61	1.50	1.33
23	3	504	BCR	C24-C23	5.61	1.50	1.33
23	A	4001	BCR	C24-C23	5.60	1.50	1.33
34	1	503	C7Z	C12-C13	5.60	1.58	1.45
23	5	503	BCR	C24-C23	5.59	1.50	1.33
23	3	503	BCR	C24-C23	5.59	1.50	1.33
23	B	4001	BCR	C24-C23	5.57	1.49	1.33
33	F	4001	RRX	C30-C25	-5.57	1.46	1.53
23	B	4006	BCR	C24-C23	5.56	1.49	1.33
23	B	4007	BCR	C24-C23	5.54	1.49	1.33
23	A	4002	BCR	C24-C23	5.54	1.49	1.33
23	K	4001	BCR	C24-C23	5.53	1.49	1.33
34	J	4002	C7Z	C12-C13	5.52	1.57	1.45
23	I	4001	BCR	C24-C23	5.51	1.49	1.33
23	3	503	BCR	C11-C12	-5.49	1.20	1.34
23	A	4003	BCR	C24-C23	5.48	1.49	1.33
23	B	4001	BCR	C11-C12	-5.46	1.20	1.34
23	8	503	BCR	C24-C23	5.46	1.49	1.33
23	B	4004	BCR	C24-C23	5.43	1.49	1.33
23	B	4004	BCR	C11-C12	-5.42	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	504	BCR	C11-C12	-5.42	1.20	1.34
23	A	4005	BCR	C11-C12	-5.39	1.20	1.34
23	A	4005	BCR	C24-C23	5.39	1.49	1.33
23	A	4004	BCR	C11-C12	-5.38	1.20	1.34
23	B	4007	BCR	C11-C12	-5.34	1.20	1.34
23	5	503	BCR	C11-C12	-5.32	1.20	1.34
19	A	1011	CL0	O2A-C1	5.32	1.61	1.46
23	B	4005	BCR	C11-C12	-5.31	1.20	1.34
23	B	4002	BCR	C11-C12	-5.31	1.20	1.34
23	5	504	BCR	C11-C12	-5.28	1.21	1.34
23	L	4002	BCR	C11-C12	-5.28	1.21	1.34
33	F	4001	RRX	C2-C1	5.27	1.66	1.54
23	7	503	BCR	C11-C12	-5.26	1.21	1.34
23	G	4001	BCR	C11-C12	-5.26	1.21	1.34
23	I	4001	BCR	C11-C12	-5.25	1.21	1.34
23	J	4001	BCR	C11-C12	-5.25	1.21	1.34
23	L	4001	BCR	C11-C12	-5.20	1.21	1.34
23	4	503	BCR	C11-C12	-5.20	1.21	1.34
23	K	4001	BCR	C11-C12	-5.20	1.21	1.34
23	A	4001	BCR	C11-C12	-5.17	1.21	1.34
34	5	505	C7Z	C28-C29	5.14	1.57	1.45
23	A	4002	BCR	C11-C12	-5.13	1.21	1.34
23	K	4002	BCR	C11-C12	-5.11	1.21	1.34
23	3	505	BCR	C11-C12	-5.11	1.21	1.34
23	B	4003	BCR	C11-C12	-5.11	1.21	1.34
23	6	503	BCR	C11-C12	-5.10	1.21	1.34
23	8	503	BCR	C11-C12	-5.10	1.21	1.34
23	7	504	BCR	C11-C12	-5.10	1.21	1.34
23	B	4006	BCR	C11-C12	-5.08	1.21	1.34
34	1	503	C7Z	C28-C29	5.03	1.56	1.45
33	F	4001	RRX	C19-C18	5.03	1.56	1.45
23	6	504	BCR	C11-C12	-5.03	1.21	1.34
23	A	4003	BCR	C11-C12	-5.02	1.21	1.34
34	5	505	C7Z	C1-C6	-4.97	1.46	1.53
23	3	506	BCR	C11-C12	-4.93	1.21	1.34
34	J	4002	C7Z	C28-C29	4.89	1.56	1.45
33	F	4001	RRX	C8-C9	4.86	1.56	1.45
34	J	4002	C7Z	C32-C33	4.81	1.56	1.45
19	A	1011	CL0	O2D-CGD	4.80	1.44	1.33
34	J	4002	C7Z	C24-C25	-4.75	1.43	1.51
39	Z	504	QTB	C17-C11	-4.74	1.50	1.55
34	1	503	C7Z	C32-C33	4.71	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	5	505	C7Z	C32-C33	4.64	1.55	1.45
34	5	505	C7Z	C8-C9	4.61	1.55	1.45
33	F	4001	RRX	C27-C26	-4.56	1.44	1.51
19	A	1011	CL0	C3D-C4D	-4.55	1.33	1.44
23	B	4005	BCR	C16-C17	-4.54	1.29	1.43
23	A	4005	BCR	C16-C17	-4.54	1.29	1.43
23	3	503	BCR	C16-C17	-4.53	1.29	1.43
34	5	505	C7Z	C24-C25	-4.53	1.44	1.51
19	A	1011	CL0	CHD-C1D	4.52	1.47	1.38
23	B	4001	BCR	C16-C17	-4.49	1.29	1.43
20	A	1128	CLA	MG-ND	-4.47	1.96	2.05
23	I	4001	BCR	C16-C17	-4.46	1.29	1.43
23	B	4004	BCR	C16-C17	-4.46	1.29	1.43
34	1	503	C7Z	C24-C25	-4.45	1.44	1.51
23	L	4002	BCR	C16-C17	-4.44	1.29	1.43
23	G	4001	BCR	C16-C17	-4.43	1.29	1.43
23	B	4007	BCR	C16-C17	-4.42	1.29	1.43
23	5	503	BCR	C16-C17	-4.40	1.29	1.43
23	8	503	BCR	C16-C17	-4.40	1.29	1.43
34	5	505	C7Z	C31-C30	4.39	1.57	1.43
37	4	613	CHL	CBB-CAB	4.39	1.52	1.30
37	6	611	CHL	CBB-CAB	4.38	1.52	1.30
23	A	4002	BCR	C16-C17	-4.37	1.29	1.43
23	A	4004	BCR	C16-C17	-4.36	1.29	1.43
19	A	1011	CL0	C3C-C2C	4.35	1.46	1.36
20	8	611	CLA	CBB-CAB	4.35	1.51	1.30
20	B	1206	CLA	CBB-CAB	4.34	1.51	1.30
34	1	503	C7Z	C31-C30	4.34	1.56	1.43
23	6	503	BCR	C16-C17	-4.34	1.30	1.43
20	Z	607	CLA	CBB-CAB	4.33	1.51	1.30
19	A	1011	CL0	CHC-C1C	4.33	1.47	1.38
20	B	1226	CLA	MG-ND	-4.33	1.97	2.05
20	B	1201	CLA	CBB-CAB	4.33	1.51	1.30
34	J	4002	C7Z	C31-C30	4.33	1.56	1.43
20	8	615	CLA	CBB-CAB	4.33	1.51	1.30
37	Z	613	CHL	CBB-CAB	4.33	1.51	1.30
20	Z	606	CLA	CBB-CAB	4.33	1.51	1.30
20	L	1503	CLA	CBB-CAB	4.33	1.51	1.30
34	J	4002	C7Z	C4-C5	-4.32	1.44	1.51
37	4	611	CHL	CBB-CAB	4.32	1.51	1.30
34	5	505	C7Z	C11-C10	4.32	1.56	1.43
23	K	4002	BCR	C16-C17	-4.32	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	605	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1221	CLA	CBB-CAB	4.32	1.51	1.30
20	A	1102	CLA	CBB-CAB	4.32	1.51	1.30
20	3	616	CLA	CBB-CAB	4.32	1.51	1.30
20	6	619	CLA	CBB-CAB	4.32	1.51	1.30
20	B	1211	CLA	CBB-CAB	4.31	1.51	1.30
20	B	1222	CLA	CBB-CAB	4.31	1.51	1.30
20	6	606	CLA	CBB-CAB	4.31	1.51	1.30
23	K	4001	BCR	C16-C17	-4.31	1.30	1.43
20	8	602	CLA	CBB-CAB	4.31	1.51	1.30
20	K	1404	CLA	CBB-CAB	4.31	1.51	1.30
20	B	1208	CLA	CBB-CAB	4.31	1.51	1.30
20	4	606	CLA	CBB-CAB	4.31	1.51	1.30
20	1	608	CLA	CBB-CAB	4.31	1.51	1.30
23	3	505	BCR	C16-C17	-4.31	1.30	1.43
20	5	603	CLA	CBB-CAB	4.31	1.51	1.30
20	1	613	CLA	CBB-CAB	4.31	1.51	1.30
37	1	610	CHL	CBB-CAB	4.30	1.51	1.30
20	6	601	CLA	CBB-CAB	4.30	1.51	1.30
20	A	1133	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1236	CLA	CBB-CAB	4.30	1.51	1.30
20	4	605	CLA	CBB-CAB	4.30	1.51	1.30
23	A	4001	BCR	C16-C17	-4.30	1.30	1.43
20	7	615	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1237	CLA	CBB-CAB	4.30	1.51	1.30
20	5	606	CLA	CBB-CAB	4.30	1.51	1.30
37	5	611	CHL	CBB-CAB	4.30	1.51	1.30
20	6	618	CLA	CBB-CAB	4.30	1.51	1.30
20	5	607	CLA	CBB-CAB	4.30	1.51	1.30
20	1	602	CLA	CBB-CAB	4.30	1.51	1.30
20	A	1012	CLA	CBB-CAB	4.30	1.51	1.30
20	B	1203	CLA	CBB-CAB	4.30	1.51	1.30
37	5	617	CHL	CBB-CAB	4.30	1.51	1.30
20	6	602	CLA	CBB-CAB	4.29	1.51	1.30
20	8	609	CLA	CBB-CAB	4.29	1.51	1.30
20	3	607	CLA	CBB-CAB	4.29	1.51	1.30
20	8	605	CLA	CBB-CAB	4.29	1.51	1.30
23	6	504	BCR	C16-C17	-4.29	1.30	1.43
20	Z	608	CLA	CBB-CAB	4.29	1.51	1.30
20	3	612	CLA	CBB-CAB	4.29	1.51	1.30
23	B	4002	BCR	C16-C17	-4.29	1.30	1.43
20	A	1141	CLA	CBB-CAB	4.29	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1013	CLA	MG-ND	-4.29	1.97	2.05
20	7	611	CLA	CBB-CAB	4.29	1.51	1.30
20	7	601	CLA	CBB-CAB	4.29	1.51	1.30
20	4	612	CLA	CBB-CAB	4.29	1.51	1.30
20	A	1118	CLA	CBB-CAB	4.29	1.51	1.30
20	A	1137	CLA	CBB-CAB	4.29	1.51	1.30
20	B	1212	CLA	CBB-CAB	4.28	1.51	1.30
20	7	602	CLA	CBB-CAB	4.28	1.51	1.30
20	B	1207	CLA	CBB-CAB	4.28	1.51	1.30
20	B	1225	CLA	CBB-CAB	4.28	1.51	1.30
20	B	1213	CLA	CBB-CAB	4.28	1.51	1.30
20	B	1235	CLA	CBB-CAB	4.28	1.51	1.30
20	B	1202	CLA	CBB-CAB	4.28	1.51	1.30
20	G	1602	CLA	CBB-CAB	4.28	1.51	1.30
20	A	1114	CLA	CBB-CAB	4.28	1.51	1.30
20	6	605	CLA	CBB-CAB	4.28	1.51	1.30
20	6	607	CLA	CBB-CAB	4.28	1.51	1.30
20	B	1215	CLA	CBB-CAB	4.28	1.51	1.30
20	Z	603	CLA	CBB-CAB	4.28	1.51	1.30
34	1	503	C7Z	C8-C9	4.28	1.55	1.45
20	4	615	CLA	CBB-CAB	4.28	1.51	1.30
20	K	1401	CLA	CBB-CAB	4.27	1.51	1.30
20	4	602	CLA	CBB-CAB	4.27	1.51	1.30
20	A	1110	CLA	CBB-CAB	4.27	1.51	1.30
20	Z	601	CLA	CBB-CAB	4.27	1.51	1.30
20	B	1223	CLA	CBB-CAB	4.27	1.51	1.30
20	3	618	CLA	CBB-CAB	4.27	1.51	1.30
20	B	1205	CLA	CBB-CAB	4.27	1.51	1.30
20	A	1125	CLA	CBB-CAB	4.27	1.51	1.30
20	7	612	CLA	CBB-CAB	4.27	1.51	1.30
34	1	503	C7Z	C4-C5	-4.27	1.44	1.51
20	5	622	CLA	CBB-CAB	4.27	1.51	1.30
20	1	605	CLA	CBB-CAB	4.27	1.51	1.30
20	5	613	CLA	CBB-CAB	4.27	1.51	1.30
20	B	1219	CLA	CBB-CAB	4.27	1.51	1.30
20	7	616	CLA	CBB-CAB	4.27	1.51	1.30
20	B	1224	CLA	CBB-CAB	4.27	1.51	1.30
20	B	1240	CLA	CBB-CAB	4.27	1.51	1.30
20	B	1224	CLA	MG-ND	-4.27	1.97	2.05
20	8	612	CLA	CBB-CAB	4.26	1.51	1.30
20	Z	615	CLA	CBB-CAB	4.26	1.51	1.30
20	6	608	CLA	CBB-CAB	4.26	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	6	613	CHL	CBB-CAB	4.26	1.51	1.30
20	B	1226	CLA	CBB-CAB	4.26	1.51	1.30
20	A	1107	CLA	CBB-CAB	4.26	1.51	1.30
20	3	606	CLA	CBB-CAB	4.26	1.51	1.30
23	B	4006	BCR	C16-C17	-4.26	1.30	1.43
20	A	1121	CLA	CBB-CAB	4.26	1.51	1.30
20	B	1241	CLA	CBB-CAB	4.26	1.51	1.30
20	8	608	CLA	CBB-CAB	4.26	1.51	1.30
20	Z	602	CLA	CBB-CAB	4.26	1.51	1.30
20	7	606	CLA	CBB-CAB	4.26	1.51	1.30
20	K	1403	CLA	CBB-CAB	4.26	1.51	1.30
20	1	611	CLA	CBB-CAB	4.26	1.51	1.30
20	A	1115	CLA	CBB-CAB	4.26	1.51	1.30
20	8	606	CLA	CBB-CAB	4.25	1.51	1.30
20	5	618	CLA	CBB-CAB	4.25	1.51	1.30
20	A	1106	CLA	CBB-CAB	4.25	1.51	1.30
20	5	615	CLA	CBB-CAB	4.25	1.51	1.30
20	3	613	CLA	CBB-CAB	4.25	1.51	1.30
20	5	602	CLA	CBB-CAB	4.25	1.51	1.30
20	B	1210	CLA	CBB-CAB	4.25	1.51	1.30
20	F	1301	CLA	CBB-CAB	4.25	1.51	1.30
20	A	1122	CLA	CBB-CAB	4.25	1.51	1.30
20	A	1139	CLA	CBB-CAB	4.25	1.51	1.30
20	K	1402	CLA	CBB-CAB	4.25	1.51	1.30
37	Z	610	CHL	CBB-CAB	4.25	1.51	1.30
20	B	1232	CLA	CBB-CAB	4.25	1.51	1.30
20	5	605	CLA	CBB-CAB	4.25	1.51	1.30
20	Z	604	CLA	CBB-CAB	4.25	1.51	1.30
20	1	612	CLA	CBB-CAB	4.25	1.51	1.30
20	6	609	CLA	CBB-CAB	4.25	1.51	1.30
20	B	1204	CLA	CBB-CAB	4.25	1.51	1.30
20	Z	611	CLA	CBB-CAB	4.25	1.51	1.30
20	3	608	CLA	CBB-CAB	4.25	1.51	1.30
37	8	613	CHL	CBB-CAB	4.25	1.51	1.30
20	B	1220	CLA	CBB-CAB	4.25	1.51	1.30
20	A	1109	CLA	CBB-CAB	4.25	1.51	1.30
20	A	1116	CLA	CBB-CAB	4.25	1.51	1.30
20	6	612	CLA	CBB-CAB	4.25	1.51	1.30
20	G	1601	CLA	CBB-CAB	4.25	1.51	1.30
20	5	601	CLA	CBB-CAB	4.25	1.51	1.30
20	B	1228	CLA	CBB-CAB	4.25	1.51	1.30
23	7	503	BCR	C16-C17	-4.25	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1117	CLA	CBB-CAB	4.25	1.51	1.30
23	B	4003	BCR	C16-C17	-4.24	1.30	1.43
20	4	601	CLA	CBB-CAB	4.24	1.51	1.30
20	A	1103	CLA	CBB-CAB	4.24	1.51	1.30
20	7	608	CLA	CBB-CAB	4.24	1.51	1.30
20	B	1230	CLA	CBB-CAB	4.24	1.51	1.30
20	3	603	CLA	CBB-CAB	4.24	1.51	1.30
20	5	612	CLA	CBB-CAB	4.24	1.51	1.30
23	3	506	BCR	C16-C17	-4.24	1.30	1.43
20	A	1124	CLA	CBB-CAB	4.24	1.51	1.30
20	B	1239	CLA	CBB-CAB	4.24	1.51	1.30
33	F	4001	RRX	C12-C13	4.24	1.55	1.45
20	8	601	CLA	CBB-CAB	4.24	1.51	1.30
20	A	1128	CLA	CBB-CAB	4.24	1.51	1.30
20	4	603	CLA	CBB-CAB	4.24	1.51	1.30
20	4	607	CLA	CBB-CAB	4.24	1.51	1.30
20	A	1126	CLA	CBB-CAB	4.24	1.51	1.30
20	B	1217	CLA	CBB-CAB	4.23	1.51	1.30
20	L	1502	CLA	CBB-CAB	4.23	1.51	1.30
37	4	610	CHL	CBB-CAB	4.23	1.51	1.30
20	8	607	CLA	CBB-CAB	4.23	1.51	1.30
20	4	608	CLA	CBB-CAB	4.23	1.51	1.30
20	6	604	CLA	CBB-CAB	4.23	1.51	1.30
20	B	1216	CLA	CBB-CAB	4.23	1.51	1.30
20	3	604	CLA	CBB-CAB	4.23	1.51	1.30
20	7	609	CLA	CBB-CAB	4.23	1.51	1.30
20	A	1138	CLA	CBB-CAB	4.23	1.51	1.30
20	4	604	CLA	CBB-CAB	4.22	1.51	1.30
20	B	1023	CLA	CBB-CAB	4.22	1.51	1.30
20	6	603	CLA	CBB-CAB	4.22	1.51	1.30
20	5	609	CLA	CBB-CAB	4.22	1.51	1.30
20	B	1209	CLA	CBB-CAB	4.22	1.51	1.30
20	1	604	CLA	CBB-CAB	4.22	1.51	1.30
20	A	1123	CLA	CBB-CAB	4.22	1.51	1.30
20	1	615	CLA	CBB-CAB	4.22	1.51	1.30
37	8	610	CHL	CBB-CAB	4.22	1.51	1.30
20	A	1132	CLA	CBB-CAB	4.22	1.51	1.30
34	5	505	C7Z	C4-C5	-4.22	1.44	1.51
20	A	1105	CLA	CBB-CAB	4.22	1.51	1.30
20	Z	612	CLA	CBB-CAB	4.22	1.51	1.30
20	B	1021	CLA	CBB-CAB	4.22	1.51	1.30
20	B	1234	CLA	CBB-CAB	4.22	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	601	CLA	CBB-CAB	4.22	1.51	1.30
20	A	1111	CLA	CBB-CAB	4.22	1.51	1.30
20	1	606	CLA	CBB-CAB	4.22	1.51	1.30
20	A	1134	CLA	CBB-CAB	4.22	1.51	1.30
20	7	607	CLA	CBB-CAB	4.22	1.51	1.30
20	J	1901	CLA	CBB-CAB	4.21	1.51	1.30
20	B	1231	CLA	CBB-CAB	4.21	1.51	1.30
20	3	602	CLA	CBB-CAB	4.21	1.51	1.30
20	A	1127	CLA	MG-ND	-4.21	1.97	2.05
20	B	1214	CLA	CBB-CAB	4.21	1.51	1.30
20	B	1218	CLA	CBB-CAB	4.21	1.51	1.30
23	5	504	BCR	C16-C17	-4.21	1.30	1.43
20	A	1101	CLA	CBB-CAB	4.21	1.51	1.30
20	8	603	CLA	CBB-CAB	4.21	1.51	1.30
20	B	1238	CLA	CBB-CAB	4.21	1.51	1.30
20	5	608	CLA	CBB-CAB	4.21	1.51	1.30
20	7	613	CLA	CBB-CAB	4.21	1.51	1.30
23	A	4003	BCR	C16-C17	-4.21	1.30	1.43
20	A	1113	CLA	CBB-CAB	4.20	1.51	1.30
20	4	609	CLA	CBB-CAB	4.20	1.51	1.30
20	3	610	CLA	CBB-CAB	4.20	1.51	1.30
20	A	1119	CLA	CBB-CAB	4.20	1.51	1.30
20	6	615	CLA	CBB-CAB	4.20	1.51	1.30
20	A	1129	CLA	CBB-CAB	4.20	1.51	1.30
23	J	4001	BCR	C16-C17	-4.20	1.30	1.43
20	B	1021	CLA	MG-ND	-4.20	1.97	2.05
20	3	601	CLA	CBB-CAB	4.20	1.51	1.30
20	A	1108	CLA	CBB-CAB	4.20	1.51	1.30
20	A	1120	CLA	CBB-CAB	4.19	1.51	1.30
20	1	607	CLA	CBB-CAB	4.19	1.51	1.30
20	A	1127	CLA	CBB-CAB	4.19	1.51	1.30
20	A	1013	CLA	CBB-CAB	4.19	1.51	1.30
23	L	4001	BCR	C16-C17	-4.19	1.30	1.43
20	1	603	CLA	CBB-CAB	4.19	1.51	1.30
23	4	503	BCR	C16-C17	-4.18	1.30	1.43
20	A	1140	CLA	CBB-CAB	4.18	1.51	1.30
20	A	1131	CLA	CBB-CAB	4.18	1.51	1.30
20	A	1112	CLA	CBB-CAB	4.18	1.51	1.30
31	B	5003	DGD	O1G-C1A	4.18	1.45	1.33
20	7	604	CLA	CBB-CAB	4.18	1.51	1.30
20	7	605	CLA	CBB-CAB	4.17	1.51	1.30
37	6	617	CHL	CBB-CAB	4.17	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	605	CLA	CBB-CAB	4.17	1.51	1.30
20	8	604	CLA	CBB-CAB	4.16	1.50	1.30
20	A	1136	CLA	CBB-CAB	4.16	1.50	1.30
37	1	609	CHL	CBB-CAB	4.15	1.50	1.30
20	B	1022	CLA	CBB-CAB	4.15	1.50	1.30
20	7	603	CLA	CBB-CAB	4.15	1.50	1.30
20	B	1229	CLA	CBB-CAB	4.15	1.50	1.30
37	7	610	CHL	CBB-CAB	4.15	1.50	1.30
20	B	1227	CLA	CBB-CAB	4.15	1.50	1.30
37	Z	609	CHL	CBB-CAB	4.15	1.50	1.30
20	A	1130	CLA	CBB-CAB	4.15	1.50	1.30
37	6	610	CHL	CBB-CAB	4.15	1.50	1.30
20	A	1124	CLA	MG-ND	-4.14	1.97	2.05
34	J	4002	C7Z	C8-C9	4.14	1.54	1.45
20	4	608	CLA	MG-ND	-4.14	1.97	2.05
20	A	1141	CLA	MG-ND	-4.13	1.97	2.05
20	5	604	CLA	CBB-CAB	4.13	1.50	1.30
37	4	617	CHL	CBB-CAB	4.13	1.50	1.30
20	B	1022	CLA	MG-ND	-4.13	1.97	2.05
23	3	504	BCR	C16-C17	-4.13	1.30	1.43
20	A	1104	CLA	CBB-CAB	4.12	1.50	1.30
20	B	1211	CLA	MG-ND	-4.12	1.97	2.05
20	B	1023	CLA	MG-ND	-4.12	1.97	2.05
33	F	4001	RRX	C3-C4	4.12	1.65	1.52
20	A	1135	CLA	CBB-CAB	4.10	1.50	1.30
20	F	1302	CLA	CBB-CAB	4.10	1.50	1.30
20	B	1220	CLA	MG-ND	-4.07	1.97	2.05
34	1	503	C7Z	C11-C10	4.06	1.56	1.43
20	3	618	CLA	MG-ND	-4.06	1.97	2.05
20	B	1202	CLA	MG-ND	-4.06	1.97	2.05
20	B	1225	CLA	MG-ND	-4.06	1.97	2.05
20	4	612	CLA	MG-ND	-4.05	1.97	2.05
20	3	608	CLA	MG-ND	-4.05	1.97	2.05
20	1	606	CLA	MG-ND	-4.04	1.97	2.05
20	A	1125	CLA	MG-ND	-4.04	1.97	2.05
20	A	1126	CLA	MG-ND	-4.04	1.97	2.05
20	B	1219	CLA	MG-ND	-4.04	1.97	2.05
20	1	615	CLA	MG-ND	-4.03	1.97	2.05
20	F	1302	CLA	MG-ND	-4.02	1.97	2.05
20	A	1119	CLA	MG-ND	-4.02	1.97	2.05
20	4	607	CLA	MG-ND	-4.02	1.97	2.05
23	7	504	BCR	C16-C17	-4.02	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	8	605	CLA	MG-ND	-4.02	1.97	2.05
39	Z	504	QTB	C11-C10	-4.02	1.44	1.50
37	5	610	CHL	CBB-CAB	4.01	1.50	1.30
20	A	1137	CLA	MG-ND	-4.01	1.97	2.05
20	B	1206	CLA	MG-ND	-4.01	1.97	2.05
20	7	612	CLA	MG-ND	-4.01	1.97	2.05
20	B	1232	CLA	MG-ND	-4.01	1.97	2.05
20	6	619	CLA	MG-ND	-4.00	1.97	2.05
20	B	1237	CLA	MG-ND	-4.00	1.97	2.05
20	B	1222	CLA	MG-ND	-4.00	1.97	2.05
20	5	607	CLA	MG-ND	-4.00	1.97	2.05
20	B	1227	CLA	MG-ND	-4.00	1.97	2.05
20	A	1012	CLA	MG-ND	-4.00	1.97	2.05
34	J	4002	C7Z	C11-C10	4.00	1.55	1.43
20	6	615	CLA	MG-ND	-4.00	1.97	2.05
33	F	4001	RRX	C20-C21	3.99	1.55	1.43
20	B	1239	CLA	MG-ND	-3.99	1.97	2.05
20	L	1502	CLA	MG-ND	-3.99	1.97	2.05
20	A	1136	CLA	MG-ND	-3.99	1.97	2.05
20	3	613	CLA	MG-ND	-3.98	1.97	2.05
20	1	607	CLA	MG-ND	-3.98	1.97	2.05
20	6	601	CLA	MG-ND	-3.98	1.97	2.05
20	B	1223	CLA	MG-ND	-3.97	1.97	2.05
20	7	608	CLA	MG-ND	-3.97	1.97	2.05
20	6	608	CLA	MG-ND	-3.97	1.97	2.05
20	8	607	CLA	MG-ND	-3.97	1.97	2.05
20	A	1116	CLA	MG-ND	-3.97	1.97	2.05
20	A	1139	CLA	MG-ND	-3.97	1.97	2.05
20	K	1402	CLA	MG-ND	-3.97	1.97	2.05
20	B	1217	CLA	MG-ND	-3.97	1.97	2.05
20	B	1221	CLA	MG-ND	-3.97	1.97	2.05
34	1	503	C7Z	C22-C21	3.97	1.67	1.54
20	A	1133	CLA	MG-ND	-3.96	1.97	2.05
20	A	1104	CLA	MG-ND	-3.96	1.97	2.05
19	A	1011	CL0	CHB-C1B	3.96	1.48	1.39
20	Z	608	CLA	MG-ND	-3.95	1.98	2.05
20	1	601	CLA	MG-ND	-3.95	1.98	2.05
20	Z	603	CLA	MG-ND	-3.95	1.98	2.05
20	B	1213	CLA	MG-ND	-3.94	1.98	2.05
20	A	1117	CLA	MG-ND	-3.94	1.98	2.05
20	Z	612	CLA	MG-ND	-3.94	1.98	2.05
20	5	609	CLA	MG-ND	-3.94	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1131	CLA	MG-ND	-3.94	1.98	2.05
20	A	1114	CLA	MG-ND	-3.94	1.98	2.05
20	F	1301	CLA	MG-ND	-3.93	1.98	2.05
20	8	601	CLA	MG-ND	-3.93	1.98	2.05
20	A	1111	CLA	MG-ND	-3.93	1.98	2.05
20	A	1123	CLA	MG-ND	-3.93	1.98	2.05
20	7	611	CLA	MG-ND	-3.93	1.98	2.05
20	3	604	CLA	MG-ND	-3.92	1.98	2.05
20	4	609	CLA	MG-ND	-3.92	1.98	2.05
20	A	1109	CLA	MG-ND	-3.92	1.98	2.05
20	K	1401	CLA	MG-ND	-3.92	1.98	2.05
20	A	1108	CLA	MG-ND	-3.92	1.98	2.05
20	7	609	CLA	MG-ND	-3.92	1.98	2.05
20	3	610	CLA	MG-ND	-3.92	1.98	2.05
20	7	604	CLA	MG-ND	-3.92	1.98	2.05
20	Z	607	CLA	MG-ND	-3.91	1.98	2.05
20	7	601	CLA	MG-ND	-3.91	1.98	2.05
20	7	613	CLA	MG-ND	-3.91	1.98	2.05
20	5	622	CLA	MG-ND	-3.91	1.98	2.05
20	B	1218	CLA	MG-ND	-3.91	1.98	2.05
20	8	608	CLA	MG-ND	-3.91	1.98	2.05
20	A	1112	CLA	MG-ND	-3.91	1.98	2.05
20	B	1214	CLA	MG-ND	-3.91	1.98	2.05
20	3	602	CLA	MG-ND	-3.91	1.98	2.05
20	5	613	CLA	MG-ND	-3.91	1.98	2.05
20	A	1130	CLA	MG-ND	-3.90	1.98	2.05
20	5	601	CLA	MG-ND	-3.90	1.98	2.05
20	6	618	CLA	MG-ND	-3.90	1.98	2.05
20	A	1106	CLA	C1C-NC	-3.90	1.32	1.37
20	B	1201	CLA	MG-ND	-3.89	1.98	2.05
20	B	1210	CLA	MG-ND	-3.89	1.98	2.05
20	5	615	CLA	MG-ND	-3.89	1.98	2.05
20	1	602	CLA	MG-ND	-3.89	1.98	2.05
20	B	1216	CLA	MG-ND	-3.89	1.98	2.05
20	5	605	CLA	MG-ND	-3.89	1.98	2.05
20	8	609	CLA	MG-ND	-3.89	1.98	2.05
20	A	1118	CLA	MG-ND	-3.89	1.98	2.05
20	1	612	CLA	MG-ND	-3.88	1.98	2.05
20	5	608	CLA	MG-ND	-3.88	1.98	2.05
20	6	612	CLA	MG-ND	-3.88	1.98	2.05
20	A	1129	CLA	MG-ND	-3.88	1.98	2.05
20	5	606	CLA	MG-ND	-3.88	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1011	CL0	CHD-C4C	3.88	1.48	1.39
20	B	1212	CLA	MG-ND	-3.87	1.98	2.05
20	7	615	CLA	MG-ND	-3.87	1.98	2.05
20	8	612	CLA	MG-ND	-3.87	1.98	2.05
20	A	1135	CLA	MG-ND	-3.87	1.98	2.05
20	B	1231	CLA	MG-ND	-3.87	1.98	2.05
20	A	1128	CLA	C1C-NC	-3.87	1.32	1.37
37	3	611	CHL	CBB-CAB	3.86	1.49	1.30
20	K	1403	CLA	MG-ND	-3.86	1.98	2.05
20	K	1404	CLA	MG-ND	-3.86	1.98	2.05
20	A	1134	CLA	MG-ND	-3.86	1.98	2.05
20	6	605	CLA	MG-ND	-3.86	1.98	2.05
20	J	1901	CLA	MG-ND	-3.86	1.98	2.05
20	B	1205	CLA	MG-ND	-3.86	1.98	2.05
20	3	612	CLA	MG-ND	-3.86	1.98	2.05
20	6	609	CLA	MG-ND	-3.86	1.98	2.05
20	6	607	CLA	MG-ND	-3.86	1.98	2.05
20	Z	615	CLA	MG-ND	-3.86	1.98	2.05
20	7	606	CLA	MG-ND	-3.86	1.98	2.05
20	4	615	CLA	MG-ND	-3.85	1.98	2.05
20	1	613	CLA	MG-ND	-3.85	1.98	2.05
20	6	603	CLA	MG-ND	-3.85	1.98	2.05
20	B	1234	CLA	MG-ND	-3.85	1.98	2.05
20	3	604	CLA	C1C-NC	-3.85	1.32	1.37
20	A	1140	CLA	MG-ND	-3.85	1.98	2.05
20	A	1101	CLA	MG-ND	-3.85	1.98	2.05
20	B	1209	CLA	MG-ND	-3.85	1.98	2.05
20	7	607	CLA	MG-ND	-3.85	1.98	2.05
20	5	612	CLA	MG-ND	-3.85	1.98	2.05
20	7	616	CLA	MG-ND	-3.84	1.98	2.05
20	1	611	CLA	MG-ND	-3.84	1.98	2.05
20	4	604	CLA	MG-ND	-3.84	1.98	2.05
20	Z	605	CLA	MG-ND	-3.84	1.98	2.05
20	4	603	CLA	MG-ND	-3.83	1.98	2.05
20	3	616	CLA	MG-ND	-3.83	1.98	2.05
20	6	602	CLA	MG-ND	-3.83	1.98	2.05
20	4	605	CLA	MG-ND	-3.83	1.98	2.05
20	A	1102	CLA	MG-ND	-3.83	1.98	2.05
34	J	4002	C7Z	C22-C21	3.83	1.66	1.54
20	A	1138	CLA	MG-ND	-3.83	1.98	2.05
20	B	1215	CLA	MG-ND	-3.83	1.98	2.05
20	B	1241	CLA	MG-ND	-3.83	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	602	CLA	MG-ND	-3.82	1.98	2.05
20	6	606	CLA	MG-ND	-3.82	1.98	2.05
20	A	1110	CLA	MG-ND	-3.82	1.98	2.05
20	Z	602	CLA	MG-ND	-3.82	1.98	2.05
20	B	1235	CLA	MG-ND	-3.82	1.98	2.05
34	5	505	C7Z	C27-C26	3.82	1.58	1.45
20	B	1207	CLA	MG-ND	-3.82	1.98	2.05
34	5	505	C7Z	C22-C21	3.82	1.66	1.54
20	3	606	CLA	MG-ND	-3.81	1.98	2.05
20	1	604	CLA	MG-ND	-3.81	1.98	2.05
34	5	505	C7Z	C15-C14	3.81	1.55	1.43
20	A	1120	CLA	MG-ND	-3.81	1.98	2.05
20	4	601	CLA	MG-ND	-3.80	1.98	2.05
20	A	1103	CLA	MG-ND	-3.80	1.98	2.05
20	B	1225	CLA	C1C-NC	-3.80	1.32	1.37
20	B	1230	CLA	MG-ND	-3.80	1.98	2.05
20	A	1132	CLA	MG-ND	-3.79	1.98	2.05
20	1	603	CLA	MG-ND	-3.79	1.98	2.05
20	8	611	CLA	MG-ND	-3.79	1.98	2.05
20	A	1121	CLA	MG-ND	-3.79	1.98	2.05
20	8	604	CLA	MG-ND	-3.79	1.98	2.05
20	A	1113	CLA	MG-ND	-3.79	1.98	2.05
20	1	605	CLA	MG-ND	-3.78	1.98	2.05
20	3	603	CLA	MG-ND	-3.78	1.98	2.05
20	5	604	CLA	MG-ND	-3.78	1.98	2.05
20	Z	606	CLA	MG-ND	-3.78	1.98	2.05
20	B	1228	CLA	MG-ND	-3.78	1.98	2.05
20	A	1107	CLA	MG-ND	-3.78	1.98	2.05
20	6	609	CLA	C1C-NC	-3.78	1.32	1.37
20	B	1240	CLA	MG-ND	-3.78	1.98	2.05
20	B	1230	CLA	C1C-NC	-3.78	1.32	1.37
20	5	618	CLA	MG-ND	-3.78	1.98	2.05
33	F	4001	RRX	C15-C14	3.78	1.55	1.43
20	B	1203	CLA	MG-ND	-3.77	1.98	2.05
20	B	1236	CLA	MG-ND	-3.77	1.98	2.05
20	7	603	CLA	MG-ND	-3.77	1.98	2.05
20	6	604	CLA	MG-ND	-3.77	1.98	2.05
20	8	606	CLA	MG-ND	-3.76	1.98	2.05
20	B	1205	CLA	C1C-NC	-3.76	1.32	1.37
20	Z	601	CLA	MG-ND	-3.76	1.98	2.05
20	A	1106	CLA	MG-ND	-3.76	1.98	2.05
20	A	1105	CLA	MG-ND	-3.75	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	604	CLA	MG-ND	-3.75	1.98	2.05
33	F	4001	RRX	C23-C22	3.75	1.54	1.45
20	A	1115	CLA	MG-ND	-3.75	1.98	2.05
20	3	601	CLA	MG-ND	-3.75	1.98	2.05
20	7	602	CLA	MG-ND	-3.75	1.98	2.05
20	5	603	CLA	MG-ND	-3.75	1.98	2.05
20	3	610	CLA	C1C-NC	-3.74	1.32	1.37
20	4	606	CLA	MG-ND	-3.74	1.98	2.05
20	G	1602	CLA	MG-ND	-3.73	1.98	2.05
20	B	1238	CLA	MG-ND	-3.72	1.98	2.05
20	B	1207	CLA	C1C-NC	-3.72	1.32	1.37
20	1	608	CLA	MG-ND	-3.72	1.98	2.05
34	1	503	C7Z	C15-C14	3.72	1.55	1.43
20	3	607	CLA	MG-ND	-3.70	1.98	2.05
19	A	1011	CL0	C1D-ND	-3.70	1.33	1.37
20	A	1122	CLA	MG-ND	-3.70	1.98	2.05
20	B	1229	CLA	MG-ND	-3.69	1.98	2.05
34	1	503	C7Z	C27-C26	3.69	1.58	1.45
34	5	505	C7Z	C35-C34	3.69	1.54	1.43
20	A	1109	CLA	C1C-NC	-3.69	1.32	1.37
19	A	1011	CL0	CHC-C4B	3.68	1.47	1.39
20	8	603	CLA	MG-ND	-3.68	1.98	2.05
20	B	1208	CLA	MG-ND	-3.68	1.98	2.05
20	8	615	CLA	MG-ND	-3.67	1.98	2.05
20	A	1108	CLA	C1C-NC	-3.67	1.32	1.37
20	G	1601	CLA	MG-ND	-3.67	1.98	2.05
20	3	605	CLA	MG-ND	-3.66	1.98	2.05
20	Z	611	CLA	MG-ND	-3.66	1.98	2.05
20	8	602	CLA	MG-ND	-3.66	1.98	2.05
20	7	612	CLA	C1C-NC	-3.65	1.32	1.37
20	B	1210	CLA	C1C-NC	-3.65	1.32	1.37
20	A	1113	CLA	C1C-NC	-3.65	1.32	1.37
20	7	605	CLA	MG-ND	-3.65	1.98	2.05
20	B	1234	CLA	C1C-NC	-3.65	1.32	1.37
20	B	1204	CLA	MG-ND	-3.64	1.98	2.05
20	B	1214	CLA	C1C-NC	-3.64	1.32	1.37
20	A	1127	CLA	C1C-NC	-3.64	1.32	1.37
20	B	1220	CLA	C1C-NC	-3.64	1.32	1.37
20	B	1202	CLA	C1C-NC	-3.62	1.32	1.37
20	4	602	CLA	MG-ND	-3.62	1.98	2.05
20	A	1133	CLA	C1C-NC	-3.61	1.32	1.37
20	A	1114	CLA	C1C-NC	-3.61	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1021	CLA	C1C-NC	-3.60	1.32	1.37
20	B	1212	CLA	C1C-NC	-3.60	1.32	1.37
20	B	1223	CLA	C1C-NC	-3.60	1.32	1.37
20	8	609	CLA	C1C-NC	-3.60	1.32	1.37
20	J	1901	CLA	C1C-NC	-3.59	1.32	1.37
20	A	1124	CLA	C1C-NC	-3.59	1.32	1.37
20	A	1117	CLA	C1C-NC	-3.59	1.32	1.37
20	B	1209	CLA	C1C-NC	-3.59	1.32	1.37
20	A	1125	CLA	C1C-NC	-3.58	1.32	1.37
20	B	1236	CLA	C1C-NC	-3.58	1.32	1.37
34	J	4002	C7Z	C27-C26	3.57	1.57	1.45
20	A	1140	CLA	C1C-NC	-3.57	1.32	1.37
34	J	4002	C7Z	C15-C14	3.57	1.54	1.43
34	1	503	C7Z	C35-C34	3.56	1.54	1.43
20	B	1222	CLA	C1C-NC	-3.56	1.32	1.37
20	4	612	CLA	C1C-NC	-3.55	1.32	1.37
20	B	1201	CLA	C1C-NC	-3.55	1.32	1.37
20	3	616	CLA	C1C-NC	-3.54	1.32	1.37
20	F	1301	CLA	C1C-NC	-3.54	1.32	1.37
20	3	605	CLA	C1C-NC	-3.54	1.32	1.37
34	J	4002	C7Z	C35-C34	3.54	1.54	1.43
20	B	1239	CLA	C1C-NC	-3.54	1.32	1.37
20	A	1105	CLA	C1C-NC	-3.53	1.32	1.37
20	6	612	CLA	C1C-NC	-3.52	1.32	1.37
34	5	505	C7Z	C7-C6	3.52	1.57	1.45
20	7	609	CLA	C1C-NC	-3.52	1.32	1.37
20	7	611	CLA	C1C-NC	-3.52	1.32	1.37
20	A	1119	CLA	C1C-NC	-3.52	1.32	1.37
20	6	603	CLA	C1C-NC	-3.51	1.32	1.37
20	1	601	CLA	C1C-NC	-3.51	1.32	1.37
20	L	1503	CLA	MG-ND	-3.51	1.98	2.05
20	B	1228	CLA	C1C-NC	-3.51	1.32	1.37
20	B	1226	CLA	C1C-NC	-3.51	1.32	1.37
20	5	608	CLA	C1C-NC	-3.51	1.32	1.37
20	A	1132	CLA	C1C-NC	-3.50	1.32	1.37
20	B	1222	CLA	C4B-NB	-3.50	1.33	1.37
20	3	613	CLA	C1C-NC	-3.49	1.32	1.37
20	8	601	CLA	C1C-NC	-3.49	1.32	1.37
20	8	615	CLA	C1C-NC	-3.49	1.32	1.37
20	A	1111	CLA	C1C-NC	-3.49	1.32	1.37
20	B	1208	CLA	C1C-NC	-3.49	1.32	1.37
20	3	601	CLA	C1C-NC	-3.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	607	CLA	C1C-NC	-3.48	1.32	1.37
20	Z	601	CLA	C1C-NC	-3.48	1.32	1.37
20	A	1126	CLA	C1C-NC	-3.47	1.32	1.37
20	A	1122	CLA	C1C-NC	-3.47	1.32	1.37
19	A	1011	CL0	OBD-CAD	3.47	1.28	1.22
20	A	1101	CLA	C1C-NC	-3.47	1.32	1.37
20	8	608	CLA	C1C-NC	-3.47	1.32	1.37
20	A	1103	CLA	C1C-NC	-3.47	1.32	1.37
20	B	1224	CLA	C1C-NC	-3.47	1.32	1.37
20	B	1216	CLA	C1C-NC	-3.46	1.32	1.37
20	3	604	CLA	C4B-NB	-3.46	1.33	1.37
20	B	1229	CLA	C1C-NC	-3.46	1.32	1.37
20	4	609	CLA	C1C-NC	-3.46	1.32	1.37
30	A	5005	DGA	OG1-CA1	3.46	1.43	1.33
20	A	1107	CLA	C1C-NC	-3.45	1.32	1.37
20	6	619	CLA	C1C-NC	-3.45	1.32	1.37
20	K	1401	CLA	C1C-NC	-3.45	1.32	1.37
20	A	1135	CLA	C1C-NC	-3.44	1.32	1.37
34	1	503	C7Z	C2-C1	3.44	1.65	1.54
20	A	1130	CLA	C1C-NC	-3.44	1.32	1.37
20	A	1121	CLA	C1C-NC	-3.44	1.32	1.37
20	5	605	CLA	C1C-NC	-3.44	1.32	1.37
20	1	615	CLA	C1C-NC	-3.44	1.32	1.37
20	B	1204	CLA	C1C-NC	-3.44	1.32	1.37
20	B	1227	CLA	C1C-NC	-3.43	1.32	1.37
20	7	601	CLA	C1C-NC	-3.43	1.32	1.37
20	6	618	CLA	C1C-NC	-3.43	1.32	1.37
33	F	4001	RRX	C11-C10	3.43	1.54	1.43
20	1	604	CLA	C1C-NC	-3.43	1.32	1.37
20	3	603	CLA	C1C-NC	-3.43	1.32	1.37
20	B	1218	CLA	C1C-NC	-3.42	1.32	1.37
20	5	615	CLA	C1C-NC	-3.42	1.32	1.37
34	5	505	C7Z	C2-C1	3.42	1.65	1.54
20	1	606	CLA	C1C-NC	-3.42	1.32	1.37
20	Z	615	CLA	C1C-NC	-3.41	1.32	1.37
20	B	1231	CLA	C1C-NC	-3.41	1.32	1.37
20	8	606	CLA	C1C-NC	-3.41	1.32	1.37
20	A	1139	CLA	C1C-NC	-3.41	1.32	1.37
20	L	1502	CLA	C1C-NC	-3.40	1.32	1.37
20	A	1138	CLA	C1C-NC	-3.40	1.32	1.37
20	7	604	CLA	C1C-NC	-3.40	1.32	1.37
20	4	602	CLA	C1C-NC	-3.40	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1129	CLA	C1C-NC	-3.40	1.32	1.37
20	B	1235	CLA	C1C-NC	-3.40	1.32	1.37
20	A	1114	CLA	C4B-NB	-3.40	1.33	1.37
20	A	1137	CLA	C1C-NC	-3.39	1.32	1.37
20	5	612	CLA	C1C-NC	-3.39	1.32	1.37
20	7	606	CLA	C1C-NC	-3.39	1.32	1.37
20	3	606	CLA	C1C-NC	-3.39	1.32	1.37
20	8	603	CLA	C1C-NC	-3.38	1.32	1.37
20	8	605	CLA	C1C-NC	-3.38	1.32	1.37
20	B	1203	CLA	C1C-NC	-3.38	1.32	1.37
20	A	1136	CLA	C1C-NC	-3.38	1.32	1.37
20	Z	603	CLA	C1C-NC	-3.38	1.32	1.37
20	3	612	CLA	C1C-NC	-3.38	1.32	1.37
20	1	603	CLA	C1C-NC	-3.37	1.32	1.37
20	A	1118	CLA	C1C-NC	-3.37	1.32	1.37
20	B	1237	CLA	C1C-NC	-3.37	1.32	1.37
33	F	4001	RRX	C4-C5	-3.37	1.44	1.51
20	K	1404	CLA	C1C-NC	-3.37	1.32	1.37
20	8	607	CLA	C1C-NC	-3.37	1.32	1.37
20	5	618	CLA	C1C-NC	-3.37	1.32	1.37
20	A	1110	CLA	C1C-NC	-3.37	1.32	1.37
33	F	4001	RRX	C24-C25	3.36	1.57	1.45
20	6	605	CLA	C1C-NC	-3.36	1.32	1.37
33	F	4001	RRX	C29-C30	3.36	1.65	1.54
20	4	603	CLA	C1C-NC	-3.36	1.32	1.37
20	4	605	CLA	C1C-NC	-3.36	1.32	1.37
20	B	1211	CLA	C4B-NB	-3.36	1.33	1.37
20	Z	612	CLA	C1C-NC	-3.35	1.32	1.37
20	B	1213	CLA	C1C-NC	-3.35	1.32	1.37
20	A	1102	CLA	C1C-NC	-3.34	1.32	1.37
20	1	602	CLA	C1C-NC	-3.34	1.32	1.37
34	1	503	C7Z	C38-C25	3.34	1.56	1.50
20	6	602	CLA	C1C-NC	-3.34	1.32	1.37
20	7	613	CLA	C1C-NC	-3.34	1.32	1.37
20	A	1104	CLA	C1C-NC	-3.33	1.32	1.37
34	J	4002	C7Z	C2-C1	3.33	1.65	1.54
20	B	1211	CLA	C1C-NC	-3.33	1.32	1.37
20	5	622	CLA	C1C-NC	-3.33	1.32	1.37
30	A	5005	DGA	OG2-CB1	3.33	1.43	1.34
20	5	602	CLA	C1C-NC	-3.33	1.32	1.37
31	B	5003	DGD	CDB-CCB	-3.33	1.32	1.51
20	7	608	CLA	C1C-NC	-3.33	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	603	CLA	C1C-NC	-3.32	1.32	1.37
20	A	1131	CLA	C1C-NC	-3.32	1.32	1.37
31	B	5003	DGD	CGB-CFB	-3.32	1.32	1.51
20	4	601	CLA	C1C-NC	-3.32	1.32	1.37
20	B	1219	CLA	C1C-NC	-3.32	1.32	1.37
20	B	1217	CLA	C1C-NC	-3.32	1.32	1.37
20	5	604	CLA	C1C-NC	-3.32	1.32	1.37
20	1	608	CLA	C1C-NC	-3.32	1.32	1.37
20	B	1215	CLA	C1C-NC	-3.31	1.32	1.37
20	A	1134	CLA	C1C-NC	-3.31	1.32	1.37
20	3	618	CLA	C1C-NC	-3.31	1.32	1.37
20	B	1023	CLA	C1C-NC	-3.31	1.32	1.37
19	A	1011	CL0	C1B-NB	-3.31	1.33	1.37
24	3	801	LHG	O7-C5	-3.31	1.42	1.46
20	8	611	CLA	C1C-NC	-3.31	1.32	1.37
20	F	1302	CLA	C1C-NC	-3.31	1.32	1.37
20	6	608	CLA	C1C-NC	-3.31	1.32	1.37
31	B	5003	DGD	CAB-C9B	-3.30	1.33	1.51
20	B	1206	CLA	C1C-NC	-3.30	1.32	1.37
20	1	607	CLA	C1C-NC	-3.30	1.32	1.37
20	5	609	CLA	C1C-NC	-3.30	1.32	1.37
20	8	604	CLA	C1C-NC	-3.30	1.32	1.37
20	B	1201	CLA	C4B-NB	-3.29	1.33	1.37
20	7	605	CLA	C1C-NC	-3.29	1.32	1.37
20	A	1136	CLA	C4B-NB	-3.29	1.33	1.37
20	B	1238	CLA	C1C-NC	-3.29	1.32	1.37
20	5	601	CLA	C1C-NC	-3.29	1.32	1.37
20	G	1601	CLA	C1C-NC	-3.28	1.32	1.37
34	5	505	C7Z	C38-C25	3.28	1.56	1.50
20	A	1129	CLA	C4B-NB	-3.28	1.33	1.37
20	6	619	CLA	C4B-NB	-3.28	1.33	1.37
20	1	611	CLA	C1C-NC	-3.28	1.32	1.37
20	6	601	CLA	C1C-NC	-3.28	1.32	1.37
20	6	615	CLA	C1C-NC	-3.28	1.32	1.37
20	7	602	CLA	C1C-NC	-3.28	1.32	1.37
20	Z	604	CLA	C1C-NC	-3.28	1.32	1.37
34	1	503	C7Z	C7-C6	3.27	1.56	1.45
33	F	4001	RRX	C16-C17	3.27	1.53	1.43
20	Z	606	CLA	C1C-NC	-3.27	1.32	1.37
20	4	604	CLA	C1C-NC	-3.27	1.32	1.37
20	8	612	CLA	C1C-NC	-3.27	1.32	1.37
20	A	1113	CLA	C4B-NB	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	4002	C7Z	C7-C6	3.26	1.56	1.45
31	B	5003	DGD	CGA-CFA	-3.26	1.33	1.51
20	Z	605	CLA	C1C-NC	-3.26	1.32	1.37
20	6	606	CLA	C1C-NC	-3.26	1.32	1.37
20	1	613	CLA	C1C-NC	-3.26	1.32	1.37
37	4	613	CHL	C1B-NB	-3.26	1.33	1.37
20	5	606	CLA	C1C-NC	-3.25	1.32	1.37
20	4	615	CLA	C1C-NC	-3.25	1.33	1.37
20	A	1126	CLA	C4B-NB	-3.25	1.33	1.37
20	Z	602	CLA	C1C-NC	-3.25	1.33	1.37
20	B	1232	CLA	C1C-NC	-3.25	1.33	1.37
20	1	607	CLA	C4B-NB	-3.24	1.33	1.37
20	4	607	CLA	C1C-NC	-3.24	1.33	1.37
20	7	615	CLA	C1C-NC	-3.24	1.33	1.37
20	K	1403	CLA	C1C-NC	-3.24	1.33	1.37
20	B	1228	CLA	C4B-NB	-3.23	1.33	1.37
20	7	616	CLA	C1C-NC	-3.23	1.33	1.37
20	4	606	CLA	C1C-NC	-3.23	1.33	1.37
20	A	1112	CLA	C1C-NC	-3.23	1.33	1.37
31	B	5003	DGD	CDA-CCA	-3.23	1.33	1.51
20	7	603	CLA	C1C-NC	-3.23	1.33	1.37
31	B	5003	DGD	CAA-C9A	-3.22	1.33	1.51
20	B	1224	CLA	C4B-NB	-3.22	1.33	1.37
20	A	1115	CLA	C1C-NC	-3.22	1.33	1.37
20	A	1108	CLA	C4B-NB	-3.22	1.33	1.37
19	A	1011	CL0	MG-NC	3.22	2.13	2.06
20	5	607	CLA	C1C-NC	-3.22	1.33	1.37
20	1	612	CLA	C1C-NC	-3.21	1.33	1.37
20	A	1141	CLA	C1C-NC	-3.21	1.33	1.37
20	8	602	CLA	C1C-NC	-3.21	1.33	1.37
20	B	1022	CLA	C1C-NC	-3.21	1.33	1.37
20	8	605	CLA	C4B-NB	-3.21	1.33	1.37
20	A	1120	CLA	C1C-NC	-3.21	1.33	1.37
34	J	4002	C7Z	C38-C25	3.20	1.56	1.50
20	1	605	CLA	C1C-NC	-3.20	1.33	1.37
20	A	1124	CLA	C4B-NB	-3.20	1.33	1.37
20	A	1116	CLA	C1C-NC	-3.20	1.33	1.37
20	B	1240	CLA	C1C-NC	-3.20	1.33	1.37
20	5	622	CLA	C4B-NB	-3.19	1.33	1.37
20	B	1241	CLA	C1C-NC	-3.19	1.33	1.37
20	4	612	CLA	C4B-NB	-3.19	1.33	1.37
20	4	608	CLA	C1C-NC	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1023	CLA	C4B-NB	-3.18	1.33	1.37
20	B	1218	CLA	C4B-NB	-3.18	1.33	1.37
20	L	1503	CLA	C1C-NC	-3.17	1.33	1.37
20	4	604	CLA	C4B-NB	-3.17	1.33	1.37
20	A	1013	CLA	C1C-NC	-3.17	1.33	1.37
20	Z	607	CLA	C1C-NC	-3.17	1.33	1.37
20	A	1012	CLA	C1C-NC	-3.17	1.33	1.37
20	6	604	CLA	C1C-NC	-3.17	1.33	1.37
20	Z	611	CLA	C1C-NC	-3.16	1.33	1.37
20	3	608	CLA	C1C-NC	-3.16	1.33	1.37
20	A	1123	CLA	C1C-NC	-3.16	1.33	1.37
34	J	4002	C7Z	C21-C26	-3.16	1.49	1.53
20	8	608	CLA	C4B-NB	-3.16	1.33	1.37
20	1	606	CLA	C4B-NB	-3.15	1.33	1.37
20	A	1133	CLA	C4B-NB	-3.15	1.33	1.37
20	8	612	CLA	C4B-NB	-3.15	1.33	1.37
20	6	607	CLA	C1C-NC	-3.15	1.33	1.37
20	A	1135	CLA	C4B-NB	-3.13	1.33	1.37
20	3	607	CLA	C1C-NC	-3.13	1.33	1.37
20	A	1012	CLA	C4B-NB	-3.13	1.33	1.37
20	1	602	CLA	C4B-NB	-3.13	1.33	1.37
20	7	612	CLA	C4B-NB	-3.12	1.33	1.37
20	5	608	CLA	C4B-NB	-3.12	1.33	1.37
20	6	612	CLA	C4B-NB	-3.12	1.33	1.37
20	6	605	CLA	C4B-NB	-3.11	1.34	1.37
20	6	615	CLA	C4B-NB	-3.11	1.34	1.37
20	A	1103	CLA	C4B-NB	-3.11	1.34	1.37
20	A	1123	CLA	C4B-NB	-3.10	1.34	1.37
20	B	1235	CLA	C4B-NB	-3.10	1.34	1.37
20	5	605	CLA	C4B-NB	-3.10	1.34	1.37
20	4	608	CLA	C4B-NB	-3.10	1.34	1.37
20	1	601	CLA	C4B-NB	-3.09	1.34	1.37
37	8	610	CHL	C1B-NB	-3.09	1.34	1.37
20	3	602	CLA	C1C-NC	-3.09	1.33	1.37
20	B	1230	CLA	C4B-NB	-3.09	1.34	1.37
20	A	1119	CLA	C4B-NB	-3.09	1.34	1.37
20	B	1221	CLA	C1C-NC	-3.09	1.33	1.37
20	Z	601	CLA	C4B-NB	-3.09	1.34	1.37
20	K	1402	CLA	C1C-NC	-3.08	1.33	1.37
20	A	1120	CLA	C4B-NB	-3.08	1.34	1.37
20	Z	608	CLA	C1C-NC	-3.08	1.33	1.37
20	A	1117	CLA	C4B-NB	-3.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1125	CLA	C4B-NB	-3.08	1.34	1.37
20	B	1212	CLA	C4B-NB	-3.08	1.34	1.37
20	B	1220	CLA	C4B-NB	-3.07	1.34	1.37
20	7	613	CLA	C4B-NB	-3.07	1.34	1.37
20	B	1204	CLA	C4B-NB	-3.06	1.34	1.37
20	4	615	CLA	C4B-NB	-3.06	1.34	1.37
20	B	1215	CLA	C4B-NB	-3.06	1.34	1.37
20	5	613	CLA	C1C-NC	-3.06	1.33	1.37
20	3	618	CLA	C4B-NB	-3.06	1.34	1.37
20	6	602	CLA	C4B-NB	-3.06	1.34	1.37
20	A	1128	CLA	C4B-NB	-3.05	1.34	1.37
20	6	607	CLA	C4B-NB	-3.05	1.34	1.37
19	A	1011	CL0	C4B-NB	-3.05	1.34	1.37
20	B	1213	CLA	C4B-NB	-3.04	1.34	1.37
20	8	611	CLA	C4B-NB	-3.04	1.34	1.37
20	8	607	CLA	C4B-NB	-3.04	1.34	1.37
33	F	4001	RRX	C7-C6	3.04	1.55	1.45
20	G	1602	CLA	C1C-NC	-3.03	1.33	1.37
34	5	505	C7Z	C21-C26	-3.02	1.49	1.53
20	7	609	CLA	C4B-NB	-3.02	1.34	1.37
19	A	1011	CL0	C1C-NC	-3.01	1.33	1.37
20	B	1216	CLA	C4B-NB	-3.01	1.34	1.37
20	A	1115	CLA	C4B-NB	-3.01	1.34	1.37
20	A	1013	CLA	C4B-NB	-3.01	1.34	1.37
20	B	1239	CLA	C4B-NB	-3.01	1.34	1.37
20	A	1132	CLA	C4B-NB	-3.00	1.34	1.37
20	3	601	CLA	C4B-NB	-3.00	1.34	1.37
20	B	1210	CLA	C4B-NB	-3.00	1.34	1.37
20	J	1901	CLA	C4B-NB	-3.00	1.34	1.37
20	6	604	CLA	C4B-NB	-2.99	1.34	1.37
20	8	606	CLA	C4B-NB	-2.99	1.34	1.37
20	7	607	CLA	C4B-NB	-2.98	1.34	1.37
20	A	1118	CLA	C4B-NB	-2.98	1.34	1.37
20	B	1202	CLA	C4B-NB	-2.98	1.34	1.37
24	B	5002	LHG	O7-C5	-2.98	1.43	1.46
20	A	1122	CLA	C4B-NB	-2.97	1.34	1.37
20	B	1227	CLA	C4B-NB	-2.97	1.34	1.37
20	B	1214	CLA	C4B-NB	-2.96	1.34	1.37
20	Z	612	CLA	C4B-NB	-2.96	1.34	1.37
20	A	1102	CLA	C4B-NB	-2.96	1.34	1.37
20	A	1101	CLA	C4B-NB	-2.96	1.34	1.37
20	3	613	CLA	C4B-NB	-2.96	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	606	CLA	C4B-NB	-2.95	1.34	1.37
20	A	1131	CLA	C4B-NB	-2.95	1.34	1.37
20	A	1112	CLA	C4B-NB	-2.95	1.34	1.37
20	B	1234	CLA	C4B-NB	-2.94	1.34	1.37
20	L	1502	CLA	C4B-NB	-2.94	1.34	1.37
20	5	601	CLA	C4B-NB	-2.94	1.34	1.37
20	7	611	CLA	C4B-NB	-2.94	1.34	1.37
20	A	1137	CLA	C4B-NB	-2.93	1.34	1.37
20	F	1302	CLA	C4B-NB	-2.92	1.34	1.37
37	6	613	CHL	C1B-NB	-2.92	1.34	1.37
20	1	603	CLA	C4B-NB	-2.92	1.34	1.37
20	5	612	CLA	C4B-NB	-2.92	1.34	1.37
20	Z	605	CLA	C4B-NB	-2.92	1.34	1.37
20	8	604	CLA	C4B-NB	-2.91	1.34	1.37
20	4	601	CLA	C4B-NB	-2.91	1.34	1.37
20	1	605	CLA	C4B-NB	-2.91	1.34	1.37
20	Z	606	CLA	C4B-NB	-2.91	1.34	1.37
20	A	1111	CLA	C4B-NB	-2.90	1.34	1.37
20	A	1107	CLA	C4B-NB	-2.90	1.34	1.37
20	A	1138	CLA	C4B-NB	-2.89	1.34	1.37
20	A	1109	CLA	C4B-NB	-2.89	1.34	1.37
20	A	1141	CLA	C4B-NB	-2.89	1.34	1.37
20	A	1104	CLA	C4B-NB	-2.89	1.34	1.37
37	4	610	CHL	C1B-NB	-2.89	1.34	1.37
20	8	601	CLA	C4B-NB	-2.88	1.34	1.37
20	1	604	CLA	C4B-NB	-2.88	1.34	1.37
20	8	602	CLA	C4B-NB	-2.87	1.34	1.37
20	Z	602	CLA	C4B-NB	-2.87	1.34	1.37
20	B	1241	CLA	C4B-NB	-2.87	1.34	1.37
20	B	1022	CLA	C4B-NB	-2.87	1.34	1.37
20	Z	603	CLA	C4B-NB	-2.86	1.34	1.37
20	7	608	CLA	C4B-NB	-2.86	1.34	1.37
20	3	608	CLA	C4B-NB	-2.86	1.34	1.37
20	7	604	CLA	C4B-NB	-2.86	1.34	1.37
26	4	803	LMT	O3'-C3'	-2.86	1.36	1.43
20	B	1226	CLA	C4B-NB	-2.86	1.34	1.37
19	A	1011	CL0	C4D-CHA	2.86	1.48	1.38
20	5	613	CLA	C4B-NB	-2.86	1.34	1.37
20	A	1134	CLA	C4B-NB	-2.86	1.34	1.37
20	1	615	CLA	C4B-NB	-2.85	1.34	1.37
20	B	1238	CLA	C4B-NB	-2.85	1.34	1.37
20	B	1206	CLA	C4B-NB	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	612	CLA	C4B-NB	-2.85	1.34	1.37
20	B	1208	CLA	C4B-NB	-2.85	1.34	1.37
20	7	606	CLA	C4B-NB	-2.84	1.34	1.37
20	L	1503	CLA	C4B-NB	-2.84	1.34	1.37
37	Z	610	CHL	C1B-NB	-2.84	1.34	1.37
20	3	602	CLA	C4B-NB	-2.84	1.34	1.37
20	7	615	CLA	C4B-NB	-2.84	1.34	1.37
20	3	612	CLA	C4B-NB	-2.83	1.34	1.37
20	A	1106	CLA	C4B-NB	-2.83	1.34	1.37
20	B	1203	CLA	C4B-NB	-2.83	1.34	1.37
20	6	601	CLA	C4B-NB	-2.82	1.34	1.37
20	1	611	CLA	C4B-NB	-2.82	1.34	1.37
20	3	610	CLA	C4B-NB	-2.82	1.34	1.37
20	7	603	CLA	C4B-NB	-2.82	1.34	1.37
20	6	618	CLA	C4B-NB	-2.81	1.34	1.37
20	5	602	CLA	C4B-NB	-2.81	1.34	1.37
20	3	606	CLA	C4B-NB	-2.80	1.34	1.37
26	A	5006	LMT	O3'-C3'	-2.79	1.36	1.43
20	5	615	CLA	C4B-NB	-2.79	1.34	1.37
20	Z	611	CLA	C4B-NB	-2.79	1.34	1.37
37	Z	609	CHL	C3A-C2A	-2.78	1.46	1.54
20	Z	607	CLA	C4B-NB	-2.78	1.34	1.37
20	4	603	CLA	C4B-NB	-2.78	1.34	1.37
20	B	1221	CLA	C4B-NB	-2.78	1.34	1.37
20	7	602	CLA	C4B-NB	-2.78	1.34	1.37
20	5	603	CLA	C4B-NB	-2.78	1.34	1.37
20	A	1130	CLA	C4B-NB	-2.78	1.34	1.37
20	B	1205	CLA	C4B-NB	-2.78	1.34	1.37
20	B	1219	CLA	C4B-NB	-2.78	1.34	1.37
42	8	803	LPX	P1-O1	2.77	1.70	1.59
20	4	607	CLA	C4B-NB	-2.77	1.34	1.37
20	5	607	CLA	C4B-NB	-2.77	1.34	1.37
20	5	618	CLA	C4B-NB	-2.77	1.34	1.37
20	Z	604	CLA	C4B-NB	-2.77	1.34	1.37
37	6	610	CHL	C1B-NB	-2.76	1.34	1.37
19	A	1011	CL0	C3D-C2D	2.76	1.46	1.39
37	6	611	CHL	C1B-NB	-2.76	1.34	1.37
20	6	606	CLA	C4B-NB	-2.75	1.34	1.37
20	6	609	CLA	C4B-NB	-2.75	1.34	1.37
20	B	1231	CLA	C4B-NB	-2.74	1.34	1.37
26	B	5005	LMT	O3'-C3'	-2.73	1.36	1.43
20	7	605	CLA	C4B-NB	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	601	CLA	C4B-NB	-2.72	1.34	1.37
20	K	1404	CLA	C4B-NB	-2.72	1.34	1.37
20	K	1401	CLA	C4B-NB	-2.71	1.34	1.37
20	6	603	CLA	C4B-NB	-2.71	1.34	1.37
26	1	803	LMT	O3'-C3'	-2.71	1.36	1.43
20	F	1301	CLA	C4B-NB	-2.71	1.34	1.37
20	A	1105	CLA	C4B-NB	-2.71	1.34	1.37
20	4	606	CLA	C4B-NB	-2.70	1.34	1.37
26	8	805	LMT	O2'-C2'	-2.70	1.36	1.43
20	K	1403	CLA	C4B-NB	-2.69	1.34	1.37
20	7	616	CLA	C4B-NB	-2.69	1.34	1.37
26	F	5001	LMT	O3'-C3'	-2.69	1.36	1.43
26	4	803	LMT	O3B-C3B	-2.68	1.36	1.43
20	4	602	CLA	C4B-NB	-2.68	1.34	1.37
37	Z	613	CHL	C1B-NB	-2.68	1.34	1.37
37	4	611	CHL	C1B-NB	-2.68	1.34	1.37
20	1	613	CLA	C4B-NB	-2.68	1.34	1.37
20	5	609	CLA	C4B-NB	-2.67	1.34	1.37
37	8	613	CHL	C1B-NB	-2.67	1.34	1.37
20	Z	615	CLA	C4B-NB	-2.67	1.34	1.37
20	3	607	CLA	C4B-NB	-2.67	1.34	1.37
20	B	1232	CLA	C4B-NB	-2.67	1.34	1.37
20	B	1225	CLA	C4B-NB	-2.67	1.34	1.37
34	1	503	C7Z	C21-C26	-2.66	1.50	1.53
20	3	603	CLA	C4B-NB	-2.65	1.34	1.37
26	A	5006	LMT	O2B-C2B	-2.65	1.36	1.43
25	3	802	NKP	OAF-CAG	-2.65	1.34	1.44
20	8	615	CLA	C4B-NB	-2.65	1.34	1.37
20	B	1237	CLA	C4B-NB	-2.64	1.34	1.37
20	G	1601	CLA	C4B-NB	-2.64	1.34	1.37
26	B	5005	LMT	O3B-C3B	-2.64	1.36	1.43
20	6	608	CLA	C4B-NB	-2.63	1.34	1.37
25	8	802	NKP	OAF-CAG	-2.63	1.34	1.44
40	8	806	3PH	O21-C2	-2.62	1.40	1.46
20	B	1207	CLA	C4B-NB	-2.62	1.34	1.37
19	A	1011	CL0	C1B-C2B	2.62	1.49	1.43
20	K	1402	CLA	C4B-NB	-2.62	1.34	1.37
26	A	5006	LMT	O2'-C2'	-2.61	1.36	1.43
20	3	616	CLA	C4B-NB	-2.61	1.34	1.37
26	B	5005	LMT	O2'-C2'	-2.60	1.36	1.43
25	A	5004	NKP	OAF-CAG	-2.59	1.34	1.44
20	B	1223	CLA	C4B-NB	-2.59	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	609	CLA	C4B-NB	-2.58	1.34	1.37
37	1	610	CHL	C1B-NB	-2.58	1.34	1.37
37	3	611	CHL	C1B-NB	-2.58	1.34	1.37
20	Z	608	CLA	C4B-NB	-2.57	1.34	1.37
20	A	1140	CLA	C4B-NB	-2.57	1.34	1.37
39	Z	504	QTB	C14-C12	-2.57	1.47	1.53
20	B	1229	CLA	C4B-NB	-2.57	1.34	1.37
20	3	605	CLA	C4B-NB	-2.57	1.34	1.37
37	5	610	CHL	C1B-NB	-2.56	1.34	1.37
37	4	617	CHL	C1B-NB	-2.56	1.34	1.37
33	F	4001	RRX	C32-C1	2.55	1.58	1.53
20	A	1127	CLA	C4B-NB	-2.55	1.34	1.37
26	8	805	LMT	O3B-C3B	-2.54	1.37	1.43
20	1	608	CLA	C4B-NB	-2.53	1.34	1.37
37	5	617	CHL	C1B-NB	-2.53	1.34	1.37
20	A	1139	CLA	C4B-NB	-2.53	1.34	1.37
37	5	611	CHL	C1B-NB	-2.52	1.34	1.37
40	7	802	3PH	O21-C21	2.52	1.41	1.34
34	5	505	C7Z	C20-C13	2.52	1.56	1.50
20	8	603	CLA	C4B-NB	-2.51	1.34	1.37
26	F	5001	LMT	O2B-C2B	-2.51	1.37	1.43
37	1	609	CHL	C1B-NB	-2.51	1.34	1.37
40	5	802	3PH	O21-C2	-2.50	1.40	1.46
20	A	1116	CLA	C4B-NB	-2.50	1.34	1.37
26	F	5001	LMT	O2'-C2'	-2.50	1.37	1.43
20	B	1209	CLA	C4B-NB	-2.49	1.34	1.37
40	6	802	3PH	O21-C2	-2.49	1.40	1.46
26	1	803	LMT	O2B-C2B	-2.47	1.37	1.43
26	1	803	LMT	O2'-C2'	-2.47	1.37	1.43
20	5	604	CLA	C4B-NB	-2.46	1.34	1.37
20	B	1236	CLA	C4B-NB	-2.45	1.34	1.37
40	5	802	3PH	O31-C31	2.45	1.40	1.33
20	8	609	CLA	C4B-NB	-2.44	1.34	1.37
26	8	805	LMT	O3'-C3'	-2.43	1.37	1.43
20	K	1402	CLA	C1C-C2C	2.43	1.49	1.44
34	J	4002	C7Z	C20-C13	2.43	1.55	1.50
26	B	6101	LMT	O3'-C3'	-2.43	1.37	1.43
20	B	1217	CLA	C4B-NB	-2.43	1.34	1.37
20	B	1241	CLA	C1C-C2C	2.43	1.49	1.44
40	6	802	3PH	O31-C31	2.43	1.40	1.33
34	J	4002	C7Z	C10-C9	-2.43	1.32	1.35
26	8	805	LMT	O2B-C2B	-2.42	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	7	802	3PH	O31-C31	2.42	1.40	1.33
40	8	806	3PH	O31-C31	2.42	1.40	1.33
20	A	1121	CLA	C4B-NB	-2.41	1.34	1.37
26	4	803	LMT	O2'-C2'	-2.41	1.37	1.43
20	4	612	CLA	C1A-CHA	2.40	1.53	1.43
20	B	1021	CLA	C4B-NB	-2.39	1.34	1.37
39	Z	504	QTB	C03-C02	-2.39	1.32	1.35
23	5	504	BCR	C12-C13	-2.38	1.40	1.45
26	1	803	LMT	O3B-C3B	-2.38	1.37	1.43
42	8	803	LPX	P1-O2	2.37	1.68	1.59
20	Z	603	CLA	C1C-C2C	2.36	1.49	1.44
20	B	1226	CLA	C3D-C4D	-2.36	1.38	1.44
26	4	803	LMT	O2B-C2B	-2.36	1.37	1.43
20	4	605	CLA	C4B-NB	-2.36	1.34	1.37
20	K	1404	CLA	C1A-CHA	2.36	1.52	1.43
20	A	1117	CLA	C1A-CHA	2.36	1.52	1.43
26	A	5006	LMT	O3B-C3B	-2.36	1.37	1.43
34	5	505	C7Z	C18-C5	2.35	1.54	1.50
20	A	1122	CLA	C1A-CHA	2.35	1.52	1.43
26	B	5005	LMT	O2B-C2B	-2.35	1.37	1.43
26	B	6101	LMT	O2'-C2'	-2.35	1.37	1.43
26	F	5001	LMT	O3B-C3B	-2.34	1.37	1.43
37	Z	609	CHL	C1B-NB	-2.34	1.34	1.37
26	B	6101	LMT	O2B-C2B	-2.34	1.37	1.43
34	1	503	C7Z	C18-C5	2.33	1.54	1.50
20	F	1301	CLA	C1A-CHA	2.33	1.52	1.43
20	3	607	CLA	C1A-CHA	2.32	1.52	1.43
20	B	1240	CLA	C4B-NB	-2.32	1.34	1.37
20	6	605	CLA	C1A-CHA	2.32	1.52	1.43
37	6	617	CHL	C1B-NB	-2.30	1.35	1.37
30	A	5005	DGA	OG2-CG2	-2.30	1.40	1.46
20	1	612	CLA	C1A-CHA	2.30	1.52	1.43
20	A	1135	CLA	C3D-C4D	-2.29	1.39	1.44
34	1	503	C7Z	C40-C33	2.29	1.55	1.50
20	Z	606	CLA	C1C-C2C	2.29	1.49	1.44
26	A	5006	LMT	O4'-C4B	-2.29	1.37	1.43
20	5	601	CLA	C1A-CHA	2.29	1.52	1.43
34	1	503	C7Z	C20-C13	2.29	1.55	1.50
20	B	1206	CLA	C1A-CHA	2.29	1.52	1.43
20	1	601	CLA	C1A-CHA	2.28	1.52	1.43
20	4	602	CLA	C1A-CHA	2.28	1.52	1.43
20	L	1502	CLA	C1C-C2C	2.27	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	7	607	CLA	C1A-CHA	2.27	1.52	1.43
20	G	1602	CLA	C4B-NB	-2.27	1.35	1.37
20	G	1601	CLA	C1A-CHA	2.27	1.52	1.43
20	K	1404	CLA	C1C-C2C	2.27	1.49	1.44
20	G	1602	CLA	C1C-C2C	2.27	1.49	1.44
20	B	1227	CLA	C3D-C4D	-2.27	1.39	1.44
33	F	4001	RRX	C35-C13	2.27	1.55	1.50
26	8	805	LMT	O1'-C1'	-2.26	1.36	1.40
20	4	615	CLA	C1A-CHA	2.26	1.52	1.43
20	A	1125	CLA	C3D-C4D	-2.26	1.39	1.44
20	7	603	CLA	C1A-CHA	2.26	1.52	1.43
20	A	1109	CLA	C3D-C4D	-2.25	1.39	1.44
20	8	602	CLA	C1A-CHA	2.25	1.52	1.43
20	F	1302	CLA	C1C-C2C	2.25	1.48	1.44
20	3	610	CLA	C1A-CHA	2.25	1.52	1.43
20	5	607	CLA	C1A-CHA	2.25	1.52	1.43
20	5	615	CLA	C1A-CHA	2.25	1.52	1.43
23	3	504	BCR	C12-C13	-2.24	1.41	1.45
40	6	802	3PH	O21-C21	2.24	1.40	1.34
20	B	1223	CLA	C3D-C4D	-2.24	1.39	1.44
20	7	601	CLA	C3D-C4D	-2.24	1.39	1.44
20	6	619	CLA	C1A-CHA	2.24	1.52	1.43
20	A	1104	CLA	C3D-C4D	-2.24	1.39	1.44
20	4	603	CLA	C1A-CHA	2.23	1.52	1.43
20	A	1110	CLA	C4B-NB	-2.23	1.35	1.37
20	A	1110	CLA	C1A-CHA	2.23	1.52	1.43
37	7	610	CHL	C1B-NB	-2.23	1.35	1.37
20	B	1202	CLA	C3D-C4D	-2.23	1.39	1.44
20	B	1221	CLA	C1A-CHA	2.23	1.52	1.43
20	A	1126	CLA	C3D-C4D	-2.23	1.39	1.44
20	7	615	CLA	C1A-CHA	2.23	1.52	1.43
26	1	803	LMT	O4'-C4B	-2.23	1.37	1.43
20	B	1212	CLA	C1A-CHA	2.23	1.52	1.43
28	A	5007	DAO	C2-C1	2.23	1.55	1.50
20	B	1022	CLA	C3D-C4D	-2.22	1.39	1.44
20	5	604	CLA	C1C-C2C	2.21	1.48	1.44
20	7	613	CLA	C3D-C4D	-2.21	1.39	1.44
20	Z	607	CLA	C1A-CHA	2.21	1.52	1.43
20	B	1230	CLA	C1A-CHA	2.21	1.52	1.43
34	J	4002	C7Z	C18-C5	2.21	1.54	1.50
20	B	1209	CLA	C3B-C4B	2.21	1.47	1.42
20	8	607	CLA	C1A-CHA	2.21	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	7	802	3PH	O31-C3	-2.21	1.40	1.45
20	1	603	CLA	C1A-CHA	2.21	1.52	1.43
20	A	1124	CLA	C1A-CHA	2.20	1.52	1.43
20	B	1219	CLA	C1A-CHA	2.20	1.52	1.43
20	A	1141	CLA	C1A-CHA	2.20	1.52	1.43
23	A	4005	BCR	C12-C13	-2.20	1.41	1.45
40	5	802	3PH	O21-C21	2.20	1.40	1.34
20	8	609	CLA	C1A-CHA	2.20	1.52	1.43
20	7	602	CLA	C1A-CHA	2.20	1.52	1.43
20	A	1139	CLA	C1A-CHA	2.20	1.52	1.43
20	F	1302	CLA	C1A-CHA	2.20	1.52	1.43
37	8	613	CHL	C3A-C2A	-2.19	1.48	1.54
20	A	1102	CLA	C1C-C2C	2.19	1.48	1.44
20	1	608	CLA	C1A-CHA	2.19	1.52	1.43
20	7	609	CLA	C1A-CHA	2.19	1.52	1.43
20	B	1241	CLA	C1A-CHA	2.19	1.52	1.43
25	A	5004	NKP	CAG-CAH	2.19	1.58	1.51
20	J	1901	CLA	C1A-CHA	2.19	1.52	1.43
20	B	1208	CLA	C1A-CHA	2.19	1.52	1.43
20	6	602	CLA	C1A-CHA	2.19	1.52	1.43
20	B	1207	CLA	C1A-CHA	2.18	1.52	1.43
20	A	1107	CLA	C1A-CHA	2.18	1.52	1.43
20	Z	612	CLA	C1A-CHA	2.18	1.52	1.43
20	A	1134	CLA	C1A-CHA	2.18	1.52	1.43
20	B	1204	CLA	C3D-C4D	-2.18	1.39	1.44
20	3	605	CLA	C3D-C4D	-2.18	1.39	1.44
20	5	603	CLA	C1A-CHA	2.18	1.52	1.43
20	G	1602	CLA	C1A-CHA	2.18	1.52	1.43
20	B	1239	CLA	C1A-CHA	2.18	1.52	1.43
20	4	601	CLA	C1A-CHA	2.18	1.52	1.43
37	1	609	CHL	C3A-C2A	-2.18	1.48	1.54
20	L	1502	CLA	C1A-CHA	2.18	1.52	1.43
26	F	5001	LMT	O4'-C4B	-2.18	1.37	1.43
20	B	1214	CLA	C1A-CHA	2.18	1.52	1.43
20	Z	601	CLA	C1C-C2C	2.18	1.48	1.44
20	6	615	CLA	C1A-CHA	2.18	1.52	1.43
20	5	618	CLA	C1A-CHA	2.18	1.52	1.43
20	A	1104	CLA	C1C-C2C	2.18	1.48	1.44
20	A	1106	CLA	C3B-C4B	2.17	1.47	1.42
20	A	1121	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	1011	CL0	C3B-C4B	2.17	1.47	1.42
20	B	1220	CLA	C1A-CHA	2.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	603	CLA	C1A-CHA	2.17	1.52	1.43
20	K	1403	CLA	C1A-CHA	2.17	1.52	1.43
20	L	1503	CLA	C1A-CHA	2.17	1.52	1.43
20	B	1234	CLA	C3D-C4D	-2.17	1.39	1.44
20	7	616	CLA	C1A-CHA	2.17	1.52	1.43
20	5	622	CLA	C1A-CHA	2.17	1.52	1.43
20	K	1401	CLA	C1A-CHA	2.17	1.52	1.43
20	Z	605	CLA	C1A-CHA	2.16	1.52	1.43
20	A	1114	CLA	C3D-C4D	-2.16	1.39	1.44
20	B	1217	CLA	C1C-C2C	2.16	1.48	1.44
20	A	1013	CLA	C1D-ND	-2.16	1.35	1.37
20	4	601	CLA	C1C-C2C	2.16	1.48	1.44
20	B	1209	CLA	C1A-CHA	2.16	1.52	1.43
20	8	603	CLA	C1A-CHA	2.16	1.52	1.43
20	A	1108	CLA	C3D-C4D	-2.16	1.39	1.44
20	8	603	CLA	C1C-C2C	2.16	1.48	1.44
20	7	608	CLA	C3D-C4D	-2.16	1.39	1.44
20	6	608	CLA	C1A-CHA	2.16	1.52	1.43
20	B	1023	CLA	C1A-CHA	2.16	1.52	1.43
20	K	1402	CLA	C1A-CHA	2.16	1.52	1.43
40	8	806	3PH	O31-C3	-2.16	1.40	1.45
20	Z	611	CLA	C1A-CHA	2.16	1.52	1.43
20	Z	604	CLA	C1C-C2C	2.16	1.48	1.44
20	4	604	CLA	C1A-CHA	2.16	1.52	1.43
20	7	608	CLA	C1A-CHA	2.16	1.52	1.43
20	B	1210	CLA	C3D-C4D	-2.16	1.39	1.44
20	A	1113	CLA	C1A-CHA	2.16	1.52	1.43
20	1	607	CLA	C1A-CHA	2.16	1.52	1.43
20	5	602	CLA	C1C-C2C	2.15	1.48	1.44
20	1	615	CLA	C1C-C2C	2.15	1.48	1.44
20	5	608	CLA	C1A-CHA	2.15	1.52	1.43
20	8	601	CLA	C3D-C4D	-2.15	1.39	1.44
20	Z	608	CLA	C1C-C2C	2.15	1.48	1.44
20	1	605	CLA	C3D-C4D	-2.15	1.39	1.44
20	B	1203	CLA	C1A-CHA	2.15	1.52	1.43
20	3	616	CLA	C1A-CHA	2.15	1.52	1.43
20	5	606	CLA	C1A-CHA	2.15	1.52	1.43
20	A	1123	CLA	MG-NC	2.15	2.11	2.06
20	B	1224	CLA	C1A-CHA	2.15	1.52	1.43
20	8	601	CLA	C1A-CHA	2.15	1.52	1.43
20	7	604	CLA	C1C-C2C	2.15	1.48	1.44
20	A	1012	CLA	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	605	CLA	C3D-C4D	-2.15	1.39	1.44
20	8	608	CLA	C3D-C4D	-2.15	1.39	1.44
20	A	1102	CLA	C1A-CHA	2.15	1.52	1.43
20	B	1221	CLA	C1C-C2C	2.15	1.48	1.44
20	1	615	CLA	C1A-CHA	2.15	1.52	1.43
26	B	5005	LMT	O4'-C4B	-2.15	1.37	1.43
20	A	1138	CLA	C1A-CHA	2.15	1.52	1.43
20	7	605	CLA	C1A-CHA	2.14	1.52	1.43
20	8	612	CLA	C1A-CHA	2.14	1.52	1.43
20	A	1105	CLA	C1C-C2C	2.14	1.48	1.44
20	A	1123	CLA	C1A-CHA	2.14	1.52	1.43
20	B	1213	CLA	C1A-CHA	2.14	1.52	1.43
20	B	1226	CLA	C1A-CHA	2.14	1.52	1.43
20	3	613	CLA	C1A-CHA	2.14	1.52	1.43
20	B	1214	CLA	C3D-C4D	-2.14	1.39	1.44
20	Z	603	CLA	C1A-CHA	2.14	1.52	1.43
20	8	615	CLA	C1A-CHA	2.14	1.52	1.43
20	5	622	CLA	CHD-C1D	2.14	1.42	1.38
20	A	1129	CLA	C1A-CHA	2.14	1.52	1.43
20	B	1211	CLA	C3D-C4D	-2.13	1.39	1.44
20	F	1302	CLA	MG-NC	2.13	2.11	2.06
20	A	1108	CLA	C1A-CHA	2.13	1.52	1.43
20	B	1218	CLA	C1A-CHA	2.13	1.51	1.43
20	A	1104	CLA	C1A-CHA	2.13	1.51	1.43
20	Z	604	CLA	C1A-CHA	2.13	1.51	1.43
20	7	601	CLA	C1C-C2C	2.13	1.48	1.44
20	A	1109	CLA	C1A-CHA	2.13	1.51	1.43
20	4	607	CLA	C1A-CHA	2.13	1.51	1.43
20	A	1110	CLA	C3B-C4B	2.13	1.47	1.42
20	B	1229	CLA	C1C-C2C	2.13	1.48	1.44
20	B	1236	CLA	C1C-C2C	2.13	1.48	1.44
20	3	612	CLA	C1A-CHA	2.13	1.51	1.43
20	B	1237	CLA	C3D-C4D	-2.13	1.39	1.44
20	A	1133	CLA	C1A-CHA	2.13	1.51	1.43
20	3	604	CLA	C1A-CHA	2.13	1.51	1.43
20	A	1128	CLA	C1A-CHA	2.13	1.51	1.43
20	3	608	CLA	C1A-CHA	2.13	1.51	1.43
20	7	603	CLA	C1C-C2C	2.12	1.48	1.44
20	Z	601	CLA	C1A-CHA	2.12	1.51	1.43
20	A	1123	CLA	C3D-C4D	-2.12	1.39	1.44
20	A	1139	CLA	C3D-C4D	-2.12	1.39	1.44
20	3	606	CLA	C1A-CHA	2.12	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	606	CLA	C1A-CHA	2.12	1.51	1.43
20	B	1216	CLA	C3D-C4D	-2.12	1.39	1.44
20	6	601	CLA	C1A-CHA	2.12	1.51	1.43
20	5	609	CLA	C1A-CHA	2.12	1.51	1.43
20	Z	615	CLA	C1A-CHA	2.12	1.51	1.43
20	A	1119	CLA	C3D-C4D	-2.12	1.39	1.44
20	5	602	CLA	C1A-CHA	2.12	1.51	1.43
20	A	1120	CLA	C1A-CHA	2.12	1.51	1.43
20	1	602	CLA	C1A-CHA	2.12	1.51	1.43
20	5	607	CLA	C1C-C2C	2.12	1.48	1.44
20	B	1232	CLA	C1A-CHA	2.12	1.51	1.43
20	B	1231	CLA	C3D-C4D	-2.11	1.39	1.44
20	B	1238	CLA	C1A-CHA	2.11	1.51	1.43
20	J	1901	CLA	C3D-C4D	-2.11	1.39	1.44
20	5	612	CLA	C1A-CHA	2.11	1.51	1.43
20	Z	611	CLA	C1C-C2C	2.11	1.48	1.44
20	A	1107	CLA	C1C-C2C	2.11	1.48	1.44
20	3	602	CLA	C1A-CHA	2.11	1.51	1.43
20	Z	602	CLA	C1A-CHA	2.11	1.51	1.43
20	5	613	CLA	C1C-C2C	2.11	1.48	1.44
20	A	1113	CLA	C3D-C4D	-2.11	1.39	1.44
20	B	1213	CLA	C1C-C2C	2.10	1.48	1.44
20	3	601	CLA	C1C-C2C	2.10	1.48	1.44
20	A	1114	CLA	C1A-CHA	2.10	1.51	1.43
20	B	1216	CLA	CHD-C1D	2.10	1.42	1.38
20	1	602	CLA	C1C-C2C	2.10	1.48	1.44
20	6	603	CLA	C1A-CHA	2.10	1.51	1.43
40	8	806	3PH	O21-C21	2.10	1.40	1.34
20	A	1131	CLA	C3D-C4D	-2.10	1.39	1.44
20	5	609	CLA	C1C-C2C	2.10	1.48	1.44
20	A	1101	CLA	C3D-C4D	-2.10	1.39	1.44
20	8	604	CLA	C1A-CHA	2.10	1.51	1.43
34	J	4002	C7Z	C40-C33	2.10	1.55	1.50
40	6	802	3PH	O31-C3	-2.10	1.40	1.45
20	B	1201	CLA	C3B-C4B	2.10	1.47	1.42
20	Z	607	CLA	C1C-C2C	2.10	1.48	1.44
20	A	1138	CLA	C3D-C4D	-2.10	1.39	1.44
20	7	611	CLA	C1A-CHA	2.10	1.51	1.43
20	B	1225	CLA	C3B-C4B	2.10	1.47	1.42
20	1	611	CLA	C3D-C4D	-2.10	1.39	1.44
20	A	1136	CLA	C1A-CHA	2.10	1.51	1.43
20	1	611	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	618	CLA	C1A-CHA	2.10	1.51	1.43
20	6	618	CLA	C1A-CHA	2.10	1.51	1.43
20	5	609	CLA	MG-NC	2.10	2.11	2.06
20	A	1115	CLA	C3D-C4D	-2.09	1.39	1.44
20	A	1131	CLA	C1A-CHA	2.09	1.51	1.43
20	B	1205	CLA	C1A-CHA	2.09	1.51	1.43
20	Z	606	CLA	CHD-C1D	2.09	1.42	1.38
20	A	1111	CLA	C3D-C4D	-2.09	1.39	1.44
25	3	802	NKP	CAG-CAH	2.09	1.58	1.51
20	B	1238	CLA	C1C-C2C	2.09	1.48	1.44
20	6	607	CLA	C1A-CHA	2.09	1.51	1.43
20	B	1240	CLA	C3D-C4D	-2.09	1.39	1.44
20	3	612	CLA	C1C-C2C	2.09	1.48	1.44
26	B	6101	LMT	O3B-C3B	-2.09	1.38	1.43
20	B	1225	CLA	C1A-CHA	2.09	1.51	1.43
20	B	1227	CLA	C1C-C2C	2.09	1.48	1.44
20	B	1217	CLA	C1A-CHA	2.09	1.51	1.43
20	A	1013	CLA	C1A-CHA	2.09	1.51	1.43
20	6	608	CLA	C3D-C4D	-2.09	1.39	1.44
20	3	605	CLA	C1A-CHA	2.09	1.51	1.43
20	A	1137	CLA	C3D-C4D	-2.09	1.39	1.44
20	B	1238	CLA	C3D-C4D	-2.09	1.39	1.44
20	6	612	CLA	C3D-C4D	-2.09	1.39	1.44
26	B	6101	LMT	O4'-C4B	-2.09	1.38	1.43
20	8	611	CLA	C1A-CHA	2.09	1.51	1.43
20	4	608	CLA	C1C-C2C	2.09	1.48	1.44
20	8	605	CLA	C1A-CHA	2.09	1.51	1.43
20	Z	606	CLA	C1A-CHA	2.08	1.51	1.43
20	4	608	CLA	C1A-CHA	2.08	1.51	1.43
20	5	613	CLA	C1A-CHA	2.08	1.51	1.43
20	B	1240	CLA	C1A-CHA	2.08	1.51	1.43
20	A	1120	CLA	C1C-C2C	2.08	1.48	1.44
20	K	1401	CLA	C3D-C4D	-2.08	1.39	1.44
20	8	605	CLA	C3D-C4D	-2.08	1.39	1.44
20	5	604	CLA	C3B-C4B	2.08	1.47	1.42
20	A	1116	CLA	C3D-C4D	-2.08	1.39	1.44
20	1	613	CLA	C1C-C2C	2.08	1.48	1.44
20	A	1130	CLA	C1A-CHA	2.08	1.51	1.43
20	7	615	CLA	C1C-C2C	2.08	1.48	1.44
20	8	612	CLA	C1C-C2C	2.08	1.48	1.44
20	B	1241	CLA	MG-NC	2.08	2.11	2.06
34	5	505	C7Z	C40-C33	2.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1127	CLA	C3D-C4D	-2.08	1.39	1.44
20	A	1111	CLA	C1A-CHA	2.08	1.51	1.43
20	8	606	CLA	C1A-CHA	2.08	1.51	1.43
20	B	1021	CLA	C3D-C4D	-2.08	1.39	1.44
26	A	5006	LMT	O1'-C1'	-2.08	1.36	1.40
20	3	607	CLA	MG-NC	2.08	2.11	2.06
20	A	1106	CLA	C3D-C4D	-2.08	1.39	1.44
20	A	1136	CLA	C3D-C4D	-2.07	1.39	1.44
20	B	1201	CLA	C3D-C4D	-2.07	1.39	1.44
20	7	611	CLA	C1C-C2C	2.07	1.48	1.44
20	A	1117	CLA	C3D-C4D	-2.07	1.39	1.44
20	B	1236	CLA	C1A-CHA	2.07	1.51	1.43
20	A	1128	CLA	C3D-C4D	-2.07	1.39	1.44
20	4	609	CLA	C3D-C4D	-2.07	1.39	1.44
20	4	609	CLA	C1A-CHA	2.07	1.51	1.43
20	A	1137	CLA	C1A-CHA	2.07	1.51	1.43
20	6	604	CLA	C1C-C2C	2.07	1.48	1.44
20	7	601	CLA	C1A-CHA	2.07	1.51	1.43
20	8	602	CLA	C1C-C2C	2.07	1.48	1.44
20	A	1126	CLA	C1C-C2C	2.07	1.48	1.44
20	B	1241	CLA	C3D-C4D	-2.07	1.39	1.44
20	4	606	CLA	C1A-CHA	2.07	1.51	1.43
20	7	613	CLA	C1A-CHA	2.07	1.51	1.43
20	4	605	CLA	C1A-CHA	2.07	1.51	1.43
20	B	1235	CLA	C1C-C2C	2.07	1.48	1.44
20	3	601	CLA	C1A-CHA	2.07	1.51	1.43
20	A	1132	CLA	CHD-C1D	2.07	1.42	1.38
20	A	1129	CLA	C3D-C4D	-2.07	1.39	1.44
20	A	1126	CLA	C1A-CHA	2.06	1.51	1.43
20	A	1140	CLA	C1A-CHA	2.06	1.51	1.43
20	7	612	CLA	C3D-C4D	-2.06	1.39	1.44
20	B	1228	CLA	C1A-CHA	2.06	1.51	1.43
20	7	612	CLA	C1A-CHA	2.06	1.51	1.43
20	A	1133	CLA	C3D-C4D	-2.06	1.39	1.44
20	8	606	CLA	C3D-C4D	-2.06	1.39	1.44
23	3	503	BCR	C12-C13	-2.06	1.41	1.45
20	B	1208	CLA	C1C-C2C	2.06	1.48	1.44
20	5	609	CLA	C3D-C4D	-2.06	1.39	1.44
20	K	1402	CLA	C3D-C4D	-2.06	1.39	1.44
20	5	602	CLA	C3D-C4D	-2.06	1.39	1.44
20	Z	611	CLA	C3D-C4D	-2.06	1.39	1.44
20	B	1211	CLA	C1A-CHA	2.06	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1222	CLA	C1A-CHA	2.06	1.51	1.43
20	5	608	CLA	C3D-C4D	-2.06	1.39	1.44
20	A	1132	CLA	C3D-C4D	-2.06	1.39	1.44
20	3	610	CLA	C3D-C4D	-2.06	1.39	1.44
20	3	606	CLA	C3D-C4D	-2.06	1.39	1.44
20	8	615	CLA	C3D-C4D	-2.06	1.39	1.44
20	B	1229	CLA	C3D-C4D	-2.06	1.39	1.44
20	Z	608	CLA	C1A-CHA	2.06	1.51	1.43
20	B	1215	CLA	C1A-CHA	2.06	1.51	1.43
20	B	1201	CLA	C1A-CHA	2.06	1.51	1.43
20	4	604	CLA	C1C-C2C	2.06	1.48	1.44
20	Z	606	CLA	C3D-C4D	-2.05	1.39	1.44
20	A	1118	CLA	C1A-CHA	2.05	1.51	1.43
20	7	609	CLA	C3D-C4D	-2.05	1.39	1.44
20	B	1023	CLA	C3D-C4D	-2.05	1.39	1.44
20	B	1236	CLA	C3D-C4D	-2.05	1.39	1.44
20	3	618	CLA	C3D-C4D	-2.05	1.39	1.44
20	3	604	CLA	C3D-C4D	-2.05	1.39	1.44
20	4	605	CLA	C3D-C4D	-2.05	1.39	1.44
20	1	613	CLA	C1A-CHA	2.05	1.51	1.43
20	6	606	CLA	C3D-C4D	-2.05	1.39	1.44
20	B	1234	CLA	C1A-CHA	2.05	1.51	1.43
20	G	1602	CLA	MG-NC	2.05	2.11	2.06
20	3	608	CLA	C1C-C2C	2.05	1.48	1.44
20	B	1219	CLA	C3D-C4D	-2.05	1.39	1.44
20	A	1137	CLA	C1C-C2C	2.05	1.48	1.44
20	B	1218	CLA	C1C-C2C	2.05	1.48	1.44
20	6	607	CLA	C1C-C2C	2.05	1.48	1.44
20	3	602	CLA	C3D-C4D	-2.05	1.39	1.44
20	B	1215	CLA	C3D-C4D	-2.04	1.39	1.44
20	A	1103	CLA	C1A-CHA	2.04	1.51	1.43
20	6	612	CLA	C1A-CHA	2.04	1.51	1.43
40	5	802	3PH	O31-C3	-2.04	1.40	1.45
20	7	606	CLA	C1A-CHA	2.04	1.51	1.43
20	B	1229	CLA	C3B-C4B	2.04	1.47	1.42
20	B	1214	CLA	MG-NC	2.04	2.11	2.06
20	6	609	CLA	C3B-C4B	2.04	1.47	1.42
20	1	606	CLA	C1C-C2C	2.04	1.48	1.44
20	A	1112	CLA	C3D-C4D	-2.04	1.39	1.44
20	A	1105	CLA	C1A-CHA	2.04	1.51	1.43
20	B	1216	CLA	C1A-CHA	2.04	1.51	1.43
20	B	1229	CLA	C1A-CHA	2.04	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1237	CLA	C1A-CHA	2.04	1.51	1.43
20	1	606	CLA	C3D-C4D	-2.04	1.39	1.44
20	3	601	CLA	C3D-C4D	-2.03	1.39	1.44
20	1	613	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	4001	BCR	C12-C13	-2.03	1.41	1.45
20	6	605	CLA	C3D-C4D	-2.03	1.39	1.44
20	3	603	CLA	C1C-C2C	2.03	1.48	1.44
20	1	602	CLA	MG-NC	2.03	2.11	2.06
20	4	607	CLA	C1C-C2C	2.03	1.48	1.44
20	6	601	CLA	C3D-C4D	-2.03	1.39	1.44
20	7	605	CLA	C1C-C2C	2.03	1.48	1.44
20	A	1112	CLA	C1A-CHA	2.03	1.51	1.43
20	7	608	CLA	C1C-C2C	2.03	1.48	1.44
20	A	1116	CLA	C1A-CHA	2.03	1.51	1.43
20	B	1240	CLA	C3B-C4B	2.03	1.47	1.42
20	A	1132	CLA	C1A-CHA	2.03	1.51	1.43
20	B	1232	CLA	C3D-C4D	-2.03	1.39	1.44
20	3	612	CLA	C3D-C4D	-2.03	1.39	1.44
20	A	1107	CLA	C3D-C4D	-2.03	1.39	1.44
20	5	601	CLA	C1C-C2C	2.03	1.48	1.44
20	5	604	CLA	C1A-CHA	2.03	1.51	1.43
20	K	1402	CLA	MG-NC	2.03	2.11	2.06
20	7	608	CLA	MG-NC	2.03	2.11	2.06
20	B	1240	CLA	C1C-C2C	2.02	1.48	1.44
20	Z	608	CLA	C3D-C4D	-2.02	1.39	1.44
20	A	1135	CLA	C1C-C2C	2.02	1.48	1.44
20	8	612	CLA	C3D-C4D	-2.02	1.39	1.44
20	A	1130	CLA	C3D-C4D	-2.02	1.39	1.44
20	A	1106	CLA	C1A-CHA	2.02	1.51	1.43
20	B	1235	CLA	C3D-C4D	-2.02	1.39	1.44
20	A	1128	CLA	C1B-NB	-2.02	1.35	1.37
20	A	1012	CLA	C1A-CHA	2.02	1.51	1.43
20	7	615	CLA	C3D-C4D	-2.02	1.39	1.44
20	B	1235	CLA	C1A-CHA	2.02	1.51	1.43
20	A	1115	CLA	C1A-CHA	2.02	1.51	1.43
20	A	1118	CLA	C1C-C2C	2.02	1.48	1.44
20	5	606	CLA	C1C-C2C	2.02	1.48	1.44
20	3	605	CLA	C3B-C4B	2.02	1.47	1.42
20	7	602	CLA	C1C-C2C	2.02	1.48	1.44
20	5	618	CLA	C1C-C2C	2.02	1.48	1.44
20	A	1140	CLA	C3D-C4D	-2.02	1.39	1.44
20	1	604	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1222	CLA	C1C-C2C	2.01	1.48	1.44
20	6	605	CLA	C1C-C2C	2.01	1.48	1.44
26	F	5001	LMT	O1'-C1'	-2.01	1.36	1.40
20	A	1013	CLA	C1C-C2C	2.01	1.48	1.44
20	1	605	CLA	C1A-CHA	2.01	1.51	1.43
20	8	609	CLA	C3B-C4B	2.01	1.47	1.42
20	7	616	CLA	C1C-C2C	2.01	1.48	1.44
20	A	1135	CLA	C1A-CHA	2.01	1.51	1.43
20	B	1224	CLA	C3D-C4D	-2.01	1.39	1.44
20	L	1502	CLA	C3D-C4D	-2.01	1.39	1.44
20	5	605	CLA	C1A-CHA	2.01	1.51	1.43
20	1	612	CLA	C1C-C2C	2.01	1.48	1.44
20	B	1203	CLA	C1C-C2C	2.01	1.48	1.44
20	B	1225	CLA	C3D-C4D	-2.01	1.39	1.44
20	A	1118	CLA	C3D-C4D	-2.01	1.39	1.44
20	4	608	CLA	C3D-C4D	-2.01	1.39	1.44
20	6	609	CLA	C1A-CHA	2.01	1.51	1.43
20	B	1204	CLA	C1A-CHA	2.01	1.51	1.43
20	1	602	CLA	C3D-C4D	-2.01	1.39	1.44
20	Z	608	CLA	MG-NC	2.01	2.11	2.06
20	A	1102	CLA	C3D-C4D	-2.01	1.39	1.44
20	1	603	CLA	C1C-C2C	2.01	1.48	1.44
20	B	1203	CLA	C3D-C4D	-2.01	1.39	1.44
20	B	1239	CLA	C3D-C4D	-2.01	1.39	1.44
20	7	603	CLA	C3D-C4D	-2.01	1.39	1.44
20	8	611	CLA	C3D-C4D	-2.01	1.39	1.44
20	4	606	CLA	C1C-C2C	2.00	1.48	1.44
20	8	608	CLA	C1A-CHA	2.00	1.51	1.43
26	4	803	LMT	O5'-C5'	-2.00	1.39	1.44
20	4	606	CLA	C3D-C4D	-2.00	1.39	1.44
26	4	803	LMT	O4'-C4B	-2.00	1.38	1.43
20	B	1205	CLA	C3D-C4D	-2.00	1.39	1.44
20	B	1213	CLA	C3D-C4D	-2.00	1.39	1.44
20	3	613	CLA	C3D-C4D	-2.00	1.39	1.44

All (4679) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	504	BCR	C10-C11-C12	18.18	179.94	123.22
23	5	504	BCR	C16-C15-C14	17.70	159.73	123.47
23	K	4001	BCR	C10-C11-C12	17.63	178.24	123.22
23	A	4003	BCR	C10-C11-C12	17.47	177.75	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	4007	BCR	C10-C11-C12	17.47	177.72	123.22
23	7	504	BCR	C10-C11-C12	17.46	177.71	123.22
23	4	503	BCR	C10-C11-C12	17.46	177.69	123.22
23	5	503	BCR	C10-C11-C12	17.45	177.67	123.22
23	8	503	BCR	C10-C11-C12	17.42	177.58	123.22
23	I	4001	BCR	C10-C11-C12	17.39	177.48	123.22
23	3	505	BCR	C10-C11-C12	17.36	177.38	123.22
23	B	4002	BCR	C10-C11-C12	17.33	177.31	123.22
23	6	503	BCR	C10-C11-C12	17.30	177.21	123.22
23	B	4005	BCR	C10-C11-C12	17.30	177.21	123.22
23	L	4001	BCR	C10-C11-C12	17.26	177.07	123.22
23	3	503	BCR	C10-C11-C12	17.16	176.78	123.22
23	B	4004	BCR	C10-C11-C12	17.16	176.77	123.22
23	A	4001	BCR	C10-C11-C12	17.13	176.68	123.22
23	B	4001	BCR	C10-C11-C12	17.09	176.56	123.22
23	A	4002	BCR	C10-C11-C12	17.03	176.36	123.22
23	7	503	BCR	C10-C11-C12	17.02	176.33	123.22
23	G	4001	BCR	C10-C11-C12	16.78	175.58	123.22
23	A	4004	BCR	C10-C11-C12	16.77	175.56	123.22
23	3	504	BCR	C10-C11-C12	16.76	175.53	123.22
23	3	506	BCR	C10-C11-C12	16.72	175.40	123.22
23	J	4001	BCR	C10-C11-C12	16.59	174.98	123.22
23	6	504	BCR	C10-C11-C12	16.58	174.95	123.22
23	L	4002	BCR	C10-C11-C12	16.54	174.85	123.22
23	B	4003	BCR	C10-C11-C12	16.51	174.74	123.22
23	K	4002	BCR	C10-C11-C12	16.41	174.44	123.22
23	A	4005	BCR	C10-C11-C12	16.15	173.61	123.22
23	B	4006	BCR	C10-C11-C12	15.99	173.12	123.22
23	3	506	BCR	C11-C10-C9	14.92	148.61	127.31
23	6	503	BCR	C16-C15-C14	14.58	153.34	123.47
23	B	4002	BCR	C11-C10-C9	14.27	147.68	127.31
23	7	504	BCR	C16-C15-C14	14.19	152.54	123.47
23	J	4001	BCR	C11-C10-C9	14.08	147.40	127.31
23	A	4004	BCR	C11-C10-C9	13.93	147.19	127.31
23	B	4006	BCR	C11-C10-C9	13.80	147.01	127.31
23	G	4001	BCR	C21-C20-C19	13.74	166.10	123.22
23	3	505	BCR	C11-C10-C9	13.72	146.89	127.31
23	6	504	BCR	C16-C15-C14	13.71	151.56	123.47
23	B	4003	BCR	C11-C10-C9	13.61	146.74	127.31
23	6	503	BCR	C11-C10-C9	13.59	146.70	127.31
23	K	4002	BCR	C11-C10-C9	13.53	146.62	127.31
23	B	4001	BCR	C21-C20-C19	13.53	165.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	4001	BCR	C11-C10-C9	13.52	146.61	127.31
23	I	4001	BCR	C11-C10-C9	13.47	146.53	127.31
23	B	4005	BCR	C11-C10-C9	13.25	146.22	127.31
23	A	4005	BCR	C11-C10-C9	13.21	146.16	127.31
23	L	4001	BCR	C11-C10-C9	13.16	146.09	127.31
23	G	4001	BCR	C11-C10-C9	13.09	146.00	127.31
23	L	4002	BCR	C11-C10-C9	13.09	145.99	127.31
23	B	4005	BCR	C21-C20-C19	13.02	163.84	123.22
23	K	4001	BCR	C16-C15-C14	13.02	150.14	123.47
23	3	506	BCR	C21-C20-C19	13.00	163.79	123.22
23	3	506	BCR	C16-C15-C14	12.85	149.79	123.47
23	7	503	BCR	C11-C10-C9	12.84	145.64	127.31
23	7	503	BCR	C16-C15-C14	12.77	149.64	123.47
23	8	503	BCR	C16-C15-C14	12.77	149.63	123.47
23	K	4001	BCR	C11-C10-C9	12.71	145.45	127.31
23	A	4003	BCR	C21-C20-C19	12.69	162.82	123.22
23	3	504	BCR	C16-C15-C14	12.63	149.35	123.47
23	L	4001	BCR	C16-C15-C14	12.62	149.33	123.47
23	B	4004	BCR	C11-C10-C9	12.62	145.32	127.31
23	K	4001	BCR	C21-C20-C19	12.57	162.44	123.22
23	K	4002	BCR	C21-C20-C19	12.54	162.36	123.22
23	7	504	BCR	C21-C20-C19	12.54	162.36	123.22
23	J	4001	BCR	C21-C20-C19	12.53	162.32	123.22
23	7	504	BCR	C11-C10-C9	12.50	145.14	127.31
23	5	503	BCR	C11-C10-C9	12.48	145.12	127.31
23	B	4007	BCR	C16-C15-C14	12.38	148.82	123.47
23	5	503	BCR	C16-C15-C14	12.36	148.79	123.47
23	A	4005	BCR	C11-C12-C13	12.32	161.03	126.42
23	L	4002	BCR	C21-C20-C19	12.26	161.49	123.22
23	8	503	BCR	C11-C10-C9	12.23	144.76	127.31
23	3	504	BCR	C11-C10-C9	12.18	144.69	127.31
23	4	503	BCR	C16-C15-C14	12.17	148.41	123.47
23	B	4004	BCR	C16-C15-C14	12.16	148.38	123.47
23	A	4003	BCR	C11-C10-C9	12.15	144.64	127.31
23	3	504	BCR	C21-C20-C19	12.09	160.95	123.22
23	3	503	BCR	C16-C15-C14	12.05	148.15	123.47
23	3	505	BCR	C16-C15-C14	12.04	148.13	123.47
23	K	4002	BCR	C11-C12-C13	12.03	160.22	126.42
23	A	4004	BCR	C21-C20-C19	12.03	160.76	123.22
23	L	4002	BCR	C11-C12-C13	12.03	160.21	126.42
23	B	4006	BCR	C21-C20-C19	12.03	160.75	123.22
23	5	503	BCR	C21-C20-C19	12.02	160.71	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	505	BCR	C21-C20-C19	11.99	160.62	123.22
23	4	503	BCR	C11-C10-C9	11.95	144.37	127.31
23	B	4003	BCR	C11-C12-C13	11.95	159.99	126.42
23	4	503	BCR	C21-C20-C19	11.94	160.48	123.22
23	B	4001	BCR	C11-C10-C9	11.89	144.28	127.31
23	B	4002	BCR	C16-C15-C14	11.89	147.82	123.47
23	7	503	BCR	C21-C20-C19	11.87	160.25	123.22
23	I	4001	BCR	C16-C15-C14	11.85	147.75	123.47
23	L	4002	BCR	C16-C15-C14	11.77	147.59	123.47
23	B	4007	BCR	C11-C10-C9	11.77	144.10	127.31
23	A	4001	BCR	C21-C20-C19	11.72	159.78	123.22
23	G	4001	BCR	C11-C12-C13	11.65	159.14	126.42
23	B	4006	BCR	C11-C12-C13	11.59	158.98	126.42
23	A	4002	BCR	C11-C10-C9	11.58	143.84	127.31
23	A	4002	BCR	C16-C15-C14	11.56	147.16	123.47
23	A	4004	BCR	C16-C15-C14	11.45	146.94	123.47
23	3	503	BCR	C11-C12-C13	11.39	158.40	126.42
23	B	4001	BCR	C11-C12-C13	11.37	158.35	126.42
23	B	4002	BCR	C21-C20-C19	11.37	158.68	123.22
23	A	4002	BCR	C21-C20-C19	11.33	158.57	123.22
23	3	503	BCR	C11-C10-C9	11.27	143.39	127.31
23	A	4004	BCR	C11-C12-C13	11.25	158.03	126.42
23	G	4001	BCR	C16-C15-C14	11.17	146.36	123.47
23	A	4003	BCR	C16-C15-C14	11.12	146.25	123.47
23	B	4003	BCR	C16-C15-C14	11.11	146.23	123.47
23	B	4003	BCR	C21-C20-C19	11.03	157.63	123.22
23	L	4001	BCR	C21-C20-C19	11.03	157.63	123.22
23	B	4004	BCR	C21-C20-C19	10.97	157.46	123.22
23	B	4004	BCR	C11-C12-C13	10.97	157.22	126.42
23	K	4002	BCR	C16-C15-C14	10.96	145.92	123.47
23	L	4001	BCR	C11-C12-C13	10.95	157.17	126.42
23	J	4001	BCR	C11-C12-C13	10.92	157.09	126.42
23	6	504	BCR	C11-C12-C13	10.79	156.73	126.42
23	B	4001	BCR	C16-C15-C14	10.78	145.55	123.47
23	J	4001	BCR	C16-C15-C14	10.74	145.48	123.47
23	K	4001	BCR	C11-C12-C13	10.72	156.53	126.42
23	7	503	BCR	C11-C12-C13	10.71	156.51	126.42
23	A	4003	BCR	C11-C12-C13	10.71	156.49	126.42
20	K	1404	CLA	C4A-NA-C1A	10.70	111.52	106.71
23	8	503	BCR	C11-C12-C13	10.67	156.39	126.42
23	B	4005	BCR	C16-C15-C14	10.62	145.23	123.47
23	3	503	BCR	C21-C20-C19	10.61	156.33	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	503	BCR	C21-C20-C19	10.61	156.31	123.22
23	B	4007	BCR	C11-C12-C13	10.49	155.89	126.42
23	B	4005	BCR	C11-C12-C13	10.46	155.80	126.42
23	3	506	BCR	C11-C12-C13	10.37	155.56	126.42
23	3	505	BCR	C11-C12-C13	10.33	155.43	126.42
23	A	4001	BCR	C11-C12-C13	10.32	155.42	126.42
23	A	4002	BCR	C11-C12-C13	10.32	155.41	126.42
23	4	503	BCR	C11-C12-C13	10.32	155.41	126.42
23	I	4001	BCR	C11-C12-C13	10.28	155.28	126.42
23	A	4005	BCR	C16-C15-C14	10.25	144.47	123.47
23	8	503	BCR	C21-C20-C19	10.23	155.14	123.22
23	B	4006	BCR	C16-C15-C14	10.20	144.37	123.47
23	I	4001	BCR	C21-C20-C19	10.19	155.01	123.22
23	B	4007	BCR	C21-C20-C19	10.14	154.86	123.22
23	A	4005	BCR	C21-C20-C19	10.11	154.76	123.22
20	F	1301	CLA	C4A-NA-C1A	10.08	111.24	106.71
20	7	616	CLA	C4A-NA-C1A	10.07	111.23	106.71
20	5	618	CLA	C4A-NA-C1A	10.07	111.23	106.71
23	6	504	BCR	C11-C10-C9	10.03	141.63	127.31
23	B	4002	BCR	C11-C12-C13	10.01	154.53	126.42
20	4	603	CLA	C4A-NA-C1A	9.99	111.20	106.71
20	A	1103	CLA	C4A-NA-C1A	9.97	111.19	106.71
23	5	504	BCR	C21-C20-C19	9.93	154.20	123.22
20	3	606	CLA	C4A-NA-C1A	9.92	111.17	106.71
23	A	4001	BCR	C16-C15-C14	9.92	143.80	123.47
20	8	611	CLA	C4A-NA-C1A	9.88	111.15	106.71
23	7	504	BCR	C11-C12-C13	9.87	154.14	126.42
20	B	1208	CLA	C4A-NA-C1A	9.85	111.13	106.71
20	7	611	CLA	C4A-NA-C1A	9.83	111.13	106.71
23	6	504	BCR	C21-C20-C19	9.80	153.80	123.22
20	L	1502	CLA	C4A-NA-C1A	9.78	111.10	106.71
20	B	1219	CLA	C4A-NA-C1A	9.77	111.10	106.71
20	A	1102	CLA	C4A-NA-C1A	9.76	111.09	106.71
20	A	1138	CLA	C4A-NA-C1A	9.75	111.09	106.71
20	3	603	CLA	C4A-NA-C1A	9.74	111.08	106.71
20	B	1230	CLA	C4A-NA-C1A	9.73	111.08	106.71
20	B	1205	CLA	C4A-NA-C1A	9.72	111.08	106.71
20	B	1221	CLA	C4A-NA-C1A	9.72	111.08	106.71
20	1	603	CLA	C4A-NA-C1A	9.71	111.07	106.71
20	B	1239	CLA	C4A-NA-C1A	9.70	111.07	106.71
20	5	601	CLA	C4A-NA-C1A	9.68	111.06	106.71
20	4	612	CLA	C4A-NA-C1A	9.67	111.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	607	CLA	C4A-NA-C1A	9.64	111.04	106.71
23	3	504	BCR	C11-C12-C13	9.64	153.49	126.42
20	5	603	CLA	C4A-NA-C1A	9.61	111.03	106.71
20	6	615	CLA	C4A-NA-C1A	9.60	111.02	106.71
20	A	1141	CLA	C4A-NA-C1A	9.59	111.02	106.71
20	A	1117	CLA	C4A-NA-C1A	9.58	111.01	106.71
20	4	602	CLA	C4A-NA-C1A	9.57	111.01	106.71
20	A	1110	CLA	C4A-NA-C1A	9.55	111.00	106.71
20	8	615	CLA	C4A-NA-C1A	9.49	110.97	106.71
23	5	504	BCR	C11-C10-C9	9.48	140.84	127.31
20	8	602	CLA	C4A-NA-C1A	9.47	110.96	106.71
20	3	604	CLA	C4A-NA-C1A	9.46	110.96	106.71
20	B	1214	CLA	C4A-NA-C1A	9.44	110.95	106.71
23	A	4005	BCR	C20-C19-C18	9.43	152.90	126.42
20	B	1206	CLA	C4A-NA-C1A	9.43	110.94	106.71
23	5	503	BCR	C11-C12-C13	9.39	152.80	126.42
20	A	1012	CLA	C4A-NA-C1A	9.38	110.92	106.71
23	5	504	BCR	C11-C12-C13	9.38	152.76	126.42
20	5	606	CLA	C4A-NA-C1A	9.37	110.92	106.71
20	A	1113	CLA	C4A-NA-C1A	9.35	110.91	106.71
20	6	618	CLA	C4A-NA-C1A	9.35	110.91	106.71
20	Z	604	CLA	C4A-NA-C1A	9.34	110.91	106.71
20	A	1123	CLA	C4A-NA-C1A	9.33	110.90	106.71
20	A	1139	CLA	C4A-NA-C1A	9.33	110.90	106.71
20	B	1213	CLA	C4A-NA-C1A	9.33	110.90	106.71
20	4	615	CLA	C4A-NA-C1A	9.33	110.90	106.71
20	1	601	CLA	C4A-NA-C1A	9.32	110.90	106.71
20	3	616	CLA	C4A-NA-C1A	9.32	110.90	106.71
20	B	1218	CLA	C4A-NA-C1A	9.32	110.89	106.71
20	1	608	CLA	C4A-NA-C1A	9.31	110.89	106.71
20	A	1118	CLA	C4A-NA-C1A	9.31	110.89	106.71
20	A	1115	CLA	C4A-NA-C1A	9.30	110.89	106.71
20	B	1236	CLA	C4A-NA-C1A	9.29	110.88	106.71
20	7	603	CLA	C4A-NA-C1A	9.28	110.88	106.71
20	B	1231	CLA	C4A-NA-C1A	9.28	110.88	106.71
20	B	1021	CLA	C4A-NA-C1A	9.27	110.87	106.71
20	8	607	CLA	C4A-NA-C1A	9.27	110.87	106.71
20	1	612	CLA	C4A-NA-C1A	9.27	110.87	106.71
20	3	618	CLA	C4A-NA-C1A	9.26	110.87	106.71
20	7	609	CLA	C4A-NA-C1A	9.25	110.87	106.71
20	4	601	CLA	C4A-NA-C1A	9.24	110.86	106.71
20	B	1235	CLA	C4A-NA-C1A	9.24	110.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1134	CLA	C4A-NA-C1A	9.22	110.85	106.71
20	A	1137	CLA	C4A-NA-C1A	9.22	110.85	106.71
20	J	1901	CLA	C4A-NA-C1A	9.22	110.85	106.71
20	B	1023	CLA	C4A-NA-C1A	9.22	110.85	106.71
20	B	1212	CLA	C4A-NA-C1A	9.21	110.85	106.71
20	3	612	CLA	C4A-NA-C1A	9.20	110.84	106.71
20	L	1503	CLA	C4A-NA-C1A	9.20	110.84	106.71
20	Z	603	CLA	C4A-NA-C1A	9.18	110.83	106.71
20	B	1217	CLA	C4A-NA-C1A	9.18	110.83	106.71
20	8	606	CLA	C4A-NA-C1A	9.17	110.83	106.71
20	5	608	CLA	C4A-NA-C1A	9.16	110.83	106.71
20	4	606	CLA	C4A-NA-C1A	9.16	110.82	106.71
20	B	1204	CLA	C4A-NA-C1A	9.15	110.82	106.71
20	8	603	CLA	C4A-NA-C1A	9.15	110.82	106.71
20	A	1122	CLA	C4A-NA-C1A	9.15	110.82	106.71
20	A	1120	CLA	C4A-NA-C1A	9.14	110.81	106.71
20	6	608	CLA	C4A-NA-C1A	9.14	110.81	106.71
20	A	1136	CLA	C4A-NA-C1A	9.13	110.81	106.71
20	A	1107	CLA	C4A-NA-C1A	9.12	110.81	106.71
20	B	1224	CLA	C4A-NA-C1A	9.12	110.81	106.71
20	G	1601	CLA	C4A-NA-C1A	9.12	110.80	106.71
20	8	604	CLA	C4A-NA-C1A	9.10	110.80	106.71
20	6	603	CLA	C4A-NA-C1A	9.08	110.79	106.71
20	7	602	CLA	C4A-NA-C1A	9.08	110.79	106.71
20	6	612	CLA	C4A-NA-C1A	9.08	110.79	106.71
20	K	1403	CLA	C4A-NA-C1A	9.07	110.78	106.71
20	3	613	CLA	C4A-NA-C1A	9.05	110.78	106.71
23	I	4001	BCR	C20-C19-C18	9.05	151.83	126.42
20	B	1228	CLA	C4A-NA-C1A	9.01	110.76	106.71
20	5	607	CLA	C4A-NA-C1A	9.01	110.76	106.71
20	B	1215	CLA	C4A-NA-C1A	9.00	110.75	106.71
20	1	607	CLA	C4A-NA-C1A	9.00	110.75	106.71
20	5	615	CLA	C4A-NA-C1A	9.00	110.75	106.71
20	B	1207	CLA	C4A-NA-C1A	8.98	110.74	106.71
23	B	4005	BCR	C20-C19-C18	8.96	151.59	126.42
20	B	1203	CLA	C4A-NA-C1A	8.96	110.73	106.71
20	6	605	CLA	C4A-NA-C1A	8.96	110.73	106.71
20	3	607	CLA	C4A-NA-C1A	8.95	110.73	106.71
20	A	1104	CLA	C4A-NA-C1A	8.94	110.73	106.71
20	4	605	CLA	C4A-NA-C1A	8.94	110.73	106.71
20	Z	607	CLA	C4A-NA-C1A	8.94	110.72	106.71
20	Z	612	CLA	C4A-NA-C1A	8.92	110.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1133	CLA	C4A-NA-C1A	8.91	110.71	106.71
20	7	601	CLA	C4A-NA-C1A	8.89	110.70	106.71
20	B	1232	CLA	C4A-NA-C1A	8.89	110.70	106.71
20	B	1237	CLA	C4A-NA-C1A	8.89	110.70	106.71
20	A	1129	CLA	C4A-NA-C1A	8.88	110.70	106.71
20	Z	608	CLA	C4A-NA-C1A	8.88	110.70	106.71
20	B	1226	CLA	C4A-NA-C1A	8.87	110.70	106.71
20	1	611	CLA	C4A-NA-C1A	8.87	110.70	106.71
20	A	1124	CLA	C4A-NA-C1A	8.87	110.69	106.71
20	7	605	CLA	C4A-NA-C1A	8.85	110.69	106.71
20	A	1105	CLA	C4A-NA-C1A	8.85	110.69	106.71
20	A	1131	CLA	C4A-NA-C1A	8.84	110.68	106.71
20	Z	601	CLA	C4A-NA-C1A	8.84	110.68	106.71
20	3	608	CLA	C4A-NA-C1A	8.84	110.68	106.71
20	8	609	CLA	C4A-NA-C1A	8.83	110.68	106.71
20	6	619	CLA	C4A-NA-C1A	8.83	110.68	106.71
20	B	1220	CLA	C4A-NA-C1A	8.82	110.67	106.71
23	6	503	BCR	C20-C19-C18	8.82	151.18	126.42
20	A	1106	CLA	C4A-NA-C1A	8.81	110.67	106.71
20	A	1108	CLA	C4A-NA-C1A	8.81	110.67	106.71
20	B	1202	CLA	C4A-NA-C1A	8.80	110.66	106.71
20	B	1201	CLA	C4A-NA-C1A	8.76	110.64	106.71
20	6	606	CLA	C4A-NA-C1A	8.76	110.64	106.71
20	Z	605	CLA	C4A-NA-C1A	8.76	110.64	106.71
20	A	1112	CLA	C4A-NA-C1A	8.75	110.64	106.71
20	A	1114	CLA	C4A-NA-C1A	8.75	110.64	106.71
20	7	615	CLA	C4A-NA-C1A	8.75	110.64	106.71
20	Z	611	CLA	C4A-NA-C1A	8.75	110.64	106.71
20	1	604	CLA	C4A-NA-C1A	8.75	110.64	106.71
20	3	601	CLA	C4A-NA-C1A	8.75	110.64	106.71
23	6	503	BCR	C11-C12-C13	8.74	150.98	126.42
20	7	606	CLA	C4A-NA-C1A	8.72	110.62	106.71
20	B	1234	CLA	C4A-NA-C1A	8.70	110.62	106.71
20	3	610	CLA	C4A-NA-C1A	8.69	110.61	106.71
20	Z	602	CLA	C4A-NA-C1A	8.68	110.61	106.71
20	4	604	CLA	C4A-NA-C1A	8.68	110.61	106.71
20	1	615	CLA	C4A-NA-C1A	8.66	110.60	106.71
20	K	1402	CLA	C4A-NA-C1A	8.66	110.60	106.71
20	A	1135	CLA	C4A-NA-C1A	8.66	110.60	106.71
20	A	1111	CLA	C4A-NA-C1A	8.65	110.59	106.71
20	B	1229	CLA	C4A-NA-C1A	8.65	110.59	106.71
23	3	506	BCR	C20-C19-C18	8.65	150.70	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	8	503	BCR	C20-C19-C18	8.64	150.70	126.42
20	A	1128	CLA	C4A-NA-C1A	8.64	110.59	106.71
20	1	606	CLA	C4A-NA-C1A	8.64	110.59	106.71
20	A	1127	CLA	C4A-NA-C1A	8.64	110.59	106.71
20	B	1222	CLA	C4A-NA-C1A	8.64	110.59	106.71
20	5	612	CLA	C4A-NA-C1A	8.63	110.59	106.71
20	A	1125	CLA	C4A-NA-C1A	8.62	110.58	106.71
20	6	602	CLA	C4A-NA-C1A	8.62	110.58	106.71
23	3	503	BCR	C20-C19-C18	8.60	150.59	126.42
20	6	601	CLA	C4A-NA-C1A	8.59	110.57	106.71
20	7	608	CLA	C4A-NA-C1A	8.58	110.56	106.71
20	G	1602	CLA	C4A-NA-C1A	8.58	110.56	106.71
20	B	1209	CLA	C4A-NA-C1A	8.55	110.55	106.71
20	4	607	CLA	C4A-NA-C1A	8.51	110.53	106.71
20	5	602	CLA	C4A-NA-C1A	8.51	110.53	106.71
20	1	602	CLA	C4A-NA-C1A	8.51	110.53	106.71
20	7	604	CLA	C4A-NA-C1A	8.51	110.53	106.71
20	4	608	CLA	C4A-NA-C1A	8.51	110.53	106.71
20	5	605	CLA	C4A-NA-C1A	8.51	110.53	106.71
20	6	604	CLA	C4A-NA-C1A	8.49	110.52	106.71
20	B	1223	CLA	C4A-NA-C1A	8.49	110.52	106.71
23	5	504	BCR	C15-C14-C13	-8.48	115.21	127.31
20	B	1211	CLA	C4A-NA-C1A	8.47	110.51	106.71
20	B	1238	CLA	C4A-NA-C1A	8.46	110.51	106.71
20	A	1121	CLA	C4A-NA-C1A	8.45	110.50	106.71
20	8	605	CLA	C4A-NA-C1A	8.45	110.50	106.71
20	Z	615	CLA	C4A-NA-C1A	8.44	110.50	106.71
20	8	608	CLA	C4A-NA-C1A	8.44	110.50	106.71
20	7	612	CLA	C4A-NA-C1A	8.44	110.50	106.71
20	A	1140	CLA	C4A-NA-C1A	8.43	110.50	106.71
20	B	1241	CLA	C4A-NA-C1A	8.43	110.50	106.71
20	8	601	CLA	C4A-NA-C1A	8.43	110.50	106.71
20	B	1210	CLA	C4A-NA-C1A	8.41	110.48	106.71
20	5	622	CLA	C4A-NA-C1A	8.41	110.48	106.71
23	B	4004	BCR	C20-C19-C18	8.40	150.02	126.42
20	7	613	CLA	C4A-NA-C1A	8.40	110.48	106.71
20	8	612	CLA	C4A-NA-C1A	8.40	110.48	106.71
20	A	1109	CLA	C4A-NA-C1A	8.40	110.48	106.71
23	B	4003	BCR	C20-C19-C18	8.38	149.96	126.42
23	L	4001	BCR	C20-C19-C18	8.38	149.95	126.42
20	A	1126	CLA	C4A-NA-C1A	8.38	110.47	106.71
20	3	602	CLA	C4A-NA-C1A	8.36	110.47	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1227	CLA	C4A-NA-C1A	8.33	110.45	106.71
20	5	609	CLA	C4A-NA-C1A	8.33	110.45	106.71
20	6	607	CLA	C4A-NA-C1A	8.33	110.45	106.71
20	B	1216	CLA	C4A-NA-C1A	8.32	110.45	106.71
20	F	1302	CLA	C4A-NA-C1A	8.31	110.44	106.71
20	4	609	CLA	C4A-NA-C1A	8.31	110.44	106.71
20	A	1132	CLA	C4A-NA-C1A	8.30	110.44	106.71
20	A	1101	CLA	C4A-NA-C1A	8.30	110.44	106.71
20	B	1022	CLA	C4A-NA-C1A	8.23	110.40	106.71
20	A	1119	CLA	C4A-NA-C1A	8.21	110.40	106.71
23	B	4002	BCR	C20-C19-C18	8.18	149.40	126.42
20	A	1013	CLA	C4A-NA-C1A	8.17	110.38	106.71
20	5	604	CLA	C4A-NA-C1A	8.16	110.37	106.71
20	B	1225	CLA	C4A-NA-C1A	8.16	110.37	106.71
20	1	613	CLA	C4A-NA-C1A	8.15	110.37	106.71
20	5	613	CLA	C4A-NA-C1A	8.14	110.37	106.71
20	1	605	CLA	C4A-NA-C1A	8.11	110.35	106.71
23	3	505	BCR	C20-C19-C18	7.97	148.80	126.42
23	B	4007	BCR	C20-C19-C18	7.87	148.52	126.42
20	A	1130	CLA	C4A-NA-C1A	7.87	110.24	106.71
23	L	4002	BCR	C20-C19-C18	7.85	148.47	126.42
19	A	1011	CL0	CMD-C2D-C1D	7.75	138.37	124.71
20	K	1401	CLA	C4A-NA-C1A	7.72	110.18	106.71
20	3	605	CLA	C4A-NA-C1A	7.70	110.17	106.71
23	7	504	BCR	C20-C19-C18	7.70	148.04	126.42
20	B	1240	CLA	C4A-NA-C1A	7.67	110.15	106.71
20	Z	606	CLA	C4A-NA-C1A	7.66	110.15	106.71
20	6	609	CLA	C4A-NA-C1A	7.64	110.14	106.71
23	A	4001	BCR	C20-C19-C18	7.63	147.85	126.42
23	4	503	BCR	C20-C19-C18	7.62	147.81	126.42
23	J	4001	BCR	C20-C19-C18	7.57	147.69	126.42
23	A	4002	BCR	C20-C19-C18	7.57	147.68	126.42
23	A	4004	BCR	C20-C19-C18	7.47	147.41	126.42
20	A	1116	CLA	C4A-NA-C1A	7.44	110.05	106.71
19	A	1011	CL0	C4A-NA-C1A	7.39	110.03	106.71
34	1	503	C7Z	C35-C34-C33	-7.30	116.90	127.31
23	5	503	BCR	C20-C19-C18	7.29	146.90	126.42
23	K	4001	BCR	C20-C19-C18	7.23	146.74	126.42
23	K	4002	BCR	C20-C19-C18	7.23	146.72	126.42
23	B	4006	BCR	C20-C19-C18	7.14	146.48	126.42
23	7	503	BCR	C20-C19-C18	7.08	146.30	126.42
23	3	504	BCR	C20-C19-C18	7.04	146.18	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	603	CLA	O2A-C1-C2	6.71	126.27	108.64
20	B	1213	CLA	O2A-C1-C2	6.68	126.18	108.64
23	A	4003	BCR	C20-C19-C18	6.63	145.03	126.42
36	5	501	LUT	C21-C26-C27	6.60	121.04	112.70
30	A	5005	DGA	CDB-CCB-CBB	-6.57	81.09	114.42
20	A	1012	CLA	O2A-C1-C2	6.51	125.75	108.64
20	G	1602	CLA	O2D-CGD-CBD	6.49	122.79	111.27
23	B	4001	BCR	C20-C19-C18	6.42	144.44	126.42
20	6	603	CLA	O2A-C1-C2	6.40	125.46	108.64
20	A	1110	CLA	O2A-C1-C2	6.40	125.45	108.64
19	A	1011	CL0	C2C-C1C-NC	6.39	115.96	109.97
20	3	601	CLA	O2A-C1-C2	6.38	125.41	108.64
20	8	603	CLA	O2A-C1-C2	6.37	125.39	108.64
34	5	505	C7Z	C7-C8-C9	-6.35	116.64	126.23
20	B	1205	CLA	O2A-C1-C2	6.34	125.31	108.64
20	B	1238	CLA	O2A-C1-C2	6.34	125.29	108.64
23	6	504	BCR	C20-C19-C18	6.28	144.07	126.42
20	A	1106	CLA	O2D-CGD-CBD	6.27	122.41	111.27
34	J	4002	C7Z	C27-C28-C29	-6.26	116.78	126.23
23	5	504	BCR	C20-C19-C18	6.26	143.99	126.42
20	Z	606	CLA	O2D-CGD-CBD	6.25	122.37	111.27
20	A	1105	CLA	O2A-C1-C2	6.24	125.04	108.64
20	B	1210	CLA	O2D-CGD-CBD	6.24	122.36	111.27
20	A	1111	CLA	O2D-CGD-CBD	6.21	122.30	111.27
20	A	1121	CLA	CMD-C2D-C1D	6.20	135.64	124.71
20	1	613	CLA	CMD-C2D-C1D	6.17	135.59	124.71
20	3	606	CLA	O2A-C1-C2	6.16	124.81	108.64
20	A	1137	CLA	O2A-C1-C2	6.14	124.78	108.64
20	5	603	CLA	O2A-C1-C2	6.09	124.65	108.64
20	B	1204	CLA	O2A-C1-C2	6.09	124.64	108.64
20	8	601	CLA	O2A-C1-C2	6.07	124.60	108.64
20	B	1226	CLA	CMD-C2D-C1D	6.07	135.42	124.71
20	B	1021	CLA	O2D-CGD-CBD	6.07	122.05	111.27
20	A	1138	CLA	O2A-C1-C2	6.06	124.57	108.64
20	A	1130	CLA	O2A-C1-C2	6.04	124.52	108.64
20	6	605	CLA	O2A-C1-C2	6.03	124.49	108.64
20	5	605	CLA	CMD-C2D-C1D	6.02	135.32	124.71
20	A	1135	CLA	CMD-C2D-C1D	6.01	135.31	124.71
20	K	1404	CLA	O2D-CGD-CBD	6.01	121.94	111.27
20	8	601	CLA	CMD-C2D-C1D	5.98	135.25	124.71
20	5	608	CLA	CMD-C2D-C1D	5.97	135.24	124.71
20	6	601	CLA	O2A-C1-C2	5.97	124.31	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	615	CLA	CMD-C2D-C1D	5.95	135.20	124.71
20	B	1224	CLA	O2A-C1-C2	5.95	124.28	108.64
20	A	1109	CLA	CMD-C2D-C1D	5.94	135.18	124.71
20	1	605	CLA	CMD-C2D-C1D	5.94	135.18	124.71
20	7	609	CLA	O2D-CGD-CBD	5.93	121.81	111.27
20	7	603	CLA	O2A-C1-C2	5.93	124.21	108.64
20	B	1204	CLA	CMD-C2D-C1D	5.91	135.13	124.71
20	6	609	CLA	O2D-CGD-CBD	5.91	121.77	111.27
20	B	1227	CLA	CMD-C2D-C1D	5.89	135.09	124.71
20	8	605	CLA	O2D-CGD-CBD	5.89	121.73	111.27
20	A	1134	CLA	O2A-C1-C2	5.88	124.09	108.64
20	A	1128	CLA	O2A-C1-C2	5.87	124.05	108.64
20	B	1224	CLA	O2D-CGD-CBD	5.86	121.69	111.27
20	7	601	CLA	CMD-C2D-C1D	5.86	135.04	124.71
20	8	602	CLA	O2A-C1-C2	5.86	124.03	108.64
20	B	1231	CLA	CMD-C2D-C1D	5.86	135.03	124.71
20	A	1116	CLA	CMD-C2D-C1D	5.86	135.03	124.71
20	5	604	CLA	O2A-C1-C2	5.84	123.99	108.64
20	L	1503	CLA	CMD-C2D-C1D	5.83	134.98	124.71
20	G	1602	CLA	CMD-C2D-C1D	5.81	134.96	124.71
20	7	605	CLA	CMD-C2D-C1D	5.81	134.95	124.71
20	3	607	CLA	O2A-C1-C2	5.81	123.89	108.64
20	B	1226	CLA	O2A-C1-C2	5.80	123.87	108.64
20	Z	611	CLA	CMD-C2D-C1D	5.80	134.93	124.71
20	8	602	CLA	CMD-C2D-C1D	5.80	134.93	124.71
20	4	604	CLA	CMD-C2D-C1D	5.79	134.92	124.71
20	B	1211	CLA	O2A-C1-C2	5.79	123.84	108.64
20	7	601	CLA	O2A-C1-C2	5.79	123.84	108.64
20	A	1108	CLA	O2A-C1-C2	5.78	123.83	108.64
20	3	604	CLA	O2A-C1-C2	5.78	123.82	108.64
20	4	603	CLA	O2A-C1-C2	5.77	123.80	108.64
20	A	1112	CLA	O2D-CGD-CBD	5.76	121.50	111.27
20	6	608	CLA	CMD-C2D-C1D	5.75	134.85	124.71
20	A	1126	CLA	CMD-C2D-C1D	5.75	134.85	124.71
20	B	1023	CLA	O2A-C1-C2	5.74	123.73	108.64
20	A	1103	CLA	O2D-CGD-CBD	5.74	121.47	111.27
20	6	604	CLA	O2A-C1-C2	5.74	123.72	108.64
23	B	4005	BCR	C37-C22-C21	-5.74	114.89	122.92
20	A	1138	CLA	O2D-CGD-CBD	5.73	121.46	111.27
20	B	1219	CLA	CMD-C2D-C1D	5.73	134.81	124.71
20	6	609	CLA	O2A-C1-C2	5.73	123.69	108.64
20	A	1117	CLA	O2A-C1-C2	5.73	123.69	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1229	CLA	O2D-CGD-CBD	5.73	121.44	111.27
19	A	1011	CL0	C1C-C2C-C3C	-5.73	100.94	106.96
39	Z	504	QTB	C09-C02-C03	5.72	127.72	118.94
20	A	1116	CLA	O2A-C1-C2	5.72	123.66	108.64
20	8	611	CLA	CMD-C2D-C1D	5.72	134.79	124.71
20	7	615	CLA	CMD-C2D-C1D	5.70	134.77	124.71
20	4	603	CLA	CMD-C2D-C1D	5.70	134.76	124.71
20	B	1238	CLA	CMD-C2D-C1D	5.70	134.76	124.71
20	B	1213	CLA	O2D-CGD-CBD	5.70	121.39	111.27
20	B	1203	CLA	CMD-C2D-C1D	5.69	134.75	124.71
20	8	609	CLA	O2A-C1-C2	5.69	123.58	108.64
39	Z	504	QTB	C04-C03-C02	5.68	135.42	127.31
20	6	615	CLA	O2A-C1-C2	5.68	123.56	108.64
20	A	1110	CLA	O2D-CGD-CBD	5.68	121.35	111.27
19	A	1011	CL0	O2D-CGD-CBD	5.67	121.35	111.27
20	A	1120	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	G	4001	BCR	C20-C19-C18	5.67	142.34	126.42
20	A	1135	CLA	O2D-CGD-CBD	5.67	121.34	111.27
20	5	622	CLA	CMD-C2D-C1D	5.66	134.69	124.71
20	6	606	CLA	CMD-C2D-C1D	5.66	134.69	124.71
33	F	4001	RRX	C11-C10-C9	-5.66	119.23	127.31
20	7	606	CLA	CMD-C2D-C1D	5.66	134.69	124.71
36	3	502	LUT	C21-C26-C27	5.66	119.85	112.70
20	8	603	CLA	CMD-C2D-C1D	5.66	134.68	124.71
20	4	601	CLA	CMD-C2D-C1D	5.66	134.68	124.71
20	4	606	CLA	CMD-C2D-C1D	5.65	134.68	124.71
20	6	606	CLA	O2A-C1-C2	5.65	123.49	108.64
20	1	608	CLA	CMD-C2D-C1D	5.65	134.67	124.71
20	5	605	CLA	O2A-C1-C2	5.64	123.47	108.64
20	A	1131	CLA	O2D-CGD-CBD	5.64	121.30	111.27
20	A	1111	CLA	CMD-C2D-C1D	5.64	134.65	124.71
20	A	1125	CLA	O2A-C1-C2	5.64	123.45	108.64
20	F	1301	CLA	CMD-C2D-C1D	5.64	134.65	124.71
20	B	1240	CLA	CMD-C2D-C1D	5.64	134.65	124.71
20	B	1212	CLA	O2D-CGD-CBD	5.63	121.28	111.27
20	B	1207	CLA	O2A-C1-C2	5.63	123.44	108.64
20	B	1214	CLA	CMD-C2D-C1D	5.63	134.64	124.71
20	6	608	CLA	O2A-C1-C2	5.63	123.43	108.64
20	A	1105	CLA	O2D-CGD-CBD	5.63	121.27	111.27
20	Z	606	CLA	CMD-C2D-C1D	5.63	134.63	124.71
20	A	1114	CLA	CMD-C2D-C1D	5.62	134.62	124.71
20	A	1106	CLA	O2A-C1-C2	5.62	123.40	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	606	CLA	O2D-CGD-CBD	5.61	121.24	111.27
20	A	1106	CLA	CMD-C2D-C1D	5.61	134.60	124.71
20	B	1023	CLA	O2D-CGD-CBD	5.59	121.21	111.27
20	B	1202	CLA	O2D-CGD-CBD	5.59	121.20	111.27
20	B	1216	CLA	CMD-C2D-C1D	5.59	134.56	124.71
20	1	611	CLA	CMD-C2D-C1D	5.59	134.56	124.71
20	4	606	CLA	O2D-CGD-CBD	5.59	121.19	111.27
20	A	1134	CLA	O2D-CGD-CBD	5.58	121.19	111.27
20	B	1218	CLA	O2D-CGD-CBD	5.58	121.19	111.27
20	Z	611	CLA	O2A-C1-C2	5.58	123.31	108.64
20	A	1132	CLA	CMD-C2D-C1D	5.58	134.54	124.71
20	6	605	CLA	CMD-C2D-C1D	5.57	134.54	124.71
19	A	1011	CL0	C2D-C1D-ND	5.57	114.21	110.10
20	A	1137	CLA	O2D-CGD-CBD	5.57	121.17	111.27
20	7	608	CLA	O2D-CGD-CBD	5.57	121.17	111.27
20	B	1230	CLA	O2D-CGD-CBD	5.57	121.17	111.27
20	6	619	CLA	O2D-CGD-CBD	5.56	121.15	111.27
20	5	618	CLA	O2A-C1-C2	5.56	123.25	108.64
20	B	1239	CLA	O2D-CGD-CBD	5.55	121.14	111.27
20	B	1229	CLA	CMD-C2D-C1D	5.55	134.50	124.71
20	B	1221	CLA	O2D-CGD-CBD	5.55	121.13	111.27
36	7	501	LUT	C21-C26-C25	5.55	121.36	111.42
20	A	1101	CLA	O2A-C1-C2	5.55	123.21	108.64
20	3	603	CLA	CMD-C2D-C1D	5.54	134.48	124.71
20	1	612	CLA	CMD-C2D-C1D	5.54	134.48	124.71
20	A	1115	CLA	CMD-C2D-C1D	5.54	134.48	124.71
20	K	1403	CLA	CMD-C2D-C1D	5.54	134.48	124.71
20	7	604	CLA	O2A-C1-C2	5.54	123.19	108.64
20	B	1209	CLA	O2A-C1-C2	5.54	123.18	108.64
20	B	1231	CLA	O2A-C1-C2	5.53	123.17	108.64
20	3	601	CLA	CMD-C2D-C1D	5.53	134.46	124.71
20	B	1202	CLA	CMD-C2D-C1D	5.53	134.45	124.71
20	8	609	CLA	CMD-C2D-C1D	5.52	134.45	124.71
24	3	801	LHG	O7-C7-O9	-5.52	118.54	125.57
20	Z	612	CLA	O2A-C1-C2	5.52	123.15	108.64
20	3	605	CLA	CMD-C2D-C1D	5.52	134.44	124.71
20	5	601	CLA	CMD-C2D-C1D	5.52	134.44	124.71
36	Z	502	LUT	C21-C26-C25	5.52	121.30	111.42
20	1	601	CLA	O2A-C1-C2	5.51	123.13	108.64
20	3	613	CLA	CMD-C2D-C1D	5.51	134.43	124.71
20	1	613	CLA	O2D-CGD-CBD	5.51	121.06	111.27
20	A	1130	CLA	CMD-C2D-C1D	5.51	134.43	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	605	CLA	CMD-C2D-C1D	5.51	134.42	124.71
20	3	612	CLA	CMD-C2D-C1D	5.51	134.42	124.71
20	Z	608	CLA	O2D-CGD-CBD	5.51	121.06	111.27
20	B	1221	CLA	O2A-C1-C2	5.51	123.11	108.64
20	4	609	CLA	O2D-CGD-CBD	5.51	121.05	111.27
20	3	616	CLA	O2A-C1-C2	5.50	123.10	108.64
20	1	606	CLA	CMD-C2D-C1D	5.50	134.41	124.71
20	B	1216	CLA	O2A-C1-C2	5.50	123.09	108.64
20	B	1213	CLA	CMD-C2D-C1D	5.50	134.41	124.71
20	A	1102	CLA	O2D-CGD-CBD	5.50	121.03	111.27
20	Z	608	CLA	CMD-C2D-C1D	5.49	134.40	124.71
20	5	603	CLA	CMD-C2D-C1D	5.49	134.40	124.71
20	B	1212	CLA	O2A-C1-C2	5.49	123.08	108.64
20	A	1101	CLA	CMD-C2D-C1D	5.49	134.40	124.71
20	A	1131	CLA	CMD-C2D-C1D	5.49	134.40	124.71
20	B	1218	CLA	CMD-C2D-C1D	5.49	134.39	124.71
20	K	1402	CLA	O2D-CGD-CBD	5.49	121.03	111.27
20	1	604	CLA	O2D-CGD-CBD	5.49	121.02	111.27
20	B	1208	CLA	CMD-C2D-C1D	5.49	134.38	124.71
20	7	607	CLA	CMD-C2D-C1D	5.48	134.38	124.71
20	A	1120	CLA	O2A-C1-C2	5.48	123.05	108.64
20	Z	615	CLA	CMD-C2D-C1D	5.48	134.38	124.71
20	7	616	CLA	O2A-C1-C2	5.48	123.03	108.64
20	5	606	CLA	O2D-CGD-CBD	5.48	121.00	111.27
20	A	1113	CLA	CMD-C2D-C1D	5.47	134.36	124.71
20	G	1601	CLA	CMD-C2D-C1D	5.47	134.35	124.71
20	7	616	CLA	CMD-C2D-C1D	5.47	134.34	124.71
20	7	609	CLA	CMD-C2D-C1D	5.46	134.34	124.71
36	4	502	LUT	C21-C26-C25	5.46	121.20	111.42
20	A	1120	CLA	CMD-C2D-C1D	5.46	134.33	124.71
20	1	602	CLA	O2D-CGD-CBD	5.45	120.96	111.27
20	A	1125	CLA	O2D-CGD-CBD	5.45	120.96	111.27
20	7	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
36	3	501	LUT	C21-C26-C25	5.45	121.17	111.42
20	1	605	CLA	O2D-CGD-CBD	5.45	120.94	111.27
20	5	613	CLA	CMD-C2D-C1D	5.45	134.31	124.71
20	A	1141	CLA	O2A-C1-C2	5.44	122.92	108.64
20	4	609	CLA	CMD-C2D-C1D	5.43	134.29	124.71
20	1	606	CLA	O2A-C1-C2	5.43	122.91	108.64
20	L	1502	CLA	O2A-C1-C2	5.43	122.90	108.64
20	A	1137	CLA	CMD-C2D-C1D	5.43	134.28	124.71
20	5	612	CLA	O2A-C1-C2	5.42	122.89	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	8	501	LUT	C21-C26-C25	5.42	121.12	111.42
20	A	1139	CLA	O2D-CGD-CBD	5.42	120.89	111.27
20	5	605	CLA	O2D-CGD-CBD	5.42	120.89	111.27
20	7	602	CLA	CMD-C2D-C1D	5.41	134.24	124.71
20	B	1241	CLA	O2A-C1-C2	5.40	122.84	108.64
20	Z	604	CLA	CMD-C2D-C1D	5.40	134.23	124.71
20	6	601	CLA	CMD-C2D-C1D	5.40	134.22	124.71
20	B	1223	CLA	O2A-C1-C2	5.39	122.81	108.64
36	7	502	LUT	C21-C26-C27	5.39	119.52	112.70
36	1	501	LUT	C21-C26-C25	5.39	121.07	111.42
20	8	611	CLA	O2A-C1-C2	5.39	122.79	108.64
20	7	613	CLA	CMD-C2D-C1D	5.38	134.20	124.71
20	4	601	CLA	O2A-C1-C2	5.38	122.78	108.64
20	7	611	CLA	CMD-C2D-C1D	5.38	134.19	124.71
20	K	1401	CLA	CMD-C2D-C1D	5.38	134.19	124.71
34	5	505	C7Z	C11-C10-C9	-5.37	119.64	127.31
20	B	1241	CLA	CMD-C2D-C1D	5.37	134.19	124.71
20	4	608	CLA	CMD-C2D-C1D	5.37	134.18	124.71
20	6	606	CLA	O2D-CGD-CBD	5.37	120.82	111.27
20	6	615	CLA	O2D-CGD-CBD	5.37	120.81	111.27
20	K	1401	CLA	O2D-CGD-CBD	5.37	120.81	111.27
20	B	1235	CLA	O2A-C1-C2	5.37	122.74	108.64
20	A	1115	CLA	O2A-C1-C2	5.37	122.74	108.64
20	B	1217	CLA	O2A-C1-C2	5.37	122.74	108.64
20	A	1116	CLA	O2D-CGD-CBD	5.36	120.80	111.27
20	3	606	CLA	CMD-C2D-C1D	5.36	134.16	124.71
20	7	616	CLA	O2D-CGD-CBD	5.36	120.80	111.27
20	3	607	CLA	CMD-C2D-C1D	5.35	134.15	124.71
20	8	609	CLA	O2D-CGD-CBD	5.35	120.78	111.27
20	B	1220	CLA	O2A-C1-C2	5.35	122.68	108.64
20	J	1901	CLA	CMD-C2D-C1D	5.35	134.13	124.71
20	6	615	CLA	CMD-C2D-C1D	5.35	134.13	124.71
20	6	603	CLA	CMD-C2D-C1D	5.34	134.13	124.71
20	1	604	CLA	CMD-C2D-C1D	5.34	134.12	124.71
20	B	1214	CLA	O2A-C1-C2	5.34	122.66	108.64
20	Z	605	CLA	O2D-CGD-CBD	5.34	120.75	111.27
20	3	616	CLA	CMD-C2D-C1D	5.34	134.12	124.71
20	B	1214	CLA	O2D-CGD-CBD	5.34	120.75	111.27
20	A	1104	CLA	CMD-C2D-C1D	5.34	134.12	124.71
20	6	607	CLA	CMD-C2D-C1D	5.33	134.11	124.71
20	6	612	CLA	O2A-C1-C2	5.33	122.64	108.64
20	Z	605	CLA	CMD-C2D-C1D	5.33	134.10	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	622	CLA	O2D-CGD-CBD	5.33	120.73	111.27
20	7	606	CLA	O2A-C1-C2	5.31	122.60	108.64
20	8	605	CLA	CMD-C2D-C1D	5.31	134.07	124.71
20	A	1139	CLA	CMD-C2D-C1D	5.31	134.07	124.71
20	6	619	CLA	CMD-C2D-C1D	5.31	134.07	124.71
20	B	1239	CLA	CMD-C2D-C1D	5.31	134.07	124.71
20	B	1223	CLA	CMD-C2D-C1D	5.31	134.06	124.71
23	B	4005	BCR	C23-C22-C21	5.30	127.07	118.94
20	A	1138	CLA	CMD-C2D-C1D	5.30	134.05	124.71
20	1	611	CLA	O2A-C1-C2	5.30	122.55	108.64
20	B	1208	CLA	O2A-C1-C2	5.29	122.55	108.64
20	4	607	CLA	CMD-C2D-C1D	5.29	134.03	124.71
20	A	1126	CLA	O2D-CGD-CBD	5.29	120.67	111.27
20	B	1210	CLA	O2A-C1-C2	5.29	122.53	108.64
20	B	1234	CLA	O2A-C1-C2	5.29	122.53	108.64
20	A	1129	CLA	CMD-C2D-C1D	5.28	134.02	124.71
20	B	1228	CLA	CMD-C2D-C1D	5.28	134.02	124.71
20	B	1238	CLA	O2D-CGD-CBD	5.28	120.65	111.27
20	A	1125	CLA	CMD-C2D-C1D	5.28	134.02	124.71
20	6	612	CLA	CMD-C2D-C1D	5.28	134.01	124.71
20	B	1201	CLA	CMD-C2D-C1D	5.28	134.01	124.71
20	3	610	CLA	CMD-C2D-C1D	5.27	134.01	124.71
20	B	1203	CLA	O2D-CGD-CBD	5.27	120.64	111.27
20	J	1901	CLA	O2D-CGD-CBD	5.27	120.63	111.27
20	1	601	CLA	CMD-C2D-C1D	5.27	133.99	124.71
20	B	1222	CLA	CMD-C2D-C1D	5.26	133.99	124.71
20	8	607	CLA	O2A-C1-C2	5.26	122.47	108.64
20	A	1101	CLA	O2D-CGD-CBD	5.26	120.62	111.27
36	1	502	LUT	C21-C26-C25	5.26	120.84	111.42
20	3	602	CLA	CMD-C2D-C1D	5.26	133.98	124.71
20	G	1601	CLA	O2A-C1-C2	5.26	122.45	108.64
20	7	607	CLA	O2D-CGD-CBD	5.26	120.61	111.27
20	B	1022	CLA	O2A-C1-C2	5.25	122.44	108.64
20	A	1141	CLA	CMD-C2D-C1D	5.25	133.97	124.71
20	B	1212	CLA	CMD-C2D-C1D	5.25	133.97	124.71
20	Z	602	CLA	CMD-C2D-C1D	5.25	133.97	124.71
20	8	604	CLA	O2A-C1-C2	5.25	122.43	108.64
20	Z	604	CLA	O2D-CGD-CBD	5.25	120.59	111.27
20	A	1103	CLA	CMD-C2D-C1D	5.25	133.96	124.71
20	A	1107	CLA	CMD-C2D-C1D	5.24	133.96	124.71
20	3	613	CLA	O2D-CGD-CBD	5.24	120.59	111.27
20	8	615	CLA	O2D-CGD-CBD	5.24	120.58	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	604	CLA	CMD-C2D-C1D	5.24	133.95	124.71
20	5	608	CLA	O2D-CGD-CBD	5.23	120.57	111.27
20	3	608	CLA	O2D-CGD-CBD	5.23	120.57	111.27
20	A	1135	CLA	O2A-C1-C2	5.23	122.39	108.64
20	Z	604	CLA	O2A-C1-C2	5.23	122.39	108.64
20	B	1235	CLA	CMD-C2D-C1D	5.23	133.93	124.71
20	A	1118	CLA	CMD-C2D-C1D	5.23	133.93	124.71
20	B	1215	CLA	O2D-CGD-CBD	5.23	120.56	111.27
36	Z	501	LUT	C21-C26-C25	5.23	120.78	111.42
20	5	613	CLA	O2D-CGD-CBD	5.22	120.55	111.27
20	K	1402	CLA	O2A-C1-C2	5.22	122.35	108.64
20	4	612	CLA	O2A-C1-C2	5.22	122.35	108.64
20	A	1132	CLA	O2A-C1-C2	5.22	122.35	108.64
20	7	611	CLA	O2A-C1-C2	5.22	122.34	108.64
20	A	1119	CLA	CMD-C2D-C1D	5.21	133.90	124.71
20	B	1236	CLA	O2A-C1-C2	5.21	122.32	108.64
20	A	1012	CLA	O2D-CGD-CBD	5.21	120.52	111.27
20	B	1221	CLA	CMD-C2D-C1D	5.20	133.88	124.71
20	A	1112	CLA	CMD-C2D-C1D	5.20	133.88	124.71
20	B	1234	CLA	O2D-CGD-CBD	5.19	120.50	111.27
20	A	1134	CLA	CMD-C2D-C1D	5.19	133.86	124.71
20	Z	601	CLA	CMD-C2D-C1D	5.19	133.86	124.71
20	A	1133	CLA	CMD-C2D-C1D	5.19	133.86	124.71
20	5	602	CLA	CMD-C2D-C1D	5.19	133.86	124.71
20	B	1209	CLA	CMD-C2D-C1D	5.19	133.85	124.71
20	A	1136	CLA	O2A-C1-C2	5.18	122.26	108.64
20	3	616	CLA	O2D-CGD-CBD	5.18	120.48	111.27
20	5	618	CLA	O2D-CGD-CBD	5.18	120.48	111.27
20	6	607	CLA	O2A-C1-C2	5.18	122.25	108.64
20	7	612	CLA	CMD-C2D-C1D	5.18	133.84	124.71
20	5	607	CLA	O2A-C1-C2	5.18	122.24	108.64
20	3	610	CLA	O2D-CGD-CBD	5.18	120.47	111.27
20	5	609	CLA	CMD-C2D-C1D	5.18	133.83	124.71
20	7	603	CLA	O2D-CGD-CBD	5.17	120.46	111.27
20	8	605	CLA	O2A-C1-C2	5.17	122.23	108.64
20	A	1128	CLA	O2D-CGD-CBD	5.17	120.46	111.27
20	8	611	CLA	O2D-CGD-CBD	5.17	120.46	111.27
20	Z	603	CLA	CMD-C2D-C1D	5.17	133.82	124.71
20	1	607	CLA	O2A-C1-C2	5.17	122.22	108.64
20	4	606	CLA	O2A-C1-C2	5.16	122.21	108.64
20	7	608	CLA	CMD-C2D-C1D	5.16	133.81	124.71
33	F	4001	RRX	C33-C5-C6	-5.16	118.73	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	612	CLA	O2A-C1-C2	5.16	122.19	108.64
20	A	1108	CLA	CMD-C2D-C1D	5.16	133.81	124.71
20	1	612	CLA	O2A-C1-C2	5.16	122.19	108.64
20	5	607	CLA	CMD-C2D-C1D	5.16	133.80	124.71
20	5	601	CLA	O2D-CGD-CBD	5.15	120.43	111.27
20	B	1231	CLA	O2D-CGD-CBD	5.15	120.42	111.27
20	B	1228	CLA	O2A-C1-C2	5.15	122.17	108.64
20	8	606	CLA	CMD-C2D-C1D	5.15	133.79	124.71
20	A	1122	CLA	CMD-C2D-C1D	5.15	133.79	124.71
20	1	603	CLA	CMD-C2D-C1D	5.15	133.78	124.71
20	Z	607	CLA	CMD-C2D-C1D	5.15	133.78	124.71
20	1	615	CLA	CMD-C2D-C1D	5.14	133.78	124.71
36	5	502	LUT	C21-C26-C25	5.14	120.63	111.42
34	1	503	C7Z	C21-C26-C25	-5.14	115.37	122.61
20	8	615	CLA	CMD-C2D-C1D	5.14	133.77	124.71
20	7	602	CLA	O2A-C1-C2	5.14	122.14	108.64
20	F	1302	CLA	CMD-C2D-C1D	5.14	133.77	124.71
20	4	608	CLA	O2D-CGD-CBD	5.14	120.39	111.27
20	3	605	CLA	O2A-C1-C2	5.13	122.12	108.64
20	A	1110	CLA	CMD-C2D-C1D	5.13	133.76	124.71
20	3	608	CLA	CMD-C2D-C1D	5.13	133.75	124.71
20	8	607	CLA	O2D-CGD-CBD	5.13	120.38	111.27
20	5	606	CLA	O2A-C1-C2	5.13	122.11	108.64
20	B	1241	CLA	O2D-CGD-CBD	5.12	120.37	111.27
20	A	1121	CLA	O2A-C1-C2	5.12	122.10	108.64
20	5	604	CLA	CMD-C2D-C1D	5.12	133.74	124.71
20	6	604	CLA	O2D-CGD-CBD	5.12	120.36	111.27
20	3	607	CLA	O2D-CGD-CBD	5.12	120.36	111.27
20	4	609	CLA	O2A-C1-C2	5.11	122.08	108.64
20	5	618	CLA	CMD-C2D-C1D	5.11	133.73	124.71
20	8	608	CLA	O2D-CGD-CBD	5.11	120.35	111.27
20	5	615	CLA	O2A-C1-C2	5.11	122.06	108.64
20	4	605	CLA	O2A-C1-C2	5.11	122.06	108.64
20	4	615	CLA	CMD-C2D-C1D	5.11	133.71	124.71
20	5	612	CLA	CMD-C2D-C1D	5.11	133.71	124.71
20	B	1239	CLA	O2A-C1-C2	5.10	122.05	108.64
20	4	612	CLA	CMD-C2D-C1D	5.10	133.71	124.71
20	1	602	CLA	CMD-C2D-C1D	5.10	133.70	124.71
20	B	1234	CLA	CMD-C2D-C1D	5.10	133.70	124.71
20	B	1210	CLA	CMD-C2D-C1D	5.09	133.69	124.71
20	Z	612	CLA	CMD-C2D-C1D	5.09	133.69	124.71
19	A	1011	CL0	O2A-CGA-O1A	-5.09	110.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	7	502	LUT	C21-C26-C25	5.09	120.54	111.42
20	4	607	CLA	O2A-C1-C2	5.09	122.01	108.64
20	B	1220	CLA	CMD-C2D-C1D	5.09	133.68	124.71
20	B	1201	CLA	O2D-CGD-CBD	5.09	120.31	111.27
20	A	1102	CLA	CMD-C2D-C1D	5.09	133.68	124.71
20	A	1104	CLA	O2A-C1-C2	5.09	122.01	108.64
20	K	1402	CLA	CMD-C2D-C1D	5.09	133.68	124.71
20	B	1206	CLA	O2A-C1-C2	5.08	122.00	108.64
20	1	607	CLA	O2D-CGD-CBD	5.08	120.30	111.27
20	Z	607	CLA	O2A-C1-C2	5.08	121.98	108.64
20	5	602	CLA	O2D-CGD-CBD	5.08	120.29	111.27
36	4	501	LUT	C21-C26-C25	5.08	120.51	111.42
20	B	1223	CLA	O2D-CGD-CBD	5.08	120.29	111.27
20	Z	615	CLA	O2D-CGD-CBD	5.07	120.28	111.27
20	K	1403	CLA	O2A-C1-C2	5.06	120.81	108.97
20	A	1104	CLA	O2D-CGD-CBD	5.06	120.26	111.27
20	B	1227	CLA	O2D-CGD-CBD	5.06	120.26	111.27
20	B	1202	CLA	O2A-C1-C2	5.06	121.93	108.64
20	4	612	CLA	O2D-CGD-CBD	5.06	120.25	111.27
20	B	1217	CLA	CMD-C2D-C1D	5.06	133.63	124.71
20	8	608	CLA	O2A-C1-C2	5.06	121.93	108.64
20	B	1022	CLA	CMD-C2D-C1D	5.06	133.62	124.71
20	B	1207	CLA	CMD-C2D-C1D	5.05	133.61	124.71
20	3	601	CLA	O2D-CGD-CBD	5.05	120.24	111.27
20	4	605	CLA	O2D-CGD-CBD	5.05	120.24	111.27
20	8	607	CLA	CMD-C2D-C1D	5.05	133.61	124.71
20	A	1118	CLA	O2D-CGD-CBD	5.04	120.23	111.27
20	5	609	CLA	O2D-CGD-CBD	5.04	120.23	111.27
20	A	1136	CLA	CMD-C2D-C1D	5.04	133.60	124.71
20	B	1205	CLA	CMD-C2D-C1D	5.04	133.60	124.71
20	1	603	CLA	O2D-CGD-CBD	5.04	120.22	111.27
20	6	609	CLA	CMD-C2D-C1D	5.04	133.59	124.71
20	6	602	CLA	O2D-CGD-CBD	5.04	120.22	111.27
20	B	1208	CLA	O2D-CGD-CBD	5.04	120.22	111.27
20	6	601	CLA	O2D-CGD-CBD	5.04	120.22	111.27
20	B	1205	CLA	O2D-CGD-CBD	5.03	120.21	111.27
20	B	1225	CLA	O2A-C1-C2	5.03	121.87	108.64
20	3	610	CLA	O2A-C1-C2	5.03	121.85	108.64
20	A	1107	CLA	O2A-C1-C2	5.03	121.85	108.64
20	B	1209	CLA	O2D-CGD-CBD	5.03	120.20	111.27
36	7	501	LUT	C21-C26-C27	5.02	119.05	112.70
20	A	1114	CLA	O2D-CGD-CBD	5.02	120.19	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	608	CLA	CMD-C2D-C1D	5.02	133.56	124.71
20	4	601	CLA	O2D-CGD-CBD	5.02	120.19	111.27
20	4	602	CLA	CMD-C2D-C1D	5.02	133.56	124.71
20	A	1123	CLA	CMD-C2D-C1D	5.02	133.56	124.71
20	A	1119	CLA	O2D-CGD-CBD	5.02	120.19	111.27
20	1	611	CLA	O2D-CGD-CBD	5.02	120.19	111.27
20	B	1236	CLA	O2D-CGD-CBD	5.02	120.18	111.27
20	A	1112	CLA	O2A-C1-C2	5.01	121.81	108.64
20	7	604	CLA	O2D-CGD-CBD	5.01	120.17	111.27
20	Z	603	CLA	O2D-CGD-CBD	5.01	120.17	111.27
20	Z	601	CLA	O2D-CGD-CBD	5.01	120.17	111.27
20	8	606	CLA	O2D-CGD-CBD	5.00	120.15	111.27
20	Z	606	CLA	O2A-C1-C2	5.00	121.77	108.64
36	8	502	LUT	C21-C26-C25	5.00	120.37	111.42
20	A	1129	CLA	O2D-CGD-CBD	4.99	120.13	111.27
20	B	1211	CLA	CMD-C2D-C1D	4.99	133.50	124.71
20	5	602	CLA	O2A-C1-C2	4.99	121.74	108.64
20	8	612	CLA	CMD-C2D-C1D	4.98	133.50	124.71
20	A	1131	CLA	O2A-C1-C2	4.98	121.72	108.64
20	B	1226	CLA	O2D-CGD-CBD	4.98	120.12	111.27
20	6	618	CLA	CMD-C2D-C1D	4.98	133.49	124.71
20	4	602	CLA	O2A-C1-C2	4.98	121.72	108.64
20	A	1121	CLA	O2D-CGD-CBD	4.98	120.11	111.27
20	3	613	CLA	O2A-C1-C2	4.98	121.71	108.64
34	1	503	C7Z	C31-C30-C29	-4.98	120.21	127.31
20	A	1117	CLA	CMD-C2D-C1D	4.98	133.48	124.71
20	7	609	CLA	O2A-C1-C2	4.98	121.71	108.64
20	B	1237	CLA	CMD-C2D-C1D	4.98	133.48	124.71
20	7	601	CLA	O2D-CGD-CBD	4.97	120.11	111.27
20	B	1236	CLA	CMD-C2D-C1D	4.97	133.48	124.71
20	5	606	CLA	CMD-C2D-C1D	4.97	133.48	124.71
20	A	1136	CLA	O2D-CGD-CBD	4.97	120.09	111.27
20	B	1237	CLA	O2A-C1-C2	4.96	121.67	108.64
20	B	1219	CLA	O2A-C1-C2	4.96	121.66	108.64
20	3	604	CLA	CMD-C2D-C1D	4.95	133.44	124.71
20	A	1129	CLA	O2A-C1-C2	4.95	121.64	108.64
20	1	608	CLA	O2D-CGD-CBD	4.94	120.05	111.27
20	Z	601	CLA	O2A-C1-C2	4.94	121.62	108.64
20	3	602	CLA	O2D-CGD-CBD	4.93	120.04	111.27
20	8	604	CLA	CMD-C2D-C1D	4.93	133.41	124.71
20	7	605	CLA	O2A-C1-C2	4.93	121.60	108.64
20	7	613	CLA	O2D-CGD-CBD	4.93	120.03	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1237	CLA	O2D-CGD-CBD	4.93	120.02	111.27
20	B	1230	CLA	O2A-C1-C2	4.92	121.58	108.64
20	B	1215	CLA	O2A-C1-C2	4.92	121.57	108.64
20	B	1240	CLA	O2A-C1-C2	4.92	121.57	108.64
20	B	1022	CLA	O2D-CGD-CBD	4.92	120.01	111.27
20	6	602	CLA	CMD-C2D-C1D	4.92	133.38	124.71
20	L	1502	CLA	O2D-CGD-CBD	4.91	120.00	111.27
20	B	1228	CLA	O2D-CGD-CBD	4.91	120.00	111.27
36	3	501	LUT	C21-C26-C27	4.91	118.91	112.70
20	A	1127	CLA	O2A-C1-C2	4.91	121.54	108.64
20	Z	607	CLA	O2D-CGD-CBD	4.90	119.97	111.27
20	B	1218	CLA	O2A-C1-C2	4.90	121.50	108.64
20	B	1232	CLA	CMD-C2D-C1D	4.90	133.34	124.71
20	A	1113	CLA	O2D-CGD-CBD	4.89	119.97	111.27
20	4	604	CLA	O2A-C1-C2	4.89	121.50	108.64
20	A	1130	CLA	O2D-CGD-CBD	4.89	119.96	111.27
20	1	604	CLA	O2A-C1-C2	4.89	121.48	108.64
19	A	1011	CL0	O2A-C1-C2	4.88	121.47	108.64
20	7	615	CLA	O2D-CGD-CBD	4.88	119.94	111.27
20	4	607	CLA	O2D-CGD-CBD	4.87	119.93	111.27
20	A	1111	CLA	O2A-C1-C2	4.87	121.44	108.64
20	B	1021	CLA	O2A-C1-C2	4.87	121.44	108.64
20	7	607	CLA	O2A-C1-C2	4.87	121.44	108.64
20	B	1232	CLA	O2D-CGD-CBD	4.87	119.92	111.27
20	5	612	CLA	O2D-CGD-CBD	4.87	119.92	111.27
20	A	1105	CLA	CMD-C2D-C1D	4.87	133.29	124.71
20	A	1012	CLA	CMD-C2D-C1D	4.86	133.28	124.71
20	3	604	CLA	O2D-CGD-CBD	4.85	119.89	111.27
20	A	1140	CLA	CMD-C2D-C1D	4.85	133.26	124.71
34	J	4002	C7Z	C35-C34-C33	-4.85	120.39	127.31
20	3	612	CLA	O2D-CGD-CBD	4.85	119.88	111.27
20	7	602	CLA	O2D-CGD-CBD	4.85	119.88	111.27
20	5	607	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	Z	602	CLA	O2D-CGD-CBD	4.84	119.87	111.27
20	5	613	CLA	O2A-C1-C2	4.84	121.35	108.64
34	J	4002	C7Z	C38-C25-C26	-4.84	119.09	124.53
20	B	1206	CLA	CMD-C2D-C1D	4.84	133.24	124.71
20	7	604	CLA	CMD-C2D-C1D	4.84	133.24	124.71
20	6	618	CLA	O2D-CGD-CBD	4.83	119.85	111.27
36	3	502	LUT	C21-C26-C25	4.83	120.06	111.42
24	B	5002	LHG	O7-C7-O9	-4.82	119.43	125.57
20	A	1013	CLA	O2D-CGD-CBD	4.82	119.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	604	CLA	O2D-CGD-CBD	4.82	119.84	111.27
36	6	502	LUT	C21-C26-C27	4.82	118.80	112.70
24	4	801	LHG	O7-C7-C8	4.82	121.89	111.50
39	Z	504	QTB	C01-C02-C09	-4.81	110.50	118.08
20	A	1140	CLA	O2D-CGD-CBD	4.81	119.81	111.27
20	B	1240	CLA	O2D-CGD-CBD	4.81	119.81	111.27
20	A	1113	CLA	O2A-C1-C2	4.81	121.27	108.64
20	B	1216	CLA	O2D-CGD-CBD	4.81	119.81	111.27
20	3	612	CLA	O2A-C1-C2	4.81	121.26	108.64
20	6	619	CLA	O2A-C1-C2	4.80	121.25	108.64
36	6	502	LUT	C21-C26-C25	4.80	120.01	111.42
20	L	1502	CLA	CMD-C2D-C1D	4.79	133.16	124.71
20	A	1123	CLA	O2D-CGD-CBD	4.79	119.78	111.27
20	B	1215	CLA	CMD-C2D-C1D	4.78	133.14	124.71
20	A	1132	CLA	O2D-CGD-CBD	4.78	119.76	111.27
33	F	4001	RRX	C30-C25-C26	-4.78	115.88	122.61
20	8	606	CLA	O2A-C1-C2	4.78	121.19	108.64
20	3	618	CLA	CMD-C2D-C1D	4.77	133.13	124.71
20	A	1119	CLA	O2A-C1-C2	4.77	121.18	108.64
20	B	1207	CLA	O2D-CGD-CBD	4.77	119.75	111.27
20	4	608	CLA	O2A-C1-C2	4.77	121.17	108.64
20	A	1133	CLA	O2D-CGD-CBD	4.77	119.74	111.27
20	L	1503	CLA	O2A-C1-C2	4.77	121.17	108.64
20	A	1107	CLA	O2D-CGD-CBD	4.77	119.74	111.27
20	6	608	CLA	O2D-CGD-CBD	4.75	119.71	111.27
20	B	1224	CLA	CMD-C2D-C1D	4.75	133.08	124.71
20	B	1217	CLA	O2D-CGD-CBD	4.74	119.69	111.27
20	A	1114	CLA	O2A-C1-C2	4.73	121.08	108.64
20	5	601	CLA	O2A-C1-C2	4.73	121.08	108.64
36	8	501	LUT	C22-C23-C24	-4.73	106.35	111.74
20	3	618	CLA	O2D-CGD-CBD	4.73	119.67	111.27
20	5	609	CLA	O2A-C1-C2	4.72	121.05	108.64
20	G	1601	CLA	O2D-CGD-CBD	4.72	119.66	111.27
20	Z	605	CLA	O2A-C1-C2	4.72	121.04	108.64
20	A	1117	CLA	O2D-CGD-CBD	4.72	119.65	111.27
39	Z	504	QTB	C13-C12-C11	4.72	121.90	112.60
20	B	1225	CLA	O2D-CGD-CBD	4.72	119.65	111.27
20	3	605	CLA	O2D-CGD-CBD	4.71	119.64	111.27
19	A	1011	CL0	C3D-C2D-C1D	-4.71	99.40	105.83
20	B	1206	CLA	O2D-CGD-CBD	4.70	119.63	111.27
20	Z	608	CLA	O2A-C1-C2	4.70	121.00	108.64
36	Z	503	LUT	C21-C26-C27	4.70	118.64	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	6	501	LUT	C21-C26-C25	4.70	119.83	111.42
20	B	1235	CLA	O2D-CGD-CBD	4.70	119.61	111.27
20	A	1122	CLA	O2A-C1-C2	4.69	120.96	108.64
20	8	602	CLA	O2D-CGD-CBD	4.69	119.60	111.27
20	A	1109	CLA	O2A-C1-C2	4.68	120.95	108.64
33	F	4001	RRX	C16-C17-C18	-4.68	120.63	127.31
19	A	1011	CL0	C3B-C2B-C1B	-4.68	101.51	107.16
20	6	603	CLA	O2D-CGD-CBD	4.68	119.58	111.27
34	5	505	C7Z	C38-C25-C26	-4.68	119.28	124.53
20	Z	612	CLA	O2D-CGD-CBD	4.67	119.57	111.27
36	5	501	LUT	C35-C34-C33	-4.67	120.64	127.31
20	1	615	CLA	O2D-CGD-CBD	4.67	119.57	111.27
20	4	602	CLA	O2D-CGD-CBD	4.67	119.56	111.27
20	A	1127	CLA	O2D-CGD-CBD	4.66	119.54	111.27
20	B	1204	CLA	O2D-CGD-CBD	4.65	119.53	111.27
20	6	602	CLA	O2A-C1-C2	4.65	120.85	108.64
20	B	1230	CLA	CMD-C2D-C1D	4.65	132.90	124.71
20	A	1122	CLA	O2D-CGD-CBD	4.64	119.52	111.27
20	1	612	CLA	O2D-CGD-CBD	4.64	119.52	111.27
20	1	607	CLA	CMD-C2D-C1D	4.64	132.89	124.71
20	A	1140	CLA	O2A-C1-C2	4.64	120.83	108.64
20	B	1229	CLA	O2A-C1-C2	4.64	120.83	108.64
23	3	504	BCR	C4-C5-C6	-4.64	116.00	122.73
23	3	504	BCR	C1-C6-C5	-4.63	116.10	122.61
20	B	1227	CLA	O2A-C1-C2	4.62	120.78	108.64
20	A	1109	CLA	O2D-CGD-CBD	4.62	119.48	111.27
20	7	611	CLA	O2D-CGD-CBD	4.62	119.48	111.27
20	7	615	CLA	O2A-C1-C2	4.62	120.77	108.64
20	6	605	CLA	O2D-CGD-CBD	4.61	119.46	111.27
20	6	612	CLA	O2D-CGD-CBD	4.61	119.46	111.27
36	6	501	LUT	C35-C34-C33	-4.60	120.75	127.31
20	A	1126	CLA	O2A-C1-C2	4.60	120.71	108.64
24	Z	801	LHG	O7-C7-C8	4.59	121.40	111.50
33	F	4001	RRX	C24-C23-C22	-4.59	119.30	126.23
20	A	1123	CLA	O2A-C1-C2	4.59	120.69	108.64
20	7	606	CLA	O2D-CGD-CBD	4.58	119.41	111.27
20	A	1124	CLA	CMD-C2D-C1D	4.58	132.79	124.71
34	J	4002	C7Z	C11-C10-C9	-4.58	120.78	127.31
19	A	1011	CL0	O2A-CGA-CBA	4.58	126.27	111.91
36	Z	501	LUT	C21-C26-C27	4.57	118.48	112.70
20	K	1403	CLA	O2D-CGD-CBD	4.57	119.39	111.27
20	8	601	CLA	O2D-CGD-CBD	4.57	119.39	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	503	C7Z	C38-C25-C26	-4.57	119.40	124.53
20	3	606	CLA	O2D-CGD-CBD	4.57	119.38	111.27
20	A	1139	CLA	O2A-C1-C2	4.57	120.63	108.64
20	A	1118	CLA	O2A-C1-C2	4.56	120.63	108.64
36	5	502	LUT	C21-C26-C27	4.56	118.46	112.70
20	5	618	CLA	C2D-C1D-ND	4.55	113.45	110.10
20	1	601	CLA	O2D-CGD-CBD	4.55	119.35	111.27
20	A	1102	CLA	O2A-C1-C2	4.54	120.56	108.64
20	4	615	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	A	1124	CLA	O2D-CGD-CBD	4.53	119.33	111.27
20	K	1404	CLA	CMD-C2D-C1D	4.53	132.70	124.71
20	A	1115	CLA	O2D-CGD-CBD	4.53	119.32	111.27
20	4	603	CLA	O2D-CGD-CBD	4.51	119.29	111.27
20	7	605	CLA	O2D-CGD-CBD	4.51	119.28	111.27
36	8	502	LUT	C35-C34-C33	-4.50	120.89	127.31
36	Z	503	LUT	C35-C34-C33	-4.50	120.89	127.31
20	L	1503	CLA	O2D-CGD-CBD	4.50	119.27	111.27
19	A	1011	CL0	CHD-C1D-ND	-4.50	120.32	124.45
20	Z	611	CLA	O2D-CGD-CBD	4.49	119.25	111.27
20	Z	603	CLA	O2A-C1-C2	4.49	120.45	108.64
20	1	605	CLA	O2A-C1-C2	4.49	120.44	108.64
20	B	1222	CLA	O2A-C1-C2	4.49	120.43	108.64
33	F	4001	RRX	C4-C5-C6	-4.48	116.23	122.73
36	4	501	LUT	C35-C34-C33	-4.48	120.92	127.31
20	1	608	CLA	O2A-C1-C2	4.46	120.36	108.64
20	7	603	CLA	CAA-C2A-C3A	-4.46	100.56	112.78
39	Z	504	QTB	C19-C17-C11	-4.46	104.18	110.60
20	4	604	CLA	O2D-CGD-CBD	4.45	119.17	111.27
29	A	5003	LMG	O7-C10-C11	4.45	121.08	111.50
19	A	1011	CL0	C2B-C1B-NB	4.45	113.21	110.23
40	6	802	3PH	O21-C21-C22	4.44	121.08	111.50
36	Z	503	LUT	C15-C14-C13	-4.44	120.98	127.31
20	F	1301	CLA	O2D-CGD-CBD	4.43	119.14	111.27
20	B	1219	CLA	O2D-CGD-CBD	4.43	119.14	111.27
36	6	501	LUT	C35-C15-C14	-4.43	114.41	123.47
23	A	4004	BCR	C27-C26-C25	-4.42	116.32	122.73
24	A	5002	LHG	O7-C7-C8	4.42	121.02	111.50
20	F	1302	CLA	O2D-CGD-CBD	4.41	119.11	111.27
36	5	501	LUT	C22-C23-C24	-4.41	106.72	111.74
20	6	607	CLA	O2D-CGD-CBD	4.41	119.10	111.27
20	3	603	CLA	O2D-CGD-CBD	4.40	119.08	111.27
36	Z	503	LUT	C21-C26-C25	4.40	119.29	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1222	CLA	O2D-CGD-CBD	4.39	119.08	111.27
20	A	1103	CLA	O2A-C1-C2	4.38	120.14	108.64
20	8	612	CLA	O2D-CGD-CBD	4.37	119.04	111.27
20	A	1013	CLA	O2A-C1-C2	4.36	120.10	108.64
20	1	615	CLA	O2A-C1-C2	4.36	120.10	108.64
36	8	502	LUT	C21-C26-C27	4.35	118.21	112.70
20	5	604	CLA	O2D-CGD-CBD	4.35	119.00	111.27
36	Z	503	LUT	C11-C10-C9	-4.35	121.11	127.31
20	K	1404	CLA	O2A-C1-C2	4.34	120.05	108.64
24	5	801	LHG	O7-C7-C8	4.34	120.85	111.50
20	1	603	CLA	O2A-C1-C2	4.32	120.00	108.64
34	5	505	C7Z	C21-C26-C25	-4.32	116.53	122.61
33	F	4001	RRX	C1-C6-C5	-4.30	116.55	122.61
29	J	5001	LMG	O7-C10-C11	4.30	120.77	111.50
40	5	802	3PH	O21-C21-C22	4.30	120.76	111.50
20	8	603	CLA	CAA-C2A-C3A	-4.29	101.04	112.78
20	B	1203	CLA	O2A-C1-C2	4.28	119.89	108.64
20	B	1023	CLA	CMD-C2D-C1D	4.28	132.25	124.71
33	F	4001	RRX	C20-C21-C22	-4.27	121.21	127.31
20	B	1225	CLA	CMD-C2D-C1D	4.27	132.24	124.71
36	6	502	LUT	C15-C14-C13	-4.27	121.22	127.31
20	7	612	CLA	O2D-CGD-CBD	4.27	118.85	111.27
20	A	1141	CLA	O2D-CGD-CBD	4.27	118.85	111.27
36	Z	501	LUT	C22-C23-C24	-4.27	106.89	111.74
34	J	4002	C7Z	C31-C30-C29	-4.26	121.23	127.31
24	B	5006	LHG	O7-C7-C8	4.26	120.68	111.50
34	5	505	C7Z	C18-C5-C6	-4.22	119.79	124.53
24	1	801	LHG	O7-C7-C8	4.22	120.59	111.50
24	8	801	LHG	O7-C7-C8	4.19	120.52	111.50
24	7	801	LHG	O7-C7-C8	4.18	120.50	111.50
34	J	4002	C7Z	C1-C6-C5	-4.17	116.74	122.61
23	A	4003	BCR	C27-C26-C25	-4.17	116.68	122.73
24	B	5001	LHG	O7-C7-C8	4.17	120.49	111.50
36	Z	502	LUT	C35-C34-C33	-4.17	121.36	127.31
20	B	1021	CLA	CMD-C2D-C1D	4.16	132.05	124.71
33	F	4001	RRX	C15-C14-C13	-4.13	121.42	127.31
23	A	4004	BCR	C28-C27-C26	-4.12	106.72	114.08
20	B	1211	CLA	O2D-CGD-CBD	4.12	118.59	111.27
40	7	802	3PH	O21-C21-C22	4.11	120.37	111.50
20	5	603	CLA	O2D-CGD-CBD	4.11	118.58	111.27
36	1	502	LUT	C21-C26-C27	4.10	117.88	112.70
20	5	615	CLA	O2D-CGD-CBD	4.10	118.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	4003	BCR	C28-C27-C26	-4.09	106.78	114.08
34	J	4002	C7Z	C31-C32-C33	-4.09	114.94	126.42
36	8	501	LUT	C21-C26-C27	4.08	117.86	112.70
34	5	505	C7Z	C31-C30-C29	-4.07	121.50	127.31
34	J	4002	C7Z	C18-C5-C6	-4.06	119.97	124.53
36	Z	502	LUT	C21-C26-C27	4.03	117.80	112.70
20	A	1128	CLA	CMD-C2D-C1D	4.02	131.80	124.71
19	A	1011	CL0	CAA-C2A-C3A	-4.02	101.78	112.78
36	Z	501	LUT	C7-C8-C9	-4.01	120.17	126.23
37	6	611	CHL	C4A-NA-C1A	4.01	108.51	106.71
24	A	5001	LHG	O7-C7-C8	4.00	120.13	111.50
34	1	503	C7Z	C2-C3-C4	4.00	115.78	110.30
23	I	4001	BCR	C23-C24-C25	-4.00	115.97	127.20
23	5	503	BCR	C15-C14-C13	-3.99	121.61	127.31
36	1	502	LUT	C35-C34-C33	-3.99	121.62	127.31
20	A	1133	CLA	O2A-C1-C2	3.99	119.11	108.64
36	7	502	LUT	C35-C34-C33	-3.98	121.63	127.31
20	B	1220	CLA	O2D-CGD-CBD	3.98	118.34	111.27
36	3	501	LUT	C7-C8-C9	-3.97	120.23	126.23
30	A	5005	DGA	OG2-CB1-CB2	3.96	120.04	111.50
20	A	1108	CLA	O2D-CGD-CBD	3.96	118.30	111.27
37	5	611	CHL	CHD-C1D-ND	-3.95	120.83	124.45
36	1	502	LUT	C22-C23-C24	-3.94	107.25	111.74
34	J	4002	C7Z	C8-C7-C6	-3.94	116.13	127.20
34	1	503	C7Z	C27-C28-C29	-3.94	120.28	126.23
37	4	613	CHL	CHD-C1D-ND	-3.94	120.84	124.45
36	3	501	LUT	C35-C34-C33	-3.93	121.70	127.31
37	3	611	CHL	C2B-C1B-NB	-3.92	107.60	110.23
24	4	802	LHG	O7-C7-C8	3.92	119.95	111.50
31	B	5003	DGD	O2G-C1B-C2B	3.91	119.92	111.50
20	A	1128	CLA	C2C-C1C-NC	3.90	113.63	109.97
20	A	1109	CLA	CHD-C1D-ND	-3.90	120.87	124.45
23	6	503	BCR	C15-C14-C13	-3.89	121.75	127.31
33	F	4001	RRX	C38-C26-C25	-3.89	120.16	124.53
34	1	503	C7Z	C15-C14-C13	-3.89	121.76	127.31
20	B	1239	CLA	C1-C2-C3	-3.88	119.32	126.04
34	1	503	C7Z	C18-C5-C6	-3.87	120.18	124.53
36	6	501	LUT	C21-C26-C27	3.87	117.59	112.70
36	1	502	LUT	C7-C8-C9	-3.86	120.40	126.23
24	6	801	LHG	O7-C7-C8	3.86	119.82	111.50
36	Z	501	LUT	C35-C34-C33	-3.86	121.81	127.31
36	4	501	LUT	C22-C23-C24	-3.86	107.35	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	603	CLA	CBA-CAA-C2A	3.86	125.25	113.86
20	B	1239	CLA	C2C-C1C-NC	3.86	113.58	109.97
20	5	604	CLA	CMA-C3A-C4A	3.86	122.14	111.77
37	4	611	CHL	C4A-NA-C1A	3.85	108.44	106.71
36	7	502	LUT	C15-C14-C13	-3.84	121.83	127.31
23	A	4005	BCR	C12-C13-C14	-3.84	113.05	118.94
20	B	1236	CLA	C2D-C1D-ND	3.84	112.93	110.10
25	3	802	NKP	OAA-PAC-OAF	-3.84	96.53	106.73
23	6	504	BCR	C33-C5-C6	-3.82	120.23	124.53
36	4	501	LUT	C35-C15-C14	-3.82	115.64	123.47
36	Z	502	LUT	C7-C8-C9	-3.82	120.46	126.23
34	5	505	C7Z	C15-C14-C13	-3.82	121.86	127.31
20	L	1502	CLA	C2D-C1D-ND	3.81	112.92	110.10
20	4	615	CLA	CAA-C2A-C3A	-3.81	107.20	116.10
20	5	622	CLA	C2C-C1C-NC	3.81	113.55	109.97
36	3	502	LUT	C15-C14-C13	-3.80	121.88	127.31
36	5	501	LUT	C35-C15-C14	-3.80	115.69	123.47
36	1	501	LUT	C21-C26-C27	3.80	117.50	112.70
36	Z	503	LUT	C7-C8-C9	-3.79	120.50	126.23
36	4	502	LUT	C21-C26-C27	3.79	117.49	112.70
23	3	504	BCR	C33-C5-C4	3.78	120.88	113.62
20	8	603	CLA	O2D-CGD-CBD	3.77	117.97	111.27
20	B	1238	CLA	C1-C2-C3	-3.77	119.52	126.04
36	6	501	LUT	C7-C8-C9	-3.75	120.56	126.23
33	F	4001	RRX	C2-C1-C6	3.75	116.26	110.48
23	B	4007	BCR	C23-C24-C25	-3.75	116.68	127.20
36	7	502	LUT	C7-C8-C9	-3.75	120.57	126.23
37	4	611	CHL	CHD-C1D-ND	-3.74	121.01	124.45
23	3	506	BCR	C37-C22-C21	-3.74	117.68	122.92
20	1	606	CLA	C1-C2-C3	-3.74	119.58	126.04
20	G	1601	CLA	C1-C2-C3	-3.74	120.70	126.75
20	5	615	CLA	C1-C2-C3	-3.73	120.72	126.75
23	A	4003	BCR	C19-C18-C17	3.73	124.66	118.94
23	A	4003	BCR	C1-C6-C5	-3.73	117.37	122.61
37	3	611	CHL	C3B-C4B-NB	-3.72	107.06	110.52
37	1	610	CHL	CHD-C1D-ND	-3.72	121.04	124.45
20	B	1226	CLA	C2C-C1C-NC	3.71	113.45	109.97
20	A	1127	CLA	CMD-C2D-C1D	3.70	131.23	124.71
36	7	501	LUT	C22-C23-C24	-3.69	107.54	111.74
20	8	603	CLA	C1-C2-C3	-3.68	119.68	126.04
20	Z	612	CLA	C2C-C1C-NC	3.68	113.42	109.97
34	1	503	C7Z	C8-C7-C6	-3.67	116.88	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1013	CLA	CMD-C2D-C1D	3.67	131.18	124.71
23	L	4002	BCR	C33-C5-C6	-3.67	120.41	124.53
23	B	4007	BCR	C33-C5-C6	-3.66	120.42	124.53
23	I	4001	BCR	C27-C26-C25	-3.66	117.42	122.73
36	4	501	LUT	C15-C14-C13	-3.65	122.09	127.31
20	7	612	CLA	CHD-C1D-ND	-3.65	121.10	124.45
23	B	4003	BCR	C23-C22-C21	3.65	124.55	118.94
37	8	613	CHL	CHD-C1D-ND	-3.65	121.10	124.45
36	8	502	LUT	C15-C14-C13	-3.65	122.10	127.31
20	A	1123	CLA	C2C-C1C-NC	3.65	113.39	109.97
20	B	1201	CLA	CHD-C1D-ND	-3.64	121.11	124.45
37	8	610	CHL	CHD-C1D-ND	-3.64	121.11	124.45
20	A	1120	CLA	C2D-C1D-ND	3.64	112.78	110.10
20	3	616	CLA	C2C-C1C-NC	3.63	113.37	109.97
20	7	616	CLA	C1-C2-C3	-3.63	119.76	126.04
23	B	4006	BCR	C19-C18-C17	3.63	124.51	118.94
20	1	607	CLA	C2C-C1C-NC	3.62	113.36	109.97
20	3	604	CLA	CAA-C2A-C3A	-3.62	102.86	112.78
20	F	1301	CLA	O2A-C1-C2	3.62	118.14	108.64
20	5	603	CLA	CHD-C1D-ND	-3.61	121.14	124.45
23	3	504	BCR	C23-C24-C25	-3.61	117.07	127.20
20	3	613	CLA	C1-C2-C3	-3.61	119.81	126.04
37	8	613	CHL	CMA-C3A-C4A	3.60	121.46	111.77
20	6	618	CLA	C2D-C1D-ND	3.60	112.76	110.10
20	7	611	CLA	C2D-C1D-ND	3.60	112.76	110.10
20	B	1227	CLA	CHD-C1D-ND	-3.60	121.15	124.45
20	B	1235	CLA	CHD-C1D-ND	-3.59	121.15	124.45
36	6	502	LUT	C22-C23-C24	-3.59	107.65	111.74
36	Z	503	LUT	C18-C5-C6	-3.59	120.50	124.53
20	4	606	CLA	CHD-C1D-ND	-3.59	121.16	124.45
23	5	503	BCR	C36-C18-C17	-3.58	117.90	122.92
23	G	4001	BCR	C33-C5-C6	-3.58	120.51	124.53
36	5	502	LUT	C15-C14-C13	-3.58	122.20	127.31
33	F	4001	RRX	C7-C8-C9	-3.58	120.83	126.23
20	A	1115	CLA	CHD-C1D-ND	-3.57	121.17	124.45
37	4	610	CHL	C4A-NA-C1A	3.57	108.31	106.71
20	A	1117	CLA	C1-C2-C3	-3.57	119.87	126.04
20	A	1114	CLA	C2C-C1C-NC	3.57	113.32	109.97
20	A	1140	CLA	C1-C2-C3	-3.57	119.87	126.04
36	3	502	LUT	C35-C34-C33	-3.57	122.22	127.31
23	A	4004	BCR	C30-C25-C26	-3.56	117.59	122.61
23	A	4005	BCR	C23-C24-C25	-3.56	117.20	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1104	CLA	C2D-C1D-ND	3.56	112.72	110.10
20	B	1210	CLA	CHD-C1D-ND	-3.56	121.19	124.45
20	Z	601	CLA	C1-C2-C3	-3.55	119.91	126.04
20	4	605	CLA	C1-C2-C3	-3.55	119.91	126.04
20	8	601	CLA	CHD-C1D-ND	-3.54	121.20	124.45
20	A	1102	CLA	C2D-C1D-ND	3.54	112.72	110.10
37	4	617	CHL	CHD-C1D-ND	-3.54	121.20	124.45
36	3	502	LUT	C18-C5-C6	-3.54	120.55	124.53
20	3	612	CLA	CHD-C1D-ND	-3.54	121.20	124.45
20	8	604	CLA	CMA-C3A-C4A	3.54	121.28	111.77
23	A	4004	BCR	C33-C5-C6	-3.53	120.56	124.53
20	B	1230	CLA	C2D-C1D-ND	3.53	112.71	110.10
20	A	1103	CLA	C2D-C1D-ND	3.52	112.70	110.10
20	A	1125	CLA	C1-C2-C3	-3.52	119.95	126.04
23	B	4005	BCR	C35-C13-C12	3.52	123.62	118.08
34	5	505	C7Z	C22-C23-C24	3.52	115.12	110.30
37	7	610	CHL	CHD-C1D-ND	-3.51	121.22	124.45
20	5	612	CLA	CHD-C1D-ND	-3.51	121.23	124.45
37	5	617	CHL	CHD-C1D-ND	-3.51	121.23	124.45
20	8	603	CLA	CHD-C1D-ND	-3.51	121.23	124.45
20	K	1404	CLA	CMA-C3A-C4A	3.51	121.20	111.77
20	4	601	CLA	CHD-C1D-ND	-3.51	121.23	124.45
20	3	610	CLA	C2C-C1C-NC	3.51	113.26	109.97
25	A	5004	NKP	OAF-PAC-OAD	-3.50	96.64	106.47
36	4	501	LUT	C21-C26-C27	3.50	117.13	112.70
37	5	611	CHL	C4A-NA-C1A	3.50	108.28	106.71
20	7	601	CLA	CHD-C1D-ND	-3.50	121.24	124.45
20	Z	602	CLA	C2C-C1C-NC	3.50	113.25	109.97
20	6	612	CLA	C2C-C1C-NC	3.49	113.24	109.97
23	B	4001	BCR	C33-C5-C6	-3.49	120.61	124.53
20	A	1113	CLA	C2C-C1C-NC	3.49	113.24	109.97
20	B	1229	CLA	C3B-C4B-NB	-3.49	107.28	110.52
20	4	603	CLA	CHD-C1D-ND	-3.49	121.25	124.45
38	1	802	SQD	O7-S-C6	-3.49	102.80	106.94
20	A	1124	CLA	O2A-C1-C2	3.48	117.79	108.64
23	B	4003	BCR	C37-C22-C21	-3.48	118.05	122.92
25	8	802	NKP	OAF-PAC-OAD	-3.48	96.72	106.47
37	Z	609	CHL	C3B-C4B-NB	-3.48	107.29	110.52
23	B	4002	BCR	C33-C5-C6	-3.48	120.62	124.53
37	Z	609	CHL	CHD-C1D-ND	-3.48	121.26	124.45
37	4	610	CHL	CMA-C3A-C4A	3.47	121.11	111.77
20	A	1113	CLA	C1-C2-C3	-3.47	120.04	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1127	CLA	C1-C2-C3	-3.47	120.04	126.04
23	5	504	BCR	C34-C9-C10	-3.47	118.07	122.92
20	A	1013	CLA	C2D-C1D-ND	3.47	112.66	110.10
20	A	1124	CLA	C2C-C1C-NC	3.46	113.22	109.97
36	8	501	LUT	C7-C8-C9	-3.46	121.01	126.23
37	4	610	CHL	CHD-C1D-ND	-3.45	121.28	124.45
20	B	1207	CLA	C2C-C1C-NC	3.45	113.21	109.97
20	A	1120	CLA	CHD-C1D-ND	-3.45	121.28	124.45
20	4	602	CLA	C2C-C1C-NC	3.45	113.20	109.97
20	7	609	CLA	C1-C2-C3	-3.45	120.08	126.04
20	B	1218	CLA	C2D-C1D-ND	3.45	112.64	110.10
36	Z	502	LUT	C22-C23-C24	-3.45	107.82	111.74
20	3	606	CLA	CHD-C1D-ND	-3.45	121.29	124.45
36	4	502	LUT	C22-C23-C24	-3.44	107.82	111.74
20	1	608	CLA	CHD-C1D-ND	-3.44	121.29	124.45
36	1	501	LUT	C35-C34-C33	-3.44	122.40	127.31
20	A	1132	CLA	CHD-C1D-ND	-3.44	121.29	124.45
36	7	501	LUT	C35-C34-C33	-3.44	122.40	127.31
20	4	612	CLA	C1-C2-C3	-3.43	121.20	126.75
20	A	1109	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
36	5	502	LUT	C22-C23-C24	-3.43	107.84	111.74
20	7	607	CLA	C2C-C1C-NC	3.43	113.19	109.97
20	7	611	CLA	CHD-C1D-ND	-3.43	121.30	124.45
23	K	4001	BCR	C28-C27-C26	-3.43	107.96	114.08
20	L	1503	CLA	CHD-C1D-ND	-3.43	121.31	124.45
36	3	502	LUT	C31-C30-C29	-3.42	122.42	127.31
20	Z	601	CLA	CHD-C1D-ND	-3.42	121.31	124.45
20	B	1022	CLA	CHD-C1D-ND	-3.42	121.31	124.45
20	G	1601	CLA	C2C-C1C-NC	3.42	113.18	109.97
20	B	1224	CLA	C2C-C1C-NC	3.42	113.18	109.97
20	3	607	CLA	C2C-C1C-NC	3.42	113.17	109.97
34	J	4002	C7Z	C11-C12-C13	-3.42	116.82	126.42
36	8	501	LUT	C35-C34-C33	-3.41	122.44	127.31
20	4	601	CLA	C1-C2-C3	-3.41	120.14	126.04
20	B	1228	CLA	CHD-C1D-ND	-3.41	121.32	124.45
20	B	1221	CLA	O2A-CGA-CBA	3.41	122.62	111.91
20	A	1125	CLA	C2D-C1D-ND	3.41	112.62	110.10
37	5	610	CHL	C4A-NA-C1A	3.41	108.24	106.71
20	A	1121	CLA	CHD-C1D-ND	-3.41	121.32	124.45
20	8	602	CLA	CHD-C1D-ND	-3.41	121.32	124.45
20	8	607	CLA	C2C-C1C-NC	3.41	113.17	109.97
20	B	1235	CLA	O2A-CGA-CBA	3.41	122.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1229	CLA	CHD-C1D-ND	-3.40	121.33	124.45
20	A	1110	CLA	CMA-C3A-C4A	3.40	120.92	111.77
20	A	1139	CLA	CMA-C3A-C4A	3.40	120.91	111.77
23	A	4003	BCR	C33-C5-C4	3.40	120.14	113.62
20	A	1121	CLA	CMA-C3A-C4A	3.40	120.91	111.77
20	B	1227	CLA	C1-C2-C3	-3.39	121.26	126.75
20	7	616	CLA	C2D-C1D-ND	3.39	112.60	110.10
20	7	605	CLA	CHD-C1D-ND	-3.39	121.34	124.45
20	B	1215	CLA	CHD-C1D-ND	-3.39	121.34	124.45
20	B	1219	CLA	C2C-C1C-NC	3.39	113.15	109.97
36	8	502	LUT	C22-C23-C24	-3.39	107.89	111.74
20	A	1013	CLA	CAA-C2A-C3A	-3.39	103.50	112.78
36	1	502	LUT	C35-C15-C14	-3.39	116.54	123.47
20	7	605	CLA	C1-C2-C3	-3.39	120.19	126.04
20	B	1220	CLA	C1-C2-C3	-3.38	120.20	126.04
23	6	504	BCR	C33-C5-C4	3.38	120.11	113.62
20	3	601	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	Z	603	CLA	CMA-C3A-C4A	3.38	120.85	111.77
20	4	608	CLA	C1-C2-C3	-3.38	120.20	126.04
20	A	1101	CLA	CHD-C1D-ND	-3.38	121.35	124.45
20	7	608	CLA	C2C-C1C-NC	3.37	113.13	109.97
37	8	613	CHL	C3B-C4B-NB	-3.37	107.39	110.52
20	B	1202	CLA	CAA-C2A-C3A	-3.37	103.54	112.78
20	6	603	CLA	O2A-CGA-CBA	3.37	122.49	111.91
20	A	1116	CLA	CHD-C1D-ND	-3.37	121.36	124.45
23	G	4001	BCR	C19-C18-C17	3.37	124.11	118.94
20	A	1103	CLA	CHD-C1D-ND	-3.37	121.36	124.45
20	A	1109	CLA	CMA-C3A-C4A	3.37	120.83	111.77
20	A	1129	CLA	C2C-C1C-NC	3.37	113.13	109.97
37	4	610	CHL	C4B-CHC-C1C	3.37	134.32	126.34
20	5	601	CLA	C2D-C1D-ND	3.37	112.58	110.10
20	B	1202	CLA	CHD-C1D-ND	-3.36	121.36	124.45
20	B	1204	CLA	CHD-C1D-ND	-3.36	121.36	124.45
23	8	503	BCR	C33-C5-C6	-3.36	120.75	124.53
20	8	615	CLA	C2C-C1C-NC	3.36	113.12	109.97
20	B	1225	CLA	C2C-C1C-NC	3.36	113.12	109.97
20	5	603	CLA	O2A-CGA-CBA	3.35	122.43	111.91
37	6	611	CHL	CHD-C1D-ND	-3.35	121.37	124.45
36	6	501	LUT	C18-C5-C6	-3.35	120.76	124.53
20	7	606	CLA	CHD-C1D-ND	-3.35	121.38	124.45
20	3	603	CLA	CMA-C3A-C4A	3.35	120.78	111.77
20	F	1302	CLA	C2D-C1D-ND	3.35	112.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	603	CLA	C2D-C1D-ND	3.35	112.57	110.10
20	A	1134	CLA	C2C-C1C-NC	3.35	113.11	109.97
36	7	502	LUT	C22-C23-C24	-3.35	107.93	111.74
20	6	608	CLA	C2C-C1C-NC	3.35	113.11	109.97
20	A	1126	CLA	CHD-C1D-ND	-3.34	121.38	124.45
20	7	613	CLA	CHD-C1D-ND	-3.34	121.38	124.45
36	3	501	LUT	C22-C23-C24	-3.34	107.93	111.74
20	A	1130	CLA	CHD-C1D-ND	-3.34	121.38	124.45
36	8	501	LUT	C38-C25-C24	-3.34	116.41	123.56
20	3	604	CLA	C2D-C1D-ND	3.34	112.57	110.10
20	B	1022	CLA	C2C-C1C-NC	3.34	113.10	109.97
20	A	1102	CLA	O2A-CGA-CBA	3.34	122.39	111.91
20	4	606	CLA	C1-C2-C3	-3.34	121.35	126.75
20	4	609	CLA	C2C-C1C-NC	3.34	113.10	109.97
20	6	615	CLA	C1-C2-C3	-3.34	120.27	126.04
31	B	5003	DGD	O1G-C1A-C2A	3.34	122.38	111.91
36	8	501	LUT	C15-C14-C13	-3.34	122.55	127.31
33	F	4001	RRX	C38-C26-C27	3.34	120.53	114.36
36	1	502	LUT	C15-C14-C13	-3.34	122.55	127.31
20	8	611	CLA	CHD-C1D-ND	-3.33	121.39	124.45
37	3	611	CHL	CHD-C1D-ND	-3.33	121.39	124.45
20	6	615	CLA	C2C-C1C-NC	3.33	113.09	109.97
20	A	1137	CLA	C2C-C1C-NC	3.33	113.09	109.97
20	4	612	CLA	C2C-C1C-NC	3.33	113.09	109.97
20	8	609	CLA	C2C-C1C-NC	3.33	113.09	109.97
20	A	1135	CLA	CHD-C1D-ND	-3.33	121.40	124.45
20	B	1203	CLA	C2D-C1D-ND	3.33	112.56	110.10
23	A	4002	BCR	C27-C26-C25	-3.33	117.90	122.73
20	4	603	CLA	C1-C2-C3	-3.32	120.29	126.04
20	7	605	CLA	C2D-C1D-ND	3.32	112.55	110.10
20	7	609	CLA	CHD-C1D-ND	-3.32	121.41	124.45
20	1	611	CLA	CHD-C1D-ND	-3.32	121.41	124.45
20	7	615	CLA	CHD-C1D-ND	-3.32	121.41	124.45
20	Z	603	CLA	C2D-C1D-ND	3.32	112.55	110.10
20	Z	604	CLA	CHD-C1D-ND	-3.32	121.41	124.45
20	A	1129	CLA	C1-C2-C3	-3.31	121.39	126.75
37	6	610	CHL	CHD-C1D-ND	-3.31	121.41	124.45
20	B	1238	CLA	CHD-C1D-ND	-3.31	121.41	124.45
20	A	1115	CLA	C2D-C1D-ND	3.31	112.55	110.10
20	1	601	CLA	C2D-C1D-ND	3.31	112.54	110.10
20	5	605	CLA	CHD-C1D-ND	-3.31	121.41	124.45
20	A	1114	CLA	CMA-C3A-C4A	3.31	120.66	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	3	501	LUT	C15-C14-C13	-3.31	122.59	127.31
20	A	1110	CLA	C1-C2-C3	-3.30	120.33	126.04
20	5	618	CLA	CHD-C1D-ND	-3.30	121.42	124.45
20	3	618	CLA	C2D-C1D-ND	3.30	112.54	110.10
20	6	612	CLA	CHD-C1D-ND	-3.30	121.42	124.45
23	L	4001	BCR	C33-C5-C6	-3.30	120.82	124.53
20	7	613	CLA	C2C-C1C-NC	3.30	113.06	109.97
20	A	1118	CLA	CHD-C1D-ND	-3.30	121.42	124.45
20	A	1138	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
20	1	613	CLA	CHD-C1D-ND	-3.29	121.43	124.45
23	J	4001	BCR	C38-C26-C25	-3.29	120.83	124.53
20	A	1136	CLA	C2C-C1C-NC	3.29	113.06	109.97
37	5	610	CHL	CHB-C4A-NA	3.29	129.06	124.51
20	6	604	CLA	CHD-C1D-ND	-3.29	121.43	124.45
20	6	609	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	6	503	BCR	C33-C5-C6	-3.29	120.83	124.53
20	A	1107	CLA	C2D-C1D-ND	3.29	112.53	110.10
33	F	4001	RRX	C30-C25-C24	3.29	125.08	115.78
20	B	1218	CLA	CMA-C3A-C4A	3.29	120.61	111.77
20	6	608	CLA	CHD-C1D-ND	-3.29	121.43	124.45
23	7	504	BCR	C15-C14-C13	-3.28	122.62	127.31
23	6	504	BCR	C36-C18-C17	-3.28	118.33	122.92
20	A	1113	CLA	CHD-C1D-ND	-3.28	121.44	124.45
20	B	1239	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
20	4	602	CLA	O2A-CGA-CBA	3.28	122.20	111.91
20	5	608	CLA	C2C-C1C-NC	3.28	113.04	109.97
20	B	1213	CLA	CHD-C1D-ND	-3.28	121.44	124.45
20	B	1236	CLA	CHD-C1D-ND	-3.28	121.44	124.45
20	4	603	CLA	CAA-C2A-C3A	-3.28	103.80	112.78
20	8	602	CLA	C2D-C1D-ND	3.28	112.52	110.10
20	G	1602	CLA	CHD-C1D-ND	-3.27	121.44	124.45
34	J	4002	C7Z	C22-C23-C24	3.27	114.78	110.30
37	6	610	CHL	C3C-C4C-NC	-3.27	106.90	110.57
20	7	603	CLA	C1-C2-C3	-3.27	120.39	126.04
20	8	603	CLA	CMA-C3A-C4A	3.27	120.55	111.77
20	J	1901	CLA	C2C-C1C-NC	3.27	113.03	109.97
20	Z	615	CLA	CHD-C1D-ND	-3.26	121.45	124.45
23	5	504	BCR	C37-C22-C23	3.26	123.22	118.08
20	A	1138	CLA	O2A-CGA-CBA	3.26	122.14	111.91
20	7	615	CLA	C2C-C1C-NC	3.26	113.03	109.97
20	4	604	CLA	CHD-C1D-ND	-3.26	121.46	124.45
37	4	610	CHL	C4D-CHA-C1A	3.26	125.22	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	605	CLA	C2C-C1C-NC	3.26	113.03	109.97
20	5	604	CLA	CHD-C1D-ND	-3.26	121.46	124.45
20	5	607	CLA	CMA-C3A-C4A	3.26	120.53	111.77
20	A	1122	CLA	C1-C2-C3	-3.26	120.41	126.04
19	A	1011	CL0	C1D-ND-C4D	-3.25	104.02	106.33
20	B	1236	CLA	C1D-ND-C4D	-3.25	104.02	106.33
20	A	1138	CLA	CHD-C1D-ND	-3.25	121.46	124.45
20	3	608	CLA	CHD-C1D-ND	-3.25	121.46	124.45
23	5	503	BCR	C33-C5-C4	3.25	119.87	113.62
20	3	613	CLA	C2C-C1C-NC	3.25	113.02	109.97
23	5	504	BCR	C12-C13-C14	3.25	123.93	118.94
20	6	602	CLA	C2C-C1C-NC	3.25	113.02	109.97
23	B	4002	BCR	C23-C24-C25	-3.25	118.08	127.20
20	L	1503	CLA	C1-C2-C3	-3.25	121.49	126.75
23	B	4004	BCR	C33-C5-C6	-3.25	120.88	124.53
20	5	608	CLA	CHD-C1D-ND	-3.24	121.47	124.45
20	6	609	CLA	C2C-C1C-NC	3.24	113.01	109.97
20	A	1110	CLA	O2A-CGA-CBA	3.24	122.08	111.91
37	6	613	CHL	CHD-C1D-ND	-3.24	121.48	124.45
20	A	1110	CLA	C2D-C1D-ND	3.24	112.49	110.10
20	7	616	CLA	CHD-C1D-ND	-3.24	121.48	124.45
20	F	1301	CLA	C2C-C1C-NC	3.24	113.00	109.97
36	Z	501	LUT	C35-C15-C14	-3.24	116.84	123.47
20	6	612	CLA	C2D-C1D-ND	3.24	112.49	110.10
20	A	1106	CLA	C1-C2-C3	-3.24	120.45	126.04
20	3	618	CLA	C2C-C1C-NC	3.23	113.00	109.97
20	B	1232	CLA	C2C-C1C-NC	3.23	113.00	109.97
20	A	1108	CLA	CHD-C1D-ND	-3.23	121.48	124.45
20	6	606	CLA	CHD-C1D-ND	-3.23	121.49	124.45
20	3	603	CLA	C2C-C1C-NC	3.23	113.00	109.97
20	A	1122	CLA	C2C-C1C-NC	3.23	113.00	109.97
20	K	1403	CLA	CHD-C1D-ND	-3.23	121.49	124.45
34	1	503	C7Z	C35-C15-C14	-3.23	116.86	123.47
20	B	1234	CLA	C2C-C1C-NC	3.22	112.99	109.97
20	3	606	CLA	C2D-C1D-ND	3.22	112.48	110.10
20	6	618	CLA	C2C-C1C-NC	3.22	112.99	109.97
36	Z	502	LUT	C35-C15-C14	-3.22	116.87	123.47
37	7	610	CHL	C3B-C4B-NB	-3.22	107.53	110.52
20	Z	603	CLA	C1-C2-C3	-3.22	121.54	126.75
20	A	1111	CLA	CHD-C1D-ND	-3.22	121.49	124.45
20	A	1135	CLA	C3B-C4B-NB	-3.22	107.53	110.52
36	1	502	LUT	C11-C10-C9	-3.22	122.71	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1012	CLA	C1-O2A-CGA	3.22	124.89	116.44
20	B	1219	CLA	C1-C2-C3	-3.22	120.48	126.04
20	A	1141	CLA	C2C-C1C-NC	3.22	112.99	109.97
20	A	1130	CLA	C2C-C1C-NC	3.22	112.98	109.97
23	7	503	BCR	C19-C18-C17	3.22	123.88	118.94
37	4	610	CHL	C1-C2-C3	-3.22	121.55	126.75
20	B	1222	CLA	CHD-C1D-ND	-3.22	121.50	124.45
37	1	609	CHL	C3B-C4B-NB	-3.22	107.53	110.52
23	K	4001	BCR	C3-C4-C5	-3.22	108.34	114.08
20	A	1112	CLA	CHD-C1D-ND	-3.21	121.50	124.45
37	7	610	CHL	C4A-NA-C1A	3.21	108.15	106.71
20	B	1223	CLA	CMA-C3A-C4A	3.21	120.40	111.77
20	K	1404	CLA	C2D-C1D-ND	3.21	112.47	110.10
20	Z	605	CLA	C1-C2-C3	-3.21	120.49	126.04
20	G	1602	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
20	B	1226	CLA	CMD-C2D-C3D	-3.21	120.23	127.61
20	5	605	CLA	C1-C2-C3	-3.21	120.49	126.04
20	A	1124	CLA	C2D-C1D-ND	3.21	112.47	110.10
20	8	601	CLA	C1-C2-C3	-3.21	120.50	126.04
20	1	612	CLA	C2C-C1C-NC	3.21	112.98	109.97
20	1	605	CLA	CHD-C1D-ND	-3.21	121.51	124.45
20	B	1208	CLA	CHD-C1D-ND	-3.20	121.51	124.45
20	1	606	CLA	CHD-C1D-ND	-3.20	121.51	124.45
20	1	602	CLA	C2C-C1C-NC	3.20	112.97	109.97
20	5	612	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
20	7	603	CLA	CMA-C3A-C4A	3.20	120.37	111.77
34	1	503	C7Z	C1-C6-C5	-3.20	118.11	122.61
20	A	1123	CLA	CMA-C3A-C4A	3.20	120.37	111.77
20	B	1204	CLA	C2C-C1C-NC	3.20	112.97	109.97
20	4	605	CLA	C2C-C1C-NC	3.20	112.97	109.97
20	A	1104	CLA	C3B-C4B-NB	-3.19	107.55	110.52
20	Z	605	CLA	C2C-C1C-NC	3.19	112.97	109.97
20	B	1218	CLA	CHD-C1D-ND	-3.19	121.52	124.45
20	7	603	CLA	CHD-C1D-ND	-3.19	121.52	124.45
20	6	604	CLA	O2A-CGA-CBA	3.19	121.93	111.91
20	A	1119	CLA	CHD-C1D-ND	-3.19	121.52	124.45
20	6	618	CLA	CHD-C1D-ND	-3.19	121.52	124.45
20	A	1106	CLA	C4B-CHC-C1C	3.19	133.91	126.34
23	B	4005	BCR	C27-C26-C25	-3.19	118.10	122.73
20	8	605	CLA	C2C-C1C-NC	3.19	112.96	109.97
20	7	604	CLA	CHD-C1D-ND	-3.19	121.52	124.45
21	A	2001	PQN	C14-C13-C15	3.19	120.63	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1011	CL0	O2D-CGD-O1D	-3.19	117.61	123.84
20	3	602	CLA	C2C-C1C-NC	3.19	112.96	109.97
20	8	606	CLA	C2C-C1C-NC	3.19	112.96	109.97
20	7	615	CLA	C2D-C1D-ND	3.18	112.45	110.10
23	5	503	BCR	C19-C18-C17	3.18	123.83	118.94
20	5	609	CLA	C2C-C1C-NC	3.18	112.95	109.97
20	4	607	CLA	CHD-C1D-ND	-3.18	121.53	124.45
20	A	1131	CLA	CHD-C1D-ND	-3.18	121.53	124.45
20	A	1108	CLA	C2C-C1C-NC	3.18	112.95	109.97
20	B	1231	CLA	CHD-C1D-ND	-3.18	121.53	124.45
20	A	1137	CLA	CHD-C1D-ND	-3.18	121.53	124.45
23	3	503	BCR	C23-C24-C25	-3.18	118.28	127.20
20	B	1216	CLA	CHD-C1D-ND	-3.18	121.54	124.45
20	1	611	CLA	C2C-C1C-NC	3.17	112.95	109.97
20	B	1238	CLA	CMA-C3A-C4A	3.17	120.30	111.77
20	A	1106	CLA	C2C-C1C-NC	3.17	112.94	109.97
36	4	501	LUT	C18-C5-C6	-3.17	120.97	124.53
37	1	609	CHL	CHD-C1D-ND	-3.17	121.54	124.45
20	A	1117	CLA	CMA-C3A-C4A	3.17	120.30	111.77
20	8	604	CLA	C2C-C1C-NC	3.17	112.94	109.97
34	5	505	C7Z	C38-C25-C24	3.17	120.23	114.36
20	5	618	CLA	C1-C2-C3	-3.17	120.56	126.04
20	8	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
20	B	1210	CLA	C2C-C1C-NC	3.17	112.94	109.97
20	B	1237	CLA	C1-C2-C3	-3.17	120.56	126.04
20	4	608	CLA	C2C-C1C-NC	3.17	112.94	109.97
20	F	1301	CLA	CHD-C1D-ND	-3.17	121.54	124.45
20	Z	611	CLA	CMA-C3A-C4A	3.17	120.28	111.77
20	3	604	CLA	CMA-C3A-C4A	3.17	120.28	111.77
23	7	504	BCR	C4-C5-C6	-3.17	118.14	122.73
20	A	1127	CLA	C2C-C1C-NC	3.16	112.94	109.97
20	B	1227	CLA	C2C-C1C-NC	3.16	112.94	109.97
20	A	1012	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	5	622	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	7	611	CLA	C1-C2-C3	-3.16	121.63	126.75
20	B	1021	CLA	C2D-C1D-ND	3.16	112.44	110.10
20	4	606	CLA	C2D-C1D-ND	3.16	112.44	110.10
36	7	501	LUT	C7-C8-C9	-3.16	121.46	126.23
20	4	615	CLA	C2C-C1C-NC	3.16	112.93	109.97
20	B	1229	CLA	C2D-C1D-ND	3.16	112.43	110.10
20	Z	606	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
20	6	609	CLA	C1-C2-C3	-3.16	120.58	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1203	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	1	612	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	A	1102	CLA	CHD-C1D-ND	-3.15	121.56	124.45
20	6	601	CLA	CHD-C1D-ND	-3.15	121.56	124.45
20	A	1135	CLA	C2C-C1C-NC	3.15	112.93	109.97
20	4	603	CLA	C2C-C1C-NC	3.15	112.93	109.97
20	A	1128	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
20	B	1021	CLA	C1-C2-C3	-3.15	120.59	126.04
20	A	1139	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	B	2002	PQN	C11-C12-C13	-3.15	121.55	126.79
20	5	615	CLA	C2C-C1C-NC	3.15	112.92	109.97
20	A	1108	CLA	C1-C2-C3	-3.15	120.59	126.04
20	A	1138	CLA	C1-C2-C3	-3.15	120.59	126.04
20	B	1240	CLA	CHD-C1D-ND	-3.15	121.56	124.45
20	Z	611	CLA	C2C-C1C-NC	3.15	112.92	109.97
20	7	602	CLA	C2C-C1C-NC	3.15	112.92	109.97
20	A	1117	CLA	C2C-C1C-NC	3.15	112.92	109.97
20	5	604	CLA	C3B-C4B-NB	-3.15	107.60	110.52
20	3	604	CLA	O2A-CGA-CBA	3.15	121.78	111.91
20	7	616	CLA	O2A-CGA-CBA	3.14	121.78	111.91
20	5	605	CLA	C2C-C1C-NC	3.14	112.92	109.97
20	3	610	CLA	CHD-C1D-ND	-3.14	121.56	124.45
20	7	613	CLA	CAA-C2A-C3A	-3.14	106.41	114.26
37	Z	609	CHL	CMA-C3A-C4A	3.14	120.22	111.77
20	3	610	CLA	C1-C2-C3	-3.14	120.61	126.04
20	B	1208	CLA	C2C-C1C-NC	3.14	112.92	109.97
20	5	605	CLA	C1C-C2C-C3C	-3.14	103.65	106.96
37	4	611	CHL	CMA-C3A-C4A	3.14	120.22	111.77
20	8	608	CLA	CHD-C1D-ND	-3.14	121.57	124.45
20	B	1235	CLA	C2D-C1D-ND	3.14	112.42	110.10
20	B	1023	CLA	C3B-C4B-NB	-3.14	107.60	110.52
20	4	603	CLA	CMA-C3A-C4A	3.14	120.21	111.77
23	6	504	BCR	C19-C18-C17	3.14	123.76	118.94
20	8	615	CLA	CMA-C3A-C4A	3.14	120.21	111.77
20	B	1215	CLA	C2C-C1C-NC	3.14	112.91	109.97
37	3	611	CHL	C2C-C3C-C4C	3.14	108.73	106.49
20	8	611	CLA	O2A-CGA-CBA	3.14	121.75	111.91
20	G	1601	CLA	CHD-C1D-ND	-3.14	121.57	124.45
20	5	613	CLA	CHD-C1D-ND	-3.14	121.57	124.45
20	Z	607	CLA	C2C-C1C-NC	3.14	112.91	109.97
20	5	601	CLA	CHD-C1D-ND	-3.13	121.57	124.45
20	3	616	CLA	C2D-C1D-ND	3.13	112.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	613	CLA	CMA-C3A-C4A	3.13	120.19	111.77
20	Z	611	CLA	C1-C2-C3	-3.13	120.62	126.04
20	1	611	CLA	C1-C2-C3	-3.13	120.63	126.04
20	7	604	CLA	C2D-C1D-ND	3.13	112.41	110.10
20	Z	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
23	B	4003	BCR	C33-C5-C4	3.13	119.63	113.62
37	4	610	CHL	CHC-C1C-NC	3.13	128.95	124.20
37	6	610	CHL	C1-O2A-CGA	3.13	124.65	116.44
20	1	611	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
20	B	1236	CLA	C1-C2-C3	-3.13	120.63	126.04
36	1	501	LUT	C22-C23-C24	-3.13	108.18	111.74
23	7	504	BCR	C33-C5-C4	3.12	119.62	113.62
20	5	618	CLA	C1D-ND-C4D	-3.12	104.12	106.33
20	7	612	CLA	C1-C2-C3	-3.12	121.70	126.75
20	6	603	CLA	C2C-C1C-NC	3.12	112.90	109.97
20	B	1240	CLA	C3B-C4B-NB	-3.12	107.62	110.52
20	4	607	CLA	C2C-C1C-NC	3.12	112.90	109.97
23	7	504	BCR	C1-C6-C5	-3.12	118.22	122.61
20	8	612	CLA	C2C-C1C-NC	3.12	112.89	109.97
20	1	601	CLA	CHD-C1D-ND	-3.12	121.59	124.45
20	B	1206	CLA	C1-O2A-CGA	3.12	124.62	116.44
20	Z	608	CLA	CHD-C1D-ND	-3.12	121.59	124.45
20	B	1022	CLA	C3B-C4B-NB	-3.12	107.62	110.52
37	1	610	CHL	CMA-C3A-C4A	3.11	120.14	111.77
20	B	1226	CLA	CAA-C2A-C3A	-3.11	104.25	112.78
20	A	1136	CLA	O2A-CGA-CBA	3.11	121.68	111.91
20	7	601	CLA	C2D-C1D-ND	3.11	112.40	110.10
20	B	1241	CLA	CMA-C3A-C4A	3.11	120.14	111.77
23	3	504	BCR	C15-C14-C13	-3.11	122.87	127.31
20	1	605	CLA	C1-C2-C3	-3.11	120.66	126.04
23	A	4004	BCR	C36-C18-C17	-3.11	118.56	122.92
20	8	604	CLA	O2A-CGA-CBA	3.11	121.67	111.91
20	3	603	CLA	O2A-CGA-CBA	3.11	121.67	111.91
20	7	604	CLA	O2A-CGA-CBA	3.11	121.67	111.91
20	6	602	CLA	C1-C2-C3	-3.11	120.67	126.04
20	4	612	CLA	CHD-C1D-ND	-3.11	121.60	124.45
20	1	604	CLA	C2C-C1C-NC	3.11	112.88	109.97
20	B	1223	CLA	C1-C2-C3	-3.11	120.67	126.04
20	B	1021	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
20	8	611	CLA	C2D-C1D-ND	3.11	112.39	110.10
36	4	502	LUT	C35-C34-C33	-3.11	122.88	127.31
34	5	505	C7Z	C1-C6-C5	-3.10	118.24	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1113	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
20	B	1234	CLA	CMA-C3A-C4A	3.10	120.11	111.77
20	8	608	CLA	C2C-C1C-NC	3.10	112.88	109.97
20	5	606	CLA	CHD-C1D-ND	-3.10	121.60	124.45
23	A	4005	BCR	C35-C13-C12	3.10	122.96	118.08
20	A	1140	CLA	C2C-C1C-NC	3.10	112.88	109.97
20	A	1118	CLA	C2D-C1D-ND	3.10	112.39	110.10
20	A	1105	CLA	C4B-CHC-C1C	3.10	133.69	126.34
20	A	1131	CLA	C1-C2-C3	-3.10	120.69	126.04
20	8	602	CLA	C2C-C1C-NC	3.10	112.87	109.97
20	Z	604	CLA	CMA-C3A-C4A	3.10	120.10	111.77
20	6	619	CLA	CHD-C1D-ND	-3.10	121.61	124.45
20	5	603	CLA	C2C-C1C-NC	3.10	112.87	109.97
20	A	1136	CLA	CHD-C1D-ND	-3.09	121.61	124.45
20	A	1131	CLA	C2C-C1C-NC	3.09	112.87	109.97
37	Z	613	CHL	CHD-C1D-ND	-3.09	121.61	124.45
23	7	503	BCR	C33-C5-C6	-3.09	121.06	124.53
20	A	1122	CLA	CHD-C1D-ND	-3.09	121.61	124.45
20	B	1023	CLA	CHD-C1D-ND	-3.09	121.61	124.45
36	Z	502	LUT	C38-C25-C24	-3.09	116.94	123.56
23	7	504	BCR	C36-C18-C17	-3.09	118.59	122.92
20	A	1105	CLA	CHD-C1D-ND	-3.09	121.62	124.45
20	5	618	CLA	C2C-C1C-NC	3.09	112.86	109.97
23	B	4006	BCR	C36-C18-C17	-3.09	118.60	122.92
20	1	604	CLA	CHD-C1D-ND	-3.09	121.62	124.45
20	Z	601	CLA	C2D-C1D-ND	3.09	112.38	110.10
40	8	806	3PH	O21-C21-C22	3.08	119.40	110.80
20	3	604	CLA	CHD-C1D-ND	-3.08	121.62	124.45
20	B	1215	CLA	C2D-C1D-ND	3.08	112.38	110.10
20	4	609	CLA	C1-C2-C3	-3.08	120.71	126.04
20	B	1241	CLA	C3B-C4B-NB	-3.08	107.66	110.52
20	Z	611	CLA	CHD-C1D-ND	-3.08	121.62	124.45
20	A	1120	CLA	C1-C2-C3	-3.08	120.71	126.04
20	B	1226	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
36	4	502	LUT	C38-C25-C24	-3.08	116.97	123.56
36	3	502	LUT	C22-C23-C24	-3.08	108.23	111.74
20	B	1205	CLA	C1-C2-C3	-3.08	120.72	126.04
20	6	603	CLA	CHD-C1D-ND	-3.08	121.62	124.45
20	A	1101	CLA	C2C-C1C-NC	3.08	112.86	109.97
20	5	622	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
20	B	1206	CLA	C2D-C1D-ND	3.08	112.37	110.10
26	B	6101	LMT	C1'-O5'-C5'	-3.08	107.65	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1224	CLA	O1D-CGD-CBD	-3.07	118.19	124.48
20	B	1212	CLA	C2D-C1D-ND	3.07	112.37	110.10
20	B	1205	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	B	4005	BCR	C33-C5-C4	3.07	119.52	113.62
20	5	604	CLA	O2A-CGA-CBA	3.07	121.55	111.91
20	Z	604	CLA	C2D-C1D-ND	3.07	112.37	110.10
20	1	601	CLA	C1-C2-C3	-3.07	120.73	126.04
20	6	615	CLA	CHD-C1D-ND	-3.07	121.63	124.45
20	B	1021	CLA	C3B-C4B-NB	-3.07	107.67	110.52
20	A	1133	CLA	CHD-C1D-ND	-3.07	121.63	124.45
20	A	1118	CLA	C2C-C1C-NC	3.07	112.84	109.97
20	A	1132	CLA	C2C-C1C-NC	3.06	112.84	109.97
20	3	616	CLA	CMA-C3A-C4A	3.06	120.01	111.77
20	B	1232	CLA	CMA-C3A-C4A	3.06	120.00	111.77
20	B	1223	CLA	C2D-C1D-ND	3.06	112.36	110.10
20	3	616	CLA	CHD-C1D-ND	-3.06	121.64	124.45
20	8	603	CLA	O2A-CGA-CBA	3.06	121.51	111.91
20	B	1205	CLA	C2C-C1C-NC	3.06	112.84	109.97
36	5	501	LUT	C21-C26-C25	3.06	116.90	111.42
20	5	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
20	A	1121	CLA	C2C-C1C-NC	3.06	112.84	109.97
23	5	503	BCR	C33-C5-C6	-3.06	121.10	124.53
36	3	501	LUT	C18-C5-C6	-3.06	121.10	124.53
20	1	603	CLA	CHD-C1D-ND	-3.06	121.65	124.45
20	A	1132	CLA	CMA-C3A-C4A	3.06	119.98	111.77
20	7	609	CLA	C2C-C1C-NC	3.06	112.83	109.97
20	A	1141	CLA	CHD-C1D-ND	-3.05	121.65	124.45
20	A	1104	CLA	CHD-C1D-ND	-3.05	121.65	124.45
20	A	1108	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
20	G	1601	CLA	C2D-C1D-ND	3.05	112.35	110.10
20	F	1301	CLA	C1-C2-C3	-3.05	120.77	126.04
20	A	1124	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
37	3	611	CHL	C3C-C4C-NC	-3.05	107.15	110.57
20	K	1404	CLA	C2C-C1C-NC	3.05	112.83	109.97
37	Z	609	CHL	C3C-C4C-NC	-3.05	107.15	110.57
20	A	1138	CLA	C2D-C1D-ND	3.05	112.35	110.10
20	B	1239	CLA	C2D-C1D-ND	3.05	112.35	110.10
23	8	503	BCR	C23-C24-C25	-3.05	118.64	127.20
20	B	1219	CLA	CHD-C1D-ND	-3.05	121.65	124.45
20	4	603	CLA	CBA-CAA-C2A	3.05	122.86	113.86
20	B	1223	CLA	C2C-C1C-NC	3.05	112.83	109.97
23	3	503	BCR	C34-C9-C10	-3.05	118.66	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1121	CLA	C1-C2-C3	-3.05	120.78	126.04
20	B	1209	CLA	C3B-C4B-NB	-3.05	107.69	110.52
20	K	1402	CLA	C2D-C1D-ND	3.05	112.35	110.10
21	B	2002	PQN	C14-C13-C15	3.04	120.39	115.27
23	B	4005	BCR	C33-C5-C6	-3.04	121.11	124.53
20	L	1502	CLA	CMA-C3A-C4A	3.04	119.95	111.77
37	8	610	CHL	CMA-C3A-C4A	3.04	119.95	111.77
23	3	504	BCR	C19-C18-C17	3.04	123.61	118.94
20	B	1207	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
37	5	610	CHL	C3B-C4B-NB	-3.04	107.69	110.52
20	A	1116	CLA	C3B-C4B-NB	-3.04	107.69	110.52
20	B	1213	CLA	C2D-C1D-ND	3.04	112.34	110.10
20	A	1107	CLA	CHD-C1D-ND	-3.04	121.66	124.45
20	3	608	CLA	C2C-C1C-NC	3.04	112.82	109.97
37	4	613	CHL	C1-O2A-CGA	3.04	124.41	116.44
20	A	1013	CLA	C1-C2-C3	-3.03	120.79	126.04
37	8	610	CHL	C4B-CHC-C1C	3.03	133.54	126.34
20	K	1402	CLA	C1-C2-C3	-3.03	120.80	126.04
37	Z	609	CHL	C4B-CHC-C1C	3.03	133.53	126.34
37	1	609	CHL	C3C-C4C-NC	-3.03	107.17	110.57
20	B	1226	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	4	608	CLA	CHD-C1D-ND	-3.03	121.67	124.45
20	5	607	CLA	C2C-C1C-NC	3.03	112.81	109.97
20	4	606	CLA	C2C-C1C-NC	3.03	112.81	109.97
23	K	4002	BCR	C36-C18-C17	-3.03	118.68	122.92
37	4	617	CHL	C4B-CHC-C1C	3.03	133.52	126.34
37	Z	610	CHL	C3C-C4C-NC	-3.03	107.17	110.57
20	B	1213	CLA	C1-O2A-CGA	3.03	124.39	116.44
20	5	606	CLA	C2C-C1C-NC	3.03	112.81	109.97
36	5	502	LUT	C31-C30-C29	-3.03	122.99	127.31
20	7	602	CLA	C2D-C1D-ND	3.03	112.33	110.10
36	8	502	LUT	C7-C8-C9	-3.03	121.66	126.23
20	A	1119	CLA	C1-C2-C3	-3.03	120.81	126.04
36	7	502	LUT	C11-C10-C9	-3.02	122.99	127.31
20	1	612	CLA	C2D-C1D-ND	3.02	112.33	110.10
37	1	609	CHL	CMA-C3A-C4A	3.02	119.90	111.77
20	A	1123	CLA	CHD-C1D-ND	-3.02	121.67	124.45
23	5	504	BCR	C33-C5-C4	3.02	119.42	113.62
20	F	1301	CLA	C2D-C1D-ND	3.02	112.33	110.10
37	8	610	CHL	C4A-NA-C1A	3.02	108.06	106.71
20	7	607	CLA	CHD-C1D-ND	-3.02	121.68	124.45
20	5	603	CLA	C1C-C2C-C3C	-3.02	103.78	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	607	CLA	C2C-C1C-NC	3.02	112.80	109.97
20	6	609	CLA	CHD-C1D-ND	-3.02	121.68	124.45
37	8	610	CHL	CHC-C1C-NC	3.02	128.78	124.20
20	8	605	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
20	A	1012	CLA	C3B-C4B-NB	-3.02	107.72	110.52
20	B	1201	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	6	504	BCR	C35-C13-C12	3.02	122.83	118.08
20	B	1215	CLA	C1C-C2C-C3C	-3.02	103.79	106.96
20	1	615	CLA	CHD-C1D-ND	-3.02	121.68	124.45
20	3	605	CLA	C1-C2-C3	-3.01	120.83	126.04
20	K	1401	CLA	C2C-C1C-NC	3.01	112.80	109.97
37	Z	610	CHL	CHB-C4A-NA	3.01	128.68	124.51
20	1	603	CLA	C2D-C1D-ND	3.01	112.32	110.10
20	F	1302	CLA	C2C-C1C-NC	3.01	112.79	109.97
20	G	1602	CLA	C2C-C1C-NC	3.01	112.79	109.97
20	A	1106	CLA	CHD-C1D-ND	-3.01	121.69	124.45
20	B	1222	CLA	O2A-CGA-CBA	3.01	121.36	111.91
37	Z	613	CHL	CMA-C3A-C4A	3.01	119.86	111.77
20	A	1121	CLA	CMD-C2D-C3D	-3.01	120.69	127.61
20	Z	612	CLA	CHD-C1D-ND	-3.01	121.69	124.45
20	4	615	CLA	CHD-C1D-ND	-3.01	121.69	124.45
20	5	602	CLA	C2D-C1D-ND	3.01	112.32	110.10
20	A	1105	CLA	C2C-C1C-NC	3.01	112.79	109.97
20	A	1132	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
20	A	1124	CLA	CHD-C1D-ND	-3.00	121.69	124.45
20	A	1105	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
20	Z	615	CLA	C2C-C1C-NC	3.00	112.78	109.97
20	7	602	CLA	CHD-C1D-ND	-3.00	121.69	124.45
20	A	1115	CLA	C1-C2-C3	-3.00	120.85	126.04
20	6	615	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
20	5	603	CLA	C2D-C1D-ND	3.00	112.31	110.10
37	5	610	CHL	CHD-C1D-ND	-3.00	121.70	124.45
23	A	4002	BCR	C38-C26-C27	3.00	119.38	113.62
36	Z	502	LUT	C3-C4-C5	-3.00	105.88	111.85
20	A	1110	CLA	CHD-C1D-ND	-3.00	121.70	124.45
20	7	603	CLA	C2D-C1D-ND	3.00	112.31	110.10
20	A	1125	CLA	CHD-C1D-ND	-3.00	121.70	124.45
20	L	1502	CLA	C2C-C1C-NC	2.99	112.78	109.97
20	A	1109	CLA	C2C-C1C-NC	2.99	112.78	109.97
37	5	611	CHL	C1-C2-C3	-2.99	121.91	126.75
37	6	611	CHL	CMA-C3A-C4A	2.99	119.81	111.77
20	1	607	CLA	CAA-C2A-C3A	-2.99	104.59	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1206	CLA	C2C-C1C-NC	2.99	112.77	109.97
36	Z	501	LUT	C38-C25-C24	-2.99	117.16	123.56
37	Z	613	CHL	CHB-C4A-NA	2.99	128.65	124.51
20	A	1105	CLA	C2D-C1D-ND	2.99	112.31	110.10
20	A	1112	CLA	C2D-C1D-ND	2.99	112.31	110.10
20	B	1216	CLA	C2C-C1C-NC	2.99	112.77	109.97
20	A	1110	CLA	C3B-C4B-NB	-2.99	107.74	110.52
20	1	603	CLA	CMA-C3A-C4A	2.99	119.80	111.77
20	6	606	CLA	C2C-C1C-NC	2.98	112.77	109.97
36	4	502	LUT	C35-C15-C14	-2.98	117.36	123.47
23	J	4001	BCR	C36-C18-C17	-2.98	118.75	122.92
23	L	4002	BCR	C36-C18-C17	-2.98	118.75	122.92
20	8	607	CLA	CHD-C1D-ND	-2.98	121.72	124.45
20	7	602	CLA	C1-C2-C3	-2.98	121.93	126.75
20	B	1220	CLA	C2D-C1D-ND	2.98	112.30	110.10
20	F	1302	CLA	C3B-C4B-NB	-2.98	107.75	110.52
20	B	1211	CLA	C2C-C1C-NC	2.98	112.76	109.97
20	8	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
20	A	1140	CLA	CHD-C1D-ND	-2.97	121.72	124.45
20	6	619	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
20	7	609	CLA	C2D-C1D-ND	2.97	112.30	110.10
23	G	4001	BCR	C35-C13-C12	2.97	122.76	118.08
20	3	607	CLA	CMA-C3A-C4A	2.97	119.76	111.77
20	B	1226	CLA	CAC-C3C-C4C	2.97	128.67	124.81
37	5	611	CHL	CMA-C3A-C4A	2.97	119.76	111.77
20	Z	607	CLA	CMA-C3A-C4A	2.97	119.75	111.77
20	6	601	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
20	A	1013	CLA	C3B-C4B-NB	-2.97	107.76	110.52
23	G	4001	BCR	C37-C22-C21	-2.97	118.77	122.92
20	7	601	CLA	CAA-C2A-C3A	-2.96	104.66	112.78
20	A	1141	CLA	C6-C5-C3	-2.96	109.77	114.62
20	B	1236	CLA	C2C-C1C-NC	2.96	112.75	109.97
23	3	503	BCR	C33-C5-C6	-2.96	121.20	124.53
20	1	608	CLA	C2C-C1C-NC	2.96	112.75	109.97
33	F	4001	RRX	C29-C28-C27	2.96	114.36	110.30
20	5	607	CLA	C2D-C1D-ND	2.96	112.28	110.10
20	4	604	CLA	C2C-C1C-NC	2.96	112.74	109.97
20	A	1130	CLA	C1-C2-C3	-2.96	120.93	126.04
37	Z	610	CHL	CHD-C1D-ND	-2.96	121.74	124.45
20	7	603	CLA	C2C-C1C-NC	2.96	112.74	109.97
23	6	503	BCR	C33-C5-C4	2.96	119.30	113.62
23	5	504	BCR	C8-C9-C10	2.96	123.48	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1111	CLA	C1-C2-C3	-2.96	120.93	126.04
20	5	615	CLA	CHD-C1D-ND	-2.96	121.74	124.45
20	3	608	CLA	CMA-C3A-C4A	2.95	119.71	111.77
20	3	606	CLA	C2C-C1C-NC	2.95	112.74	109.97
20	A	1106	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
20	B	1209	CLA	C2D-C1D-ND	2.95	112.28	110.10
20	8	602	CLA	O2A-CGA-CBA	2.95	121.16	111.91
20	3	605	CLA	C3B-C4B-NB	-2.95	107.78	110.52
20	5	604	CLA	C2D-C1D-ND	2.95	112.28	110.10
20	B	1230	CLA	C1-C2-C3	-2.95	120.95	126.04
20	B	1237	CLA	CHD-C1D-ND	-2.95	121.75	124.45
20	3	613	CLA	CHD-C1D-ND	-2.95	121.75	124.45
20	5	615	CLA	CMA-C3A-C4A	2.95	119.69	111.77
20	K	1402	CLA	C3B-C4B-NB	-2.94	107.78	110.52
20	A	1129	CLA	CHD-C1D-ND	-2.94	121.75	124.45
36	7	502	LUT	C10-C11-C12	-2.94	114.03	123.22
20	B	1021	CLA	O1D-CGD-CBD	-2.94	118.46	124.48
20	4	609	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	7	608	CLA	CMA-C3A-C4A	2.94	119.68	111.77
20	Z	601	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
20	A	1122	CLA	CMA-C3A-C4A	2.94	119.68	111.77
20	A	1117	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	6	608	CLA	C1-O2A-CGA	2.94	124.16	116.44
23	5	504	BCR	C36-C18-C17	-2.94	118.81	122.92
20	6	607	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	B	1203	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
20	B	1205	CLA	C1-O2A-CGA	2.94	124.15	116.44
20	B	1214	CLA	C2C-C1C-NC	2.94	112.72	109.97
20	A	1134	CLA	C1-C2-C3	-2.94	120.96	126.04
23	4	503	BCR	C33-C5-C4	2.94	119.26	113.62
20	Z	606	CLA	CHD-C1D-ND	-2.94	121.75	124.45
20	7	606	CLA	C2C-C1C-NC	2.94	112.72	109.97
20	A	1013	CLA	CMB-C2B-C3B	2.94	133.70	126.59
20	8	615	CLA	C2D-C1D-ND	2.93	112.27	110.10
20	4	608	CLA	CMA-C3A-C4A	2.93	119.66	111.77
20	4	612	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
20	3	616	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
20	A	1137	CLA	C2D-C1D-ND	2.93	112.26	110.10
20	B	1223	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	B	1206	CLA	O2A-CGA-CBA	2.93	121.10	111.91
20	Z	608	CLA	C2C-C1C-NC	2.93	112.72	109.97
20	8	611	CLA	C1C-C2C-C3C	-2.93	103.88	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1236	CLA	C3B-C4B-NB	-2.93	107.80	110.52
20	7	613	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
36	4	502	LUT	C10-C11-C12	-2.93	114.09	123.22
20	6	612	CLA	CMA-C3A-C4A	2.93	119.64	111.77
20	B	1239	CLA	CHD-C1D-ND	-2.92	121.77	124.45
20	B	1203	CLA	C2C-C1C-NC	2.92	112.71	109.97
37	Z	613	CHL	C3C-C4C-NC	-2.92	107.29	110.57
36	8	501	LUT	C35-C15-C14	-2.92	117.48	123.47
20	8	612	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
23	B	4006	BCR	C35-C13-C12	2.92	122.68	118.08
20	8	611	CLA	C2C-C1C-NC	2.92	112.71	109.97
23	B	4007	BCR	C19-C18-C17	2.92	123.42	118.94
20	7	611	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
37	8	610	CHL	C1-O2A-CGA	2.92	124.10	116.44
20	8	612	CLA	CHD-C1D-ND	-2.92	121.77	124.45
20	7	607	CLA	CMA-C3A-C4A	2.92	119.62	111.77
20	K	1404	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	K	4002	BCR	C19-C18-C17	2.92	123.42	118.94
20	5	603	CLA	CMA-C3A-C4A	2.92	119.61	111.77
34	1	503	C7Z	C38-C25-C24	2.92	119.76	114.36
37	6	610	CHL	C2C-C3C-C4C	2.92	108.57	106.49
39	Z	504	QTB	C11-C10-C09	2.92	131.80	125.47
37	4	610	CHL	C1-O2A-CGA	2.92	124.09	116.44
20	3	601	CLA	C1-O2A-CGA	2.92	124.09	116.44
20	3	601	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
20	A	1127	CLA	C2D-C1D-ND	2.91	112.25	110.10
20	3	608	CLA	C2D-C1D-ND	2.91	112.25	110.10
20	B	1240	CLA	C1-C2-C3	-2.91	121.01	126.04
20	3	601	CLA	O2A-CGA-CBA	2.91	121.04	111.91
20	B	1214	CLA	OBD-CAD-C3D	-2.91	121.52	128.52
20	6	603	CLA	CMA-C3A-C4A	2.91	119.59	111.77
20	Z	602	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
20	5	602	CLA	C1-C2-C3	-2.91	121.01	126.04
36	Z	502	LUT	C15-C14-C13	-2.91	123.16	127.31
20	6	612	CLA	C1-C2-C3	-2.91	122.05	126.75
20	3	607	CLA	CHD-C1D-ND	-2.90	121.78	124.45
20	B	1228	CLA	C1-C2-C3	-2.90	121.02	126.04
20	B	1221	CLA	C2D-C1D-ND	2.90	112.24	110.10
37	4	613	CHL	CMA-C3A-C4A	2.90	119.58	111.77
20	B	1209	CLA	CHD-C1D-ND	-2.90	121.79	124.45
20	A	1120	CLA	C2C-C1C-NC	2.90	112.69	109.97
37	Z	610	CHL	C2C-C3C-C4C	2.90	108.56	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1126	CLA	C1-C2-C3	-2.90	121.03	126.04
20	5	618	CLA	CMA-C3A-C4A	2.90	119.57	111.77
20	8	606	CLA	C1-C2-C3	-2.90	121.03	126.04
20	B	1214	CLA	C1-C2-C3	-2.90	121.03	126.04
20	A	1109	CLA	O2A-CGA-CBA	2.90	121.01	111.91
20	A	1134	CLA	CMA-C3A-C4A	2.90	119.56	111.77
40	8	806	3PH	O31-C31-C32	2.90	121.00	111.91
20	1	605	CLA	C2C-C1C-NC	2.90	112.69	109.97
20	B	1022	CLA	C2D-C1D-ND	2.90	112.24	110.10
20	7	612	CLA	C2D-C1D-ND	2.90	112.24	110.10
20	B	1209	CLA	C4B-CHC-C1C	2.90	133.21	126.34
20	B	1208	CLA	C2D-C1D-ND	2.90	112.24	110.10
20	3	603	CLA	C2D-C1D-ND	2.90	112.24	110.10
37	7	610	CHL	C4B-CHC-C1C	2.90	133.21	126.34
36	6	502	LUT	C35-C34-C33	-2.89	123.18	127.31
23	7	503	BCR	C36-C18-C17	-2.89	118.87	122.92
20	6	605	CLA	O2A-CGA-CBA	2.89	120.98	111.91
37	1	609	CHL	C4B-CHC-C1C	2.89	133.20	126.34
20	6	609	CLA	C4B-CHC-C1C	2.89	133.20	126.34
20	A	1120	CLA	CMA-C3A-C4A	2.89	119.54	111.77
20	5	605	CLA	CMA-C3A-C4A	2.89	119.54	111.77
20	3	601	CLA	C2C-C1C-NC	2.89	112.68	109.97
20	B	1221	CLA	CHD-C1D-ND	-2.89	121.80	124.45
20	6	604	CLA	C2D-C1D-ND	2.89	112.23	110.10
20	6	619	CLA	C2C-C1C-NC	2.89	112.68	109.97
26	B	5005	LMT	O5'-C1'-C2'	-2.89	104.23	110.35
37	4	617	CHL	C3B-C4B-NB	-2.89	107.84	110.52
33	F	4001	RRX	C35-C13-C14	-2.89	118.88	122.92
20	B	1222	CLA	C2D-C1D-ND	2.89	112.23	110.10
20	A	1103	CLA	C1-C2-C3	-2.89	121.05	126.04
20	A	1130	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
20	6	605	CLA	C2D-C1D-ND	2.89	112.23	110.10
20	Z	607	CLA	CHD-C1D-ND	-2.88	121.80	124.45
23	B	4005	BCR	C38-C26-C27	2.88	119.16	113.62
23	A	4001	BCR	C19-C18-C17	2.88	123.37	118.94
20	Z	605	CLA	CHD-C1D-ND	-2.88	121.80	124.45
20	6	612	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
20	A	1139	CLA	CAA-C2A-C3A	-2.88	104.88	112.78
37	8	613	CHL	C4B-CHC-C1C	2.88	133.18	126.34
37	5	617	CHL	C4B-CHC-C1C	2.88	133.18	126.34
20	Z	602	CLA	CHD-C1D-ND	-2.88	121.81	124.45
33	F	4001	RRX	C33-C5-C4	2.88	119.15	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	612	CLA	CMA-C3A-C4A	2.88	119.52	111.77
20	7	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	A	1135	CLA	C1-C2-C3	-2.88	121.06	126.04
37	6	613	CHL	CMA-C3A-C4A	2.88	119.52	111.77
20	K	1403	CLA	C2C-C1C-NC	2.88	112.67	109.97
20	6	601	CLA	C2D-C1D-ND	2.88	112.23	110.10
20	8	605	CLA	CHD-C1D-ND	-2.88	121.81	124.45
37	6	610	CHL	C4B-CHC-C1C	2.88	133.17	126.34
23	B	4004	BCR	C33-C5-C4	2.88	119.15	113.62
20	B	1241	CLA	C2C-C1C-NC	2.88	112.67	109.97
37	7	610	CHL	CMA-C3A-C4A	2.88	119.51	111.77
37	8	610	CHL	C4D-CHA-C1A	2.88	124.75	121.25
23	A	4003	BCR	C33-C5-C6	-2.88	121.30	124.53
36	1	502	LUT	C38-C25-C24	-2.88	117.40	123.56
20	A	1117	CLA	C2D-C1D-ND	2.88	112.22	110.10
23	A	4003	BCR	C4-C5-C6	-2.88	118.56	122.73
20	K	1402	CLA	CMA-C3A-C4A	2.88	119.50	111.77
20	Z	605	CLA	C2D-C1D-ND	2.88	112.22	110.10
20	B	1230	CLA	CMA-C3A-C4A	2.88	119.50	111.77
24	8	801	LHG	O8-C23-C24	2.87	120.93	111.91
20	7	616	CLA	C2C-C1C-NC	2.87	112.67	109.97
20	A	1102	CLA	C1-O2A-CGA	2.87	123.99	116.44
20	8	606	CLA	CHD-C1D-ND	-2.87	121.81	124.45
37	6	617	CHL	CMA-C3A-C4A	2.87	119.50	111.77
20	A	1132	CLA	C1-C2-C3	-2.87	121.07	126.04
36	4	502	LUT	C18-C5-C6	-2.87	121.30	124.53
20	7	605	CLA	C3B-C4B-NB	-2.87	107.85	110.52
20	A	1110	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	B	1212	CLA	C1-C2-C3	-2.87	121.08	126.04
20	A	1128	CLA	CHD-C1D-ND	-2.87	121.82	124.45
20	5	602	CLA	C2C-C1C-NC	2.87	112.66	109.97
20	B	1213	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
20	6	603	CLA	C2D-C1D-ND	2.87	112.22	110.10
20	A	1126	CLA	O1D-CGD-CBD	-2.87	118.62	124.48
20	5	601	CLA	O1D-CGD-CBD	-2.87	118.62	124.48
20	8	609	CLA	CHD-C1D-ND	-2.87	121.82	124.45
20	A	1112	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
20	B	1210	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	5	501	LUT	C7-C8-C9	-2.86	121.91	126.23
20	A	1115	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
20	1	613	CLA	CMD-C2D-C3D	-2.86	121.03	127.61
20	B	1210	CLA	CMA-C3A-C4A	2.86	119.47	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1124	CLA	C1-C2-C3	-2.86	121.09	126.04
20	5	613	CLA	C3B-C4B-NB	-2.86	107.86	110.52
20	3	602	CLA	CHD-C1D-ND	-2.86	121.83	124.45
36	1	502	LUT	C10-C11-C12	-2.86	114.29	123.22
20	3	606	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
37	1	609	CHL	C2C-C3C-C4C	2.86	108.53	106.49
20	B	1023	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	K	1402	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	3	605	CLA	CHD-C1D-ND	-2.86	121.83	124.45
20	B	1217	CLA	C2C-C1C-NC	2.86	112.65	109.97
20	B	1230	CLA	C2C-C1C-NC	2.86	112.65	109.97
36	3	502	LUT	C38-C25-C24	-2.86	117.44	123.56
20	4	602	CLA	C1-C2-C3	-2.86	121.10	126.04
20	Z	612	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
20	A	1140	CLA	C3B-C4B-NB	-2.86	107.86	110.52
20	A	1012	CLA	C2D-C1D-ND	2.86	112.21	110.10
20	7	603	CLA	O2A-CGA-CBA	2.86	120.87	111.91
20	4	602	CLA	C6-C5-C3	-2.85	109.95	114.62
20	3	618	CLA	CHD-C1D-ND	-2.85	121.83	124.45
37	3	611	CHL	CMA-C3A-C4A	2.85	119.44	111.77
20	7	607	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
20	B	1207	CLA	CHD-C1D-ND	-2.85	121.83	124.45
20	5	603	CLA	C1-C2-C3	-2.85	121.12	126.04
20	A	1140	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
20	6	607	CLA	CMA-C3A-C4A	2.85	119.42	111.77
37	5	611	CHL	C3C-C4C-NC	-2.85	107.38	110.57
20	A	1120	CLA	C3B-C4B-NB	-2.85	107.88	110.52
25	8	802	NKP	OAB-PAC-OAA	2.85	118.51	107.64
20	B	1227	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	A	4003	BCR	C36-C18-C17	-2.84	118.94	122.92
20	A	1136	CLA	CMA-C3A-C4A	2.84	119.41	111.77
20	5	613	CLA	C2C-C1C-NC	2.84	112.63	109.97
40	5	802	3PH	O31-C31-C32	2.84	120.82	111.91
20	B	1209	CLA	C2C-C1C-NC	2.84	112.63	109.97
34	1	503	C7Z	C31-C32-C33	-2.84	118.44	126.42
20	A	1122	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
20	1	601	CLA	C2C-C1C-NC	2.84	112.63	109.97
20	1	613	CLA	C2C-C1C-NC	2.84	112.63	109.97
20	Z	605	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
20	B	1226	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
20	5	606	CLA	C2D-C1D-ND	2.84	112.19	110.10
20	6	604	CLA	C2C-C1C-NC	2.84	112.63	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1222	CLA	C1-C2-C3	-2.83	121.14	126.04
20	B	1207	CLA	CMA-C3A-C4A	2.83	119.39	111.77
26	B	5005	LMT	C1'-O5'-C5'	-2.83	108.12	113.69
20	A	1123	CLA	C1-C2-C3	-2.83	121.14	126.04
20	A	1127	CLA	C3B-C4B-NB	-2.83	107.89	110.52
20	B	1202	CLA	C2C-C1C-NC	2.83	112.62	109.97
20	B	1221	CLA	C2C-C1C-NC	2.83	112.62	109.97
20	B	1231	CLA	C2C-C1C-NC	2.83	112.62	109.97
20	A	1139	CLA	C2C-C1C-NC	2.83	112.62	109.97
36	8	502	LUT	C10-C11-C12	-2.83	114.39	123.22
37	Z	613	CHL	C2C-C3C-C4C	2.83	108.51	106.49
23	B	4007	BCR	C37-C22-C23	2.83	122.53	118.08
20	B	1224	CLA	CHD-C1D-ND	-2.83	121.86	124.45
20	6	607	CLA	C1-C2-C3	-2.83	121.15	126.04
20	1	615	CLA	C2C-C1C-NC	2.83	112.62	109.97
24	4	801	LHG	O8-C23-C24	2.83	120.78	111.91
34	J	4002	C7Z	C21-C26-C25	-2.83	118.63	122.61
20	7	608	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
20	B	1212	CLA	CMA-C3A-C4A	2.83	119.37	111.77
37	4	617	CHL	CHB-C4A-NA	2.82	128.42	124.51
23	B	4002	BCR	C27-C26-C25	-2.82	118.63	122.73
20	A	1114	CLA	CHD-C1D-ND	-2.82	121.86	124.45
20	B	1239	CLA	CMA-C3A-C4A	2.82	119.36	111.77
20	B	1238	CLA	C2C-C1C-NC	2.82	112.62	109.97
37	6	617	CHL	CHB-C4A-NA	2.82	128.42	124.51
20	A	1126	CLA	C2C-C1C-NC	2.82	112.62	109.97
20	4	609	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
36	7	501	LUT	C35-C15-C14	-2.82	117.70	123.47
37	6	611	CHL	C1-O2A-CGA	2.82	123.84	116.44
20	B	1241	CLA	C1-C2-C3	-2.82	121.17	126.04
20	B	1214	CLA	CMA-C3A-C4A	2.82	119.35	111.77
20	5	604	CLA	C2C-C1C-NC	2.82	112.61	109.97
26	A	5006	LMT	C1'-O5'-C5'	-2.82	108.16	113.69
20	A	1122	CLA	C2D-C1D-ND	2.82	112.18	110.10
20	B	1223	CLA	C3B-C4B-NB	-2.82	107.90	110.52
20	B	1229	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
20	4	603	CLA	C2D-C1D-ND	2.81	112.18	110.10
20	7	607	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
36	4	501	LUT	C7-C8-C9	-2.81	121.98	126.23
20	A	1012	CLA	C2C-C1C-NC	2.81	112.61	109.97
20	A	1139	CLA	C2D-C1D-ND	2.81	112.18	110.10
20	B	1218	CLA	C2C-C1C-NC	2.81	112.61	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1118	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
20	3	603	CLA	CHD-C1D-ND	-2.81	121.87	124.45
20	A	1104	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
20	K	1403	CLA	C2D-C1D-ND	2.81	112.17	110.10
23	6	503	BCR	C38-C26-C25	-2.81	121.38	124.53
20	B	1202	CLA	C1-C2-C3	-2.81	121.19	126.04
20	1	608	CLA	C1-C2-C3	-2.81	121.19	126.04
33	F	4001	RRX	C20-C19-C18	-2.81	118.53	126.42
20	A	1115	CLA	C2C-C1C-NC	2.81	112.60	109.97
36	3	502	LUT	C7-C8-C9	-2.81	122.00	126.23
36	8	502	LUT	C31-C30-C29	-2.81	123.31	127.31
20	1	606	CLA	C2C-C1C-NC	2.81	112.60	109.97
37	5	617	CHL	CMA-C3A-C4A	2.80	119.31	111.77
20	A	1120	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
20	B	1225	CLA	C4B-CHC-C1C	2.80	132.99	126.34
20	A	1138	CLA	C2C-C1C-NC	2.80	112.60	109.97
36	8	501	LUT	C10-C11-C12	-2.80	114.47	123.22
20	A	1112	CLA	CMA-C3A-C4A	2.80	119.31	111.77
23	G	4001	BCR	C36-C18-C17	-2.80	119.00	122.92
25	A	5004	NKP	OAB-PAC-OAA	2.80	118.35	107.64
20	A	1112	CLA	C2C-C1C-NC	2.80	112.60	109.97
20	K	1403	CLA	CMA-C3A-C4A	2.80	119.30	111.77
36	1	501	LUT	C38-C25-C24	-2.80	117.56	123.56
20	5	604	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
20	B	1231	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
20	A	1127	CLA	CMA-C3A-C4A	2.80	119.30	111.77
37	4	613	CHL	C3C-C4C-NC	-2.80	107.43	110.57
23	B	4003	BCR	C33-C5-C6	-2.80	121.39	124.53
20	7	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	Z	608	CLA	CMA-C3A-C4A	2.80	119.29	111.77
20	B	1228	CLA	C2C-C1C-NC	2.80	112.59	109.97
20	3	605	CLA	C2C-C1C-NC	2.80	112.59	109.97
20	B	1232	CLA	CHD-C1D-ND	-2.80	121.89	124.45
20	7	608	CLA	CHD-C1D-ND	-2.80	121.89	124.45
20	3	616	CLA	C4B-CHC-C1C	2.80	132.97	126.34
20	4	604	CLA	C1-C2-C3	-2.79	121.21	126.04
20	8	602	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
20	5	604	CLA	C4B-CHC-C1C	2.79	132.96	126.34
23	5	504	BCR	C19-C18-C17	2.79	123.23	118.94
20	7	608	CLA	C3B-C4B-NB	-2.79	107.92	110.52
20	1	607	CLA	CMA-C3A-C4A	2.79	119.28	111.77
20	L	1502	CLA	C1-C2-C3	-2.79	121.21	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1226	CLA	CHA-C4D-ND	2.79	138.34	132.50
20	A	1135	CLA	C2D-C1D-ND	2.79	112.16	110.10
20	A	1012	CLA	OBD-CAD-C3D	-2.79	121.80	128.52
20	A	1111	CLA	C2C-C1C-NC	2.79	112.59	109.97
20	A	1125	CLA	C2C-C1C-NC	2.79	112.59	109.97
20	L	1503	CLA	C2C-C1C-NC	2.79	112.59	109.97
20	4	605	CLA	C2D-C1D-ND	2.79	112.16	110.10
20	B	1218	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
23	7	503	BCR	C33-C5-C4	2.79	118.97	113.62
20	8	604	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
20	G	1602	CLA	C2D-C1D-ND	2.79	112.16	110.10
20	B	1241	CLA	CHD-C1D-ND	-2.79	121.89	124.45
20	7	616	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
20	5	601	CLA	C1-O2A-CGA	2.79	123.75	116.44
20	7	603	CLA	CBA-CAA-C2A	2.79	122.08	113.86
20	1	602	CLA	CAC-C3C-C4C	2.79	128.42	124.81
20	A	1120	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
20	A	1116	CLA	CMA-C3A-C4A	2.79	119.26	111.77
23	A	4002	BCR	C23-C24-C25	-2.78	119.38	127.20
20	A	1013	CLA	C1-O2A-CGA	2.78	123.75	116.44
23	5	504	BCR	C33-C5-C6	-2.78	121.40	124.53
20	1	604	CLA	C1-C2-C3	-2.78	121.23	126.04
20	5	601	CLA	C1-C2-C3	-2.78	121.23	126.04
20	3	602	CLA	C2D-C1D-ND	2.78	112.15	110.10
20	4	607	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
20	B	1207	CLA	C2D-C1D-ND	2.78	112.15	110.10
20	Z	612	CLA	C1-O2A-CGA	2.78	123.73	116.44
36	4	501	LUT	C38-C25-C24	-2.78	117.61	123.56
20	1	602	CLA	CHD-C1D-ND	-2.78	121.90	124.45
20	3	607	CLA	C1-O2A-CGA	2.78	123.73	116.44
20	4	605	CLA	CHD-C1D-ND	-2.78	121.90	124.45
19	A	1011	CL0	CMC-C2C-C1C	2.78	129.27	125.04
20	8	609	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
20	Z	603	CLA	C3B-C4B-NB	-2.78	107.94	110.52
20	B	1210	CLA	C1-C2-C3	-2.78	121.24	126.04
20	1	615	CLA	C2D-C1D-ND	2.78	112.15	110.10
20	Z	607	CLA	C2D-C1D-ND	2.78	112.15	110.10
20	B	1208	CLA	O2A-CGA-CBA	2.78	120.62	111.91
20	Z	606	CLA	C1-C2-C3	-2.78	121.24	126.04
20	5	622	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
20	5	622	CLA	CMA-C3A-C4A	2.77	119.23	111.77
20	A	1111	CLA	O2D-CGD-O1D	-2.77	118.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1107	CLA	C1-C2-C3	-2.77	121.25	126.04
20	B	1219	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
20	B	1227	CLA	C3B-C4B-NB	-2.77	107.94	110.52
20	3	603	CLA	C1-O2A-CGA	2.77	123.72	116.44
20	7	607	CLA	C2D-C1D-ND	2.77	112.15	110.10
34	J	4002	C7Z	C18-C5-C4	2.77	119.49	114.36
20	A	1114	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
20	A	1104	CLA	C2C-C1C-NC	2.77	112.57	109.97
20	B	1217	CLA	C2D-C1D-ND	2.77	112.15	110.10
20	A	1134	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	B	1205	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	B	1239	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
20	A	1104	CLA	C1-O2A-CGA	2.77	123.71	116.44
20	1	603	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
20	A	1101	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
20	A	1135	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
20	A	1137	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
20	1	608	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
20	B	1209	CLA	C1-C2-C3	-2.77	121.26	126.04
20	B	1217	CLA	C1-O2A-CGA	2.77	123.70	116.44
23	3	503	BCR	C38-C26-C25	-2.77	121.42	124.53
23	3	506	BCR	C4-C5-C6	-2.77	118.72	122.73
20	A	1136	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
20	L	1502	CLA	CHD-C1D-ND	-2.77	121.91	124.45
20	B	1223	CLA	OBD-CAD-C3D	-2.76	121.87	128.52
20	L	1503	CLA	CMA-C3A-C4A	2.76	119.20	111.77
20	A	1123	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
20	1	612	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
37	6	613	CHL	C1-O2A-CGA	2.76	123.69	116.44
20	6	601	CLA	C2C-C1C-NC	2.76	112.56	109.97
20	B	1209	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
20	8	603	CLA	C2C-C1C-NC	2.76	112.56	109.97
20	5	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
20	G	1601	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
20	B	1223	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
20	B	1207	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
20	G	1602	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
20	B	1215	CLA	CMA-C3A-C4A	2.76	119.19	111.77
20	A	1133	CLA	O2A-CGA-CBA	2.76	120.56	111.91
20	F	1301	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
37	4	611	CHL	C1-C2-C3	-2.76	122.29	126.75
20	6	618	CLA	C1D-ND-C4D	-2.76	104.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1107	CLA	C2C-C1C-NC	2.76	112.55	109.97
20	B	1224	CLA	C2D-C1D-ND	2.76	112.14	110.10
20	5	602	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
37	6	611	CHL	CHB-C4A-NA	2.76	128.32	124.51
20	K	1402	CLA	CHD-C1D-ND	-2.76	121.92	124.45
37	Z	609	CHL	C2C-C3C-C4C	2.76	108.45	106.49
20	B	1204	CLA	O2A-CGA-CBA	2.76	120.55	111.91
20	1	603	CLA	C2C-C1C-NC	2.76	112.55	109.97
20	A	1128	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
20	A	1138	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
20	8	603	CLA	C1D-ND-C4D	-2.75	104.38	106.33
20	A	1107	CLA	CMA-C3A-C4A	2.75	119.18	111.77
20	A	1137	CLA	C1-O2A-CGA	2.75	123.67	116.44
20	6	615	CLA	C2D-C1D-ND	2.75	112.13	110.10
20	K	1401	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
20	4	602	CLA	CHD-C1D-ND	-2.75	121.92	124.45
20	B	1225	CLA	C3B-C4B-NB	-2.75	107.96	110.52
20	6	605	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
20	A	1102	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	J	5001	LMG	O8-C28-C29	2.75	120.55	111.91
20	B	1237	CLA	CMA-C3A-C4A	2.75	119.17	111.77
20	7	601	CLA	O2A-CGA-CBA	2.75	120.54	111.91
20	8	608	CLA	C2D-C1D-ND	2.75	112.13	110.10
20	6	602	CLA	C2D-C1D-ND	2.75	112.13	110.10
20	5	612	CLA	C1-C2-C3	-2.75	121.28	126.04
20	B	1237	CLA	C2C-C1C-NC	2.75	112.55	109.97
20	4	607	CLA	C1-C2-C3	-2.75	121.29	126.04
31	B	5003	DGD	C2G-O2G-C1B	-2.75	111.02	117.79
20	1	615	CLA	C3B-C4B-NB	-2.75	107.96	110.52
20	A	1121	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
20	A	1108	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
20	5	609	CLA	C3B-C4B-NB	-2.75	107.97	110.52
20	B	1214	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	K	1402	CLA	C2C-C1C-NC	2.75	112.55	109.97
20	B	1217	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	B	1228	CLA	C2D-C1D-ND	2.75	112.13	110.10
20	4	604	CLA	C2D-C1D-ND	2.75	112.13	110.10
20	1	607	CLA	CHD-C1D-ND	-2.75	121.93	124.45
20	B	1023	CLA	C2D-C1D-ND	2.75	112.13	110.10
20	Z	601	CLA	O2A-CGA-CBA	2.74	120.52	111.91
20	5	606	CLA	C1-C2-C3	-2.74	122.31	126.75
20	3	604	CLA	C2C-C1C-NC	2.74	112.54	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	801	LHG	C5-O7-C7	-2.74	111.04	117.79
20	B	1215	CLA	C1-C2-C3	-2.74	121.30	126.04
20	Z	601	CLA	C2C-C1C-NC	2.74	112.54	109.97
20	3	610	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
20	3	618	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
20	7	601	CLA	C3B-C4B-NB	-2.74	107.97	110.52
20	A	1101	CLA	C1-C2-C3	-2.74	121.30	126.04
34	1	503	C7Z	C28-C27-C26	-2.74	119.51	127.20
36	Z	501	LUT	C10-C11-C12	-2.74	114.67	123.22
20	B	1211	CLA	CHD-C1D-ND	-2.74	121.94	124.45
20	3	605	CLA	C4B-CHC-C1C	2.74	132.83	126.34
20	8	607	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
20	5	613	CLA	C2D-C1D-ND	2.74	112.12	110.10
20	3	612	CLA	C2C-C1C-NC	2.74	112.54	109.97
20	B	1216	CLA	C1-C2-C3	-2.74	121.31	126.04
20	F	1301	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
20	B	1224	CLA	C1-O2A-CGA	2.74	123.63	116.44
36	3	502	LUT	C37-C21-C26	2.74	113.69	109.55
40	7	802	3PH	O31-C31-C32	2.74	120.50	111.91
24	A	5002	LHG	O8-C23-C24	2.74	120.49	111.91
20	A	1141	CLA	C2D-C1D-ND	2.74	112.12	110.10
20	3	605	CLA	C2D-C1D-ND	2.74	112.12	110.10
23	A	4003	BCR	C1-C6-C7	2.74	123.52	115.78
20	7	615	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
36	8	502	LUT	C31-C32-C33	-2.73	118.73	126.42
20	8	608	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
20	B	1201	CLA	C2D-C1D-ND	2.73	112.12	110.10
20	B	1207	CLA	C4B-CHC-C1C	2.73	132.82	126.34
20	8	615	CLA	CHD-C1D-ND	-2.73	121.94	124.45
23	3	505	BCR	C38-C26-C25	-2.73	121.46	124.53
37	6	617	CHL	C4A-NA-C1A	2.73	107.93	106.71
20	1	605	CLA	CMA-C3A-C4A	2.73	119.11	111.77
36	Z	501	LUT	C18-C5-C6	-2.73	121.46	124.53
20	A	1116	CLA	C1-C2-C3	-2.73	121.32	126.04
20	B	1212	CLA	C2C-C1C-NC	2.73	112.53	109.97
20	A	1123	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	A	4002	BCR	C19-C18-C17	2.73	123.13	118.94
20	7	604	CLA	C3B-C4B-NB	-2.73	107.98	110.52
20	B	1208	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
23	3	504	BCR	C36-C18-C17	-2.73	119.10	122.92
20	A	1141	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
20	5	602	CLA	CHD-C1D-ND	-2.73	121.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1126	CLA	C3B-C4B-NB	-2.73	107.98	110.52
20	B	1202	CLA	CAA-C2A-C1A	-2.73	103.04	111.97
23	3	506	BCR	C23-C22-C21	2.73	123.12	118.94
20	B	1205	CLA	C2D-C1D-ND	2.73	112.11	110.10
20	3	603	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
20	A	1129	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	I	4001	BCR	C38-C26-C27	2.72	118.85	113.62
20	Z	612	CLA	O2A-CGA-CBA	2.72	120.46	111.91
20	7	606	CLA	C1-C2-C3	-2.72	121.33	126.04
20	5	612	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
20	B	1222	CLA	C1-O2A-CGA	2.72	123.58	116.44
20	A	1133	CLA	C2C-C1C-NC	2.72	112.52	109.97
20	B	1213	CLA	C2C-C1C-NC	2.72	112.52	109.97
23	A	4001	BCR	C36-C18-C17	-2.72	119.11	122.92
20	B	1022	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
20	7	602	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
36	5	501	LUT	C18-C5-C6	-2.72	121.47	124.53
20	B	1224	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
20	1	613	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	L	4001	BCR	C36-C18-C17	-2.72	119.12	122.92
37	Z	609	CHL	CAA-C2A-C3A	-2.72	105.34	112.78
37	4	613	CHL	CHB-C4A-NA	2.72	128.27	124.51
20	B	1240	CLA	O2A-CGA-CBA	2.71	120.43	111.91
40	6	802	3PH	O31-C31-C32	2.71	120.43	111.91
20	A	1135	CLA	C4B-CHC-C1C	2.71	132.78	126.34
20	6	618	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
20	B	1231	CLA	C1-C2-C3	-2.71	121.35	126.04
20	7	603	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
20	B	1021	CLA	C2C-C1C-NC	2.71	112.51	109.97
23	4	503	BCR	C36-C18-C17	-2.71	119.13	122.92
20	Z	601	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
20	7	605	CLA	C1D-ND-C4D	-2.71	104.41	106.33
20	A	1134	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	A	1105	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
20	5	618	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
20	A	1103	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
20	B	1234	CLA	C1-C2-C3	-2.71	121.36	126.04
20	A	1129	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
20	K	1404	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
20	A	1119	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
20	7	616	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
20	8	606	CLA	C1C-C2C-C3C	-2.70	104.11	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	1901	CLA	CHD-C1D-ND	-2.70	121.97	124.45
20	B	1217	CLA	C3B-C4B-NB	-2.70	108.01	110.52
20	B	1234	CLA	C2D-C1D-ND	2.70	112.10	110.10
20	B	1228	CLA	CMA-C3A-C4A	2.70	119.04	111.77
20	3	604	CLA	C4B-CHC-C1C	2.70	132.75	126.34
20	Z	615	CLA	CMA-C3A-C4A	2.70	119.04	111.77
20	B	1214	CLA	C6-C5-C3	-2.70	106.37	113.45
20	6	608	CLA	C1-C2-C3	-2.70	121.37	126.04
20	B	1227	CLA	CMD-C2D-C3D	-2.70	121.40	127.61
20	6	619	CLA	O2A-CGA-CBA	2.70	120.38	111.91
20	4	602	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
20	3	612	CLA	C1-C2-C3	-2.70	121.37	126.04
20	B	1223	CLA	CHD-C1D-ND	-2.70	121.97	124.45
20	6	602	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
20	1	602	CLA	C2D-C1D-ND	2.70	112.09	110.10
20	B	1217	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
20	A	1101	CLA	C3B-C4B-NB	-2.70	108.01	110.52
20	4	603	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
20	A	1134	CLA	C1-O2A-CGA	2.70	123.52	116.44
20	B	1212	CLA	CHD-C1D-ND	-2.70	121.98	124.45
20	A	1130	CLA	CMA-C3A-C4A	2.70	119.02	111.77
37	6	610	CHL	C1-C2-C3	-2.69	121.39	126.04
20	A	1104	CLA	O2A-CGA-CBA	2.69	120.36	111.91
20	B	1232	CLA	C2D-C1D-ND	2.69	112.09	110.10
20	K	1401	CLA	CHD-C1D-ND	-2.69	121.98	124.45
34	5	505	C7Z	C28-C27-C26	-2.69	119.64	127.20
20	3	605	CLA	CHA-C4D-ND	2.69	138.13	132.50
20	B	1229	CLA	C4B-CHC-C1C	2.69	132.72	126.34
20	B	1206	CLA	CHD-C1D-ND	-2.69	121.98	124.45
37	5	610	CHL	C1-O2A-CGA	2.69	123.50	116.44
20	7	608	CLA	C2D-C1D-ND	2.69	112.09	110.10
20	8	609	CLA	C2D-C1D-ND	2.69	112.09	110.10
20	6	603	CLA	C3B-C4B-NB	-2.69	108.02	110.52
20	A	1101	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
20	5	613	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
20	A	1109	CLA	CMD-C2D-C3D	-2.69	121.43	127.61
20	5	609	CLA	O2A-CGA-CBA	2.69	120.35	111.91
20	A	1113	CLA	CMA-C3A-C4A	2.69	119.00	111.77
37	6	610	CHL	CMA-C3A-C4A	2.69	119.00	111.77
20	J	1901	CLA	C2D-C1D-ND	2.69	112.09	110.10
20	Z	608	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	A	1117	CLA	C1C-C2C-C3C	-2.69	104.13	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	605	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
20	A	1101	CLA	O2A-CGA-CBA	2.69	120.34	111.91
20	B	1208	CLA	CMA-C3A-C4A	2.69	118.99	111.77
20	3	602	CLA	C3B-C4B-NB	-2.69	108.02	110.52
23	L	4002	BCR	C35-C13-C12	2.69	122.31	118.08
37	6	613	CHL	C4B-CHC-C1C	2.68	132.71	126.34
20	8	605	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
33	F	4001	RRX	C16-C15-C14	-2.68	117.97	123.47
20	4	609	CLA	C2D-C1D-ND	2.68	112.08	110.10
23	K	4002	BCR	C35-C13-C12	2.68	122.31	118.08
20	1	607	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
20	5	607	CLA	CHD-C1D-ND	-2.68	121.99	124.45
37	5	611	CHL	CHB-C4A-NA	2.68	128.22	124.51
20	B	1231	CLA	C2D-C1D-ND	2.68	112.08	110.10
20	8	601	CLA	CHA-C4D-ND	2.68	138.11	132.50
37	6	617	CHL	C4B-CHC-C1C	2.68	132.70	126.34
20	4	606	CLA	C1D-ND-C4D	-2.68	104.43	106.33
20	Z	604	CLA	C1-C2-C3	-2.68	121.41	126.04
20	A	1112	CLA	C3B-C4B-NB	-2.68	108.03	110.52
20	A	1132	CLA	C3B-C4B-NB	-2.68	108.03	110.52
37	6	617	CHL	C3B-C4B-NB	-2.68	108.03	110.52
20	1	608	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
37	8	613	CHL	CHB-C4A-NA	2.68	128.22	124.51
37	5	617	CHL	C3B-C4B-NB	-2.68	108.03	110.52
20	4	615	CLA	C2D-C1D-ND	2.68	112.08	110.10
20	A	1113	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
20	5	613	CLA	C1-C2-C3	-2.68	121.42	126.04
20	7	611	CLA	C2C-C1C-NC	2.68	112.48	109.97
20	B	1229	CLA	C2C-C1C-NC	2.67	112.47	109.97
20	B	1235	CLA	C1D-ND-C4D	-2.67	104.44	106.33
20	6	601	CLA	O2A-CGA-CBA	2.67	120.28	111.91
20	B	1023	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
20	5	609	CLA	CHD-C1D-ND	-2.67	122.00	124.45
20	6	602	CLA	O2A-CGA-CBA	2.67	120.28	111.91
20	7	613	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	L	4002	BCR	C37-C22-C21	-2.67	119.19	122.92
20	4	605	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
36	Z	502	LUT	C11-C10-C9	-2.67	123.50	127.31
23	8	503	BCR	C38-C26-C27	2.67	118.74	113.62
20	L	1503	CLA	C2D-C1D-ND	2.67	112.07	110.10
20	1	604	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
20	B	1221	CLA	O2D-CGD-O1D	-2.67	118.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	615	CLA	C2D-C1D-ND	2.67	112.07	110.10
20	8	609	CLA	C1-C2-C3	-2.66	121.43	126.04
20	B	1240	CLA	C2C-C1C-NC	2.66	112.47	109.97
20	B	1202	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
20	A	1013	CLA	CHD-C1D-ND	-2.66	122.01	124.45
20	Z	607	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
20	B	1204	CLA	C2D-C1D-ND	2.66	112.07	110.10
20	A	1110	CLA	C2C-C1C-NC	2.66	112.47	109.97
20	Z	608	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
20	5	609	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
23	L	4001	BCR	C34-C9-C10	-2.66	119.19	122.92
37	8	610	CHL	CHB-C4A-NA	2.66	128.19	124.51
37	4	611	CHL	CHB-C4A-NA	2.66	128.19	124.51
20	6	609	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
20	1	607	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
20	6	606	CLA	C1-C2-C3	-2.66	121.45	126.04
20	B	1207	CLA	C1-C2-C3	-2.66	121.45	126.04
20	8	606	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
20	7	605	CLA	O2A-CGA-CBA	2.66	120.24	111.91
20	4	602	CLA	C2D-C1D-ND	2.66	112.06	110.10
37	7	610	CHL	C1-O2A-CGA	2.66	123.41	116.44
37	Z	609	CHL	CHB-C4A-NA	2.65	128.18	124.51
20	5	605	CLA	CHA-C4D-ND	2.65	138.05	132.50
42	8	803	LPX	O3-P1-O4	2.65	125.36	112.24
20	8	608	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
20	B	1231	CLA	C1-O2A-CGA	2.65	123.41	116.44
37	1	609	CHL	C1-O2A-CGA	2.65	123.41	116.44
20	B	1216	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
20	3	610	CLA	C3B-C4B-NB	-2.65	108.05	110.52
20	A	1137	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
20	5	606	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
36	8	501	LUT	C2-C3-C4	-2.65	106.67	110.30
20	B	1235	CLA	C2C-C1C-NC	2.65	112.46	109.97
20	3	612	CLA	C2D-C1D-ND	2.65	112.06	110.10
20	A	1104	CLA	C1-C2-C3	-2.65	121.46	126.04
20	A	1107	CLA	O2A-CGA-CBA	2.65	120.22	111.91
20	B	1230	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	5	606	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	3	602	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
20	A	1103	CLA	C1D-ND-C4D	-2.65	104.45	106.33
20	B	1236	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
37	8	610	CHL	C3C-C4C-NC	-2.65	107.60	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	607	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
20	B	1206	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
20	A	1125	CLA	OBD-CAD-C3D	-2.65	122.15	128.52
23	A	4003	BCR	C30-C25-C26	-2.65	118.89	122.61
20	6	608	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
20	8	603	CLA	C3B-C4B-NB	-2.65	108.06	110.52
20	A	1134	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
20	3	607	CLA	C1-C2-C3	-2.64	121.47	126.04
20	8	609	CLA	C4B-CHC-C1C	2.64	132.61	126.34
23	G	4001	BCR	C34-C9-C10	-2.64	119.22	122.92
20	B	1214	CLA	C2D-C1D-ND	2.64	112.05	110.10
20	B	1240	CLA	CMA-C3A-C4A	2.64	118.87	111.77
20	1	605	CLA	CHA-C4D-ND	2.64	138.03	132.50
36	1	501	LUT	C10-C11-C12	-2.64	114.97	123.22
20	B	1227	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
20	A	1125	CLA	CMA-C3A-C4A	2.64	118.87	111.77
20	B	1202	CLA	O2A-CGA-CBA	2.64	120.19	111.91
20	Z	606	CLA	CHA-C4D-ND	2.64	138.02	132.50
20	A	1137	CLA	C1-C2-C3	-2.64	121.48	126.04
37	Z	610	CHL	C4B-CHC-C1C	2.64	132.60	126.34
20	4	605	CLA	CHA-C4D-ND	2.64	138.02	132.50
37	4	617	CHL	CMA-C3A-C4A	2.64	118.86	111.77
20	K	1401	CLA	C2D-C1D-ND	2.64	112.05	110.10
20	8	606	CLA	C2D-C1D-ND	2.64	112.05	110.10
20	6	619	CLA	C2D-C1D-ND	2.64	112.05	110.10
20	B	1213	CLA	O2A-CGA-CBA	2.64	120.19	111.91
20	B	1231	CLA	CHA-C4D-ND	2.64	138.01	132.50
37	Z	610	CHL	C4A-NA-C1A	2.64	107.89	106.71
20	B	1202	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
20	B	1229	CLA	C1D-ND-C4D	-2.64	104.46	106.33
20	B	1232	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
20	4	609	CLA	C3B-C4B-NB	-2.63	108.07	110.52
20	B	1211	CLA	O2A-CGA-CBA	2.63	120.17	111.91
37	8	613	CHL	C3C-C4C-NC	-2.63	107.62	110.57
20	G	1602	CLA	C3B-C4B-NB	-2.63	108.07	110.52
20	4	608	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
20	4	607	CLA	CMA-C3A-C4A	2.63	118.85	111.77
20	A	1114	CLA	CHA-C4D-ND	2.63	138.00	132.50
20	B	1021	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
20	1	608	CLA	C2D-C1D-ND	2.63	112.04	110.10
20	4	601	CLA	C2D-C1D-ND	2.63	112.04	110.10
20	A	1116	CLA	CHA-C4D-ND	2.63	138.00	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	1301	CLA	C4B-CHC-C1C	2.63	132.58	126.34
23	4	503	BCR	C1-C6-C5	-2.63	118.91	122.61
20	6	618	CLA	CMA-C3A-C4A	2.63	118.84	111.77
20	B	1238	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
23	3	506	BCR	C33-C5-C4	2.63	118.67	113.62
20	7	604	CLA	CMA-C3A-C4A	2.63	118.84	111.77
37	5	617	CHL	C3C-C4C-NC	-2.63	107.62	110.57
20	1	615	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
20	A	1119	CLA	C3B-C4B-NB	-2.63	108.08	110.52
20	1	605	CLA	CMD-C2D-C3D	-2.63	121.57	127.61
20	A	1126	CLA	CHA-C4D-ND	2.63	137.99	132.50
37	6	617	CHL	C2B-C1B-NB	-2.63	108.47	110.23
37	Z	610	CHL	CMA-C3A-C4A	2.63	118.83	111.77
37	1	609	CHL	CHB-C4A-NA	2.62	128.14	124.51
20	7	609	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
20	8	611	CLA	CMA-C3A-C4A	2.62	118.82	111.77
20	A	1136	CLA	C1-C2-C3	-2.62	121.51	126.04
20	A	1136	CLA	C2D-C1D-ND	2.62	112.04	110.10
20	A	1133	CLA	C1-O2A-CGA	2.62	123.32	116.44
20	B	1219	CLA	CHA-C4D-ND	2.62	137.98	132.50
24	6	801	LHG	O8-C23-C24	2.62	120.14	111.91
20	6	603	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
20	B	1238	CLA	C2D-C1D-ND	2.62	112.04	110.10
23	4	503	BCR	C33-C5-C6	-2.62	121.58	124.53
20	B	1238	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
20	5	605	CLA	C1-O2A-CGA	2.62	123.31	116.44
24	5	801	LHG	O8-C23-C24	2.62	120.13	111.91
24	A	5001	LHG	O8-C23-C24	2.62	120.12	111.91
37	4	613	CHL	C4B-CHC-C1C	2.62	132.55	126.34
20	6	605	CLA	CHD-C1D-ND	-2.62	122.05	124.45
36	7	502	LUT	C2-C3-C4	-2.62	106.72	110.30
20	A	1101	CLA	C1-O2A-CGA	2.62	123.31	116.44
23	B	4001	BCR	C23-C24-C25	-2.62	119.86	127.20
20	B	1240	CLA	CHA-C4D-ND	2.62	137.97	132.50
20	F	1302	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
20	6	604	CLA	CMA-C3A-C4A	2.61	118.80	111.77
37	1	610	CHL	C3C-C4C-NC	-2.61	107.64	110.57
20	B	1236	CLA	C4B-CHC-C1C	2.61	132.54	126.34
20	J	1901	CLA	CMA-C3A-C4A	2.61	118.80	111.77
20	7	603	CLA	C3B-C4B-NB	-2.61	108.09	110.52
20	G	1602	CLA	CHA-C4D-ND	2.61	137.96	132.50
20	4	604	CLA	C1C-C2C-C3C	-2.61	104.21	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	608	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
20	5	615	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
23	B	4001	BCR	C36-C18-C17	-2.61	119.27	122.92
34	J	4002	C7Z	C2-C3-C4	2.61	113.88	110.30
20	4	606	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
20	1	601	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
20	5	605	CLA	CMD-C2D-C3D	-2.61	121.61	127.61
20	1	613	CLA	CHA-C4D-ND	2.61	137.96	132.50
20	8	615	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
20	6	608	CLA	CHA-C4D-ND	2.61	137.96	132.50
20	Z	607	CLA	C3B-C4B-NB	-2.61	108.10	110.52
23	3	506	BCR	C38-C26-C25	-2.61	121.60	124.53
20	B	1219	CLA	CMA-C3A-C4A	2.61	118.78	111.77
20	A	1106	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
20	B	1216	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
20	A	1115	CLA	CMA-C3A-C4A	2.61	118.78	111.77
20	1	611	CLA	C2D-C1D-ND	2.61	112.03	110.10
20	3	613	CLA	CHA-C4D-ND	2.61	137.95	132.50
20	Z	608	CLA	C1-C2-C3	-2.61	121.54	126.04
36	7	501	LUT	C37-C21-C22	-2.60	104.50	109.44
23	A	4005	BCR	C34-C9-C10	-2.60	119.27	122.92
20	1	612	CLA	CMA-C3A-C4A	2.60	118.77	111.77
20	3	606	CLA	C1-C2-C3	-2.60	121.54	126.04
23	3	506	BCR	C34-C9-C10	-2.60	119.28	122.92
37	4	613	CHL	C4A-NA-C1A	2.60	107.88	106.71
20	F	1301	CLA	CHA-C4D-ND	2.60	137.94	132.50
20	J	1901	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
20	7	613	CLA	CMA-C3A-C4A	2.60	118.77	111.77
20	5	615	CLA	CHA-C4D-ND	2.60	137.94	132.50
20	5	607	CLA	CHA-C4D-ND	2.60	137.94	132.50
20	B	1240	CLA	C2D-C1D-ND	2.60	112.02	110.10
20	B	1214	CLA	CHA-C4D-ND	2.60	137.94	132.50
20	7	602	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	B	4005	BCR	C12-C13-C14	-2.60	114.95	118.94
20	Z	603	CLA	C2C-C1C-NC	2.60	112.41	109.97
20	A	1129	CLA	CHA-C4D-ND	2.60	137.94	132.50
20	1	601	CLA	C3B-C4B-NB	-2.60	108.10	110.52
20	A	1131	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
20	8	605	CLA	C2D-C1D-ND	2.60	112.02	110.10
20	5	608	CLA	C2D-C1D-ND	2.60	112.02	110.10
20	A	1107	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
20	B	1211	CLA	CHA-C4D-ND	2.60	137.93	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	610	CLA	C4B-CHC-C1C	2.60	132.50	126.34
23	B	4004	BCR	C23-C24-C25	-2.60	119.91	127.20
20	A	1109	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
20	Z	608	CLA	CHA-C4D-ND	2.60	137.93	132.50
20	3	612	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
37	3	611	CHL	C4B-CHC-C1C	2.60	132.49	126.34
23	B	4002	BCR	C36-C18-C17	-2.59	119.29	122.92
20	5	615	CLA	C3B-C4B-NB	-2.59	108.11	110.52
20	8	612	CLA	C2D-C1D-ND	2.59	112.02	110.10
20	6	606	CLA	CHA-C4D-ND	2.59	137.93	132.50
37	5	610	CHL	C2B-C1B-NB	-2.59	108.49	110.23
20	A	1106	CLA	C3B-C4B-NB	-2.59	108.11	110.52
20	A	1013	CLA	CMB-C2B-C1B	-2.59	121.42	125.37
20	B	1021	CLA	C1-O2A-CGA	2.59	123.24	116.44
20	1	603	CLA	C1-O2A-CGA	2.59	123.24	116.44
36	5	502	LUT	C11-C10-C9	-2.59	123.61	127.31
20	7	603	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
20	A	1119	CLA	C2D-C1D-ND	2.59	112.01	110.10
20	Z	602	CLA	C2D-C1D-ND	2.59	112.01	110.10
37	6	610	CHL	CHB-C4A-NA	2.59	128.09	124.51
24	Z	801	LHG	O8-C23-C24	2.59	120.03	111.91
20	6	619	CLA	CHA-C4D-ND	2.59	137.91	132.50
20	Z	606	CLA	C3B-C4B-NB	-2.59	108.11	110.52
20	B	1223	CLA	C4B-CHC-C1C	2.59	132.47	126.34
20	B	1227	CLA	CMA-C3A-C4A	2.59	118.72	111.77
20	B	1235	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
20	3	607	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
37	4	610	CHL	CHD-C4C-C3C	2.59	128.64	124.84
23	A	4004	BCR	C38-C26-C27	2.59	118.58	113.62
20	A	1106	CLA	C2D-C1D-ND	2.59	112.01	110.10
20	L	1502	CLA	C1D-ND-C4D	-2.58	104.50	106.33
20	Z	604	CLA	C2C-C1C-NC	2.58	112.39	109.97
20	5	612	CLA	C2C-C1C-NC	2.58	112.39	109.97
20	7	608	CLA	C4B-CHC-C1C	2.58	132.47	126.34
20	5	602	CLA	CHA-C4D-ND	2.58	137.90	132.50
20	L	1502	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
20	B	1231	CLA	CMD-C2D-C3D	-2.58	121.67	127.61
20	A	1139	CLA	C3B-C4B-NB	-2.58	108.12	110.52
20	B	1232	CLA	C3B-C4B-NB	-2.58	108.12	110.52
20	B	1235	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
20	6	601	CLA	CHA-C4D-ND	2.58	137.90	132.50
20	A	1118	CLA	C3B-C4B-NB	-2.58	108.12	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	609	CLA	C3B-C4B-NB	-2.58	108.12	110.52
20	5	615	CLA	C4B-CHC-C1C	2.58	132.46	126.34
20	A	1135	CLA	CMA-C3A-C4A	2.58	118.71	111.77
20	5	608	CLA	CHA-C4D-ND	2.58	137.90	132.50
20	4	607	CLA	O2A-CGA-CBA	2.58	120.01	111.91
23	K	4002	BCR	C33-C5-C6	-2.58	121.63	124.53
37	6	613	CHL	CHB-C4A-NA	2.58	128.08	124.51
34	5	505	C7Z	C35-C34-C33	-2.58	123.63	127.31
37	4	611	CHL	C4B-CHC-C1C	2.58	132.46	126.34
20	B	1211	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
20	4	612	CLA	C2D-C1D-ND	2.58	112.00	110.10
20	8	605	CLA	CHA-C4D-ND	2.58	137.90	132.50
23	B	4003	BCR	C4-C5-C6	-2.58	118.99	122.73
20	4	605	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
20	A	1121	CLA	CHA-C4D-ND	2.58	137.89	132.50
20	Z	615	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
20	7	611	CLA	CMA-C3A-C4A	2.58	118.70	111.77
20	5	618	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
20	3	601	CLA	CMA-C3A-C4A	2.58	118.70	111.77
20	6	609	CLA	C2D-C1D-ND	2.58	112.00	110.10
20	Z	611	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
20	A	1102	CLA	C1D-ND-C4D	-2.58	104.50	106.33
20	K	1401	CLA	C4B-CHC-C1C	2.58	132.45	126.34
20	5	615	CLA	C2D-C1D-ND	2.58	112.00	110.10
20	B	1021	CLA	CHD-C1D-ND	-2.58	122.09	124.45
20	Z	601	CLA	C4B-CHC-C1C	2.58	132.45	126.34
20	8	609	CLA	C3B-C4B-NB	-2.58	108.12	110.52
20	8	603	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
37	7	610	CHL	CHB-C4A-NA	2.58	128.07	124.51
20	B	1204	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
36	7	501	LUT	C38-C25-C24	-2.57	118.05	123.56
20	6	606	CLA	C2D-C1D-ND	2.57	112.00	110.10
37	4	611	CHL	C1-O2A-CGA	2.57	123.20	116.44
20	5	609	CLA	CMA-C3A-C4A	2.57	118.69	111.77
20	8	609	CLA	CHA-C4D-ND	2.57	137.88	132.50
20	A	1118	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
20	A	1120	CLA	C1D-ND-C4D	-2.57	104.51	106.33
20	6	612	CLA	C1D-ND-C4D	-2.57	104.51	106.33
20	B	1204	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
20	8	605	CLA	C1-C2-C3	-2.57	121.60	126.04
20	A	1140	CLA	C4B-CHC-C1C	2.57	132.43	126.34
20	A	1128	CLA	C1-C2-C3	-2.57	121.60	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1202	CLA	C2D-C1D-ND	2.57	112.00	110.10
20	B	1215	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
20	5	608	CLA	CMD-C2D-C3D	-2.57	121.71	127.61
20	B	1217	CLA	CMA-C3A-C4A	2.57	118.67	111.77
20	K	1401	CLA	CMA-C3A-C4A	2.57	118.67	111.77
20	7	601	CLA	C1-O2A-CGA	2.57	123.18	116.44
23	3	503	BCR	C36-C18-C17	-2.57	119.33	122.92
20	Z	607	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
20	B	1210	CLA	C2D-C1D-ND	2.56	111.99	110.10
20	5	609	CLA	C2D-C1D-ND	2.56	111.99	110.10
20	B	1209	CLA	O2A-CGA-CBA	2.56	119.96	111.91
24	B	5001	LHG	C5-O7-C7	-2.56	111.48	117.79
20	B	1211	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
23	B	4007	BCR	C34-C9-C10	-2.56	119.33	122.92
20	A	1130	CLA	C3B-C4B-NB	-2.56	108.14	110.52
20	7	616	CLA	C3B-C4B-NB	-2.56	108.14	110.52
20	A	1106	CLA	CHA-C4D-ND	2.56	137.86	132.50
20	4	607	CLA	CHA-C4D-ND	2.56	137.86	132.50
36	3	501	LUT	C38-C25-C24	-2.56	118.08	123.56
20	A	1125	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
20	B	1240	CLA	CHA-C1A-NA	-2.56	120.53	126.40
20	7	601	CLA	CMA-C3A-C4A	2.56	118.66	111.77
20	3	603	CLA	C3B-C4B-NB	-2.56	108.14	110.52
20	5	608	CLA	CMA-C3A-C4A	2.56	118.66	111.77
20	A	1101	CLA	C4B-CHC-C1C	2.56	132.41	126.34
20	A	1111	CLA	CHA-C4D-ND	2.56	137.85	132.50
20	8	602	CLA	CHA-C4D-ND	2.56	137.85	132.50
20	A	1121	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
23	A	4004	BCR	C19-C18-C17	2.56	122.87	118.94
20	5	601	CLA	C2C-C1C-NC	2.56	112.37	109.97
20	B	1221	CLA	CHA-C4D-ND	2.56	137.85	132.50
20	1	606	CLA	CHA-C4D-ND	2.56	137.85	132.50
37	6	610	CHL	C4D-CHA-C1A	2.56	124.36	121.25
20	A	1119	CLA	CHA-C4D-ND	2.56	137.85	132.50
20	7	602	CLA	CHA-C4D-ND	2.56	137.85	132.50
36	4	502	LUT	C15-C14-C13	-2.56	123.66	127.31
20	B	1223	CLA	CHA-C4D-ND	2.56	137.85	132.50
20	7	615	CLA	CHA-C4D-ND	2.56	137.84	132.50
37	5	610	CHL	C4B-CHC-C1C	2.56	132.40	126.34
20	3	607	CLA	C2D-C1D-ND	2.56	111.99	110.10
20	B	1205	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
20	3	618	CLA	CMA-C3A-C4A	2.55	118.64	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	604	CLA	C1D-ND-C4D	-2.55	104.52	106.33
20	B	1204	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
37	5	617	CHL	CHB-C4A-NA	2.55	128.04	124.51
20	B	1220	CLA	CHD-C1D-ND	-2.55	122.11	124.45
20	B	1203	CLA	C1-C2-C3	-2.55	121.63	126.04
20	7	611	CLA	C1D-ND-C4D	-2.55	104.52	106.33
20	B	1221	CLA	CHA-C1A-NA	-2.55	120.55	126.40
36	1	501	LUT	C35-C15-C14	-2.55	118.25	123.47
20	1	603	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
20	B	1216	CLA	CHA-C4D-ND	2.55	137.84	132.50
20	A	1116	CLA	CHA-C1A-NA	-2.55	120.56	126.40
23	B	4006	BCR	C12-C13-C14	-2.55	115.03	118.94
20	7	606	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
20	7	601	CLA	CHA-C4D-ND	2.55	137.83	132.50
20	B	1205	CLA	O2A-CGA-CBA	2.55	119.91	111.91
20	B	1229	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
20	8	601	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
23	8	503	BCR	C27-C26-C25	-2.55	119.03	122.73
20	B	1231	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
20	B	1234	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
20	B	1220	CLA	C3B-C4B-NB	-2.55	108.15	110.52
20	1	605	CLA	C3B-C4B-NB	-2.55	108.15	110.52
20	4	608	CLA	C2D-C1D-ND	2.55	111.98	110.10
20	5	604	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	L	4002	BCR	C29-C28-C27	2.55	117.07	111.38
23	5	503	BCR	C4-C5-C6	-2.55	119.03	122.73
20	A	1123	CLA	C2D-C1D-ND	2.55	111.98	110.10
20	3	601	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
20	B	1022	CLA	CHA-C4D-ND	2.55	137.82	132.50
24	7	801	LHG	O8-C23-C24	2.55	119.90	111.91
20	7	616	CLA	C1D-ND-C4D	-2.55	104.53	106.33
20	A	1105	CLA	C3B-C4B-NB	-2.54	108.15	110.52
20	B	1226	CLA	C1-C2-C3	-2.54	121.64	126.04
36	1	502	LUT	C18-C5-C6	-2.54	121.67	124.53
20	J	1901	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
20	Z	607	CLA	CHA-C4D-ND	2.54	137.82	132.50
20	B	1212	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
20	A	1141	CLA	C1-O2A-CGA	2.54	123.12	116.44
20	5	622	CLA	CHA-C4D-ND	2.54	137.82	132.50
20	B	1230	CLA	CHD-C1D-ND	-2.54	122.12	124.45
20	A	1131	CLA	C2D-C1D-ND	2.54	111.98	110.10
20	1	604	CLA	C2D-C1D-ND	2.54	111.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	605	CLA	C2D-C1D-ND	2.54	111.98	110.10
20	7	607	CLA	C1-C2-C3	-2.54	121.64	126.04
34	1	503	C7Z	C18-C5-C4	2.54	119.07	114.36
20	B	1234	CLA	CHD-C1D-ND	-2.54	122.12	124.45
20	6	608	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
20	B	1230	CLA	C1D-ND-C4D	-2.54	104.53	106.33
20	6	605	CLA	CHA-C4D-ND	2.54	137.81	132.50
20	1	606	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
24	1	801	LHG	O8-C23-C24	2.54	119.88	111.91
20	A	1111	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
20	6	604	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
20	B	1241	CLA	C2D-C1D-ND	2.54	111.97	110.10
20	B	1203	CLA	CHA-C4D-ND	2.54	137.81	132.50
20	B	1235	CLA	C3B-C4B-NB	-2.54	108.16	110.52
20	7	604	CLA	C2C-C1C-NC	2.54	112.35	109.97
20	F	1301	CLA	O2A-CGA-CBA	2.54	119.87	111.91
30	A	5005	DGA	OG1-CA1-CA2	2.54	119.87	111.91
20	A	1129	CLA	C2D-C1D-ND	2.54	111.97	110.10
20	5	607	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
20	7	605	CLA	CHA-C4D-ND	2.54	137.81	132.50
23	3	505	BCR	C36-C18-C17	-2.54	119.37	122.92
20	5	618	CLA	CAA-CBA-CGA	-2.54	105.84	113.25
20	B	1219	CLA	O2A-CGA-CBA	2.54	119.86	111.91
20	A	1012	CLA	CHA-C4D-ND	2.54	137.80	132.50
20	7	613	CLA	CHA-C4D-ND	2.54	137.80	132.50
20	4	609	CLA	C4B-CHC-C1C	2.54	132.35	126.34
20	K	1401	CLA	CHA-C4D-ND	2.54	137.80	132.50
20	6	602	CLA	CHD-C1D-ND	-2.53	122.12	124.45
20	6	603	CLA	C4B-CHC-C1C	2.53	132.35	126.34
20	5	602	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
20	A	1107	CLA	C1D-ND-C4D	-2.53	104.54	106.33
20	F	1302	CLA	CHD-C1D-ND	-2.53	122.13	124.45
20	B	1214	CLA	C1-O2A-CGA	2.53	123.09	116.44
23	5	504	BCR	C28-C27-C26	-2.53	109.56	114.08
36	4	501	LUT	C10-C11-C12	-2.53	115.32	123.22
20	B	1209	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
20	7	601	CLA	C1D-ND-C4D	-2.53	104.54	106.33
20	A	1116	CLA	C2D-C1D-ND	2.53	111.97	110.10
23	B	4001	BCR	C34-C9-C10	-2.53	119.38	122.92
20	A	1125	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
20	6	615	CLA	CHA-C4D-ND	2.53	137.79	132.50
20	A	1103	CLA	C2C-C1C-NC	2.53	112.34	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	616	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
36	7	501	LUT	C15-C14-C13	-2.53	123.70	127.31
20	A	1133	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
20	K	1402	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
20	Z	606	CLA	C4B-CHC-C1C	2.53	132.34	126.34
20	A	1131	CLA	CHA-C4D-ND	2.53	137.79	132.50
20	1	606	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	B	1225	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
20	4	612	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	4	609	CLA	CHA-C4D-ND	2.53	137.79	132.50
20	Z	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
20	B	1022	CLA	CHA-C1A-NA	-2.53	120.61	126.40
20	6	606	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
20	A	1125	CLA	CHA-C4D-ND	2.53	137.78	132.50
20	3	608	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
20	B	1231	CLA	C3B-C4B-NB	-2.53	108.17	110.52
20	6	609	CLA	O2A-CGA-CBA	2.53	119.83	111.91
20	A	1101	CLA	C2D-C1D-ND	2.53	111.97	110.10
20	1	607	CLA	C2D-C1D-ND	2.53	111.97	110.10
20	3	603	CLA	CHA-C4D-ND	2.52	137.78	132.50
20	8	604	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
20	1	602	CLA	CHA-C4D-ND	2.52	137.78	132.50
20	7	616	CLA	CMA-C3A-C4A	2.52	118.56	111.77
20	B	1204	CLA	C1-C2-C3	-2.52	121.68	126.04
20	5	605	CLA	O2A-CGA-CBA	2.52	119.83	111.91
20	6	602	CLA	CHA-C4D-ND	2.52	137.78	132.50
36	8	502	LUT	C35-C15-C14	-2.52	118.31	123.47
20	B	1238	CLA	C3B-C4B-NB	-2.52	108.17	110.52
20	A	1110	CLA	C4B-CHC-C1C	2.52	132.32	126.34
20	A	1124	CLA	CMA-C3A-C4A	2.52	118.55	111.77
20	B	1222	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
20	A	1135	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
20	5	615	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
20	A	1140	CLA	C2D-C1D-ND	2.52	111.96	110.10
20	A	1110	CLA	C1D-ND-C4D	-2.52	104.54	106.33
20	6	615	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
20	L	1503	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
20	Z	611	CLA	C2D-C1D-ND	2.52	111.96	110.10
23	6	504	BCR	C38-C26-C25	-2.52	121.70	124.53
33	F	4001	RRX	C34-C9-C10	-2.52	119.39	122.92
20	4	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
20	7	607	CLA	CHA-C4D-ND	2.52	137.77	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1135	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
20	B	1232	CLA	CHA-C4D-ND	2.52	137.77	132.50
23	B	4001	BCR	C35-C13-C12	2.52	122.04	118.08
24	4	802	LHG	O8-C23-C24	2.52	119.81	111.91
20	B	1220	CLA	CMA-C3A-C4A	2.52	118.54	111.77
20	B	1218	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
20	G	1602	CLA	CMD-C2D-C3D	-2.52	121.83	127.61
20	6	607	CLA	CHA-C4D-ND	2.52	137.76	132.50
20	1	615	CLA	CHA-C4D-ND	2.51	137.76	132.50
20	A	1125	CLA	C3D-C2D-C1D	-2.51	102.40	105.83
20	3	612	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
37	4	617	CHL	C4D-CHA-C1A	2.51	124.31	121.25
20	B	1237	CLA	CHA-C4D-ND	2.51	137.76	132.50
20	B	1239	CLA	CHA-C4D-ND	2.51	137.76	132.50
20	3	602	CLA	CHA-C4D-ND	2.51	137.76	132.50
20	6	618	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
20	B	1220	CLA	O2A-CGA-CBA	2.51	119.80	111.91
20	B	1218	CLA	CHA-C4D-ND	2.51	137.76	132.50
20	B	1232	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
20	A	1126	CLA	O2A-CGA-CBA	2.51	119.79	111.91
20	7	604	CLA	C1-O2A-CGA	2.51	123.03	116.44
20	G	1601	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
20	5	613	CLA	CHA-C4D-ND	2.51	137.75	132.50
23	B	4003	BCR	C34-C9-C10	-2.51	119.41	122.92
20	B	1219	CLA	C2D-C1D-ND	2.51	111.95	110.10
20	4	608	CLA	CHA-C4D-ND	2.51	137.75	132.50
36	Z	501	LUT	C15-C14-C13	-2.51	123.73	127.31
23	B	4006	BCR	C28-C27-C26	-2.51	109.60	114.08
20	7	608	CLA	CHA-C4D-ND	2.51	137.75	132.50
37	4	617	CHL	C3C-C4C-NC	-2.51	107.76	110.57
20	K	1403	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
20	1	607	CLA	CHA-C4D-ND	2.51	137.74	132.50
20	B	1222	CLA	C4B-CHC-C1C	2.51	132.28	126.34
20	8	602	CLA	C1D-ND-C4D	-2.51	104.56	106.33
20	6	618	CLA	CAA-C2A-C3A	-2.51	105.92	112.78
20	4	612	CLA	CHA-C4D-ND	2.51	137.74	132.50
20	4	601	CLA	CMD-C2D-C3D	-2.51	121.85	127.61
23	B	4003	BCR	C35-C13-C12	2.51	122.02	118.08
23	4	503	BCR	C38-C26-C25	-2.51	121.72	124.53
20	B	1202	CLA	CHA-C4D-ND	2.50	137.74	132.50
20	6	608	CLA	CMD-C2D-C3D	-2.50	121.85	127.61
20	1	613	CLA	C1C-C2C-C3C	-2.50	104.32	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1213	CLA	CHA-C4D-ND	2.50	137.74	132.50
36	7	502	LUT	C38-C25-C24	-2.50	118.20	123.56
26	4	803	LMT	C3'-C4'-C5'	-2.50	105.19	110.93
20	A	1118	CLA	CMA-C3A-C4A	2.50	118.50	111.77
20	1	611	CLA	CMA-C3A-C4A	2.50	118.50	111.77
20	3	610	CLA	C2D-C1D-ND	2.50	111.95	110.10
20	A	1124	CLA	C4B-CHC-C1C	2.50	132.28	126.34
20	K	1404	CLA	CHA-C4D-ND	2.50	137.74	132.50
20	3	606	CLA	C1-O2A-CGA	2.50	123.01	116.44
20	A	1119	CLA	C2C-C1C-NC	2.50	112.32	109.97
20	7	606	CLA	CHA-C4D-ND	2.50	137.73	132.50
20	6	609	CLA	C3B-C4B-NB	-2.50	108.19	110.52
20	5	607	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
20	B	1212	CLA	CHA-C4D-ND	2.50	137.73	132.50
20	4	602	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
20	B	1208	CLA	C1D-ND-C4D	-2.50	104.56	106.33
20	7	605	CLA	C2C-C1C-NC	2.50	112.31	109.97
20	B	1224	CLA	C1-C2-C3	-2.50	121.72	126.04
20	8	607	CLA	O2A-CGA-CBA	2.50	119.75	111.91
20	A	1121	CLA	C3B-C4B-NB	-2.50	108.20	110.52
20	A	1135	CLA	CHA-C4D-ND	2.50	137.72	132.50
20	A	1130	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
36	3	501	LUT	C35-C15-C14	-2.50	118.36	123.47
34	1	503	C7Z	C10-C11-C12	-2.50	115.42	123.22
20	B	1217	CLA	C4B-CHC-C1C	2.50	132.26	126.34
20	A	1132	CLA	O2A-CGA-CBA	2.50	119.74	111.91
23	B	4001	BCR	C12-C13-C14	-2.50	115.11	118.94
20	Z	612	CLA	CHA-C4D-ND	2.50	137.72	132.50
20	8	601	CLA	O2A-CGA-CBA	2.50	119.74	111.91
20	5	612	CLA	C2D-C1D-ND	2.50	111.94	110.10
26	B	5005	LMT	O1'-C1'-C2'	2.50	112.20	108.30
20	Z	606	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
20	6	601	CLA	C1-O2A-CGA	2.49	122.99	116.44
20	B	1220	CLA	C2C-C1C-NC	2.49	112.31	109.97
20	A	1118	CLA	C1-C2-C3	-2.49	121.73	126.04
20	7	606	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
20	1	606	CLA	C3B-C4B-NB	-2.49	108.20	110.52
20	6	602	CLA	CMA-C3A-C4A	2.49	118.48	111.77
20	A	1124	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
20	B	1240	CLA	C4B-CHC-C1C	2.49	132.25	126.34
20	7	615	CLA	C3B-C4B-NB	-2.49	108.20	110.52
20	B	1022	CLA	C6-C5-C3	-2.49	106.92	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1139	CLA	C1-O2A-CGA	2.49	122.98	116.44
20	A	1117	CLA	CAA-C2A-C1A	-2.49	103.81	111.97
20	A	1012	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
20	A	1137	CLA	CHA-C4D-ND	2.49	137.71	132.50
20	5	608	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
20	B	1225	CLA	C2D-C1D-ND	2.49	111.94	110.10
20	8	601	CLA	C2D-C1D-ND	2.49	111.94	110.10
20	5	602	CLA	C3B-C4B-NB	-2.49	108.20	110.52
20	A	1141	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	A	5003	LMG	O8-C28-C29	2.49	119.72	111.91
20	G	1601	CLA	CHA-C4D-ND	2.49	137.71	132.50
20	Z	615	CLA	C3B-C4B-NB	-2.49	108.21	110.52
20	B	1206	CLA	C1-C2-C3	-2.49	121.74	126.04
20	3	616	CLA	CHA-C4D-ND	2.49	137.70	132.50
20	6	608	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
20	B	1021	CLA	C4B-CHC-C1C	2.49	132.24	126.34
20	A	1114	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
20	A	1013	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
20	B	1209	CLA	CHA-C4D-ND	2.49	137.70	132.50
20	B	1219	CLA	CMD-C2D-C3D	-2.49	121.90	127.61
20	6	604	CLA	C3B-C4B-NB	-2.48	108.21	110.52
20	6	607	CLA	C2D-C1D-ND	2.48	111.94	110.10
20	3	613	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
20	B	1210	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
20	B	1241	CLA	CHA-C4D-ND	2.48	137.69	132.50
20	3	601	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	A	1011	CL0	C4D-C3D-CAD	2.48	111.02	108.10
20	B	1204	CLA	C1D-ND-C4D	-2.48	104.57	106.33
20	4	615	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
20	B	1213	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
20	3	618	CLA	CHA-C4D-ND	2.48	137.69	132.50
20	F	1302	CLA	CHA-C1A-NA	-2.48	120.72	126.40
20	Z	602	CLA	CHA-C4D-ND	2.48	137.69	132.50
20	8	603	CLA	C4B-CHC-C1C	2.48	132.22	126.34
23	B	4007	BCR	C23-C22-C21	-2.48	115.13	118.94
36	6	501	LUT	C11-C10-C9	-2.48	123.77	127.31
37	1	610	CHL	CHB-C4A-NA	2.48	127.94	124.51
20	B	1023	CLA	O2A-CGA-CBA	2.48	119.69	111.91
20	8	608	CLA	O2A-CGA-CBA	2.48	119.69	111.91
20	7	605	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
20	B	1204	CLA	C4B-CHC-C1C	2.48	132.22	126.34
20	B	1201	CLA	C2B-C1B-NB	2.48	111.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1217	CLA	CHA-C4D-ND	2.48	137.69	132.50
23	3	503	BCR	C12-C13-C14	-2.48	115.14	118.94
20	3	610	CLA	CMA-C3A-C4A	2.48	118.43	111.77
20	3	606	CLA	C1D-ND-C4D	-2.48	104.58	106.33
20	5	609	CLA	CHA-C4D-ND	2.48	137.68	132.50
20	B	1241	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
20	A	1126	CLA	CMD-C2D-C3D	-2.48	121.92	127.61
20	K	1401	CLA	CHA-C1A-NA	-2.48	120.73	126.40
20	5	604	CLA	C1-O2A-CGA	2.48	122.94	116.44
20	4	607	CLA	C3B-C4B-NB	-2.48	108.22	110.52
20	A	1140	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
20	8	611	CLA	C1-C2-C3	-2.48	122.75	126.75
20	A	1140	CLA	O2A-CGA-CBA	2.48	119.68	111.91
20	8	609	CLA	O2A-CGA-CBA	2.48	119.68	111.91
20	A	1127	CLA	C4B-CHC-C1C	2.48	132.21	126.34
20	8	615	CLA	C4B-CHC-C1C	2.48	132.21	126.34
20	Z	608	CLA	O2A-CGA-CBA	2.47	119.67	111.91
20	3	607	CLA	CHA-C4D-ND	2.47	137.68	132.50
20	A	1104	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	B	1235	CLA	C1-O2A-CGA	2.47	122.93	116.44
20	G	1602	CLA	CMA-C3A-C4A	2.47	118.42	111.77
20	A	1134	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	A	1101	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	A	1110	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	3	601	CLA	C4B-CHC-C1C	2.47	132.20	126.34
39	Z	504	QTB	C03-C04-C05	-2.47	115.50	123.22
20	B	1210	CLA	C4B-CHC-C1C	2.47	132.20	126.34
20	J	1901	CLA	CAA-C2A-C3A	-2.47	108.08	114.26
20	6	606	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
24	B	5006	LHG	O8-C23-C24	2.47	119.66	111.91
23	B	4002	BCR	C19-C18-C17	2.47	122.73	118.94
20	J	1901	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	Z	611	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	A	1104	CLA	C1D-ND-C4D	-2.47	104.58	106.33
20	1	608	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
20	A	1116	CLA	O2A-CGA-CBA	2.47	119.66	111.91
20	8	611	CLA	CHA-C4D-ND	2.47	137.67	132.50
20	A	1136	CLA	OBD-CAD-C3D	-2.47	122.58	128.52
20	Z	605	CLA	CHA-C4D-ND	2.47	137.66	132.50
20	B	1234	CLA	CHA-C4D-ND	2.47	137.66	132.50
20	B	1204	CLA	CHA-C4D-ND	2.47	137.66	132.50
20	B	1201	CLA	C4B-CHC-C1C	2.47	132.19	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1201	CLA	CHA-C4D-ND	2.47	137.66	132.50
20	A	1105	CLA	O2A-CGA-CBA	2.47	119.65	111.91
37	1	609	CHL	C2B-C1B-NB	-2.47	108.58	110.23
20	4	604	CLA	CMA-C3A-C4A	2.47	118.40	111.77
20	1	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
20	B	1237	CLA	C2D-C1D-ND	2.47	111.92	110.10
20	Z	602	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
20	A	1130	CLA	O2A-CGA-CBA	2.47	119.65	111.91
20	4	605	CLA	C4B-CHC-C1C	2.47	132.19	126.34
37	6	611	CHL	C1-C2-C3	-2.47	122.76	126.75
20	1	604	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
20	L	1503	CLA	C4B-CHC-C1C	2.47	132.19	126.34
23	5	504	BCR	C4-C5-C6	-2.46	119.15	122.73
20	B	1235	CLA	C4B-CHC-C1C	2.46	132.18	126.34
20	5	601	CLA	C3B-C4B-NB	-2.46	108.23	110.52
20	A	1130	CLA	CHA-C4D-ND	2.46	137.65	132.50
20	K	1401	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
37	8	610	CHL	C1-C2-C3	-2.46	121.78	126.04
20	B	1241	CLA	C4B-CHC-C1C	2.46	132.18	126.34
20	5	603	CLA	C1D-ND-C4D	-2.46	104.58	106.33
20	B	1236	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
20	3	613	CLA	C2D-C1D-ND	2.46	111.92	110.10
23	B	4006	BCR	C27-C26-C25	-2.46	119.16	122.73
23	4	503	BCR	C4-C5-C6	-2.46	119.16	122.73
20	B	1206	CLA	CHA-C4D-ND	2.46	137.65	132.50
20	1	608	CLA	CHA-C4D-ND	2.46	137.65	132.50
20	5	607	CLA	C4B-CHC-C1C	2.46	132.17	126.34
20	A	1114	CLA	C2D-C1D-ND	2.46	111.92	110.10
23	3	505	BCR	C34-C9-C10	-2.46	119.48	122.92
26	B	6101	LMT	O5B-C5B-C4B	2.46	114.16	109.69
23	B	4003	BCR	C31-C1-C6	-2.46	106.31	110.30
20	A	1013	CLA	CHA-C4D-ND	2.46	137.64	132.50
20	1	604	CLA	CHA-C4D-ND	2.46	137.64	132.50
20	1	604	CLA	CMA-C3A-C4A	2.46	118.38	111.77
20	A	1131	CLA	C3B-C4B-NB	-2.46	108.23	110.52
20	5	607	CLA	C3B-C4B-NB	-2.46	108.23	110.52
20	Z	611	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
37	8	613	CHL	C1-C2-C3	-2.46	121.79	126.04
20	3	602	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
23	7	504	BCR	C19-C18-C17	2.46	122.71	118.94
20	4	601	CLA	C3B-C4B-NB	-2.46	108.23	110.52
37	4	610	CHL	C3C-C4C-NC	-2.46	107.81	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1217	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
20	K	1402	CLA	CHA-C4D-ND	2.46	137.64	132.50
20	3	612	CLA	O2A-CGA-CBA	2.46	119.61	111.91
20	8	601	CLA	C4B-CHC-C1C	2.46	132.16	126.34
37	7	610	CHL	CHC-C1C-NC	2.46	127.93	124.20
37	Z	610	CHL	C4D-CHA-C1A	2.46	124.24	121.25
20	8	607	CLA	CHA-C4D-ND	2.46	137.63	132.50
20	1	606	CLA	C2D-C1D-ND	2.45	111.91	110.10
20	4	606	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
20	A	1138	CLA	CHA-C4D-ND	2.45	137.63	132.50
20	Z	604	CLA	CHA-C4D-ND	2.45	137.63	132.50
20	B	1225	CLA	CMA-C3A-C4A	2.45	118.37	111.77
20	Z	603	CLA	C1D-ND-C4D	-2.45	104.59	106.33
20	5	601	CLA	C1D-ND-C4D	-2.45	104.59	106.33
20	6	606	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
20	3	604	CLA	CBA-CAA-C2A	2.45	121.10	113.86
20	8	612	CLA	CHA-C4D-ND	2.45	137.63	132.50
20	7	604	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
20	A	1139	CLA	CHA-C4D-ND	2.45	137.63	132.50
20	A	1112	CLA	O2A-CGA-CBA	2.45	119.60	111.91
20	4	607	CLA	C2D-C1D-ND	2.45	111.91	110.10
23	L	4002	BCR	C12-C13-C14	-2.45	115.18	118.94
20	8	609	CLA	CMA-C3A-C4A	2.45	118.36	111.77
26	1	803	LMT	C1'-O5'-C5'	-2.45	108.88	113.69
20	Z	607	CLA	C1-C2-C3	-2.45	121.81	126.04
20	7	612	CLA	O2A-CGA-CBA	2.45	119.59	111.91
23	6	504	BCR	C15-C14-C13	-2.45	123.81	127.31
20	B	1234	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
20	A	1140	CLA	CHA-C4D-ND	2.45	137.62	132.50
20	4	601	CLA	CHA-C4D-ND	2.45	137.62	132.50
20	3	610	CLA	CHA-C4D-ND	2.45	137.62	132.50
23	7	503	BCR	C35-C13-C12	2.45	121.93	118.08
23	6	503	BCR	C23-C24-C25	-2.45	120.33	127.20
20	5	622	CLA	CMD-C2D-C3D	-2.45	121.99	127.61
20	5	622	CLA	C4B-CHC-C1C	2.45	132.14	126.34
20	A	1133	CLA	CHA-C4D-ND	2.45	137.62	132.50
20	5	612	CLA	CHA-C4D-ND	2.45	137.62	132.50
20	A	1131	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
20	K	1401	CLA	C3B-C4B-NB	-2.44	108.25	110.52
20	B	1229	CLA	O2A-CGA-CBA	2.44	119.58	111.91
20	B	1216	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
20	L	1502	CLA	O2D-CGD-O1D	-2.44	119.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	1503	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
20	8	608	CLA	CHA-C4D-ND	2.44	137.61	132.50
20	3	601	CLA	C2D-C1D-ND	2.44	111.90	110.10
20	4	606	CLA	C4B-CHC-C1C	2.44	132.13	126.34
20	A	1115	CLA	CHA-C4D-ND	2.44	137.61	132.50
37	1	610	CHL	C4B-CHC-C1C	2.44	132.13	126.34
20	4	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
20	A	1113	CLA	CHA-C4D-ND	2.44	137.60	132.50
20	7	605	CLA	CMA-C3A-C4A	2.44	118.33	111.77
20	3	616	CLA	C3B-C4B-NB	-2.44	108.25	110.52
20	3	605	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
20	A	1132	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
20	B	1224	CLA	CHA-C4D-ND	2.44	137.60	132.50
20	1	608	CLA	C3B-C4B-NB	-2.44	108.25	110.52
20	Z	605	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
23	J	4001	BCR	C30-C25-C24	2.44	122.68	115.78
20	8	608	CLA	C3B-C4B-NB	-2.44	108.25	110.52
20	A	1116	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
20	5	615	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
20	3	608	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
37	1	610	CHL	C1-O2A-CGA	2.44	123.81	116.73
20	A	1111	CLA	C2D-C1D-ND	2.44	111.90	110.10
23	B	4003	BCR	C39-C30-C25	-2.44	106.35	110.30
36	5	501	LUT	C11-C10-C9	-2.44	123.83	127.31
20	A	1133	CLA	C2D-C1D-ND	2.44	111.90	110.10
20	4	609	CLA	CMA-C3A-C4A	2.44	118.32	111.77
37	7	610	CHL	C3C-C4C-NC	-2.44	107.84	110.57
20	3	608	CLA	CHA-C4D-ND	2.43	137.59	132.50
20	1	605	CLA	C2D-C1D-ND	2.43	111.90	110.10
20	A	1140	CLA	CMA-C3A-C4A	2.43	118.31	111.77
20	6	605	CLA	CHA-C1A-NA	-2.43	120.83	126.40
20	L	1503	CLA	CHA-C4D-ND	2.43	137.59	132.50
20	8	606	CLA	CHA-C4D-ND	2.43	137.59	132.50
20	1	607	CLA	CHA-C1A-NA	-2.43	120.83	126.40
20	3	607	CLA	C3B-C4B-NB	-2.43	108.26	110.52
20	3	613	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
20	8	615	CLA	CHA-C4D-ND	2.43	137.58	132.50
33	F	4001	RRX	C8-C7-C6	-2.43	120.38	127.20
20	8	601	CLA	C2C-C1C-NC	2.43	112.25	109.97
20	5	601	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
20	8	606	CLA	C4B-CHC-C1C	2.43	132.10	126.34
20	B	1203	CLA	C1D-ND-C4D	-2.43	104.61	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1231	CLA	C4B-CHC-C1C	2.43	132.10	126.34
20	Z	603	CLA	C4B-CHC-C1C	2.43	132.10	126.34
20	5	606	CLA	CHA-C4D-ND	2.43	137.58	132.50
20	3	613	CLA	O2A-CGA-CBA	2.43	119.53	111.91
36	4	502	LUT	C19-C9-C8	2.43	121.90	118.08
20	A	1127	CLA	CHA-C4D-ND	2.43	137.58	132.50
20	A	1126	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
20	A	1121	CLA	C4B-CHC-C1C	2.43	132.09	126.34
20	A	1106	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
20	B	1220	CLA	CHA-C4D-ND	2.43	137.57	132.50
20	A	1108	CLA	CMA-C3A-C4A	2.43	118.29	111.77
20	Z	608	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
20	B	1207	CLA	CHA-C4D-ND	2.43	137.57	132.50
37	5	617	CHL	CHC-C1C-NC	2.42	127.88	124.20
20	A	1124	CLA	O2A-CGA-CBA	2.42	119.51	111.91
20	A	1130	CLA	C2D-C1D-ND	2.42	111.89	110.10
20	7	606	CLA	C3B-C4B-NB	-2.42	108.27	110.52
20	F	1301	CLA	C3B-C4B-NB	-2.42	108.27	110.52
20	A	1125	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
20	3	612	CLA	CHA-C4D-ND	2.42	137.56	132.50
20	3	608	CLA	C3B-C4B-NB	-2.42	108.27	110.52
23	4	503	BCR	C19-C18-C17	2.42	122.66	118.94
20	A	1134	CLA	C2D-C1D-ND	2.42	111.89	110.10
20	4	615	CLA	CHA-C4D-ND	2.42	137.56	132.50
20	6	606	CLA	C4B-CHC-C1C	2.42	132.08	126.34
23	3	503	BCR	C35-C13-C12	2.42	121.89	118.08
20	6	607	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
26	8	805	LMT	C1'-O5'-C5'	-2.42	108.94	113.69
20	3	604	CLA	C1D-ND-C4D	-2.42	104.62	106.33
20	Z	603	CLA	O2A-CGA-CBA	2.42	119.50	111.91
20	Z	615	CLA	CHA-C4D-ND	2.42	137.56	132.50
20	B	1227	CLA	CHA-C4D-ND	2.42	137.56	132.50
20	A	1127	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
24	Z	801	LHG	C5-O7-C7	-2.42	111.84	117.79
23	J	4001	BCR	C19-C18-C17	2.42	122.65	118.94
34	J	4002	C7Z	C4-C5-C6	-2.42	115.46	120.85
20	5	607	CLA	O2A-CGA-CBA	2.42	119.49	111.91
20	7	611	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
20	8	607	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
20	8	601	CLA	OBD-CAD-C3D	-2.42	122.71	128.52
20	8	601	CLA	C2A-C1A-CHA	2.41	128.08	123.86
20	8	602	CLA	C6-C5-C3	-2.41	107.12	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	603	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
24	5	801	LHG	C5-O7-C7	-2.41	111.85	117.79
37	6	617	CHL	CHD-C1D-ND	-2.41	122.24	124.45
29	A	5003	LMG	C8-O7-C10	-2.41	111.85	117.79
20	3	610	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	A	1112	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
20	7	609	CLA	CHA-C4D-ND	2.41	137.54	132.50
37	8	613	CHL	C2B-C1B-NB	-2.41	108.61	110.23
37	4	613	CHL	C4D-CHA-C1A	2.41	124.18	121.25
19	A	1011	CL0	C1-C2-C3	-2.41	121.87	126.04
20	5	613	CLA	O2A-CGA-CBA	2.41	119.47	111.91
20	A	1132	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
20	L	1502	CLA	C1-O2A-CGA	2.41	122.77	116.44
20	6	606	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
20	1	612	CLA	C1-C2-C3	-2.41	121.88	126.04
20	6	607	CLA	C3B-C4B-NB	-2.41	108.28	110.52
20	4	604	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
20	4	615	CLA	CMA-C3A-C4A	2.41	118.25	111.77
20	B	1238	CLA	CHA-C4D-ND	2.41	137.54	132.50
20	4	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
20	A	1102	CLA	C4B-CHC-C1C	2.41	132.05	126.34
20	7	601	CLA	C2C-C1C-NC	2.41	112.23	109.97
20	8	615	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
20	B	1241	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
36	4	502	LUT	C3-C4-C5	-2.41	107.06	111.85
20	7	612	CLA	CHA-C4D-ND	2.41	137.53	132.50
20	3	618	CLA	CHA-C1A-NA	-2.41	120.89	126.40
20	4	602	CLA	C4B-CHC-C1C	2.41	132.05	126.34
20	B	1218	CLA	O2A-CGA-CBA	2.41	119.46	111.91
38	1	802	SQD	O3-C3-C2	-2.41	104.79	110.35
20	Z	612	CLA	C2D-C1D-ND	2.41	111.88	110.10
20	B	1207	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
36	6	502	LUT	C38-C25-C24	-2.41	118.41	123.56
37	4	611	CHL	C3C-C4C-NC	-2.40	107.87	110.57
20	L	1503	CLA	C1D-ND-C4D	-2.40	104.63	106.33
20	Z	606	CLA	C1-O2A-CGA	2.40	122.75	116.44
20	B	1214	CLA	CAC-C3C-C4C	2.40	127.93	124.81
20	B	1208	CLA	CHA-C4D-ND	2.40	137.53	132.50
20	B	1225	CLA	CHA-C4D-ND	2.40	137.53	132.50
20	7	603	CLA	CHA-C4D-ND	2.40	137.52	132.50
20	5	609	CLA	C4B-CHC-C1C	2.40	132.03	126.34
20	A	1125	CLA	C4B-CHC-C1C	2.40	132.03	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	601	CLA	C2C-C1C-NC	2.40	112.22	109.97
20	4	601	CLA	C4B-CHC-C1C	2.40	132.03	126.34
24	A	5002	LHG	C5-O7-C7	-2.40	111.88	117.79
20	7	601	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
20	A	1012	CLA	CHA-C1A-NA	-2.40	120.90	126.40
20	B	1230	CLA	C4B-CHC-C1C	2.40	132.03	126.34
20	4	612	CLA	C2A-C1A-CHA	2.40	128.06	123.86
36	1	502	LUT	C3-C4-C5	-2.40	107.07	111.85
20	8	607	CLA	C1-C2-C3	-2.40	121.89	126.04
20	B	1203	CLA	O2A-CGA-CBA	2.40	119.44	111.91
20	3	602	CLA	CHA-C1A-NA	-2.40	120.91	126.40
20	3	618	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
20	B	1021	CLA	CHA-C4D-ND	2.40	137.51	132.50
20	1	611	CLA	CHA-C4D-ND	2.40	137.51	132.50
20	7	609	CLA	C4B-CHC-C1C	2.40	132.03	126.34
23	B	4006	BCR	C33-C5-C6	-2.40	121.84	124.53
20	B	1205	CLA	C1D-ND-C4D	-2.40	104.63	106.33
37	4	611	CHL	C4D-CHA-C1A	2.40	124.17	121.25
20	4	603	CLA	CHA-C4D-ND	2.40	137.51	132.50
20	B	1229	CLA	CHA-C4D-ND	2.40	137.51	132.50
36	1	501	LUT	C39-C29-C28	2.40	121.85	118.08
23	8	503	BCR	C35-C13-C12	2.40	121.85	118.08
20	A	1118	CLA	O2A-CGA-CBA	2.40	119.42	111.91
20	6	609	CLA	CHA-C4D-ND	2.39	137.51	132.50
20	6	604	CLA	CHA-C4D-ND	2.39	137.51	132.50
20	1	603	CLA	CHA-C4D-ND	2.39	137.51	132.50
20	A	1111	CLA	O2A-CGA-CBA	2.39	119.42	111.91
20	4	605	CLA	C3B-C4B-NB	-2.39	108.29	110.52
20	K	1403	CLA	CHA-C4D-ND	2.39	137.51	132.50
20	B	1229	CLA	CMA-C3A-C4A	2.39	118.21	111.77
20	5	612	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
20	A	1118	CLA	CHA-C4D-ND	2.39	137.50	132.50
20	3	616	CLA	O2A-CGA-CBA	2.39	119.42	111.91
20	5	609	CLA	C1-C2-C3	-2.39	121.91	126.04
23	5	503	BCR	C34-C9-C10	-2.39	119.57	122.92
20	Z	606	CLA	C2C-C1C-NC	2.39	112.21	109.97
20	4	608	CLA	CHA-C1A-NA	-2.39	120.92	126.40
20	6	602	CLA	C6-C5-C3	-2.39	110.71	114.62
20	A	1137	CLA	CMA-C3A-C4A	2.39	118.20	111.77
20	5	601	CLA	CHA-C4D-ND	2.39	137.50	132.50
20	4	612	CLA	CMA-C3A-C4A	2.39	118.20	111.77
20	7	606	CLA	C2D-C1D-ND	2.39	111.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	503	C7Z	C20-C13-C12	2.39	121.84	118.08
20	A	1107	CLA	CHA-C4D-ND	2.39	137.50	132.50
20	6	605	CLA	C1-O2A-CGA	2.39	122.71	116.44
20	B	1228	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	3	616	CLA	C1-C2-C3	-2.39	121.91	126.04
20	A	1136	CLA	CHA-C4D-ND	2.39	137.50	132.50
20	7	611	CLA	CHA-C4D-ND	2.39	137.50	132.50
23	B	4006	BCR	C23-C24-C25	-2.39	120.50	127.20
20	8	611	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	6	607	CLA	O2A-CGA-CBA	2.39	119.40	111.91
20	6	619	CLA	C1-C2-C3	-2.39	121.91	126.04
20	5	609	CLA	CHA-C1A-NA	-2.39	120.93	126.40
20	6	604	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
20	7	602	CLA	C1D-ND-C4D	-2.39	104.64	106.33
26	B	5005	LMT	O5'-C5'-C4'	2.39	114.78	109.75
20	A	1131	CLA	O2A-CGA-CBA	2.38	119.39	111.91
20	1	606	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
20	4	607	CLA	CHA-C1A-NA	-2.38	120.94	126.40
37	3	611	CHL	C1-C2-C3	-2.38	121.92	126.04
20	4	602	CLA	CHA-C4D-ND	2.38	137.49	132.50
20	B	1230	CLA	O2A-CGA-CBA	2.38	119.39	111.91
23	3	506	BCR	C1-C6-C5	-2.38	119.26	122.61
20	A	1123	CLA	CHA-C4D-ND	2.38	137.48	132.50
20	7	616	CLA	CHA-C4D-ND	2.38	137.48	132.50
20	7	601	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
20	1	611	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
37	5	610	CHL	CMA-C3A-C4A	2.38	118.18	111.77
20	A	1106	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
20	A	1105	CLA	CHA-C4D-ND	2.38	137.48	132.50
20	Z	606	CLA	CAC-C3C-C4C	2.38	127.90	124.81
20	A	1121	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
20	3	608	CLA	CHA-C1A-NA	-2.38	120.94	126.40
36	Z	501	LUT	C37-C21-C22	-2.38	104.93	109.44
20	8	602	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
20	7	606	CLA	C1-O2A-CGA	2.38	122.69	116.44
20	A	1122	CLA	CHA-C4D-ND	2.38	137.48	132.50
20	6	603	CLA	CHA-C4D-ND	2.38	137.48	132.50
20	B	1221	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
20	5	606	CLA	C3B-C4B-NB	-2.38	108.31	110.52
20	B	1240	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
23	B	4004	BCR	C12-C13-C14	-2.38	115.29	118.94
20	B	1234	CLA	O2A-CGA-CBA	2.38	119.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1220	CLA	C4B-CHC-C1C	2.38	131.98	126.34
20	B	1234	CLA	C4B-CHC-C1C	2.38	131.98	126.34
20	B	1205	CLA	CHA-C4D-ND	2.38	137.47	132.50
20	Z	603	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
20	A	1013	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
23	L	4002	BCR	C34-C9-C10	-2.38	119.59	122.92
36	7	501	LUT	C18-C5-C6	-2.38	121.86	124.53
20	7	612	CLA	C4B-CHC-C1C	2.38	131.97	126.34
20	B	1216	CLA	C3B-C4B-NB	-2.38	108.31	110.52
20	B	1239	CLA	O2A-CGA-CBA	2.38	119.36	111.91
23	B	4007	BCR	C31-C1-C6	-2.38	106.45	110.30
20	1	601	CLA	C4B-CHC-C1C	2.38	131.97	126.34
20	B	1228	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
20	7	605	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
20	B	1228	CLA	O2A-CGA-CBA	2.37	119.36	111.91
20	A	1111	CLA	C4B-CHC-C1C	2.37	131.97	126.34
36	Z	502	LUT	C18-C5-C6	-2.37	121.86	124.53
20	7	612	CLA	C2C-C1C-NC	2.37	112.20	109.97
23	J	4001	BCR	C2-C3-C4	-2.37	106.07	111.38
20	B	1204	CLA	C1-O2A-CGA	2.37	122.67	116.44
20	7	601	CLA	C4B-CHC-C1C	2.37	131.97	126.34
20	B	1023	CLA	CAC-C3C-C4C	2.37	127.89	124.81
20	A	1120	CLA	CHA-C4D-ND	2.37	137.46	132.50
20	6	612	CLA	C4B-CHC-C1C	2.37	131.97	126.34
20	5	604	CLA	CHA-C4D-ND	2.37	137.46	132.50
20	8	605	CLA	O2A-CGA-CBA	2.37	119.35	111.91
20	6	619	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
20	B	1213	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
36	6	502	LUT	C31-C32-C33	-2.37	119.75	126.42
20	A	1113	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
20	A	1131	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
20	3	612	CLA	CHA-C1A-NA	-2.37	120.97	126.40
20	B	1219	CLA	CHA-C1A-NA	-2.37	120.97	126.40
20	B	1222	CLA	CHA-C4D-ND	2.37	137.46	132.50
20	1	615	CLA	O2A-CGA-CBA	2.37	119.35	111.91
20	A	1115	CLA	C3D-C2D-C1D	-2.37	102.60	105.83
20	6	605	CLA	C1-C2-C3	-2.37	121.94	126.04
20	4	603	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
20	6	602	CLA	C4B-CHC-C1C	2.37	131.96	126.34
20	A	1109	CLA	CHA-C4D-ND	2.37	137.45	132.50
20	A	1117	CLA	CHA-C4D-ND	2.37	137.45	132.50
20	B	1023	CLA	C2C-C1C-NC	2.37	112.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	4002	BCR	C15-C14-C13	-2.37	123.93	127.31
20	G	1602	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
20	8	602	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
20	A	1110	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
20	6	601	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
20	B	1229	CLA	C1-C2-C3	-2.36	121.95	126.04
20	A	1139	CLA	O2A-CGA-CBA	2.36	119.33	111.91
20	5	601	CLA	CMA-C3A-C4A	2.36	118.13	111.77
20	7	615	CLA	CHA-C1A-NA	-2.36	120.98	126.40
37	5	611	CHL	C4B-CHC-C1C	2.36	131.94	126.34
36	Z	503	LUT	C31-C32-C33	-2.36	119.78	126.42
20	A	1109	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
20	8	615	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
20	6	602	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
20	3	606	CLA	CHA-C4D-ND	2.36	137.44	132.50
20	A	1132	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
37	4	610	CHL	CHB-C4A-NA	2.36	127.78	124.51
23	3	505	BCR	C37-C22-C21	-2.36	119.61	122.92
20	A	1118	CLA	C1D-ND-C4D	-2.36	104.66	106.33
23	A	4002	BCR	C33-C5-C6	-2.36	121.88	124.53
37	5	617	CHL	C4D-CHA-C1A	2.36	124.12	121.25
23	7	504	BCR	C37-C22-C21	-2.36	119.62	122.92
20	F	1301	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
20	A	1136	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
20	B	1022	CLA	O2A-CGA-CBA	2.36	119.31	111.91
20	B	1213	CLA	C3B-C4B-NB	-2.36	108.33	110.52
20	Z	601	CLA	C3B-C4B-NB	-2.36	108.33	110.52
20	A	1124	CLA	C1-O2A-CGA	2.36	122.63	116.44
20	B	1226	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
20	G	1601	CLA	C3B-C4B-NB	-2.36	108.33	110.52
20	1	602	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
20	B	1207	CLA	O2A-CGA-CBA	2.36	119.30	111.91
23	B	4004	BCR	C37-C22-C23	2.36	121.79	118.08
20	B	1230	CLA	CAA-CBA-CGA	-2.36	106.37	113.25
36	4	501	LUT	C39-C29-C28	2.36	121.79	118.08
20	6	607	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
20	8	609	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
20	Z	615	CLA	C4B-CHC-C1C	2.35	131.92	126.34
20	B	1241	CLA	O2A-CGA-CBA	2.35	119.30	111.91
20	A	1108	CLA	C4B-CHC-C1C	2.35	131.92	126.34
20	1	605	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
20	A	1115	CLA	C1-O2A-CGA	2.35	122.62	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	603	CLA	C3B-C4B-NB	-2.35	108.33	110.52
20	A	1114	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
20	Z	608	CLA	C2D-C1D-ND	2.35	111.84	110.10
20	Z	606	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
19	A	1011	CL0	CBC-CAC-C3C	-2.35	105.94	112.43
37	1	609	CHL	C1-C2-C3	-2.35	121.97	126.04
20	5	603	CLA	C4B-CHC-C1C	2.35	131.92	126.34
20	1	601	CLA	CHA-C4D-ND	2.35	137.42	132.50
36	3	501	LUT	C11-C10-C9	-2.35	123.95	127.31
23	A	4001	BCR	C23-C24-C25	-2.35	120.60	127.20
37	3	611	CHL	C4D-CHA-C1A	2.35	124.11	121.25
20	5	618	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
20	8	601	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
24	A	5001	LHG	C5-O7-C7	-2.35	112.00	117.79
20	7	609	CLA	CMA-C3A-C4A	2.35	118.09	111.77
20	B	1203	CLA	C6-C5-C3	-2.35	107.30	113.45
20	1	615	CLA	CHA-C1A-NA	-2.35	121.02	126.40
23	3	504	BCR	C38-C26-C27	2.35	118.13	113.62
20	B	1237	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
20	A	1121	CLA	O2A-CGA-CBA	2.35	119.28	111.91
20	8	612	CLA	CHA-C1A-NA	-2.35	121.02	126.40
20	5	602	CLA	C4B-CHC-C1C	2.35	131.91	126.34
20	6	605	CLA	C4B-CHC-C1C	2.35	131.90	126.34
20	A	1108	CLA	CHA-C4D-ND	2.35	137.41	132.50
20	8	605	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
20	6	608	CLA	CHA-C1A-NA	-2.35	121.03	126.40
20	B	1213	CLA	CMA-C3A-C4A	2.35	118.08	111.77
20	A	1128	CLA	CHA-C4D-ND	2.35	137.41	132.50
20	8	604	CLA	C3B-C4B-NB	-2.35	108.34	110.52
23	I	4001	BCR	C35-C13-C12	2.35	121.77	118.08
20	A	1104	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
20	6	615	CLA	CHA-C1A-NA	-2.34	121.03	126.40
20	Z	611	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
20	8	605	CLA	C3B-C4B-NB	-2.34	108.34	110.52
20	Z	603	CLA	CHA-C4D-ND	2.34	137.40	132.50
20	7	605	CLA	C1-O2A-CGA	2.34	122.59	116.44
20	A	1112	CLA	CHA-C4D-ND	2.34	137.40	132.50
19	A	1011	CL0	CMD-C2D-C3D	-2.34	122.22	127.61
36	5	501	LUT	C10-C11-C12	-2.34	115.91	123.22
20	B	1023	CLA	CHA-C4D-ND	2.34	137.40	132.50
20	4	605	CLA	C1D-ND-C4D	-2.34	104.67	106.33
20	B	1210	CLA	O2A-CGA-CBA	2.34	119.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1139	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
20	5	603	CLA	C6-C5-C3	-2.34	107.31	113.45
20	Z	603	CLA	C1-O2A-CGA	2.34	122.59	116.44
20	Z	605	CLA	C1D-ND-C4D	-2.34	104.67	106.33
20	B	1206	CLA	CHA-C1A-NA	-2.34	121.04	126.40
37	Z	609	CHL	C2B-C1B-NB	-2.34	108.66	110.23
20	B	1224	CLA	O2A-CGA-CBA	2.34	119.25	111.91
20	B	1212	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
20	L	1502	CLA	CHA-C4D-ND	2.34	137.39	132.50
20	8	602	CLA	C1-C2-C3	-2.34	122.00	126.04
20	J	1901	CLA	C4B-CHC-C1C	2.34	131.89	126.34
20	8	604	CLA	CHA-C1A-NA	-2.34	121.04	126.40
20	A	1141	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	A	4003	BCR	C38-C26-C27	2.34	118.11	113.62
20	B	1221	CLA	C2A-C1A-CHA	2.34	127.95	123.86
20	3	604	CLA	C3B-C4B-NB	-2.34	108.35	110.52
20	A	1140	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
20	A	1124	CLA	CHA-C4D-ND	2.34	137.39	132.50
37	Z	613	CHL	C3B-C4B-NB	-2.34	108.35	110.52
20	B	1226	CLA	C1-O2A-CGA	2.34	122.57	116.44
23	7	504	BCR	C29-C28-C27	2.34	116.60	111.38
20	A	1122	CLA	C1-O2A-CGA	2.34	122.57	116.44
20	6	601	CLA	C3B-C4B-NB	-2.33	108.35	110.52
36	3	502	LUT	C10-C11-C12	-2.33	115.93	123.22
37	4	617	CHL	CHC-C1C-NC	2.33	127.75	124.20
20	Z	608	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
20	5	601	CLA	C4B-CHC-C1C	2.33	131.88	126.34
20	7	615	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
20	A	1102	CLA	CHA-C4D-ND	2.33	137.38	132.50
20	8	608	CLA	C4B-CHC-C1C	2.33	131.87	126.34
36	6	502	LUT	C31-C30-C29	-2.33	123.98	127.31
23	B	4004	BCR	C35-C13-C12	2.33	121.75	118.08
20	B	1201	CLA	CHA-C1A-NA	-2.33	121.05	126.40
20	A	1102	CLA	C1C-C2C-C3C	-2.33	104.50	106.96
23	6	504	BCR	C37-C22-C23	2.33	121.75	118.08
20	Z	604	CLA	C3B-C4B-NB	-2.33	108.35	110.52
20	8	612	CLA	C3B-C4B-NB	-2.33	108.35	110.52
23	A	4002	BCR	C36-C18-C17	-2.33	119.66	122.92
20	A	1128	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
20	B	1238	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
20	A	1117	CLA	C4B-CHC-C1C	2.33	131.87	126.34
20	A	1132	CLA	CHA-C4D-ND	2.33	137.38	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	612	CLA	CHA-C1A-NA	-2.33	121.06	126.40
20	B	1213	CLA	C16-C15-C13	-2.33	108.39	115.92
23	I	4001	BCR	C36-C18-C17	-2.33	119.66	122.92
20	B	1229	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
20	1	602	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
20	B	1214	CLA	CHA-C1A-NA	-2.33	121.06	126.40
20	Z	601	CLA	CHA-C4D-ND	2.33	137.37	132.50
20	6	608	CLA	C2D-C1D-ND	2.33	111.82	110.10
20	3	604	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
23	7	504	BCR	C8-C7-C6	-2.33	120.66	127.20
36	8	501	LUT	C20-C13-C12	2.33	121.75	118.08
20	4	605	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
20	7	608	CLA	CHA-C1A-NA	-2.33	121.06	126.40
36	5	502	LUT	C38-C25-C24	-2.33	118.58	123.56
20	A	1013	CLA	C2A-C1A-CHA	2.33	127.93	123.86
20	B	1214	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
20	7	607	CLA	C3B-C4B-NB	-2.33	108.36	110.52
20	B	1230	CLA	CHA-C4D-ND	2.33	137.37	132.50
23	5	503	BCR	C29-C28-C27	2.33	116.58	111.38
34	1	503	C7Z	C40-C33-C34	-2.33	119.66	122.92
20	A	1107	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
20	4	606	CLA	CHA-C4D-ND	2.33	137.37	132.50
36	6	502	LUT	C35-C15-C14	-2.33	118.71	123.47
20	3	605	CLA	O2A-CGA-CBA	2.33	119.21	111.91
20	5	604	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
20	B	1240	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
20	B	1218	CLA	C4B-CHC-C1C	2.33	131.86	126.34
20	K	1403	CLA	C3B-C4B-NB	-2.33	108.36	110.52
37	6	611	CHL	C4B-CHC-C1C	2.33	131.85	126.34
20	7	613	CLA	C2D-C1D-ND	2.33	111.82	110.10
36	6	501	LUT	C10-C11-C12	-2.33	115.96	123.22
20	8	604	CLA	CHA-C4D-ND	2.33	137.36	132.50
20	1	613	CLA	C3B-C4B-NB	-2.33	108.36	110.52
20	A	1128	CLA	O2A-CGA-CBA	2.33	119.20	111.91
20	A	1133	CLA	C4B-CHC-C1C	2.32	131.85	126.34
20	4	604	CLA	C4B-CHC-C1C	2.32	131.85	126.34
20	4	612	CLA	C4B-CHC-C1C	2.32	131.85	126.34
20	Z	601	CLA	C1D-ND-C4D	-2.32	104.68	106.33
26	B	6101	LMT	C2'-C3'-C4'	2.32	114.99	109.68
20	7	607	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
20	A	1116	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
23	B	4005	BCR	C4-C5-C6	-2.32	119.36	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	6	502	LUT	C18-C5-C4	2.32	118.66	114.36
20	6	601	CLA	C1-C2-C3	-2.32	122.03	126.04
20	7	615	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	B	1224	CLA	CHA-C1A-NA	-2.32	121.08	126.40
20	Z	607	CLA	CHA-C1A-NA	-2.32	121.08	126.40
20	A	1120	CLA	C1-O2A-CGA	2.32	122.53	116.44
20	A	1132	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	7	604	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	A	1129	CLA	C3B-C4B-NB	-2.32	108.36	110.52
20	B	1201	CLA	C3B-C4B-NB	-2.32	108.36	110.52
20	5	608	CLA	C3B-C4B-NB	-2.32	108.36	110.52
20	3	601	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
20	B	1202	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	B	1207	CLA	C1-O2A-CGA	2.32	122.53	116.44
23	5	504	BCR	C27-C26-C25	-2.32	119.36	122.73
36	7	502	LUT	C35-C15-C14	-2.32	118.72	123.47
20	L	1503	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
37	8	613	CHL	CMA-C3A-C2A	2.32	123.18	113.83
20	G	1601	CLA	CMA-C3A-C4A	2.32	118.00	111.77
23	6	504	BCR	C34-C9-C10	-2.32	119.67	122.92
20	1	608	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	7	605	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	5	613	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	Z	604	CLA	C1D-ND-C4D	-2.32	104.69	106.33
20	3	605	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
20	L	1502	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	3	603	CLA	C4B-CHC-C1C	2.32	131.84	126.34
20	G	1601	CLA	C1D-ND-C4D	-2.32	104.69	106.33
20	4	601	CLA	C1D-ND-C4D	-2.32	104.69	106.33
20	1	602	CLA	C4B-CHC-C1C	2.32	131.83	126.34
20	5	613	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
20	B	1218	CLA	C1D-ND-C4D	-2.32	104.69	106.33
20	B	1226	CLA	CHA-C1A-NA	-2.32	121.10	126.40
20	6	603	CLA	C1-C2-C3	-2.32	122.04	126.04
36	6	502	LUT	C1-C2-C3	2.31	118.87	113.64
20	5	613	CLA	CHA-C1A-NA	-2.31	121.10	126.40
20	5	607	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
20	Z	605	CLA	C3B-C4B-NB	-2.31	108.37	110.52
20	6	612	CLA	CHA-C4D-ND	2.31	137.34	132.50
23	3	506	BCR	C29-C28-C27	2.31	116.55	111.38
20	A	1114	CLA	C4B-CHC-C1C	2.31	131.82	126.34
23	3	504	BCR	C27-C26-C25	-2.31	119.37	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1135	CLA	C1D-ND-C4D	-2.31	104.69	106.33
20	B	1228	CLA	CHA-C4D-ND	2.31	137.34	132.50
20	7	616	CLA	C4B-CHC-C1C	2.31	131.82	126.34
20	7	603	CLA	CHA-C1A-NA	-2.31	121.10	126.40
20	Z	612	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
20	B	1222	CLA	C2C-C1C-NC	2.31	112.14	109.97
20	A	1141	CLA	CHA-C1A-NA	-2.31	121.11	126.40
20	A	1111	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
20	A	1109	CLA	CBA-CAA-C2A	2.31	120.68	113.86
23	A	4004	BCR	C34-C9-C10	-2.31	119.69	122.92
20	5	605	CLA	C3B-C4B-NB	-2.31	108.37	110.52
20	B	1203	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
20	Z	604	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
20	3	610	CLA	O2A-CGA-CBA	2.31	119.16	111.91
20	A	1117	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
20	7	603	CLA	C4B-CHC-C1C	2.31	131.81	126.34
20	B	1215	CLA	CHA-C4D-ND	2.31	137.33	132.50
20	A	1115	CLA	C1D-ND-C4D	-2.31	104.69	106.33
20	B	1236	CLA	CHA-C4D-ND	2.31	137.33	132.50
20	A	1135	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	B	1237	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	4	606	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
20	8	604	CLA	C4B-CHC-C1C	2.31	131.81	126.34
20	A	1124	CLA	C3B-C4B-NB	-2.31	108.37	110.52
20	4	601	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
20	B	1218	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
20	B	1208	CLA	C4B-CHC-C1C	2.31	131.81	126.34
23	K	4002	BCR	C34-C9-C10	-2.31	119.69	122.92
20	A	1127	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
20	A	1139	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
20	3	606	CLA	C4B-CHC-C1C	2.31	131.81	126.34
20	B	1022	CLA	OBD-CAD-C3D	-2.31	122.97	128.52
20	B	1212	CLA	C4B-CHC-C1C	2.31	131.81	126.34
20	7	609	CLA	O2A-CGA-CBA	2.31	119.14	111.91
20	B	1021	CLA	C1D-ND-C4D	-2.31	104.70	106.33
20	8	607	CLA	C3B-C4B-NB	-2.31	108.38	110.52
23	G	4001	BCR	C23-C24-C25	-2.30	120.73	127.20
20	K	1403	CLA	O2A-CGA-CBA	2.30	119.14	111.91
20	A	1139	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
20	A	1120	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
20	1	611	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
20	A	1136	CLA	C4B-CHC-C1C	2.30	131.80	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	618	CLA	C4B-CHC-C1C	2.30	131.80	126.34
37	6	613	CHL	C3C-C4C-NC	-2.30	107.99	110.57
20	3	612	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	4	608	CLA	C3B-C4B-NB	-2.30	108.38	110.52
23	4	503	BCR	C34-C9-C10	-2.30	119.70	122.92
34	J	4002	C7Z	C35-C15-C14	-2.30	118.76	123.47
20	4	601	CLA	O2A-CGA-CBA	2.30	119.13	111.91
20	B	1207	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	5	603	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	8	603	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
20	B	1228	CLA	C4B-CHC-C1C	2.30	131.79	126.34
20	4	609	CLA	O2A-CGA-CBA	2.30	119.12	111.91
20	6	615	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	4	604	CLA	CHA-C1A-NA	-2.30	121.13	126.40
20	1	604	CLA	C6-C5-C3	-2.30	107.43	113.45
20	7	611	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
20	1	603	CLA	C6-C5-C3	-2.30	107.43	113.45
36	5	501	LUT	C8-C7-C6	-2.30	120.75	127.20
20	A	1115	CLA	C4B-CHC-C1C	2.30	131.79	126.34
20	4	606	CLA	C3B-C4B-NB	-2.30	108.38	110.52
20	1	607	CLA	C2A-C1A-CHA	2.30	127.88	123.86
20	F	1302	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
20	B	1201	CLA	CMA-C3A-C2A	2.30	123.09	113.83
20	5	603	CLA	CHA-C4D-ND	2.30	137.30	132.50
20	A	1012	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
20	8	607	CLA	C2D-C1D-ND	2.29	111.80	110.10
20	8	611	CLA	C1D-ND-C4D	-2.29	104.70	106.33
23	B	4006	BCR	C34-C9-C10	-2.29	119.71	122.92
20	A	1134	CLA	C4B-CHC-C1C	2.29	131.78	126.34
20	B	1215	CLA	C4B-CHC-C1C	2.29	131.78	126.34
20	1	613	CLA	C4B-CHC-C1C	2.29	131.78	126.34
23	L	4002	BCR	C38-C26-C25	-2.29	121.95	124.53
20	7	606	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
20	A	1119	CLA	C4B-CHC-C1C	2.29	131.78	126.34
20	B	1222	CLA	CMA-C3A-C4A	2.29	117.94	111.77
20	K	1403	CLA	C4B-CHC-C1C	2.29	131.78	126.34
24	6	801	LHG	C5-O7-C7	-2.29	112.15	117.79
20	6	602	CLA	CHA-C1A-NA	-2.29	121.15	126.40
20	B	1235	CLA	CHA-C4D-ND	2.29	137.29	132.50
20	8	601	CLA	CHA-C1A-NA	-2.29	121.15	126.40
20	Z	607	CLA	O2A-CGA-CBA	2.29	119.10	111.91
20	A	1101	CLA	CMD-C2D-C3D	-2.29	122.34	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1013	CLA	CHA-C1A-NA	-2.29	121.15	126.40
20	A	1134	CLA	C3B-C4B-NB	-2.29	108.39	110.52
20	8	603	CLA	CMC-C2C-C1C	2.29	128.53	125.04
20	B	1237	CLA	C3B-C4B-NB	-2.29	108.39	110.52
20	B	1210	CLA	CHA-C4D-ND	2.29	137.29	132.50
36	1	501	LUT	C20-C13-C12	2.29	121.68	118.08
36	Z	503	LUT	C31-C30-C29	-2.29	124.04	127.31
20	A	1116	CLA	CAC-C3C-C4C	2.29	127.78	124.81
20	8	615	CLA	C1D-ND-C4D	-2.29	104.71	106.33
20	Z	615	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
34	5	505	C7Z	C19-C9-C10	-2.29	119.72	122.92
20	5	605	CLA	C4B-CHC-C1C	2.29	131.77	126.34
20	F	1302	CLA	CHA-C4D-ND	2.29	137.29	132.50
20	6	607	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
20	4	615	CLA	C4B-CHC-C1C	2.29	131.76	126.34
20	B	1211	CLA	C4B-CHC-C1C	2.29	131.76	126.34
20	A	1139	CLA	CHA-C1A-NA	-2.29	121.16	126.40
20	1	601	CLA	CMA-C3A-C4A	2.29	117.92	111.77
20	3	605	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
20	B	1206	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
20	6	609	CLA	CHA-C1A-NA	-2.29	121.16	126.40
20	B	1235	CLA	CMA-C3A-C4A	2.29	117.92	111.77
20	1	602	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
20	1	612	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
20	A	1135	CLA	O2A-CGA-CBA	2.28	119.08	111.91
20	5	618	CLA	O2A-CGA-CBA	2.28	119.08	111.91
20	B	1232	CLA	C4B-CHC-C1C	2.28	131.75	126.34
20	8	605	CLA	CHA-C1A-NA	-2.28	121.17	126.40
20	B	1214	CLA	C4B-CHC-C1C	2.28	131.75	126.34
20	7	609	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
20	B	1217	CLA	C1-C2-C3	-2.28	122.10	126.04
20	Z	601	CLA	CMA-C3A-C4A	2.28	117.91	111.77
20	B	1222	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
20	8	603	CLA	CHA-C4D-ND	2.28	137.27	132.50
20	A	1112	CLA	CHA-C1A-NA	-2.28	121.18	126.40
20	7	609	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
20	7	602	CLA	C4B-CHC-C1C	2.28	131.74	126.34
34	5	505	C7Z	C27-C28-C29	-2.28	122.79	126.23
20	B	1234	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
36	5	501	LUT	C15-C14-C13	-2.28	124.06	127.31
20	A	1105	CLA	CMA-C3A-C4A	2.28	117.90	111.77
20	B	1220	CLA	C2A-C1A-CHA	2.28	127.84	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Z	503	LUT	C1-C6-C7	2.28	122.22	115.78
20	6	601	CLA	C4B-CHC-C1C	2.28	131.74	126.34
20	A	1105	CLA	C1-O2A-CGA	2.28	122.42	116.44
20	F	1302	CLA	C4B-CHC-C1C	2.28	131.74	126.34
23	A	4003	BCR	C37-C22-C21	-2.28	119.73	122.92
20	6	603	CLA	C1D-ND-C4D	-2.28	104.72	106.33
20	1	605	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
20	B	1223	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
36	7	501	LUT	C10-C11-C12	-2.28	116.12	123.22
20	3	613	CLA	CHA-C1A-NA	-2.28	121.19	126.40
23	B	4004	BCR	C37-C22-C21	-2.28	119.74	122.92
20	4	615	CLA	CHA-C1A-NA	-2.27	121.19	126.40
34	5	505	C7Z	C11-C12-C13	-2.27	120.03	126.42
20	J	1901	CLA	CHA-C1A-NA	-2.27	121.19	126.40
20	B	1213	CLA	C1-C2-C3	-2.27	122.11	126.04
20	7	607	CLA	C4B-CHC-C1C	2.27	131.73	126.34
20	1	602	CLA	CHA-C1A-NA	-2.27	121.19	126.40
20	B	1208	CLA	C1-C2-C3	-2.27	122.11	126.04
36	6	501	LUT	C22-C23-C24	-2.27	109.16	111.74
20	5	604	CLA	C1D-ND-C4D	-2.27	104.72	106.33
20	7	616	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
23	K	4001	BCR	C34-C9-C10	-2.27	119.74	122.92
20	5	603	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
20	A	1116	CLA	CAA-CBA-CGA	-2.27	106.62	113.25
20	B	1201	CLA	CMB-C2B-C3B	2.27	132.08	126.59
20	1	604	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
20	A	1138	CLA	C4B-CHC-C1C	2.27	131.72	126.34
20	Z	611	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
20	A	1129	CLA	C4B-CHC-C1C	2.27	131.72	126.34
20	B	1216	CLA	O2A-CGA-CBA	2.27	119.02	111.91
20	4	606	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
20	F	1301	CLA	C6-C5-C3	-2.27	107.51	113.45
20	A	1012	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
20	A	1130	CLA	CHA-C1A-NA	-2.26	121.21	126.40
20	B	1203	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
20	7	604	CLA	O1A-CGA-CBA	-2.26	114.90	123.73
20	5	606	CLA	C4B-CHC-C1C	2.26	131.71	126.34
20	3	618	CLA	C4B-CHC-C1C	2.26	131.71	126.34
20	B	1205	CLA	C4B-CHC-C1C	2.26	131.71	126.34
23	K	4001	BCR	C15-C14-C13	-2.26	124.08	127.31
20	B	1212	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
20	6	606	CLA	C3B-C4B-NB	-2.26	108.42	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1111	CLA	CHA-C1A-NA	-2.26	121.22	126.40
20	5	615	CLA	CHA-C1A-NA	-2.26	121.22	126.40
20	3	603	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
20	A	1113	CLA	C4B-CHC-C1C	2.26	131.70	126.34
20	3	618	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
20	B	1203	CLA	C4B-CHC-C1C	2.26	131.70	126.34
20	6	607	CLA	CHA-C1A-NA	-2.26	121.22	126.40
20	5	618	CLA	CHA-C4D-ND	2.26	137.23	132.50
20	5	604	CLA	CHA-C1A-NA	-2.26	121.22	126.40
20	F	1301	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
20	1	603	CLA	C4B-CHC-C1C	2.26	131.70	126.34
37	Z	613	CHL	C4B-CHC-C1C	2.26	131.70	126.34
20	Z	608	CLA	C3B-C4B-NB	-2.26	108.42	110.52
19	A	1011	CL0	CAA-CBA-CGA	-2.26	106.65	113.25
20	A	1106	CLA	CMA-C3A-C4A	2.26	117.84	111.77
20	7	615	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
20	B	1236	CLA	O2A-CGA-CBA	2.26	118.99	111.91
20	A	1120	CLA	C4B-CHC-C1C	2.26	131.69	126.34
20	A	1139	CLA	C4B-CHC-C1C	2.26	131.69	126.34
20	B	1228	CLA	C1-O2A-CGA	2.26	122.37	116.44
20	B	1225	CLA	CHA-C1A-NA	-2.26	121.23	126.40
20	1	606	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
20	1	608	CLA	CHA-C1A-NA	-2.26	121.23	126.40
23	I	4001	BCR	C37-C22-C23	2.26	121.63	118.08
20	L	1502	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
20	8	611	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
20	A	1118	CLA	C4B-CHC-C1C	2.25	131.69	126.34
37	3	611	CHL	CHB-C4A-NA	2.25	127.63	124.51
20	B	1219	CLA	CBA-CAA-C2A	2.25	120.52	113.86
20	A	1112	CLA	C1D-ND-C4D	-2.25	104.73	106.33
20	3	603	CLA	C1D-ND-C4D	-2.25	104.73	106.33
23	L	4001	BCR	C19-C18-C17	2.25	122.40	118.94
20	1	612	CLA	C4B-CHC-C1C	2.25	131.68	126.34
20	K	1404	CLA	CMA-C3A-C2A	2.25	122.92	113.83
20	A	1105	CLA	C1D-ND-C4D	-2.25	104.73	106.33
20	1	601	CLA	C1D-ND-C4D	-2.25	104.73	106.33
29	A	5003	LMG	O7-C10-O9	-2.25	118.26	123.70
23	L	4001	BCR	C38-C26-C25	-2.25	122.00	124.53
20	B	1211	CLA	C1-O2A-CGA	2.25	122.35	116.44
20	6	618	CLA	C3B-C4B-NB	-2.25	108.43	110.52
36	1	501	LUT	C15-C14-C13	-2.25	124.10	127.31
20	4	603	CLA	C2A-C1A-CHA	2.25	127.80	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	612	CLA	C4B-CHC-C1C	2.25	131.68	126.34
20	7	612	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
20	5	607	CLA	C1-C2-C3	-2.25	122.15	126.04
20	B	1022	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
20	3	605	CLA	C1D-ND-C4D	-2.25	104.74	106.33
20	6	604	CLA	C1D-ND-C4D	-2.25	104.74	106.33
23	3	506	BCR	C15-C14-C13	-2.25	124.10	127.31
20	8	608	CLA	CMA-C3A-C4A	2.25	117.82	111.77
20	1	615	CLA	C4B-CHC-C1C	2.25	131.67	126.34
20	8	608	CLA	CHA-C1A-NA	-2.25	121.25	126.40
20	B	1241	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
36	5	502	LUT	C10-C11-C12	-2.25	116.20	123.22
36	6	502	LUT	C10-C11-C12	-2.25	116.20	123.22
20	6	601	CLA	CHA-C1A-NA	-2.25	121.25	126.40
20	B	1218	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
20	K	1402	CLA	CHA-C1A-NA	-2.25	121.25	126.40
20	1	611	CLA	C1-O2A-CGA	2.25	122.34	116.44
20	6	619	CLA	C4B-CHC-C1C	2.25	131.67	126.34
20	Z	602	CLA	CMA-C3A-C4A	2.25	117.81	111.77
20	B	1241	CLA	CHA-C1A-NA	-2.25	121.25	126.40
23	7	504	BCR	C23-C22-C21	2.25	122.39	118.94
20	6	607	CLA	C4B-CHC-C1C	2.25	131.66	126.34
20	7	612	CLA	C3B-C4B-NB	-2.25	108.43	110.52
20	3	616	CLA	C1D-ND-C4D	-2.25	104.74	106.33
20	3	612	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
20	Z	612	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
20	A	1131	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
20	A	1101	CLA	CHA-C1A-NA	-2.24	121.26	126.40
23	K	4002	BCR	C38-C26-C27	2.24	117.93	113.62
37	8	613	CHL	C1-O2A-CGA	2.24	122.33	116.44
20	K	1404	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
20	Z	606	CLA	C2D-C1D-ND	2.24	111.76	110.10
20	Z	612	CLA	CHA-C1A-NA	-2.24	121.26	126.40
20	6	606	CLA	CHA-C1A-NA	-2.24	121.26	126.40
36	7	502	LUT	C31-C32-C33	-2.24	120.12	126.42
20	5	606	CLA	O2A-CGA-CBA	2.24	118.94	111.91
20	1	605	CLA	C4B-CHC-C1C	2.24	131.66	126.34
20	5	608	CLA	C4B-CHC-C1C	2.24	131.66	126.34
20	4	603	CLA	CHA-C1A-NA	-2.24	121.26	126.40
20	7	604	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
20	K	1402	CLA	C1-O2A-CGA	2.24	122.32	116.44
20	Z	611	CLA	C4B-CHC-C1C	2.24	131.65	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	604	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
20	4	615	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
33	F	4001	RRX	C3-C4-C5	-2.24	110.08	114.08
36	5	502	LUT	C3-C4-C5	-2.24	107.39	111.85
36	6	502	LUT	C19-C9-C8	2.24	121.61	118.08
20	A	1116	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
20	B	1201	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
20	A	1102	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
20	6	619	CLA	CHA-C1A-NA	-2.24	121.27	126.40
20	4	606	CLA	O2A-CGA-CBA	2.24	118.94	111.91
20	8	611	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
20	7	605	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
20	1	604	CLA	C4B-CHC-C1C	2.24	131.65	126.34
20	5	606	CLA	CHA-C1A-NA	-2.24	121.27	126.40
23	J	4001	BCR	C35-C13-C12	2.24	121.60	118.08
20	3	612	CLA	CMA-C3A-C4A	2.24	117.79	111.77
20	3	601	CLA	C3B-C4B-NB	-2.24	108.44	110.52
20	1	603	CLA	O2A-CGA-CBA	2.24	118.93	111.91
23	4	503	BCR	C1-C6-C7	2.24	122.11	115.78
20	B	1226	CLA	CHD-C4C-C3C	2.24	128.13	124.84
20	1	608	CLA	C1D-ND-C4D	-2.24	104.75	106.33
20	A	1123	CLA	CHA-C1A-NA	-2.24	121.28	126.40
20	8	604	CLA	O1A-CGA-CBA	-2.24	115.01	123.73
20	A	1106	CLA	O2A-CGA-CBA	2.24	118.92	111.91
23	A	4001	BCR	C35-C13-C12	2.24	121.60	118.08
20	5	613	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
20	3	616	CLA	C3D-C2D-C1D	-2.23	102.78	105.83
20	6	603	CLA	CBA-CAA-C2A	2.23	120.46	113.86
37	6	610	CHL	CHD-C4C-C3C	2.23	128.12	124.84
23	A	4004	BCR	C35-C13-C12	2.23	121.60	118.08
20	7	604	CLA	CHA-C4D-ND	2.23	137.17	132.50
20	3	607	CLA	CHA-C1A-NA	-2.23	121.28	126.40
20	A	1127	CLA	CHA-C1A-NA	-2.23	121.28	126.40
36	8	502	LUT	C20-C13-C12	2.23	121.59	118.08
20	B	1209	CLA	CMA-C3A-C4A	2.23	117.77	111.77
20	7	612	CLA	C1D-ND-C4D	-2.23	104.75	106.33
20	G	1601	CLA	C4B-CHC-C1C	2.23	131.63	126.34
20	B	1022	CLA	CMA-C3A-C4A	2.23	117.77	111.77
20	6	618	CLA	CHA-C4D-ND	2.23	137.17	132.50
20	A	1127	CLA	O2A-CGA-CBA	2.23	118.91	111.91
20	6	605	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
20	L	1503	CLA	CAA-C2A-C3A	-2.23	106.67	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	8	605	CLA	CMA-C3A-C4A	2.23	117.77	111.77
19	A	1011	CL0	CMB-C2B-C1B	2.23	128.77	125.37
20	B	1021	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
20	Z	604	CLA	C4B-CHC-C1C	2.23	131.63	126.34
23	A	4003	BCR	C34-C9-C10	-2.23	119.80	122.92
20	Z	612	CLA	C3B-C4B-NB	-2.23	108.45	110.52
20	B	1226	CLA	CMA-C3A-C4A	2.23	117.76	111.77
20	B	1225	CLA	C1-O2A-CGA	2.23	122.29	116.44
20	A	1130	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
36	6	502	LUT	C8-C7-C6	-2.23	120.94	127.20
34	1	503	C7Z	C24-C25-C26	-2.23	115.88	120.85
20	B	1202	CLA	CMA-C3A-C4A	2.23	117.76	111.77
20	K	1403	CLA	CHA-C1A-NA	-2.23	121.30	126.40
20	A	1103	CLA	CHA-C4D-ND	2.23	137.16	132.50
20	6	604	CLA	C4B-CHC-C1C	2.23	131.62	126.34
20	3	613	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
20	A	1102	CLA	CHA-C1A-NA	-2.23	121.30	126.40
23	A	4004	BCR	C30-C25-C24	2.23	122.08	115.78
20	B	1220	CLA	CHA-C1A-NA	-2.23	121.30	126.40
20	1	611	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
20	1	607	CLA	C3B-C4B-NB	-2.22	108.45	110.52
20	3	613	CLA	C3B-C4B-NB	-2.22	108.45	110.52
20	A	1116	CLA	C2C-C1C-NC	2.22	112.06	109.97
20	B	1214	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
20	A	1116	CLA	C4B-CHC-C1C	2.22	131.61	126.34
20	B	1208	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
23	B	4001	BCR	C39-C30-C25	-2.22	106.69	110.30
20	A	1119	CLA	O2A-CGA-CBA	2.22	118.88	111.91
20	A	1112	CLA	C1-C2-C3	-2.22	122.20	126.04
20	8	612	CLA	C4B-CHC-C1C	2.22	131.61	126.34
20	7	604	CLA	CHA-C1A-NA	-2.22	121.31	126.40
20	6	604	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
20	B	1202	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
20	A	1126	CLA	CHA-C1A-NA	-2.22	121.31	126.40
20	Z	615	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
20	B	1203	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
20	A	1122	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	B	1232	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	8	602	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	B	1216	CLA	C4B-CHC-C1C	2.22	131.60	126.34
26	F	5001	LMT	C1'-O5'-C5'	-2.22	109.33	113.69
23	5	503	BCR	C38-C26-C25	-2.22	122.04	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1129	CLA	O2A-CGA-CBA	2.22	118.87	111.91
20	A	1108	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	A	1114	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	A	1129	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	Z	615	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
20	B	1222	CLA	CAA-C2A-C1A	-2.22	104.71	111.97
20	3	612	CLA	C4B-CHC-C1C	2.22	131.59	126.34
20	K	1403	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
20	B	1234	CLA	CHA-C1A-NA	-2.22	121.32	126.40
20	B	1222	CLA	CMB-C2B-C3B	2.22	131.95	126.59
20	B	1239	CLA	C4B-CHC-C1C	2.21	131.59	126.34
20	Z	605	CLA	C4B-CHC-C1C	2.21	131.59	126.34
20	Z	608	CLA	C4B-CHC-C1C	2.21	131.59	126.34
20	7	613	CLA	C4B-CHC-C1C	2.21	131.59	126.34
20	5	622	CLA	CHA-C1A-NA	-2.21	121.33	126.40
20	L	1503	CLA	O2A-CGA-CBA	2.21	118.86	111.91
36	6	501	LUT	C20-C13-C12	2.21	121.56	118.08
20	B	1222	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
20	Z	606	CLA	CHA-C1A-NA	-2.21	121.33	126.40
37	7	610	CHL	C1-C2-C3	-2.21	122.22	126.04
20	B	1226	CLA	C2A-C1A-CHA	2.21	127.73	123.86
37	8	610	CHL	CHD-C4C-C3C	2.21	128.09	124.84
20	1	606	CLA	C4B-CHC-C1C	2.21	131.59	126.34
20	6	615	CLA	CMA-C3A-C4A	2.21	117.72	111.77
20	B	1239	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
20	F	1302	CLA	CMA-C3A-C4A	2.21	117.72	111.77
20	3	605	CLA	CHA-C1A-NA	-2.21	121.33	126.40
20	K	1402	CLA	C4B-CHC-C1C	2.21	131.59	126.34
20	G	1601	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
20	7	613	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
20	7	601	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
23	A	4003	BCR	C31-C1-C6	-2.21	106.71	110.30
20	7	615	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
20	1	604	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
20	1	607	CLA	O2A-CGA-CBA	2.21	118.84	111.91
20	3	604	CLA	C3A-C2A-C1A	2.21	104.65	101.34
20	8	606	CLA	CMA-C3A-C4A	2.21	117.71	111.77
20	B	1224	CLA	C4B-CHC-C1C	2.21	131.58	126.34
20	8	609	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
20	A	1137	CLA	C4B-CHC-C1C	2.21	131.58	126.34
20	A	1108	CLA	C2A-C1A-CHA	2.21	127.72	123.86
20	Z	606	CLA	O1D-CGD-CBD	-2.21	119.96	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1229	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
20	B	1214	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
20	A	1125	CLA	CHA-C1A-NA	-2.21	121.34	126.40
20	A	1107	CLA	C4B-CHC-C1C	2.21	131.57	126.34
20	A	1141	CLA	CMA-C3A-C4A	2.21	117.71	111.77
20	A	1104	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
20	A	1118	CLA	CHA-C1A-NA	-2.21	121.34	126.40
20	B	1223	CLA	C1D-ND-C4D	-2.21	104.77	106.33
20	A	1130	CLA	C4B-CHC-C1C	2.21	131.57	126.34
20	Z	607	CLA	C4B-CHC-C1C	2.21	131.57	126.34
20	4	608	CLA	O2A-CGA-CBA	2.21	118.83	111.91
20	7	606	CLA	C4B-CHC-C1C	2.21	131.57	126.34
23	A	4002	BCR	C33-C5-C4	2.21	117.85	113.62
20	A	1122	CLA	C4B-CHC-C1C	2.21	131.57	126.34
20	Z	602	CLA	CHA-C1A-NA	-2.21	121.35	126.40
20	Z	612	CLA	C4B-CHC-C1C	2.21	131.57	126.34
20	8	605	CLA	C4B-CHC-C1C	2.20	131.57	126.34
23	B	4003	BCR	C1-C6-C5	-2.20	119.51	122.61
20	Z	605	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
20	Z	601	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
34	5	505	C7Z	C30-C31-C32	-2.20	116.34	123.22
20	8	608	CLA	C1-C2-C3	-2.20	122.23	126.04
20	A	1135	CLA	CHA-C1A-NA	-2.20	121.35	126.40
20	B	1237	CLA	O2A-CGA-CBA	2.20	118.82	111.91
20	8	601	CLA	C3B-C4B-NB	-2.20	108.47	110.52
20	8	607	CLA	C4B-CHC-C1C	2.20	131.56	126.34
20	K	1404	CLA	CHD-C1D-ND	-2.20	122.43	124.45
20	5	601	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
20	A	1104	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
20	7	608	CLA	CMC-C2C-C1C	2.20	128.39	125.04
34	J	4002	C7Z	C20-C13-C12	2.20	121.54	118.08
20	6	608	CLA	C4B-CHC-C1C	2.20	131.56	126.34
20	B	1223	CLA	CHA-C1A-NA	-2.20	121.36	126.40
20	A	1122	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
20	B	1229	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
20	B	1208	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
20	B	1021	CLA	O2A-CGA-CBA	2.20	118.81	111.91
20	A	1103	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
20	8	609	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
20	1	605	CLA	CHA-C1A-NA	-2.20	121.36	126.40
20	A	1121	CLA	C1D-ND-C4D	-2.20	104.77	106.33
20	6	605	CLA	C3D-C2D-C1D	-2.20	102.83	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1236	CLA	CMA-C3A-C4A	2.20	117.68	111.77
20	A	1109	CLA	C2D-C1D-ND	2.20	111.72	110.10
20	B	1226	CLA	CBA-CAA-C2A	2.19	120.34	113.86
36	4	502	LUT	C7-C8-C9	-2.19	122.92	126.23
20	A	1101	CLA	CMA-C3A-C4A	2.19	117.67	111.77
20	B	1238	CLA	CHA-C1A-NA	-2.19	121.38	126.40
20	6	615	CLA	C4B-CHC-C1C	2.19	131.54	126.34
20	A	1105	CLA	C1-C2-C3	-2.19	122.25	126.04
23	L	4002	BCR	C19-C18-C17	2.19	122.31	118.94
20	Z	606	CLA	CMC-C2C-C1C	2.19	128.38	125.04
20	L	1502	CLA	C3B-C4B-NB	-2.19	108.48	110.52
20	6	604	CLA	CHA-C1A-NA	-2.19	121.38	126.40
37	7	610	CHL	C4D-CHA-C1A	2.19	123.92	121.25
20	B	1203	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
20	3	601	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
20	3	607	CLA	C4B-CHC-C1C	2.19	131.53	126.34
20	4	602	CLA	C3B-C4B-NB	-2.19	108.48	110.52
20	5	602	CLA	C1D-ND-C4D	-2.19	104.78	106.33
23	A	4002	BCR	C34-C9-C10	-2.19	119.86	122.92
20	8	611	CLA	C4B-CHC-C1C	2.19	131.53	126.34
20	B	1209	CLA	CHA-C1A-NA	-2.19	121.39	126.40
20	3	608	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
20	A	1137	CLA	CAA-CBA-CGA	-2.19	106.86	113.25
20	8	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
20	4	612	CLA	CHA-C1A-NA	-2.19	121.39	126.40
20	5	607	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
20	A	1128	CLA	C1-O2A-CGA	2.19	122.18	116.44
20	B	1231	CLA	C1D-ND-C4D	-2.19	104.78	106.33
20	6	612	CLA	O2A-CGA-CBA	2.19	118.77	111.91
20	3	613	CLA	C4B-CHC-C1C	2.19	131.53	126.34
20	4	603	CLA	C4B-CHC-C1C	2.19	131.53	126.34
20	1	604	CLA	C1D-ND-C4D	-2.19	104.78	106.33
20	7	611	CLA	O2A-CGA-CBA	2.19	118.77	111.91
20	6	601	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
20	1	601	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
20	6	608	CLA	C3B-C4B-NB	-2.18	108.49	110.52
20	B	1238	CLA	C4B-CHC-C1C	2.18	131.52	126.34
20	7	609	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
20	6	615	CLA	O2A-CGA-CBA	2.18	118.76	111.91
20	7	607	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
36	Z	502	LUT	C10-C11-C12	-2.18	116.40	123.22
20	B	1222	CLA	CHA-C1A-NA	-2.18	121.40	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	611	CLA	C1-O2A-CGA	2.18	122.17	116.44
20	1	612	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
20	A	1125	CLA	C1D-ND-C4D	-2.18	104.78	106.33
20	K	1404	CLA	C4B-CHC-C1C	2.18	131.52	126.34
20	3	602	CLA	C4B-CHC-C1C	2.18	131.52	126.34
20	L	1502	CLA	O2A-CGA-CBA	2.18	118.76	111.91
20	4	607	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
24	8	801	LHG	C5-O7-C7	-2.18	112.42	117.79
37	1	610	CHL	CHC-C1C-NC	2.18	127.51	124.20
20	Z	606	CLA	C1C-C2C-C3C	-2.18	104.66	106.96
20	3	610	CLA	CHA-C1A-NA	-2.18	121.40	126.40
20	5	604	CLA	CAC-C3C-C4C	2.18	127.64	124.81
20	A	1137	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
20	4	609	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
20	A	1122	CLA	C2A-C1A-CHA	2.18	127.67	123.86
20	B	1229	CLA	CHA-C1A-NA	-2.18	121.40	126.40
23	J	4001	BCR	C38-C26-C27	2.18	117.81	113.62
20	3	607	CLA	CAC-C3C-C4C	2.18	127.64	124.81
20	5	622	CLA	C3B-C4B-NB	-2.18	108.49	110.52
20	1	612	CLA	C2A-C1A-CHA	2.18	127.67	123.86
20	4	602	CLA	CHA-C1A-NA	-2.18	121.41	126.40
34	5	505	C7Z	C39-C29-C30	-2.18	119.87	122.92
20	A	1102	CLA	C2C-C1C-NC	2.18	112.01	109.97
20	B	1227	CLA	C2D-C1D-ND	2.18	111.71	110.10
20	8	605	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
23	7	503	BCR	C38-C26-C25	-2.18	122.08	124.53
20	B	1214	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
20	B	1226	CLA	CAC-C3C-C2C	-2.18	123.81	127.53
23	L	4002	BCR	C33-C5-C4	2.18	117.80	113.62
20	4	609	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
20	7	601	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
20	A	1128	CLA	CHA-C1A-NA	-2.18	121.42	126.40
20	A	1131	CLA	C4B-CHC-C1C	2.18	131.50	126.34
23	B	4007	BCR	C35-C13-C12	2.18	121.50	118.08
20	B	1023	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
20	A	1102	CLA	C1-C2-C3	-2.17	122.28	126.04
20	A	1131	CLA	CHA-C1A-NA	-2.17	121.42	126.40
20	7	613	CLA	CHA-C1A-NA	-2.17	121.42	126.40
36	4	501	LUT	C19-C9-C8	2.17	121.50	118.08
20	7	613	CLA	C3B-C4B-NB	-2.17	108.50	110.52
20	1	607	CLA	C4B-CHC-C1C	2.17	131.49	126.34
23	B	4005	BCR	C1-C6-C5	-2.17	119.55	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1228	CLA	C1D-ND-C4D	-2.17	104.79	106.33
20	1	611	CLA	C1D-ND-C4D	-2.17	104.79	106.33
20	B	1022	CLA	C1-C2-C3	-2.17	122.28	126.04
20	B	1210	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
23	J	4001	BCR	C12-C13-C14	-2.17	115.61	118.94
20	7	602	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
20	7	611	CLA	CHA-C1A-NA	-2.17	121.42	126.40
36	1	502	LUT	C20-C13-C12	2.17	121.50	118.08
20	3	618	CLA	C3B-C4B-NB	-2.17	108.50	110.52
20	7	603	CLA	C1D-ND-C4D	-2.17	104.79	106.33
20	A	1126	CLA	CMA-C3A-C4A	2.17	117.61	111.77
20	Z	611	CLA	C3B-C4B-NB	-2.17	108.50	110.52
20	B	1217	CLA	C1D-ND-C4D	-2.17	104.79	106.33
36	3	502	LUT	C39-C29-C28	2.17	121.49	118.08
20	6	605	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
23	B	4002	BCR	C34-C9-C10	-2.17	119.89	122.92
20	3	603	CLA	C1-C2-C3	-2.17	122.30	126.04
20	A	1135	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
20	K	1401	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
20	A	1125	CLA	C1-O2A-CGA	2.17	122.13	116.44
20	6	619	CLA	CMB-C2B-C3B	2.17	131.83	126.59
20	B	1213	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
20	1	606	CLA	CHA-C1A-NA	-2.16	121.44	126.40
20	8	604	CLA	C1-O2A-CGA	2.16	122.12	116.44
20	4	607	CLA	C4B-CHC-C1C	2.16	131.47	126.34
20	B	1221	CLA	C4B-CHC-C1C	2.16	131.47	126.34
20	4	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
37	5	617	CHL	CHD-C4C-C3C	2.16	128.02	124.84
20	B	1214	CLA	C3B-C4B-NB	-2.16	108.51	110.52
20	K	1404	CLA	C3B-C4B-NB	-2.16	108.51	110.52
20	K	1402	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
23	B	4003	BCR	C36-C18-C17	-2.16	119.89	122.92
20	Z	611	CLA	C1-O2A-CGA	2.16	122.12	116.44
20	3	606	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
20	A	1103	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
20	6	615	CLA	C2A-C1A-CHA	2.16	127.64	123.86
20	5	608	CLA	CHA-C1A-NA	-2.16	121.45	126.40
20	A	1126	CLA	C4B-CHC-C1C	2.16	131.46	126.34
23	L	4001	BCR	C35-C13-C12	2.16	121.48	118.08
20	A	1140	CLA	CHA-C1A-NA	-2.16	121.45	126.40
20	Z	605	CLA	O2A-CGA-CBA	2.16	118.69	111.91
20	7	605	CLA	CAA-C2A-C3A	-2.16	106.86	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	604	CLA	C1-O2A-CGA	2.16	122.11	116.44
20	5	618	CLA	C4B-CHC-C1C	2.16	131.46	126.34
20	A	1138	CLA	C1D-ND-C4D	-2.16	104.80	106.33
37	5	610	CHL	CHC-C1C-NC	2.16	127.48	124.20
36	Z	503	LUT	C22-C23-C24	-2.16	109.28	111.74
20	B	1212	CLA	C1-O2A-CGA	2.16	122.10	116.44
20	A	1112	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
20	Z	605	CLA	CMA-C3A-C4A	2.16	117.57	111.77
20	1	601	CLA	C2A-C1A-CHA	2.16	127.63	123.86
34	J	4002	C7Z	C37-C21-C26	-2.16	106.80	110.30
25	8	802	NKP	OAB-PAC-OAF	-2.16	101.00	106.73
20	6	606	CLA	O2A-CGA-CBA	2.16	118.67	111.91
23	6	504	BCR	C23-C22-C21	-2.16	115.63	118.94
20	B	1225	CLA	CHD-C1D-ND	-2.16	122.47	124.45
20	4	601	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
20	A	1119	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
20	5	607	CLA	CHA-C1A-NA	-2.15	121.46	126.40
20	7	603	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
20	6	604	CLA	CBA-CAA-C2A	2.15	120.22	113.86
20	6	612	CLA	C1-O2A-CGA	2.15	122.10	116.44
20	A	1101	CLA	C1D-ND-C4D	-2.15	104.81	106.33
20	B	1212	CLA	CHA-C1A-NA	-2.15	121.47	126.40
20	3	616	CLA	CHA-C1A-NA	-2.15	121.47	126.40
20	A	1103	CLA	CHA-C1A-NA	-2.15	121.47	126.40
20	Z	602	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
20	B	1207	CLA	CHA-C1A-NA	-2.15	121.47	126.40
23	5	503	BCR	C1-C6-C5	-2.15	119.58	122.61
20	Z	615	CLA	CHA-C1A-NA	-2.15	121.47	126.40
20	6	603	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
20	J	1901	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
20	A	1113	CLA	C2D-C1D-ND	2.15	111.69	110.10
20	1	613	CLA	C2D-C1D-ND	2.15	111.69	110.10
20	4	612	CLA	O2A-CGA-CBA	2.15	118.66	111.91
20	A	1124	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
20	K	1403	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
20	7	605	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
20	B	1227	CLA	C4B-CHC-C1C	2.15	131.44	126.34
20	1	608	CLA	O2A-CGA-CBA	2.15	118.66	111.91
20	8	607	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
20	B	1021	CLA	CHA-C1A-NA	-2.15	121.47	126.40
20	7	615	CLA	C1D-ND-C4D	-2.15	104.81	106.33
20	A	1122	CLA	C3B-C4B-NB	-2.15	108.52	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	J	4002	C7Z	C24-C25-C26	-2.15	116.06	120.85
20	B	1219	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
20	A	1115	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
20	8	609	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
20	8	602	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
20	B	1230	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
33	F	4001	RRX	C7-C6-C5	-2.15	116.26	121.46
20	B	1219	CLA	C3B-C4B-NB	-2.15	108.52	110.52
20	4	607	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
20	7	602	CLA	CHA-C1A-NA	-2.15	121.48	126.40
23	K	4002	BCR	C38-C26-C25	-2.15	122.12	124.53
20	B	1211	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
20	8	604	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
37	6	613	CHL	C4D-CHA-C1A	2.14	123.86	121.25
31	B	5003	DGD	O6D-C5D-C6D	2.14	110.99	106.67
20	4	605	CLA	CHA-C1A-NA	-2.14	121.49	126.40
20	G	1602	CLA	C1D-ND-C4D	-2.14	104.81	106.33
20	1	611	CLA	C4B-CHC-C1C	2.14	131.42	126.34
20	B	1223	CLA	O2A-CGA-CBA	2.14	118.63	111.91
20	A	1114	CLA	O2A-CGA-CBA	2.14	118.63	111.91
20	B	1241	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
20	B	1201	CLA	C3B-C2B-C1B	-2.14	104.58	107.16
23	7	503	BCR	C34-C9-C10	-2.14	119.92	122.92
20	6	601	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
20	1	613	CLA	CHA-C1A-NA	-2.14	121.50	126.40
20	B	1218	CLA	CMC-C2C-C1C	2.14	128.30	125.04
20	B	1227	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
20	3	604	CLA	CHA-C4D-ND	2.14	136.97	132.50
20	A	1104	CLA	C4B-CHC-C1C	2.14	131.41	126.34
20	B	1227	CLA	C1D-ND-C4D	-2.14	104.81	106.33
20	7	606	CLA	O2A-CGA-CBA	2.14	118.62	111.91
36	8	502	LUT	C19-C9-C8	2.14	121.45	118.08
20	6	607	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
20	B	1202	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
37	8	613	CHL	C4D-CHA-C1A	2.14	123.85	121.25
20	6	603	CLA	O1A-CGA-CBA	-2.14	115.39	123.73
23	G	4001	BCR	C38-C26-C25	-2.14	122.13	124.53
20	A	1137	CLA	C1D-ND-C4D	-2.14	104.82	106.33
20	1	603	CLA	C1D-ND-C4D	-2.14	104.82	106.33
20	7	608	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
20	Z	604	CLA	CMC-C2C-C1C	2.14	128.29	125.04
20	A	1012	CLA	O1D-CGD-CBD	-2.14	120.11	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1228	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
20	B	1203	CLA	C3B-C4B-NB	-2.14	108.53	110.52
20	A	1103	CLA	O2A-CGA-CBA	2.14	118.61	111.91
20	B	1205	CLA	CMA-C3A-C4A	2.14	117.51	111.77
20	A	1123	CLA	O2A-CGA-CBA	2.14	118.61	111.91
20	B	1215	CLA	O2A-CGA-CBA	2.14	118.61	111.91
20	Z	604	CLA	O2A-CGA-CBA	2.14	118.61	111.91
23	6	503	BCR	C31-C1-C6	-2.14	106.83	110.30
20	F	1301	CLA	C1D-ND-C4D	-2.14	104.82	106.33
20	1	603	CLA	C1-C2-C3	-2.14	122.35	126.04
20	A	1129	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
25	3	802	NKP	OAB-PAC-OAF	-2.13	101.05	106.73
20	A	1124	CLA	CHA-C1A-NA	-2.13	121.51	126.40
23	6	503	BCR	C1-C6-C5	-2.13	119.61	122.61
20	5	613	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
20	B	1216	CLA	CHA-C1A-NA	-2.13	121.51	126.40
20	B	1023	CLA	C3B-C2B-C1B	-2.13	104.59	107.16
20	B	1023	CLA	CHA-C1A-NA	-2.13	121.51	126.40
20	B	1219	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
23	5	503	BCR	C31-C1-C6	-2.13	106.84	110.30
20	A	1126	CLA	C2D-C1D-ND	2.13	111.68	110.10
23	B	4006	BCR	C38-C26-C27	2.13	117.71	113.62
20	B	1022	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
23	I	4001	BCR	C33-C5-C6	-2.13	122.14	124.53
20	A	1133	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
20	4	606	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	B	5003	DGD	O2G-C1B-O1B	-2.13	118.55	123.70
20	A	1012	CLA	C4B-CHC-C1C	2.13	131.39	126.34
20	B	1210	CLA	CHA-C1A-NA	-2.13	121.52	126.40
20	B	1212	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
23	8	503	BCR	C33-C5-C4	2.13	117.71	113.62
20	8	602	CLA	C3B-C4B-NB	-2.13	108.54	110.52
20	B	1201	CLA	C2C-C1C-NC	2.13	111.97	109.97
20	B	1213	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
20	3	605	CLA	CAC-C3C-C4C	2.13	127.57	124.81
20	A	1121	CLA	CHA-C1A-NA	-2.13	121.53	126.40
20	3	607	CLA	O2A-CGA-CBA	2.13	118.58	111.91
20	5	612	CLA	CMA-C3A-C4A	2.13	117.49	111.77
20	6	604	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
25	A	5004	NKP	OAB-PAC-OAF	-2.13	101.07	106.73
20	Z	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
37	Z	609	CHL	C1-O2A-CGA	2.13	122.02	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	610	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
20	6	605	CLA	C2A-C1A-CHA	2.13	127.58	123.86
20	Z	611	CLA	CHA-C1A-NA	-2.13	121.53	126.40
20	Z	604	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
20	6	606	CLA	C1D-ND-C4D	-2.13	104.83	106.33
20	1	612	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
20	3	607	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
20	1	611	CLA	C3B-C4B-NB	-2.12	108.54	110.52
20	A	1111	CLA	C1C-C2C-C3C	-2.12	104.72	106.96
20	4	608	CLA	C4B-CHC-C1C	2.12	131.38	126.34
23	B	4004	BCR	C31-C1-C6	-2.12	106.85	110.30
36	8	502	LUT	C18-C5-C6	-2.12	122.14	124.53
36	3	502	LUT	C15-C35-C34	-2.12	119.12	123.47
20	3	606	CLA	O2A-CGA-CBA	2.12	118.57	111.91
23	6	504	BCR	C4-C5-C6	-2.12	119.65	122.73
20	5	613	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
20	5	606	CLA	C1-O2A-CGA	2.12	122.01	116.44
20	F	1301	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
20	B	1215	CLA	C3B-C4B-NB	-2.12	108.55	110.52
20	A	1013	CLA	C2C-C1C-NC	2.12	111.96	109.97
20	5	601	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
20	6	618	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
36	6	502	LUT	C3-C4-C5	-2.12	107.63	111.85
37	6	617	CHL	C3C-C4C-NC	-2.12	108.19	110.57
20	4	612	CLA	C1-O2A-CGA	2.12	122.01	116.44
37	4	611	CHL	C3B-C4B-NB	-2.12	108.55	110.52
36	5	502	LUT	C7-C8-C9	-2.12	123.03	126.23
20	B	1225	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
20	7	612	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
20	A	1012	CLA	C2A-C1A-CHA	2.12	127.56	123.86
34	J	4002	C7Z	C38-C25-C24	2.12	118.28	114.36
37	Z	610	CHL	C1-C2-C3	-2.12	122.38	126.04
20	B	1211	CLA	CHA-C1A-NA	-2.12	121.55	126.40
20	8	602	CLA	C4B-CHC-C1C	2.12	131.36	126.34
20	3	601	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
20	3	606	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
23	B	4003	BCR	C12-C13-C14	-2.12	115.69	118.94
26	B	6101	LMT	O5'-C1'-C2'	-2.12	105.87	110.35
20	1	612	CLA	C3B-C4B-NB	-2.12	108.55	110.52
20	A	1141	CLA	C4B-CHC-C1C	2.12	131.35	126.34
23	J	4001	BCR	C31-C1-C6	-2.11	106.87	110.30
20	3	608	CLA	C4B-CHC-C1C	2.11	131.35	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1222	CLA	C1D-ND-C4D	-2.11	104.83	106.33
37	4	613	CHL	C2C-C3C-C4C	2.11	108.00	106.49
37	Z	610	CHL	C1-O2A-CGA	2.11	121.99	116.44
20	8	602	CLA	C6-C7-C8	-2.11	109.09	115.92
20	A	1112	CLA	C4B-CHC-C1C	2.11	131.35	126.34
23	5	503	BCR	C8-C7-C6	-2.11	121.27	127.20
36	7	501	LUT	C20-C13-C12	2.11	121.40	118.08
20	7	609	CLA	C1D-ND-C4D	-2.11	104.84	106.33
23	3	505	BCR	C33-C5-C6	-2.11	122.16	124.53
20	4	605	CLA	O2A-CGA-CBA	2.11	118.53	111.91
20	5	602	CLA	CHA-C1A-NA	-2.11	121.57	126.40
20	5	605	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
20	B	1023	CLA	CBB-CAB-C3B	-2.11	117.13	127.62
20	G	1602	CLA	C4B-CHC-C1C	2.11	131.34	126.34
37	1	610	CHL	C4D-CHA-C1A	2.11	123.81	121.25
20	A	1122	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
20	A	1133	CLA	C3B-C4B-NB	-2.11	108.56	110.52
20	A	1104	CLA	CMA-C3A-C4A	2.11	117.44	111.77
20	7	603	CLA	C2A-C1A-CHA	2.11	127.55	123.86
20	B	1225	CLA	C1-C2-C3	-2.11	122.40	126.04
20	4	609	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
20	B	1230	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
20	6	603	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
20	7	601	CLA	CHA-C1A-NA	-2.11	121.57	126.40
20	B	1213	CLA	C4B-CHC-C1C	2.11	131.33	126.34
20	A	1137	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
20	1	601	CLA	O2A-CGA-CBA	2.11	118.52	111.91
37	5	611	CHL	CHC-C1C-NC	2.11	127.40	124.20
20	A	1013	CLA	O2A-CGA-CBA	2.11	118.51	111.91
20	B	1236	CLA	CHA-C1A-NA	-2.11	121.58	126.40
20	1	601	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
20	Z	605	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
20	B	1221	CLA	CMA-C3A-C2A	2.10	122.32	113.83
23	A	4001	BCR	C40-C30-C25	-2.10	106.89	110.30
20	A	1012	CLA	C3B-C2B-C1B	-2.10	104.62	107.16
26	4	803	LMT	C1'-O5'-C5'	-2.10	109.56	113.69
20	A	1133	CLA	CHA-C1A-NA	-2.10	121.58	126.40
23	3	503	BCR	C37-C22-C23	2.10	121.39	118.08
20	A	1116	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
20	7	602	CLA	O2A-CGA-CBA	2.10	118.50	111.91
20	4	608	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
20	6	619	CLA	CMD-C2D-C3D	-2.10	122.78	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1119	CLA	CHA-C1A-NA	-2.10	121.58	126.40
20	A	1108	CLA	C2D-C1D-ND	2.10	111.65	110.10
20	Z	604	CLA	CHA-C1A-NA	-2.10	121.58	126.40
20	A	1132	CLA	CHA-C1A-NA	-2.10	121.59	126.40
23	8	503	BCR	C19-C18-C17	2.10	122.17	118.94
23	5	504	BCR	C38-C26-C27	2.10	117.65	113.62
20	A	1121	CLA	C6-C5-C3	-2.10	107.95	113.45
20	5	605	CLA	C1D-ND-C4D	-2.10	104.84	106.33
24	8	801	LHG	O8-C23-O10	-2.10	118.29	123.59
36	3	501	LUT	C10-C11-C12	-2.10	116.66	123.22
20	4	601	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
23	3	503	BCR	C34-C9-C8	2.10	121.39	118.08
20	B	1214	CLA	O2A-CGA-CBA	2.10	118.50	111.91
20	B	1229	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
36	6	502	LUT	C18-C5-C6	-2.10	122.17	124.53
20	A	1116	CLA	C1-O2A-CGA	2.10	121.95	116.44
20	A	1108	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
20	A	1112	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
20	K	1404	CLA	O2A-CGA-CBA	2.10	118.49	111.91
23	5	504	BCR	C3-C4-C5	-2.10	110.33	114.08
21	A	2001	PQN	C11-C12-C13	-2.10	123.30	126.79
20	A	1137	CLA	CHA-C1A-NA	-2.10	121.60	126.40
20	8	607	CLA	CHA-C1A-NA	-2.10	121.60	126.40
20	B	1218	CLA	C1-O2A-CGA	2.10	121.94	116.44
20	1	604	CLA	C3B-C4B-NB	-2.10	108.57	110.52
20	1	613	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
20	B	1218	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
20	Z	603	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
20	7	609	CLA	CHA-C1A-NA	-2.09	121.60	126.40
20	7	606	CLA	CHA-C1A-NA	-2.09	121.60	126.40
23	G	4001	BCR	C12-C13-C14	-2.09	115.73	118.94
36	5	502	LUT	C35-C34-C33	-2.09	124.32	127.31
36	4	502	LUT	C31-C32-C33	-2.09	120.54	126.42
20	A	1125	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
23	I	4001	BCR	C33-C5-C4	2.09	117.63	113.62
24	4	801	LHG	O7-C7-O9	-2.09	118.65	123.70
20	7	604	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
20	A	1141	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
36	3	502	LUT	C2-C3-C4	-2.09	107.44	110.30
20	A	1128	CLA	CMA-C3A-C4A	2.09	117.39	111.77
20	6	602	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
20	B	1240	CLA	C1C-C2C-C3C	-2.09	104.76	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	7	609	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
20	A	1104	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
20	8	606	CLA	C1D-ND-C4D	-2.09	104.85	106.33
20	4	604	CLA	C1D-ND-C4D	-2.09	104.85	106.33
20	B	1023	CLA	C2A-C1A-CHA	2.09	127.51	123.86
20	A	1127	CLA	CHD-C1D-ND	-2.09	122.54	124.45
20	3	603	CLA	O1A-CGA-CBA	-2.09	115.59	123.73
20	B	1215	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
20	5	615	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
37	3	611	CHL	C3B-C2B-C1B	2.09	109.68	107.16
36	8	501	LUT	C30-C31-C32	-2.09	116.71	123.22
23	5	504	BCR	C31-C1-C6	-2.09	106.92	110.30
37	5	610	CHL	C3C-C4C-NC	-2.09	108.23	110.57
20	B	1205	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
23	B	4007	BCR	C33-C5-C4	2.08	117.62	113.62
20	3	610	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
20	5	601	CLA	C2A-C1A-CHA	2.08	127.50	123.86
20	A	1113	CLA	O2A-CGA-CBA	2.08	118.45	111.91
20	G	1601	CLA	O2A-CGA-CBA	2.08	118.45	111.91
20	3	610	CLA	C2A-C1A-CHA	2.08	127.50	123.86
23	B	4006	BCR	C33-C5-C4	2.08	117.62	113.62
20	6	608	CLA	C2A-C1A-CHA	2.08	127.50	123.86
20	3	602	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
20	A	1107	CLA	C3B-C4B-NB	-2.08	108.58	110.52
20	3	606	CLA	C3B-C4B-NB	-2.08	108.58	110.52
36	Z	502	LUT	C39-C29-C28	2.08	121.36	118.08
20	Z	615	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
20	B	1209	CLA	C1D-ND-C4D	-2.08	104.86	106.33
20	8	606	CLA	O2A-CGA-CBA	2.08	118.44	111.91
20	A	1132	CLA	C2D-C1D-ND	2.08	111.64	110.10
20	7	607	CLA	CHA-C1A-NA	-2.08	121.63	126.40
20	8	615	CLA	C3B-C4B-NB	-2.08	108.58	110.52
20	B	1238	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
20	6	601	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
20	A	1120	CLA	O2A-CGA-CBA	2.08	118.44	111.91
20	8	603	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
20	5	604	CLA	O1A-CGA-CBA	-2.08	115.62	123.73
36	8	501	LUT	C18-C5-C6	-2.08	122.19	124.53
20	5	612	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	J	1901	CLA	C2A-C1A-CHA	2.08	127.49	123.86
23	7	503	BCR	C15-C14-C13	-2.08	124.34	127.31
20	A	1115	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1201	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
20	6	609	CLA	C1D-ND-C4D	-2.08	104.86	106.33
20	B	1206	CLA	C4B-CHC-C1C	2.08	131.27	126.34
20	B	1208	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
20	4	603	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
20	B	1217	CLA	CHA-C1A-NA	-2.08	121.64	126.40
20	5	601	CLA	CHA-C1A-NA	-2.08	121.64	126.40
36	3	501	LUT	C37-C21-C22	-2.08	105.50	109.44
20	Z	608	CLA	C1D-ND-C4D	-2.07	104.86	106.33
20	8	601	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
36	1	502	LUT	C31-C30-C29	-2.07	124.35	127.31
20	B	1222	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
20	B	1213	CLA	C1D-ND-C4D	-2.07	104.86	106.33
20	A	1103	CLA	CAC-C3C-C4C	2.07	127.50	124.81
20	A	1107	CLA	CHA-C1A-NA	-2.07	121.65	126.40
20	B	1221	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
36	4	501	LUT	C40-C33-C34	-2.07	120.02	122.92
20	B	1223	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
20	A	1133	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
20	B	1239	CLA	CHA-C1A-NA	-2.07	121.65	126.40
20	6	615	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
37	4	613	CHL	CHD-C4C-C3C	2.07	127.89	124.84
20	8	612	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
20	A	1134	CLA	CHA-C1A-NA	-2.07	121.66	126.40
20	B	1215	CLA	C1D-ND-C4D	-2.07	104.86	106.33
20	B	1219	CLA	C4B-CHC-C1C	2.07	131.25	126.34
20	B	1204	CLA	CMA-C3A-C4A	2.07	117.34	111.77
20	K	1403	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
23	A	4005	BCR	C37-C22-C23	2.07	121.34	118.08
20	1	611	CLA	O2A-CGA-CBA	2.07	118.40	111.91
20	4	604	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
20	A	1127	CLA	C1D-ND-C4D	-2.07	104.86	106.33
35	7	804	SPH	O3-C3-C2	2.07	110.60	107.31
20	A	1105	CLA	CMC-C2C-C1C	2.07	128.19	125.04
20	Z	602	CLA	C4B-CHC-C1C	2.07	131.25	126.34
23	J	4001	BCR	C34-C9-C10	-2.07	120.03	122.92
20	A	1104	CLA	CHA-C1A-NA	-2.07	121.66	126.40
23	6	503	BCR	C36-C18-C17	-2.07	120.03	122.92
20	B	1237	CLA	C4B-CHC-C1C	2.07	131.24	126.34
20	8	606	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
20	5	618	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
20	A	1108	CLA	C3B-C4B-NB	-2.07	108.60	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	1302	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
20	A	1119	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
20	A	1138	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
20	1	612	CLA	O2A-CGA-CBA	2.07	118.39	111.91
20	6	615	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
20	5	607	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
20	4	615	CLA	CAC-C3C-C4C	2.07	127.49	124.81
20	G	1602	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
20	B	1222	CLA	C3B-C4B-NB	-2.07	108.60	110.52
20	K	1404	CLA	C1D-ND-C4D	-2.07	104.87	106.33
20	4	603	CLA	C1D-ND-C4D	-2.07	104.87	106.33
20	B	1227	CLA	CHA-C1A-NA	-2.06	121.67	126.40
31	B	5003	DGD	O1G-C1A-O1A	-2.06	118.38	123.59
20	A	1117	CLA	CBA-CAA-C2A	2.06	119.96	113.86
20	A	1112	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
23	K	4001	BCR	C2-C1-C6	2.06	113.66	110.48
20	5	613	CLA	C1D-ND-C4D	-2.06	104.87	106.33
23	B	4002	BCR	C38-C26-C27	2.06	117.58	113.62
20	A	1116	CLA	C2A-C1A-CHA	2.06	127.47	123.86
37	6	610	CHL	C3B-C4B-NB	-2.06	108.60	110.52
20	A	1137	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
20	B	1231	CLA	O2A-CGA-CBA	2.06	118.38	111.91
20	8	603	CLA	C11-C10-C8	-2.06	109.25	115.92
20	B	1218	CLA	CHA-C1A-NA	-2.06	121.67	126.40
20	B	1230	CLA	CHA-C1A-NA	-2.06	121.67	126.40
20	8	602	CLA	CMA-C3A-C4A	2.06	117.31	111.77
20	A	1134	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
20	1	603	CLA	CMC-C2C-C1C	2.06	128.18	125.04
20	B	1224	CLA	C2A-C1A-CHA	2.06	127.46	123.86
36	8	502	LUT	C39-C29-C28	2.06	121.33	118.08
20	5	605	CLA	CHA-C1A-NA	-2.06	121.68	126.40
20	3	604	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
20	8	609	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	A	1011	CL0	C4-C3-C5	2.06	118.74	115.27
37	4	610	CHL	CMA-C3A-C2A	2.06	122.13	113.83
23	B	4007	BCR	C36-C18-C17	-2.06	120.04	122.92
20	G	1601	CLA	CHA-C1A-NA	-2.06	121.68	126.40
26	4	803	LMT	O5B-C5B-C4B	2.06	113.43	109.69
20	8	604	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
20	1	604	CLA	CHA-C1A-NA	-2.06	121.69	126.40
20	8	603	CLA	CHA-C1A-NA	-2.06	121.69	126.40
20	A	1139	CLA	CMD-C2D-C3D	-2.06	122.88	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	K	1402	CLA	C1D-ND-C4D	-2.06	104.87	106.33
20	Z	605	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
20	5	612	CLA	CMD-C2D-C3D	-2.06	122.89	127.61
20	6	606	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
20	6	615	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
20	B	1230	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
20	3	604	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
20	5	612	CLA	C3B-C4B-NB	-2.05	108.61	110.52
20	3	618	CLA	C1D-ND-C4D	-2.05	104.88	106.33
20	L	1503	CLA	CHA-C1A-NA	-2.05	121.70	126.40
20	8	612	CLA	C2A-C1A-CHA	2.05	127.45	123.86
37	6	613	CHL	C4A-NA-C1A	2.05	107.63	106.71
36	8	501	LUT	C31-C30-C29	-2.05	124.38	127.31
37	1	609	CHL	C3A-C2A-C1A	2.05	104.41	101.34
20	B	1210	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
20	B	1224	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
20	7	603	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
20	7	607	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
23	B	4005	BCR	C36-C18-C17	-2.05	120.05	122.92
20	B	1206	CLA	C1D-ND-C4D	-2.05	104.88	106.33
34	1	503	C7Z	C22-C23-C24	2.05	113.11	110.30
20	Z	601	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
20	6	618	CLA	CHA-C1A-NA	-2.05	121.70	126.40
20	6	602	CLA	C3B-C4B-NB	-2.05	108.61	110.52
20	8	615	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
20	B	1213	CLA	O1A-CGA-CBA	-2.05	115.73	123.73
20	B	1201	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
20	K	1402	CLA	O2A-CGA-CBA	2.05	118.34	111.91
20	1	607	CLA	C1-C2-C3	-2.05	122.50	126.04
20	A	1136	CLA	CHA-C1A-NA	-2.05	121.70	126.40
37	Z	613	CHL	CHA-C1A-NA	-2.05	121.70	126.40
20	A	1141	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
20	5	606	CLA	CMA-C3A-C4A	2.05	117.28	111.77
20	A	1124	CLA	CAA-C2A-C1A	-2.05	105.26	111.97
23	7	504	BCR	C33-C5-C6	-2.05	122.23	124.53
20	7	602	CLA	C3B-C4B-NB	-2.05	108.61	110.52
20	B	1202	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
20	B	1206	CLA	C2A-C1A-CHA	2.05	127.44	123.86
20	F	1301	CLA	C2A-C1A-CHA	2.05	127.44	123.86
36	3	502	LUT	C1-C6-C5	-2.05	119.73	122.61
20	1	615	CLA	C2A-C1A-CHA	2.05	127.44	123.86
20	4	608	CLA	C3D-C2D-C1D	-2.05	103.04	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1137	CLA	O2A-CGA-CBA	2.04	118.33	111.91
20	7	611	CLA	C3B-C4B-NB	-2.04	108.62	110.52
20	5	618	CLA	CHA-C1A-NA	-2.04	121.72	126.40
23	8	503	BCR	C38-C26-C25	-2.04	122.23	124.53
20	B	1234	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
20	A	1120	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
36	4	502	LUT	C18-C5-C4	2.04	118.14	114.36
20	F	1302	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
19	A	1011	CL0	C3D-C4D-ND	2.04	113.54	110.24
20	B	1238	CLA	O2A-CGA-CBA	2.04	118.32	111.91
20	K	1403	CLA	C1D-ND-C4D	-2.04	104.88	106.33
20	Z	615	CLA	C1D-ND-C4D	-2.04	104.88	106.33
20	6	612	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
19	A	1011	CL0	CHA-C4D-ND	2.04	136.77	132.50
20	4	603	CLA	C1-O2A-CGA	2.04	121.80	116.44
20	6	607	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
20	B	1213	CLA	CHA-C1A-NA	-2.04	121.72	126.40
37	7	610	CHL	C2B-C1B-NB	-2.04	108.86	110.23
20	1	615	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
20	A	1107	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	Z	604	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	A	1139	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	A	1127	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
37	3	611	CHL	C1-O2A-CGA	2.04	121.80	116.44
20	4	615	CLA	C2A-C1A-CHA	2.04	127.42	123.85
20	6	601	CLA	C2A-C1A-CHA	2.04	127.43	123.86
20	3	603	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
20	A	1122	CLA	C1D-ND-C4D	-2.04	104.89	106.33
20	7	616	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
20	B	1237	CLA	CHA-C1A-NA	-2.04	121.73	126.40
20	Z	607	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	B	1210	CLA	C1D-ND-C4D	-2.04	104.89	106.33
20	F	1301	CLA	CMB-C2B-C1B	2.04	128.47	125.37
20	A	1115	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
20	A	1111	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	B	1218	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
23	K	4002	BCR	C12-C13-C14	-2.04	115.81	118.94
20	B	1202	CLA	CHA-C1A-NA	-2.04	121.73	126.40
20	B	1212	CLA	C3B-C4B-NB	-2.04	108.63	110.52
20	7	612	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
20	B	1220	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	4	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	5	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
20	B	1201	CLA	C2A-C1A-CHA	2.04	127.42	123.86
23	4	503	BCR	C38-C26-C27	2.04	117.53	113.62
20	5	608	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
20	K	1401	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
37	1	610	CHL	C4A-NA-C1A	2.03	107.62	106.71
20	L	1502	CLA	CMC-C2C-C1C	2.03	128.13	125.04
37	5	611	CHL	C2C-C3C-C4C	2.03	107.94	106.49
20	A	1117	CLA	C1D-ND-C4D	-2.03	104.89	106.33
20	8	604	CLA	C2A-C1A-CHA	2.03	127.41	123.86
36	3	502	LUT	C39-C29-C30	-2.03	120.08	122.92
20	Z	601	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
20	4	615	CLA	CMA-C3A-C2A	2.03	120.84	116.10
20	4	601	CLA	CAA-C2A-C1A	-2.03	105.32	111.97
20	Z	611	CLA	C1D-ND-C4D	-2.03	104.89	106.33
20	1	601	CLA	CHA-C1A-NA	-2.03	121.75	126.40
20	1	611	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
20	B	1214	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
20	A	1117	CLA	C3A-C2A-C1A	2.03	104.38	101.34
20	A	1141	CLA	C2A-C1A-CHA	2.03	127.41	123.86
20	6	612	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
20	K	1404	CLA	C1-C2-C3	-2.03	122.53	126.04
20	B	1022	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
20	B	1235	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
20	A	1102	CLA	C2A-C1A-CHA	2.03	127.41	123.86
20	B	1240	CLA	C1D-ND-C4D	-2.03	104.89	106.33
20	B	1203	CLA	CHA-C1A-NA	-2.03	121.75	126.40
20	A	1138	CLA	C3B-C4B-NB	-2.03	108.63	110.52
36	6	501	LUT	C39-C29-C28	2.03	121.27	118.08
37	8	610	CHL	CHB-C1B-NB	-2.03	122.11	124.26
20	7	605	CLA	CHA-C1A-NA	-2.03	121.76	126.40
20	4	604	CLA	C2A-C1A-CHA	2.03	127.40	123.86
39	Z	504	QTB	C19-C17-C16	2.03	113.20	109.03
20	A	1102	CLA	C3B-C4B-NB	-2.03	108.64	110.52
20	B	1229	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
20	B	1209	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
20	5	605	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
20	1	615	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
20	A	1139	CLA	C1-C2-C3	-2.03	122.54	126.04
20	5	622	CLA	C2D-C1D-ND	2.02	111.60	110.10
20	B	1240	CLA	C2A-C1A-CHA	2.02	127.40	123.86
20	B	1219	CLA	CAA-C2A-C3A	-2.02	107.23	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	605	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
20	7	604	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
20	Z	605	CLA	CHA-C1A-NA	-2.02	121.76	126.40
20	B	1219	CLA	C2A-C1A-CHA	2.02	127.40	123.86
20	5	606	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
20	6	612	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
26	B	6101	LMT	O1'-C1'-C2'	2.02	111.46	108.30
20	8	615	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
20	6	619	CLA	C2A-C1A-CHA	2.02	127.39	123.86
20	A	1119	CLA	C1D-ND-C4D	-2.02	104.90	106.33
20	3	608	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
36	1	502	LUT	C19-C9-C8	2.02	121.26	118.08
20	A	1107	CLA	C6-C5-C3	-2.02	108.16	113.45
23	K	4001	BCR	C2-C3-C4	-2.02	106.86	111.38
20	5	609	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
20	6	604	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
20	6	609	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
20	A	1118	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
36	5	502	LUT	C35-C15-C14	-2.02	119.34	123.47
20	B	1224	CLA	C3B-C4B-NB	-2.02	108.64	110.52
20	4	603	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
20	6	601	CLA	C1D-ND-C4D	-2.02	104.90	106.33
20	8	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	Z	801	LHG	O7-C7-O9	-2.02	118.83	123.70
37	Z	609	CHL	C1-C2-C3	-2.02	122.55	126.04
20	J	1901	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
37	1	610	CHL	CHD-C4C-C3C	2.02	127.81	124.84
23	I	4001	BCR	C30-C25-C26	-2.02	119.77	122.61
20	1	601	CLA	C1-O2A-CGA	2.02	121.73	116.44
20	3	613	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
20	7	611	CLA	C4B-CHC-C1C	2.02	131.12	126.34
20	B	1216	CLA	C2D-C1D-ND	2.02	111.59	110.10
20	A	1115	CLA	O2A-CGA-CBA	2.02	118.23	111.91
23	3	503	BCR	C33-C5-C4	2.02	117.49	113.62
20	8	604	CLA	CBA-CAA-C2A	2.02	119.81	113.86
20	7	615	CLA	C2A-C1A-CHA	2.02	127.38	123.86
24	4	801	LHG	C5-O7-C7	-2.02	112.83	117.79
20	A	1109	CLA	C4B-CHC-C1C	2.02	131.12	126.34
20	1	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
20	A	1102	CLA	CMA-C3A-C2A	2.02	121.96	113.83
23	A	4001	BCR	C34-C9-C10	-2.02	120.10	122.92
20	Z	608	CLA	O1D-CGD-CBD	-2.02	120.36	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1120	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
20	B	1228	CLA	C3B-C4B-NB	-2.01	108.65	110.52
23	L	4001	BCR	C38-C26-C27	2.01	117.49	113.62
20	1	602	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
23	5	503	BCR	C35-C13-C12	2.01	121.25	118.08
20	B	1237	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
20	8	611	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
20	6	604	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
20	A	1105	CLA	CHA-C1A-NA	-2.01	121.79	126.40
20	B	1228	CLA	CHA-C1A-NA	-2.01	121.79	126.40
20	4	612	CLA	C3B-C4B-NB	-2.01	108.65	110.52
20	A	1130	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
20	A	1138	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
20	6	601	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
20	G	1602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
20	8	604	CLA	C1D-ND-C4D	-2.01	104.91	106.33
36	1	502	LUT	C30-C31-C32	-2.01	116.94	123.22
20	B	1231	CLA	CHA-C1A-NA	-2.01	121.80	126.40
37	1	609	CHL	CHD-C4C-C3C	2.01	127.79	124.84
20	A	1103	CLA	C4B-CHC-C1C	2.01	131.10	126.34
20	4	605	CLA	CMA-C3A-C4A	2.01	117.17	111.77
20	B	1201	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
20	3	606	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
23	6	503	BCR	C8-C7-C6	-2.01	121.56	127.20
20	B	1240	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
20	A	1121	CLA	C2D-C1D-ND	2.01	111.58	110.10
20	A	1107	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
20	B	1221	CLA	C1-C2-C3	-2.01	122.57	126.04
20	B	1239	CLA	C3B-C4B-NB	-2.01	108.65	110.52
20	A	1139	CLA	C1D-ND-C4D	-2.01	104.91	106.33
20	A	1111	CLA	C3B-C4B-NB	-2.00	108.66	110.52
20	B	1207	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
20	3	610	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
20	B	1215	CLA	CHA-C1A-NA	-2.00	121.81	126.40
20	B	1212	CLA	C1D-ND-C4D	-2.00	104.91	106.33
20	8	615	CLA	CHA-C1A-NA	-2.00	121.81	126.40
20	B	1221	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
20	A	1110	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
20	A	1139	CLA	C2A-C1A-CHA	2.00	127.36	123.86
20	4	602	CLA	C2A-C1A-CHA	2.00	127.36	123.86
23	J	4001	BCR	C24-C25-C26	-2.00	116.61	121.46
20	A	1013	CLA	CMC-C2C-C1C	2.00	128.09	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	6	604	CLA	C1-O2A-CGA	2.00	121.70	116.44
20	4	606	CLA	CHA-C1A-NA	-2.00	121.81	126.40
20	3	606	CLA	C11-C10-C8	-2.00	109.45	115.92
20	1	605	CLA	O2A-CGA-CBA	2.00	118.19	111.91
20	5	615	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
20	A	1123	CLA	C4B-CHC-C1C	2.00	131.09	126.34
20	A	1118	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
20	7	612	CLA	CHA-C1A-NA	-2.00	121.81	126.40
20	7	601	CLA	O2D-CGD-O1D	-2.00	119.93	123.84
20	A	1109	CLA	CHA-C1A-NA	-2.00	121.82	126.40
20	A	1120	CLA	CHA-C1A-NA	-2.00	121.82	126.40
37	6	613	CHL	C1-C2-C3	-2.00	122.58	126.04
20	F	1301	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	F	4001	RRX	C28
34	J	4002	C7Z	C3
34	1	503	C7Z	C3
34	5	505	C7Z	C3
37	1	609	CHL	C8
37	Z	610	CHL	C8
37	Z	609	CHL	C8
37	3	611	CHL	C8
37	8	610	CHL	C8
37	8	613	CHL	C3A
37	8	613	CHL	C8
37	4	610	CHL	C3A
37	4	613	CHL	C8
37	5	610	CHL	C8
37	6	610	CHL	C8
37	6	613	CHL	C8
39	Z	504	QTB	C11

All (4013) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1012	CLA	CHA-CBD-CGD-O1D
20	A	1012	CLA	CBD-CGD-O2D-CED
20	A	1012	CLA	C2-C3-C5-C6
20	A	1102	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1104	CLA	C1A-C2A-CAA-CBA
20	A	1104	CLA	C4B-C3B-CAB-CBB
20	A	1105	CLA	C1A-C2A-CAA-CBA
20	A	1105	CLA	C3A-C2A-CAA-CBA
20	A	1105	CLA	C2-C1-O2A-CGA
20	A	1106	CLA	C3A-C2A-CAA-CBA
20	A	1108	CLA	C1A-C2A-CAA-CBA
20	A	1108	CLA	C2-C1-O2A-CGA
20	A	1108	CLA	CHA-CBD-CGD-O1D
20	A	1108	CLA	CHA-CBD-CGD-O2D
20	A	1109	CLA	C1A-C2A-CAA-CBA
20	A	1109	CLA	CBD-CGD-O2D-CED
20	A	1110	CLA	C1A-C2A-CAA-CBA
20	A	1110	CLA	C14-C13-C15-C16
20	A	1111	CLA	C2-C3-C5-C6
20	A	1111	CLA	C4-C3-C5-C6
20	A	1112	CLA	C2B-C3B-CAB-CBB
20	A	1112	CLA	C4B-C3B-CAB-CBB
20	A	1114	CLA	C2-C1-O2A-CGA
20	A	1115	CLA	CBD-CGD-O2D-CED
20	A	1116	CLA	C1A-C2A-CAA-CBA
20	A	1116	CLA	C3A-C2A-CAA-CBA
20	A	1116	CLA	C2-C1-O2A-CGA
20	A	1116	CLA	CBD-CGD-O2D-CED
20	A	1117	CLA	C1A-C2A-CAA-CBA
20	A	1117	CLA	C3A-C2A-CAA-CBA
20	A	1117	CLA	CHA-CBD-CGD-O1D
20	A	1117	CLA	CHA-CBD-CGD-O2D
20	A	1119	CLA	C2A-CAA-CBA-CGA
20	A	1120	CLA	C1A-C2A-CAA-CBA
20	A	1120	CLA	C3A-C2A-CAA-CBA
20	A	1121	CLA	CBD-CGD-O2D-CED
20	A	1122	CLA	C1A-C2A-CAA-CBA
20	A	1122	CLA	C2B-C3B-CAB-CBB
20	A	1122	CLA	C4B-C3B-CAB-CBB
20	A	1122	CLA	CHA-CBD-CGD-O1D
20	A	1122	CLA	CHA-CBD-CGD-O2D
20	A	1123	CLA	C1A-C2A-CAA-CBA
20	A	1123	CLA	C3A-C2A-CAA-CBA
20	A	1123	CLA	C2-C1-O2A-CGA
20	A	1123	CLA	CHA-CBD-CGD-O1D
20	A	1123	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	1124	CLA	C1A-C2A-CAA-CBA
20	A	1124	CLA	C3A-C2A-CAA-CBA
20	A	1126	CLA	C1A-C2A-CAA-CBA
20	A	1126	CLA	CHA-CBD-CGD-O1D
20	A	1126	CLA	CHA-CBD-CGD-O2D
20	A	1127	CLA	C2A-CAA-CBA-CGA
20	A	1128	CLA	C2-C1-O2A-CGA
20	A	1129	CLA	C1A-C2A-CAA-CBA
20	A	1129	CLA	C3A-C2A-CAA-CBA
20	A	1131	CLA	C2B-C3B-CAB-CBB
20	A	1131	CLA	C4B-C3B-CAB-CBB
20	A	1131	CLA	CBD-CGD-O2D-CED
20	A	1132	CLA	C2B-C3B-CAB-CBB
20	A	1132	CLA	C4B-C3B-CAB-CBB
20	A	1132	CLA	CHA-CBD-CGD-O1D
20	A	1132	CLA	CHA-CBD-CGD-O2D
20	A	1133	CLA	C4-C3-C5-C6
20	A	1134	CLA	C1A-C2A-CAA-CBA
20	A	1134	CLA	C3A-C2A-CAA-CBA
20	A	1135	CLA	C1A-C2A-CAA-CBA
20	A	1135	CLA	C3A-C2A-CAA-CBA
20	A	1136	CLA	C1A-C2A-CAA-CBA
20	A	1136	CLA	C3A-C2A-CAA-CBA
20	A	1136	CLA	CHA-CBD-CGD-O1D
20	A	1136	CLA	CHA-CBD-CGD-O2D
20	A	1137	CLA	C2-C1-O2A-CGA
20	A	1138	CLA	C1A-C2A-CAA-CBA
20	A	1138	CLA	C3A-C2A-CAA-CBA
20	A	1138	CLA	CBD-CGD-O2D-CED
20	A	1139	CLA	C1A-C2A-CAA-CBA
20	A	1139	CLA	C3A-C2A-CAA-CBA
20	A	1130	CLA	C1A-C2A-CAA-CBA
20	A	1130	CLA	C4B-C3B-CAB-CBB
20	A	1140	CLA	CHA-CBD-CGD-O1D
20	A	1140	CLA	CHA-CBD-CGD-O2D
20	A	1140	CLA	CBD-CGD-O2D-CED
20	A	1101	CLA	C2-C1-O2A-CGA
20	A	1101	CLA	C11-C10-C8-C9
20	B	1237	CLA	C2-C1-O2A-CGA
20	B	1237	CLA	CHA-CBD-CGD-O1D
20	B	1237	CLA	CHA-CBD-CGD-O2D
20	B	1021	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	1022	CLA	C2B-C3B-CAB-CBB
20	B	1022	CLA	C4B-C3B-CAB-CBB
20	B	1022	CLA	CBD-CGD-O2D-CED
20	B	1023	CLA	C2-C1-O2A-CGA
20	B	1023	CLA	CHA-CBD-CGD-O1D
20	B	1023	CLA	CHA-CBD-CGD-O2D
20	B	1023	CLA	CBD-CGD-O2D-CED
20	B	1202	CLA	C1A-C2A-CAA-CBA
20	B	1202	CLA	C3A-C2A-CAA-CBA
20	B	1202	CLA	CHA-CBD-CGD-O1D
20	B	1202	CLA	CHA-CBD-CGD-O2D
20	B	1204	CLA	C1A-C2A-CAA-CBA
20	B	1204	CLA	CHA-CBD-CGD-O1D
20	B	1204	CLA	CHA-CBD-CGD-O2D
20	B	1205	CLA	C1A-C2A-CAA-CBA
20	B	1205	CLA	C3A-C2A-CAA-CBA
20	B	1205	CLA	C2-C1-O2A-CGA
20	B	1206	CLA	C1A-C2A-CAA-CBA
20	B	1206	CLA	C3A-C2A-CAA-CBA
20	B	1206	CLA	CBD-CGD-O2D-CED
20	B	1207	CLA	CBD-CGD-O2D-CED
20	B	1208	CLA	C1A-C2A-CAA-CBA
20	B	1208	CLA	C3A-C2A-CAA-CBA
20	B	1208	CLA	CBD-CGD-O2D-CED
20	B	1209	CLA	C1A-C2A-CAA-CBA
20	B	1209	CLA	C3A-C2A-CAA-CBA
20	B	1209	CLA	C11-C12-C13-C14
20	B	1211	CLA	C2-C1-O2A-CGA
20	B	1213	CLA	CHA-CBD-CGD-O1D
20	B	1213	CLA	CHA-CBD-CGD-O2D
20	B	1213	CLA	CBD-CGD-O2D-CED
20	B	1214	CLA	C1A-C2A-CAA-CBA
20	B	1214	CLA	C3A-C2A-CAA-CBA
20	B	1214	CLA	C2-C1-O2A-CGA
20	B	1214	CLA	CBD-CGD-O2D-CED
20	B	1215	CLA	C1A-C2A-CAA-CBA
20	B	1215	CLA	C3A-C2A-CAA-CBA
20	B	1216	CLA	C1A-C2A-CAA-CBA
20	B	1216	CLA	C3A-C2A-CAA-CBA
20	B	1216	CLA	C2B-C3B-CAB-CBB
20	B	1216	CLA	C4B-C3B-CAB-CBB
20	B	1216	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	B	1216	CLA	CHA-CBD-CGD-O2D
20	B	1217	CLA	C3A-C2A-CAA-CBA
20	B	1217	CLA	CHA-CBD-CGD-O1D
20	B	1217	CLA	CHA-CBD-CGD-O2D
20	B	1217	CLA	CBD-CGD-O2D-CED
20	B	1219	CLA	C1A-C2A-CAA-CBA
20	B	1220	CLA	C3A-C2A-CAA-CBA
20	B	1220	CLA	CHA-CBD-CGD-O1D
20	B	1220	CLA	CHA-CBD-CGD-O2D
20	B	1221	CLA	CHA-CBD-CGD-O1D
20	B	1221	CLA	CHA-CBD-CGD-O2D
20	B	1222	CLA	C1A-C2A-CAA-CBA
20	B	1224	CLA	C1A-C2A-CAA-CBA
20	B	1224	CLA	C3A-C2A-CAA-CBA
20	B	1224	CLA	C2-C1-O2A-CGA
20	B	1224	CLA	CHA-CBD-CGD-O1D
20	B	1224	CLA	CHA-CBD-CGD-O2D
20	B	1225	CLA	C1A-C2A-CAA-CBA
20	B	1225	CLA	C3A-C2A-CAA-CBA
20	B	1225	CLA	C2-C3-C5-C6
20	B	1225	CLA	C4-C3-C5-C6
20	B	1226	CLA	C1A-C2A-CAA-CBA
20	B	1226	CLA	CBD-CGD-O2D-CED
20	B	1229	CLA	C2-C1-O2A-CGA
20	B	1231	CLA	C2-C1-O2A-CGA
20	B	1232	CLA	C4B-C3B-CAB-CBB
20	B	1234	CLA	CBD-CGD-O2D-CED
20	B	1235	CLA	C1A-C2A-CAA-CBA
20	B	1235	CLA	C3A-C2A-CAA-CBA
20	B	1235	CLA	C2-C3-C5-C6
20	B	1235	CLA	C4-C3-C5-C6
20	B	1236	CLA	C1A-C2A-CAA-CBA
20	B	1238	CLA	C2A-CAA-CBA-CGA
20	B	1239	CLA	CBD-CGD-O2D-CED
20	B	1240	CLA	C3A-C2A-CAA-CBA
20	B	1240	CLA	CHA-CBD-CGD-O1D
20	B	1240	CLA	CHA-CBD-CGD-O2D
20	B	1240	CLA	C2-C3-C5-C6
20	B	1240	CLA	C4-C3-C5-C6
20	B	1241	CLA	CBD-CGD-O2D-CED
20	F	1301	CLA	C1A-C2A-CAA-CBA
20	F	1301	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	F	1301	CLA	CAD-CBD-CGD-O2D
20	F	1302	CLA	C2B-C3B-CAB-CBB
20	F	1302	CLA	C4B-C3B-CAB-CBB
20	F	1302	CLA	CBD-CGD-O2D-CED
20	G	1601	CLA	C2-C1-O2A-CGA
20	G	1601	CLA	CHA-CBD-CGD-O1D
20	G	1601	CLA	CHA-CBD-CGD-O2D
20	G	1602	CLA	CBA-CGA-O2A-C1
20	G	1602	CLA	C2B-C3B-CAB-CBB
20	G	1602	CLA	C4B-C3B-CAB-CBB
20	J	1901	CLA	C1A-C2A-CAA-CBA
20	J	1901	CLA	CBD-CGD-O2D-CED
20	K	1401	CLA	CBA-CGA-O2A-C1
20	K	1401	CLA	CHA-CBD-CGD-O1D
20	K	1401	CLA	CHA-CBD-CGD-O2D
20	K	1402	CLA	C3A-C2A-CAA-CBA
20	K	1402	CLA	CAD-CBD-CGD-O2D
20	K	1404	CLA	C1A-C2A-CAA-CBA
20	K	1404	CLA	C3A-C2A-CAA-CBA
20	K	1404	CLA	CAD-CBD-CGD-O2D
20	K	1404	CLA	CBD-CGD-O2D-CED
20	L	1502	CLA	C1A-C2A-CAA-CBA
20	L	1502	CLA	C3A-C2A-CAA-CBA
20	L	1502	CLA	CHA-CBD-CGD-O1D
20	L	1502	CLA	CHA-CBD-CGD-O2D
20	L	1503	CLA	C1A-C2A-CAA-CBA
20	L	1503	CLA	CHA-CBD-CGD-O1D
20	L	1503	CLA	CHA-CBD-CGD-O2D
20	L	1503	CLA	CBD-CGD-O2D-CED
20	1	601	CLA	C1A-C2A-CAA-CBA
20	1	601	CLA	C3A-C2A-CAA-CBA
20	1	602	CLA	CBD-CGD-O2D-CED
20	1	603	CLA	CHA-CBD-CGD-O1D
20	1	603	CLA	CHA-CBD-CGD-O2D
20	1	604	CLA	C3A-C2A-CAA-CBA
20	1	606	CLA	C1A-C2A-CAA-CBA
20	1	606	CLA	C3A-C2A-CAA-CBA
20	1	607	CLA	C1A-C2A-CAA-CBA
20	1	607	CLA	C3A-C2A-CAA-CBA
20	1	607	CLA	CHA-CBD-CGD-O1D
20	1	607	CLA	CHA-CBD-CGD-O2D
20	1	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	1	608	CLA	CHA-CBD-CGD-O1D
20	1	608	CLA	CHA-CBD-CGD-O2D
20	1	608	CLA	CBD-CGD-O2D-CED
20	1	608	CLA	C2-C3-C5-C6
20	1	608	CLA	C4-C3-C5-C6
20	1	611	CLA	CHA-CBD-CGD-O1D
20	1	611	CLA	CHA-CBD-CGD-O2D
20	1	612	CLA	C1A-C2A-CAA-CBA
20	1	612	CLA	C3A-C2A-CAA-CBA
20	1	615	CLA	C2-C1-O2A-CGA
20	1	615	CLA	C2B-C3B-CAB-CBB
20	1	615	CLA	C4B-C3B-CAB-CBB
20	1	615	CLA	CHA-CBD-CGD-O1D
20	1	615	CLA	CHA-CBD-CGD-O2D
20	1	615	CLA	CBD-CGD-O2D-CED
20	Z	601	CLA	CHA-CBD-CGD-O2D
20	Z	601	CLA	CBD-CGD-O2D-CED
20	Z	602	CLA	CBD-CGD-O2D-CED
20	Z	604	CLA	C1A-C2A-CAA-CBA
20	Z	604	CLA	C3A-C2A-CAA-CBA
20	Z	605	CLA	CBD-CGD-O2D-CED
20	Z	607	CLA	CHA-CBD-CGD-O1D
20	Z	607	CLA	CHA-CBD-CGD-O2D
20	Z	611	CLA	CHA-CBD-CGD-O1D
20	Z	615	CLA	CBA-CGA-O2A-C1
20	Z	615	CLA	O1A-CGA-O2A-C1
20	Z	615	CLA	CHA-CBD-CGD-O1D
20	3	601	CLA	C1A-C2A-CAA-CBA
20	3	602	CLA	C4B-C3B-CAB-CBB
20	3	602	CLA	CBD-CGD-O2D-CED
20	3	603	CLA	C2-C1-O2A-CGA
20	3	603	CLA	CHA-CBD-CGD-O1D
20	3	603	CLA	CHA-CBD-CGD-O2D
20	3	604	CLA	C1A-C2A-CAA-CBA
20	3	604	CLA	CHA-CBD-CGD-O1D
20	3	604	CLA	CHA-CBD-CGD-O2D
20	3	605	CLA	CBD-CGD-O2D-CED
20	3	606	CLA	C3A-C2A-CAA-CBA
20	3	606	CLA	CHA-CBD-CGD-O1D
20	3	606	CLA	CHA-CBD-CGD-O2D
20	3	607	CLA	C2-C1-O2A-CGA
20	3	607	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	3	610	CLA	C2-C1-O2A-CGA
20	3	612	CLA	C3A-C2A-CAA-CBA
20	3	618	CLA	C1A-C2A-CAA-CBA
20	3	618	CLA	CBA-CGA-O2A-C1
20	3	618	CLA	CBD-CGD-O2D-CED
20	3	616	CLA	C2-C1-O2A-CGA
20	3	616	CLA	CHA-CBD-CGD-O1D
20	3	616	CLA	CHA-CBD-CGD-O2D
20	7	609	CLA	CHA-CBD-CGD-O1D
20	7	609	CLA	CHA-CBD-CGD-O2D
20	7	609	CLA	C11-C10-C8-C9
20	7	601	CLA	C1A-C2A-CAA-CBA
20	7	602	CLA	CBD-CGD-O2D-CED
20	7	603	CLA	C1A-C2A-CAA-CBA
20	7	603	CLA	C4B-C3B-CAB-CBB
20	7	603	CLA	CBD-CGD-O2D-CED
20	7	604	CLA	C1A-C2A-CAA-CBA
20	7	605	CLA	CBA-CGA-O2A-C1
20	7	605	CLA	O1A-CGA-O2A-C1
20	7	605	CLA	CHA-CBD-CGD-O1D
20	7	605	CLA	CHA-CBD-CGD-O2D
20	7	605	CLA	CBD-CGD-O2D-CED
20	7	606	CLA	C1A-C2A-CAA-CBA
20	7	606	CLA	C3A-C2A-CAA-CBA
20	7	607	CLA	C2B-C3B-CAB-CBB
20	7	607	CLA	C4B-C3B-CAB-CBB
20	7	607	CLA	CHA-CBD-CGD-O1D
20	7	607	CLA	CHA-CBD-CGD-O2D
20	7	607	CLA	CBD-CGD-O2D-CED
20	7	612	CLA	C3A-C2A-CAA-CBA
20	7	613	CLA	C1A-C2A-CAA-CBA
20	7	613	CLA	CBD-CGD-O2D-CED
20	7	615	CLA	C3A-C2A-CAA-CBA
20	7	615	CLA	C2-C1-O2A-CGA
20	7	616	CLA	CBD-CGD-O2D-CED
20	8	601	CLA	C1A-C2A-CAA-CBA
20	8	601	CLA	C3A-C2A-CAA-CBA
20	8	603	CLA	C1A-C2A-CAA-CBA
20	8	603	CLA	CBD-CGD-O2D-CED
20	8	604	CLA	C1A-C2A-CAA-CBA
20	8	606	CLA	C1A-C2A-CAA-CBA
20	8	606	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	8	606	CLA	CHA-CBD-CGD-O1D
20	8	606	CLA	CHA-CBD-CGD-O2D
20	8	607	CLA	C1A-C2A-CAA-CBA
20	8	607	CLA	C3A-C2A-CAA-CBA
20	8	607	CLA	CHA-CBD-CGD-O1D
20	8	607	CLA	CHA-CBD-CGD-O2D
20	8	607	CLA	CBD-CGD-O2D-CED
20	8	608	CLA	CHA-CBD-CGD-O1D
20	8	608	CLA	CHA-CBD-CGD-O2D
20	8	611	CLA	C2-C1-O2A-CGA
20	8	611	CLA	CBD-CGD-O2D-CED
20	8	612	CLA	C1A-C2A-CAA-CBA
20	8	612	CLA	C3A-C2A-CAA-CBA
20	8	615	CLA	CBA-CGA-O2A-C1
20	8	615	CLA	CHA-CBD-CGD-O1D
20	8	615	CLA	CHA-CBD-CGD-O2D
20	4	601	CLA	C1A-C2A-CAA-CBA
20	4	601	CLA	C3A-C2A-CAA-CBA
20	4	602	CLA	C2-C1-O2A-CGA
20	4	603	CLA	C1A-C2A-CAA-CBA
20	4	604	CLA	C1A-C2A-CAA-CBA
20	4	604	CLA	C3A-C2A-CAA-CBA
20	4	606	CLA	C2A-CAA-CBA-CGA
20	4	606	CLA	CBD-CGD-O2D-CED
20	4	607	CLA	C2B-C3B-CAB-CBB
20	4	607	CLA	C4B-C3B-CAB-CBB
20	4	607	CLA	CHA-CBD-CGD-O1D
20	4	607	CLA	CHA-CBD-CGD-O2D
20	4	607	CLA	CBD-CGD-O2D-CED
20	4	608	CLA	CBD-CGD-O2D-CED
20	4	612	CLA	C1A-C2A-CAA-CBA
20	4	612	CLA	C3A-C2A-CAA-CBA
20	4	612	CLA	CHA-CBD-CGD-O1D
20	4	612	CLA	CHA-CBD-CGD-O2D
20	4	612	CLA	CBD-CGD-O2D-CED
20	5	601	CLA	C3A-C2A-CAA-CBA
20	5	601	CLA	CBD-CGD-O2D-CED
20	5	602	CLA	CBD-CGD-O2D-CED
20	5	603	CLA	C1A-C2A-CAA-CBA
20	5	603	CLA	CHA-CBD-CGD-O1D
20	5	603	CLA	CHA-CBD-CGD-O2D
20	5	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	5	604	CLA	C1A-C2A-CAA-CBA
20	5	605	CLA	C1A-C2A-CAA-CBA
20	5	605	CLA	C3A-C2A-CAA-CBA
20	5	605	CLA	CHA-CBD-CGD-O1D
20	5	605	CLA	CHA-CBD-CGD-O2D
20	5	605	CLA	CBD-CGD-O2D-CED
20	5	606	CLA	C1A-C2A-CAA-CBA
20	5	606	CLA	C2-C1-O2A-CGA
20	5	606	CLA	CHA-CBD-CGD-O1D
20	5	606	CLA	CHA-CBD-CGD-O2D
20	5	607	CLA	CHA-CBD-CGD-O1D
20	5	607	CLA	CHA-CBD-CGD-O2D
20	5	608	CLA	C2B-C3B-CAB-CBB
20	5	608	CLA	C4B-C3B-CAB-CBB
20	5	609	CLA	CHA-CBD-CGD-O1D
20	5	609	CLA	CHA-CBD-CGD-O2D
20	5	612	CLA	C2-C1-O2A-CGA
20	5	613	CLA	C2-C3-C5-C6
20	5	613	CLA	C4-C3-C5-C6
20	5	618	CLA	C3A-C2A-CAA-CBA
20	5	618	CLA	C2-C3-C5-C6
20	5	618	CLA	C4-C3-C5-C6
20	6	608	CLA	C1A-C2A-CAA-CBA
20	6	601	CLA	C1A-C2A-CAA-CBA
20	6	601	CLA	CHA-CBD-CGD-O1D
20	6	601	CLA	CHA-CBD-CGD-O2D
20	6	603	CLA	CHA-CBD-CGD-O1D
20	6	603	CLA	CHA-CBD-CGD-O2D
20	6	604	CLA	C1A-C2A-CAA-CBA
20	6	605	CLA	C2-C1-O2A-CGA
20	6	606	CLA	C1A-C2A-CAA-CBA
20	6	606	CLA	CHA-CBD-CGD-O1D
20	6	606	CLA	CBD-CGD-O2D-CED
20	6	612	CLA	C1A-C2A-CAA-CBA
20	6	612	CLA	C3A-C2A-CAA-CBA
20	6	612	CLA	CHA-CBD-CGD-O1D
20	6	612	CLA	CHA-CBD-CGD-O2D
20	6	615	CLA	C1A-C2A-CAA-CBA
20	6	615	CLA	C3A-C2A-CAA-CBA
20	6	615	CLA	C2B-C3B-CAB-CBB
20	6	615	CLA	C4B-C3B-CAB-CBB
20	6	615	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	6	615	CLA	CHA-CBD-CGD-O2D
20	6	618	CLA	CHA-CBD-CGD-O1D
20	6	618	CLA	CHA-CBD-CGD-O2D
20	6	618	CLA	CBD-CGD-O2D-CED
20	6	619	CLA	CBD-CGD-O2D-CED
23	A	4001	BCR	C11-C10-C9-C8
23	A	4001	BCR	C11-C10-C9-C34
23	A	4001	BCR	C10-C11-C12-C13
23	A	4002	BCR	C7-C8-C9-C10
23	A	4002	BCR	C7-C8-C9-C34
23	A	4002	BCR	C11-C10-C9-C8
23	A	4002	BCR	C11-C10-C9-C34
23	A	4002	BCR	C10-C11-C12-C13
23	A	4003	BCR	C5-C6-C7-C8
23	A	4003	BCR	C7-C8-C9-C10
23	A	4003	BCR	C7-C8-C9-C34
23	A	4003	BCR	C11-C10-C9-C8
23	A	4003	BCR	C11-C10-C9-C34
23	A	4003	BCR	C23-C24-C25-C30
23	A	4004	BCR	C7-C8-C9-C10
23	A	4004	BCR	C7-C8-C9-C34
23	A	4004	BCR	C11-C10-C9-C8
23	A	4004	BCR	C11-C10-C9-C34
23	A	4004	BCR	C10-C11-C12-C13
23	A	4004	BCR	C21-C22-C23-C24
23	A	4004	BCR	C23-C24-C25-C26
23	A	4004	BCR	C23-C24-C25-C30
23	A	4005	BCR	C1-C6-C7-C8
23	A	4005	BCR	C7-C8-C9-C10
23	A	4005	BCR	C7-C8-C9-C34
23	A	4005	BCR	C11-C10-C9-C8
23	A	4005	BCR	C11-C10-C9-C34
23	A	4005	BCR	C17-C18-C19-C20
23	A	4005	BCR	C36-C18-C19-C20
23	A	4005	BCR	C21-C22-C23-C24
23	A	4005	BCR	C37-C22-C23-C24
23	B	4001	BCR	C1-C6-C7-C8
23	B	4001	BCR	C11-C10-C9-C8
23	B	4001	BCR	C11-C10-C9-C34
23	B	4001	BCR	C21-C22-C23-C24
23	B	4001	BCR	C37-C22-C23-C24
23	B	4002	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	4002	BCR	C7-C8-C9-C10
23	B	4002	BCR	C7-C8-C9-C34
23	B	4002	BCR	C11-C10-C9-C8
23	B	4002	BCR	C11-C10-C9-C34
23	B	4002	BCR	C10-C11-C12-C13
23	B	4002	BCR	C21-C22-C23-C24
23	B	4002	BCR	C37-C22-C23-C24
23	B	4004	BCR	C11-C10-C9-C8
23	B	4004	BCR	C11-C10-C9-C34
23	B	4005	BCR	C11-C10-C9-C8
23	B	4005	BCR	C11-C10-C9-C34
23	B	4005	BCR	C10-C11-C12-C13
23	B	4005	BCR	C11-C12-C13-C35
23	B	4007	BCR	C11-C10-C9-C8
23	B	4007	BCR	C11-C10-C9-C34
23	B	4007	BCR	C9-C10-C11-C12
23	B	4007	BCR	C10-C11-C12-C13
23	B	4006	BCR	C7-C8-C9-C10
23	B	4006	BCR	C7-C8-C9-C34
23	B	4006	BCR	C11-C12-C13-C14
23	B	4006	BCR	C11-C12-C13-C35
23	B	4006	BCR	C17-C18-C19-C20
23	B	4006	BCR	C36-C18-C19-C20
23	B	4006	BCR	C21-C22-C23-C24
23	B	4006	BCR	C37-C22-C23-C24
23	G	4001	BCR	C11-C10-C9-C8
23	G	4001	BCR	C11-C10-C9-C34
23	G	4001	BCR	C10-C11-C12-C13
23	I	4001	BCR	C7-C8-C9-C10
23	I	4001	BCR	C7-C8-C9-C34
23	I	4001	BCR	C11-C10-C9-C8
23	I	4001	BCR	C11-C10-C9-C34
23	I	4001	BCR	C10-C11-C12-C13
23	I	4001	BCR	C36-C18-C19-C20
23	J	4001	BCR	C7-C8-C9-C10
23	J	4001	BCR	C7-C8-C9-C34
23	J	4001	BCR	C11-C10-C9-C8
23	J	4001	BCR	C11-C10-C9-C34
23	J	4001	BCR	C10-C11-C12-C13
23	J	4001	BCR	C11-C12-C13-C35
23	J	4001	BCR	C36-C18-C19-C20
23	J	4001	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	J	4001	BCR	C37-C22-C23-C24
23	J	4001	BCR	C23-C24-C25-C26
23	J	4001	BCR	C23-C24-C25-C30
23	K	4001	BCR	C1-C6-C7-C8
23	K	4001	BCR	C7-C8-C9-C34
23	K	4001	BCR	C11-C10-C9-C8
23	K	4001	BCR	C11-C10-C9-C34
23	K	4001	BCR	C10-C11-C12-C13
23	K	4001	BCR	C19-C20-C21-C22
23	K	4001	BCR	C21-C22-C23-C24
23	K	4001	BCR	C37-C22-C23-C24
23	K	4001	BCR	C23-C24-C25-C26
23	K	4002	BCR	C11-C10-C9-C8
23	K	4002	BCR	C11-C10-C9-C34
23	L	4001	BCR	C7-C8-C9-C10
23	L	4001	BCR	C7-C8-C9-C34
23	L	4001	BCR	C11-C10-C9-C8
23	L	4001	BCR	C11-C10-C9-C34
23	L	4001	BCR	C10-C11-C12-C13
23	L	4001	BCR	C23-C24-C25-C26
23	L	4001	BCR	C23-C24-C25-C30
23	L	4002	BCR	C21-C22-C23-C24
23	L	4002	BCR	C37-C22-C23-C24
23	L	4002	BCR	C23-C24-C25-C30
23	3	503	BCR	C5-C6-C7-C8
23	3	503	BCR	C7-C8-C9-C10
23	3	503	BCR	C7-C8-C9-C34
23	3	503	BCR	C23-C24-C25-C30
23	3	504	BCR	C7-C8-C9-C10
23	3	504	BCR	C7-C8-C9-C34
23	3	504	BCR	C11-C10-C9-C8
23	3	504	BCR	C11-C10-C9-C34
23	3	504	BCR	C10-C11-C12-C13
23	3	504	BCR	C21-C22-C23-C24
23	3	504	BCR	C37-C22-C23-C24
23	3	505	BCR	C7-C8-C9-C10
23	3	505	BCR	C7-C8-C9-C34
23	3	505	BCR	C11-C10-C9-C8
23	3	505	BCR	C11-C10-C9-C34
23	3	505	BCR	C9-C10-C11-C12
23	3	505	BCR	C10-C11-C12-C13
23	3	506	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	3	506	BCR	C7-C8-C9-C34
23	3	506	BCR	C11-C10-C9-C8
23	3	506	BCR	C11-C10-C9-C34
23	3	506	BCR	C10-C11-C12-C13
23	3	506	BCR	C17-C18-C19-C20
23	3	506	BCR	C36-C18-C19-C20
23	3	506	BCR	C23-C24-C25-C26
23	3	506	BCR	C23-C24-C25-C30
23	7	503	BCR	C11-C10-C9-C8
23	7	503	BCR	C11-C10-C9-C34
23	7	503	BCR	C10-C11-C12-C13
23	7	503	BCR	C23-C24-C25-C26
23	7	503	BCR	C23-C24-C25-C30
23	7	504	BCR	C7-C8-C9-C10
23	7	504	BCR	C7-C8-C9-C34
23	7	504	BCR	C11-C10-C9-C8
23	7	504	BCR	C11-C10-C9-C34
23	7	504	BCR	C10-C11-C12-C13
23	7	504	BCR	C11-C12-C13-C35
23	7	504	BCR	C17-C18-C19-C20
23	7	504	BCR	C36-C18-C19-C20
23	7	504	BCR	C21-C22-C23-C24
23	7	504	BCR	C37-C22-C23-C24
23	8	503	BCR	C5-C6-C7-C8
23	8	503	BCR	C11-C10-C9-C8
23	8	503	BCR	C11-C10-C9-C34
23	8	503	BCR	C10-C11-C12-C13
23	8	503	BCR	C13-C14-C15-C16
23	4	503	BCR	C7-C8-C9-C10
23	4	503	BCR	C7-C8-C9-C34
23	4	503	BCR	C11-C10-C9-C8
23	4	503	BCR	C11-C10-C9-C34
23	4	503	BCR	C10-C11-C12-C13
23	4	503	BCR	C21-C22-C23-C24
23	4	503	BCR	C37-C22-C23-C24
23	4	503	BCR	C23-C24-C25-C26
23	4	503	BCR	C23-C24-C25-C30
23	5	503	BCR	C11-C10-C9-C8
23	5	503	BCR	C11-C10-C9-C34
23	5	503	BCR	C10-C11-C12-C13
23	5	503	BCR	C17-C18-C19-C20
23	5	503	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	5	503	BCR	C21-C22-C23-C24
23	5	504	BCR	C10-C11-C12-C13
23	6	504	BCR	C11-C12-C13-C14
23	6	504	BCR	C11-C12-C13-C35
23	6	504	BCR	C23-C24-C25-C26
23	6	503	BCR	C11-C10-C9-C8
23	6	503	BCR	C11-C10-C9-C34
23	6	503	BCR	C10-C11-C12-C13
23	6	503	BCR	C36-C18-C19-C20
24	A	5001	LHG	C1-C2-C3-O3
24	A	5001	LHG	C3-O3-P-O5
24	A	5001	LHG	O6-C4-C5-O7
24	A	5002	LHG	C3-O3-P-O4
24	A	5002	LHG	C4-O6-P-O3
24	A	5002	LHG	C4-O6-P-O4
24	A	5002	LHG	C4-O6-P-O5
24	B	5001	LHG	O1-C1-C2-C3
24	B	5001	LHG	C3-O3-P-O5
24	B	5001	LHG	O9-C7-O7-C5
24	B	5001	LHG	C8-C7-O7-C5
24	B	5002	LHG	C3-O3-P-O5
24	B	5002	LHG	O9-C7-O7-C5
24	B	5006	LHG	O1-C1-C2-C3
24	B	5006	LHG	C1-C2-C3-O3
24	B	5006	LHG	C4-O6-P-O4
24	B	5006	LHG	C8-C7-O7-C5
24	1	801	LHG	C8-C7-O7-C5
24	Z	801	LHG	O1-C1-C2-C3
24	Z	801	LHG	C4-O6-P-O3
24	Z	801	LHG	C4-O6-P-O5
24	Z	801	LHG	C8-C7-O7-C5
24	3	801	LHG	O9-C7-O7-C5
24	7	801	LHG	O1-C1-C2-C3
24	7	801	LHG	C3-O3-P-O5
24	7	801	LHG	C3-O3-P-O6
24	7	801	LHG	C4-O6-P-O4
24	8	801	LHG	C1-C2-C3-O3
24	8	801	LHG	C4-O6-P-O3
24	4	801	LHG	C1-C2-C3-O3
24	4	801	LHG	O6-C4-C5-O7
24	4	801	LHG	C8-C7-O7-C5
24	4	802	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	4	802	LHG	C4-O6-P-O3
24	4	802	LHG	C4-O6-P-O4
24	4	802	LHG	C4-O6-P-O5
24	5	801	LHG	O1-C1-C2-C3
24	5	801	LHG	O2-C2-C3-O3
24	5	801	LHG	C3-O3-P-O5
24	5	801	LHG	C4-O6-P-O4
24	5	801	LHG	C4-O6-P-O5
24	5	801	LHG	O7-C5-C6-O8
24	6	801	LHG	C1-C2-C3-O3
24	6	801	LHG	C3-O3-P-O5
24	6	801	LHG	C3-O3-P-O6
24	6	801	LHG	C4-O6-P-O3
24	6	801	LHG	C4-O6-P-O5
25	A	5004	NKP	CAG-OAF-PAC-OAA
25	A	5004	NKP	CAG-OAF-PAC-OAB
25	A	5004	NKP	CAG-OAF-PAC-OAD
25	A	5004	NKP	CAG-CAH-CAI-OAJ
25	8	802	NKP	OBC-CAH-CAI-OAJ
26	A	5006	LMT	C2'-C1'-O1'-C1
26	A	5006	LMT	O5'-C1'-O1'-C1
26	B	5005	LMT	C2-C1-O1'-C1'
26	8	805	LMT	C2-C1-O1'-C1'
26	4	803	LMT	O5'-C1'-O1'-C1
29	A	5003	LMG	C2-C1-O1-C7
29	A	5003	LMG	O6-C1-O1-C7
29	J	5001	LMG	C11-C10-O7-C8
31	B	5003	DGD	C2B-C1B-O2G-C2G
33	F	4001	RRX	C23-C24-C25-C30
33	F	4001	RRX	C23-C24-C25-C26
33	F	4001	RRX	C36-C18-C19-C20
33	F	4001	RRX	C17-C18-C19-C20
34	J	4002	C7Z	C31-C32-C33-C40
34	1	503	C7Z	C27-C28-C29-C30
34	1	503	C7Z	C27-C28-C29-C39
34	5	505	C7Z	C7-C8-C9-C19
34	5	505	C7Z	C7-C8-C9-C10
34	5	505	C7Z	C13-C14-C15-C35
34	5	505	C7Z	C31-C32-C33-C40
34	5	505	C7Z	C27-C28-C29-C30
34	5	505	C7Z	C27-C28-C29-C39
35	K	5001	SPH	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
35	K	5001	SPH	C1-C2-C3-C4
35	K	5001	SPH	N2-C2-C3-O3
35	K	5001	SPH	N2-C2-C3-C4
35	7	804	SPH	C1-C2-C3-O3
35	7	804	SPH	C1-C2-C3-C4
35	7	804	SPH	N2-C2-C3-O3
35	7	804	SPH	N2-C2-C3-C4
36	Z	501	LUT	C21-C26-C27-C28
36	Z	503	LUT	C1-C6-C7-C8
36	Z	503	LUT	C5-C6-C7-C8
36	7	501	LUT	C21-C26-C27-C28
36	5	501	LUT	C27-C28-C29-C39
36	6	502	LUT	C25-C26-C27-C28
37	1	609	CHL	CHA-CBD-CGD-O1D
37	1	609	CHL	CHA-CBD-CGD-O2D
37	1	609	CHL	CAD-CBD-CGD-O1D
37	Z	613	CHL	C1A-C2A-CAA-CBA
37	Z	609	CHL	C1A-C2A-CAA-CBA
37	Z	609	CHL	C14-C13-C15-C16
37	7	610	CHL	C1A-C2A-CAA-CBA
37	8	613	CHL	C1A-C2A-CAA-CBA
37	4	610	CHL	CHA-CBD-CGD-O1D
37	4	611	CHL	C2A-CAA-CBA-CGA
37	6	610	CHL	C1A-C2A-CAA-CBA
37	6	611	CHL	C1A-C2A-CAA-CBA
37	6	611	CHL	C3A-C2A-CAA-CBA
37	6	611	CHL	C2A-CAA-CBA-CGA
37	6	617	CHL	CHA-CBD-CGD-O1D
37	6	617	CHL	CHA-CBD-CGD-O2D
38	1	802	SQD	C2-C1-O6-C44
38	1	802	SQD	O5-C1-O6-C44
38	1	802	SQD	C8-C7-O47-C45
39	Z	504	QTB	C01-C02-C09-C10
39	Z	504	QTB	C03-C02-C09-C10
39	Z	504	QTB	C04-C05-C06-C08
39	Z	504	QTB	C04-C05-C06-O07
39	Z	504	QTB	C09-C10-C11-C17
40	8	806	3PH	C22-C21-O21-C2
40	5	802	3PH	C1-O11-P-O13
40	5	802	3PH	C1-O11-P-O12
40	5	802	3PH	O11-C1-C2-O21
40	5	802	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
40	6	802	3PH	C1-O11-P-O13
40	6	802	3PH	C1-O11-P-O14
40	6	802	3PH	O22-C21-O21-C2
40	6	802	3PH	C22-C21-O21-C2
42	8	803	LPX	O1-C3-C4-O5
42	8	803	LPX	C3-O1-P1-O2
42	8	803	LPX	C1-O2-P1-O1
42	8	803	LPX	C1-O2-P1-O3
42	8	803	LPX	C1-O2-P1-O4
20	A	1115	CLA	O1D-CGD-O2D-CED
20	A	1140	CLA	O1D-CGD-O2D-CED
20	B	1023	CLA	O1D-CGD-O2D-CED
20	B	1232	CLA	O1D-CGD-O2D-CED
20	K	1403	CLA	O1D-CGD-O2D-CED
20	1	612	CLA	O1D-CGD-O2D-CED
20	8	615	CLA	O1D-CGD-O2D-CED
20	4	615	CLA	O1D-CGD-O2D-CED
20	6	619	CLA	O1D-CGD-O2D-CED
20	A	1126	CLA	O1D-CGD-O2D-CED
20	A	1138	CLA	O1D-CGD-O2D-CED
20	B	1021	CLA	O1D-CGD-O2D-CED
20	B	1219	CLA	O1D-CGD-O2D-CED
20	G	1601	CLA	O1D-CGD-O2D-CED
20	1	603	CLA	O1D-CGD-O2D-CED
20	Z	615	CLA	O1D-CGD-O2D-CED
20	3	606	CLA	O1D-CGD-O2D-CED
20	7	605	CLA	O1D-CGD-O2D-CED
20	8	603	CLA	O1D-CGD-O2D-CED
20	4	605	CLA	O1D-CGD-O2D-CED
20	5	613	CLA	O1D-CGD-O2D-CED
20	6	605	CLA	O1D-CGD-O2D-CED
20	A	1114	CLA	CBD-CGD-O2D-CED
20	A	1117	CLA	CBD-CGD-O2D-CED
20	A	1119	CLA	CBD-CGD-O2D-CED
20	A	1123	CLA	CBD-CGD-O2D-CED
20	A	1124	CLA	CBD-CGD-O2D-CED
20	A	1126	CLA	CBD-CGD-O2D-CED
20	A	1128	CLA	CBD-CGD-O2D-CED
20	A	1136	CLA	CBD-CGD-O2D-CED
20	A	1139	CLA	CBD-CGD-O2D-CED
20	A	1141	CLA	CBD-CGD-O2D-CED
20	A	1130	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1237	CLA	CBD-CGD-O2D-CED
20	B	1021	CLA	CBD-CGD-O2D-CED
20	B	1201	CLA	CBD-CGD-O2D-CED
20	B	1205	CLA	CBD-CGD-O2D-CED
20	B	1209	CLA	CBD-CGD-O2D-CED
20	B	1212	CLA	CBD-CGD-O2D-CED
20	B	1215	CLA	CBD-CGD-O2D-CED
20	B	1216	CLA	CBD-CGD-O2D-CED
20	B	1219	CLA	CBD-CGD-O2D-CED
20	B	1222	CLA	CBD-CGD-O2D-CED
20	B	1223	CLA	CBD-CGD-O2D-CED
20	B	1224	CLA	CBD-CGD-O2D-CED
20	B	1228	CLA	CBD-CGD-O2D-CED
20	B	1229	CLA	CBD-CGD-O2D-CED
20	B	1231	CLA	CBD-CGD-O2D-CED
20	B	1232	CLA	CBD-CGD-O2D-CED
20	B	1235	CLA	CBD-CGD-O2D-CED
20	G	1601	CLA	CBD-CGD-O2D-CED
20	G	1602	CLA	CBD-CGD-O2D-CED
20	K	1401	CLA	CBD-CGD-O2D-CED
20	K	1402	CLA	CBD-CGD-O2D-CED
20	K	1403	CLA	CBD-CGD-O2D-CED
20	1	601	CLA	CBD-CGD-O2D-CED
20	1	603	CLA	CBD-CGD-O2D-CED
20	1	604	CLA	CBD-CGD-O2D-CED
20	1	607	CLA	CBD-CGD-O2D-CED
20	1	611	CLA	CBD-CGD-O2D-CED
20	1	612	CLA	CBD-CGD-O2D-CED
20	1	613	CLA	CBD-CGD-O2D-CED
20	Z	603	CLA	CBD-CGD-O2D-CED
20	Z	604	CLA	CBD-CGD-O2D-CED
20	Z	606	CLA	CBD-CGD-O2D-CED
20	Z	607	CLA	CBD-CGD-O2D-CED
20	Z	611	CLA	CBD-CGD-O2D-CED
20	Z	612	CLA	CBD-CGD-O2D-CED
20	Z	615	CLA	CBD-CGD-O2D-CED
20	3	606	CLA	CBD-CGD-O2D-CED
20	3	608	CLA	CBD-CGD-O2D-CED
20	3	612	CLA	CBD-CGD-O2D-CED
20	3	613	CLA	CBD-CGD-O2D-CED
20	3	616	CLA	CBD-CGD-O2D-CED
20	7	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	7	611	CLA	CBD-CGD-O2D-CED
20	7	615	CLA	CBD-CGD-O2D-CED
20	8	602	CLA	CBD-CGD-O2D-CED
20	8	606	CLA	CBD-CGD-O2D-CED
20	8	615	CLA	CBD-CGD-O2D-CED
20	4	602	CLA	CBD-CGD-O2D-CED
20	4	603	CLA	CBD-CGD-O2D-CED
20	4	605	CLA	CBD-CGD-O2D-CED
20	4	615	CLA	CBD-CGD-O2D-CED
20	5	607	CLA	CBD-CGD-O2D-CED
20	5	608	CLA	CBD-CGD-O2D-CED
20	5	609	CLA	CBD-CGD-O2D-CED
20	5	613	CLA	CBD-CGD-O2D-CED
20	5	615	CLA	CBD-CGD-O2D-CED
20	5	622	CLA	CBD-CGD-O2D-CED
20	6	608	CLA	CBD-CGD-O2D-CED
20	6	602	CLA	CBD-CGD-O2D-CED
20	6	603	CLA	CBD-CGD-O2D-CED
20	6	605	CLA	CBD-CGD-O2D-CED
20	6	612	CLA	CBD-CGD-O2D-CED
20	A	1104	CLA	O1A-CGA-O2A-C1
20	A	1101	CLA	O1A-CGA-O2A-C1
20	B	1207	CLA	O1A-CGA-O2A-C1
20	B	1228	CLA	O1A-CGA-O2A-C1
20	B	1240	CLA	O1A-CGA-O2A-C1
20	Z	612	CLA	O1A-CGA-O2A-C1
20	4	608	CLA	O1A-CGA-O2A-C1
29	A	5003	LMG	O10-C28-O8-C9
38	1	802	SQD	O10-C23-O48-C46
20	G	1602	CLA	O1A-CGA-O2A-C1
20	K	1401	CLA	O1A-CGA-O2A-C1
20	3	618	CLA	O1A-CGA-O2A-C1
20	8	615	CLA	O1A-CGA-O2A-C1
20	A	1114	CLA	O1D-CGD-O2D-CED
20	A	1116	CLA	O1D-CGD-O2D-CED
20	A	1123	CLA	O1D-CGD-O2D-CED
20	B	1022	CLA	O1D-CGD-O2D-CED
20	B	1201	CLA	O1D-CGD-O2D-CED
20	B	1228	CLA	O1D-CGD-O2D-CED
20	K	1402	CLA	O1D-CGD-O2D-CED
20	L	1503	CLA	O1D-CGD-O2D-CED
20	1	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	Z	611	CLA	O1D-CGD-O2D-CED
20	3	602	CLA	O1D-CGD-O2D-CED
20	3	616	CLA	O1D-CGD-O2D-CED
20	7	606	CLA	O1D-CGD-O2D-CED
20	4	606	CLA	O1D-CGD-O2D-CED
20	6	602	CLA	O1D-CGD-O2D-CED
20	6	603	CLA	O1D-CGD-O2D-CED
20	Z	602	CLA	CBA-CGA-O2A-C1
20	A	1012	CLA	O1D-CGD-O2D-CED
20	A	1109	CLA	O1D-CGD-O2D-CED
20	A	1121	CLA	O1D-CGD-O2D-CED
20	A	1131	CLA	O1D-CGD-O2D-CED
20	A	1141	CLA	O1D-CGD-O2D-CED
20	B	1206	CLA	O1D-CGD-O2D-CED
20	B	1207	CLA	O1D-CGD-O2D-CED
20	B	1213	CLA	O1D-CGD-O2D-CED
20	B	1217	CLA	O1D-CGD-O2D-CED
20	B	1224	CLA	O1D-CGD-O2D-CED
20	B	1226	CLA	O1D-CGD-O2D-CED
20	F	1302	CLA	O1D-CGD-O2D-CED
20	Z	601	CLA	O1D-CGD-O2D-CED
20	Z	602	CLA	O1D-CGD-O2D-CED
20	Z	605	CLA	O1D-CGD-O2D-CED
20	Z	612	CLA	O1D-CGD-O2D-CED
20	3	605	CLA	O1D-CGD-O2D-CED
20	3	618	CLA	O1D-CGD-O2D-CED
20	7	602	CLA	O1D-CGD-O2D-CED
20	7	615	CLA	O1D-CGD-O2D-CED
20	8	602	CLA	O1D-CGD-O2D-CED
20	8	611	CLA	O1D-CGD-O2D-CED
20	4	602	CLA	O1D-CGD-O2D-CED
20	4	607	CLA	O1D-CGD-O2D-CED
20	4	608	CLA	O1D-CGD-O2D-CED
20	4	612	CLA	O1D-CGD-O2D-CED
20	5	602	CLA	O1D-CGD-O2D-CED
20	5	603	CLA	O1D-CGD-O2D-CED
20	5	605	CLA	O1D-CGD-O2D-CED
20	5	615	CLA	O1D-CGD-O2D-CED
20	6	608	CLA	O1D-CGD-O2D-CED
20	B	1228	CLA	CBA-CGA-O2A-C1
20	Z	612	CLA	CBA-CGA-O2A-C1
29	A	5003	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1103	CLA	CBD-CGD-O2D-CED
20	A	1105	CLA	CBD-CGD-O2D-CED
20	A	1106	CLA	CBD-CGD-O2D-CED
20	A	1112	CLA	CBD-CGD-O2D-CED
20	A	1113	CLA	CBD-CGD-O2D-CED
20	A	1118	CLA	CBD-CGD-O2D-CED
20	A	1127	CLA	CBD-CGD-O2D-CED
20	A	1133	CLA	CBD-CGD-O2D-CED
20	B	1203	CLA	CBD-CGD-O2D-CED
20	B	1211	CLA	CBD-CGD-O2D-CED
20	B	1218	CLA	CBD-CGD-O2D-CED
20	B	1227	CLA	CBD-CGD-O2D-CED
20	B	1230	CLA	CBD-CGD-O2D-CED
20	F	1301	CLA	CBD-CGD-O2D-CED
20	L	1502	CLA	CBD-CGD-O2D-CED
20	1	606	CLA	CBD-CGD-O2D-CED
20	3	607	CLA	CBD-CGD-O2D-CED
20	7	608	CLA	CBD-CGD-O2D-CED
20	8	605	CLA	CBD-CGD-O2D-CED
20	4	601	CLA	CBD-CGD-O2D-CED
20	5	606	CLA	CBD-CGD-O2D-CED
20	6	609	CLA	CBD-CGD-O2D-CED
20	6	607	CLA	CBD-CGD-O2D-CED
20	A	1102	CLA	O1A-CGA-O2A-C1
20	A	1113	CLA	O1A-CGA-O2A-C1
20	A	1114	CLA	O1A-CGA-O2A-C1
20	A	1129	CLA	O1A-CGA-O2A-C1
20	A	1133	CLA	O1A-CGA-O2A-C1
20	B	1202	CLA	O1A-CGA-O2A-C1
20	B	1206	CLA	O1A-CGA-O2A-C1
20	B	1218	CLA	O1A-CGA-O2A-C1
20	B	1220	CLA	O1A-CGA-O2A-C1
20	B	1222	CLA	O1A-CGA-O2A-C1
20	K	1404	CLA	O1A-CGA-O2A-C1
20	1	604	CLA	O1A-CGA-O2A-C1
20	1	605	CLA	O1A-CGA-O2A-C1
20	Z	604	CLA	O1A-CGA-O2A-C1
20	7	607	CLA	O1A-CGA-O2A-C1
20	4	604	CLA	O1A-CGA-O2A-C1
20	4	605	CLA	O1A-CGA-O2A-C1
20	5	605	CLA	O1A-CGA-O2A-C1
25	3	802	NKP	OAE-CAK-OAJ-CAI

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Mol	Chain	Res	Type	Atoms
40	7	802	3PH	O32-C31-O31-C3
40	8	806	3PH	O32-C31-O31-C3
20	B	1208	CLA	O1D-CGD-O2D-CED
20	B	1241	CLA	O1D-CGD-O2D-CED
20	J	1901	CLA	O1D-CGD-O2D-CED
20	1	615	CLA	O1D-CGD-O2D-CED
20	7	603	CLA	O1D-CGD-O2D-CED
20	7	613	CLA	O1D-CGD-O2D-CED
20	8	607	CLA	O1D-CGD-O2D-CED
20	6	618	CLA	O1D-CGD-O2D-CED
20	A	1102	CLA	O1D-CGD-O2D-CED
20	B	1205	CLA	O1D-CGD-O2D-CED
20	B	1214	CLA	O1D-CGD-O2D-CED
20	B	1234	CLA	O1D-CGD-O2D-CED
20	B	1239	CLA	O1D-CGD-O2D-CED
20	1	602	CLA	O1D-CGD-O2D-CED
20	1	608	CLA	O1D-CGD-O2D-CED
20	Z	603	CLA	O1D-CGD-O2D-CED
20	5	601	CLA	O1D-CGD-O2D-CED
20	5	608	CLA	O1D-CGD-O2D-CED
20	6	606	CLA	O1D-CGD-O2D-CED
20	A	1013	CLA	CBD-CGD-O2D-CED
20	A	1101	CLA	CBD-CGD-O2D-CED
20	7	609	CLA	CBD-CGD-O2D-CED
20	6	601	CLA	CBD-CGD-O2D-CED
20	A	1128	CLA	O1D-CGD-O2D-CED
20	K	1404	CLA	O1D-CGD-O2D-CED
20	Z	604	CLA	O1D-CGD-O2D-CED
20	7	607	CLA	O1D-CGD-O2D-CED
24	B	5006	LHG	O9-C7-O7-C5
24	4	801	LHG	O9-C7-O7-C5
24	6	801	LHG	O9-C7-O7-C5
29	J	5001	LMG	O9-C10-O7-C8
31	B	5003	DGD	O1B-C1B-O2G-C2G
38	1	802	SQD	O49-C7-O47-C45
40	7	802	3PH	O22-C21-O21-C2
40	8	806	3PH	O22-C21-O21-C2
20	8	612	CLA	CBA-CGA-O2A-C1
20	8	612	CLA	O1A-CGA-O2A-C1
20	A	1104	CLA	C3-C5-C6-C7
20	A	1107	CLA	C3-C5-C6-C7
20	A	1120	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	1126	CLA	C3-C5-C6-C7
20	A	1131	CLA	C3-C5-C6-C7
20	A	1139	CLA	C3-C5-C6-C7
20	A	1130	CLA	C3-C5-C6-C7
20	B	1237	CLA	C3-C5-C6-C7
20	B	1209	CLA	C3-C5-C6-C7
20	B	1211	CLA	C3-C5-C6-C7
20	B	1212	CLA	C3-C5-C6-C7
20	B	1215	CLA	C3-C5-C6-C7
20	B	1226	CLA	C3-C5-C6-C7
20	B	1234	CLA	C3-C5-C6-C7
20	B	1236	CLA	C3-C5-C6-C7
20	B	1239	CLA	C3-C5-C6-C7
20	1	605	CLA	C3-C5-C6-C7
20	1	607	CLA	C3-C5-C6-C7
20	Z	606	CLA	C3-C5-C6-C7
20	Z	607	CLA	C3-C5-C6-C7
20	Z	611	CLA	C3-C5-C6-C7
20	3	607	CLA	C3-C5-C6-C7
20	3	610	CLA	C3-C5-C6-C7
20	7	605	CLA	C3-C5-C6-C7
20	7	615	CLA	C3-C5-C6-C7
20	8	605	CLA	C3-C5-C6-C7
20	8	608	CLA	C3-C5-C6-C7
20	4	608	CLA	C3-C5-C6-C7
20	5	601	CLA	C3-C5-C6-C7
20	A	1102	CLA	CBA-CGA-O2A-C1
20	A	1104	CLA	CBA-CGA-O2A-C1
20	A	1113	CLA	CBA-CGA-O2A-C1
20	A	1128	CLA	CBA-CGA-O2A-C1
20	A	1133	CLA	CBA-CGA-O2A-C1
20	A	1139	CLA	CBA-CGA-O2A-C1
20	A	1130	CLA	CBA-CGA-O2A-C1
20	A	1101	CLA	CBA-CGA-O2A-C1
20	B	1202	CLA	CBA-CGA-O2A-C1
20	B	1206	CLA	CBA-CGA-O2A-C1
20	B	1207	CLA	CBA-CGA-O2A-C1
20	B	1216	CLA	CBA-CGA-O2A-C1
20	K	1404	CLA	CBA-CGA-O2A-C1
20	1	605	CLA	CBA-CGA-O2A-C1
20	7	607	CLA	CBA-CGA-O2A-C1
20	4	601	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	4	605	CLA	CBA-CGA-O2A-C1
20	4	608	CLA	CBA-CGA-O2A-C1
20	5	605	CLA	CBA-CGA-O2A-C1
20	5	607	CLA	CBA-CGA-O2A-C1
20	5	613	CLA	CBA-CGA-O2A-C1
38	1	802	SQD	C24-C23-O48-C46
40	7	802	3PH	C32-C31-O31-C3
40	8	806	3PH	C32-C31-O31-C3
24	6	801	LHG	C8-C7-O7-C5
40	7	802	3PH	C22-C21-O21-C2
40	5	802	3PH	C22-C21-O21-C2
20	A	1136	CLA	O1D-CGD-O2D-CED
20	B	1237	CLA	O1D-CGD-O2D-CED
20	B	1215	CLA	O1D-CGD-O2D-CED
20	7	611	CLA	O1D-CGD-O2D-CED
20	7	616	CLA	O1D-CGD-O2D-CED
20	7	601	CLA	CBD-CGD-O2D-CED
20	A	1124	CLA	O1A-CGA-O2A-C1
20	Z	602	CLA	O1A-CGA-O2A-C1
20	6	602	CLA	C3-C5-C6-C7
20	A	1012	CLA	C4-C3-C5-C6
20	A	1122	CLA	C4-C3-C5-C6
20	B	1237	CLA	C4-C3-C5-C6
20	A	1133	CLA	C2-C3-C5-C6
20	B	1238	CLA	CBD-CGD-O2D-CED
20	3	603	CLA	CBD-CGD-O2D-CED
20	A	1111	CLA	C2A-CAA-CBA-CGA
20	A	1120	CLA	C2A-CAA-CBA-CGA
20	A	1131	CLA	C2A-CAA-CBA-CGA
20	B	1237	CLA	C2A-CAA-CBA-CGA
20	B	1206	CLA	C2A-CAA-CBA-CGA
20	B	1228	CLA	C2A-CAA-CBA-CGA
20	Z	607	CLA	C2A-CAA-CBA-CGA
20	3	610	CLA	C2A-CAA-CBA-CGA
20	7	612	CLA	C2A-CAA-CBA-CGA
20	7	615	CLA	C2A-CAA-CBA-CGA
20	8	607	CLA	C2A-CAA-CBA-CGA
20	4	608	CLA	C2A-CAA-CBA-CGA
20	5	606	CLA	C2A-CAA-CBA-CGA
20	6	606	CLA	C2A-CAA-CBA-CGA
37	1	610	CHL	C2A-CAA-CBA-CGA
37	Z	610	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	B	1215	CLA	O1A-CGA-O2A-C1
20	1	615	CLA	O1A-CGA-O2A-C1
20	1	607	CLA	O1D-CGD-O2D-CED
31	B	5003	DGD	C8A-C9A-CAA-CBA
31	B	5003	DGD	CBA-CCA-CDA-CEA
20	A	1102	CLA	C3-C5-C6-C7
20	A	1115	CLA	C3-C5-C6-C7
20	A	1118	CLA	C3-C5-C6-C7
20	A	1136	CLA	C3-C5-C6-C7
20	B	1203	CLA	C3-C5-C6-C7
20	B	1218	CLA	C3-C5-C6-C7
20	K	1402	CLA	C3-C5-C6-C7
20	1	611	CLA	C3-C5-C6-C7
20	Z	605	CLA	C3-C5-C6-C7
20	7	607	CLA	C3-C5-C6-C7
20	8	607	CLA	C3-C5-C6-C7
20	6	605	CLA	C3-C5-C6-C7
20	A	1111	CLA	CBA-CGA-O2A-C1
20	A	1114	CLA	CBA-CGA-O2A-C1
20	A	1123	CLA	CBA-CGA-O2A-C1
20	A	1126	CLA	CBA-CGA-O2A-C1
20	A	1129	CLA	CBA-CGA-O2A-C1
20	B	1237	CLA	CBA-CGA-O2A-C1
20	B	1203	CLA	CBA-CGA-O2A-C1
20	B	1215	CLA	CBA-CGA-O2A-C1
20	B	1218	CLA	CBA-CGA-O2A-C1
20	B	1220	CLA	CBA-CGA-O2A-C1
20	B	1222	CLA	CBA-CGA-O2A-C1
20	B	1227	CLA	CBA-CGA-O2A-C1
20	B	1240	CLA	CBA-CGA-O2A-C1
20	B	1230	CLA	CBA-CGA-O2A-C1
20	1	604	CLA	CBA-CGA-O2A-C1
20	Z	604	CLA	CBA-CGA-O2A-C1
20	3	613	CLA	CBA-CGA-O2A-C1
20	8	601	CLA	CBA-CGA-O2A-C1
20	4	602	CLA	CBA-CGA-O2A-C1
20	4	604	CLA	CBA-CGA-O2A-C1
20	5	601	CLA	CBA-CGA-O2A-C1
20	5	606	CLA	CBA-CGA-O2A-C1
25	3	802	NKP	CAL-CAK-OAJ-CAI
26	B	6101	LMT	O5B-C5B-C6B-O6B
26	4	803	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	1	601	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	O1D-CGD-O2D-CED
20	4	603	CLA	O1D-CGD-O2D-CED
20	A	1129	CLA	CBD-CGD-O2D-CED
20	A	1117	CLA	O1D-CGD-O2D-CED
20	A	1119	CLA	O1D-CGD-O2D-CED
20	A	1124	CLA	O1D-CGD-O2D-CED
20	A	1139	CLA	O1D-CGD-O2D-CED
20	B	1216	CLA	O1D-CGD-O2D-CED
20	B	1229	CLA	O1D-CGD-O2D-CED
20	B	1231	CLA	O1D-CGD-O2D-CED
20	B	1235	CLA	O1D-CGD-O2D-CED
20	K	1401	CLA	O1D-CGD-O2D-CED
20	1	604	CLA	O1D-CGD-O2D-CED
20	Z	607	CLA	O1D-CGD-O2D-CED
20	3	608	CLA	O1D-CGD-O2D-CED
20	3	613	CLA	O1D-CGD-O2D-CED
20	5	607	CLA	O1D-CGD-O2D-CED
20	5	609	CLA	O1D-CGD-O2D-CED
20	5	622	CLA	O1D-CGD-O2D-CED
26	4	803	LMT	O5B-C5B-C6B-O6B
24	1	801	LHG	O9-C7-O7-C5
24	Z	801	LHG	O9-C7-O7-C5
26	F	5001	LMT	C4B-C5B-C6B-O6B
20	A	1111	CLA	O1A-CGA-O2A-C1
20	A	1119	CLA	O1A-CGA-O2A-C1
20	A	1126	CLA	O1A-CGA-O2A-C1
20	A	1128	CLA	O1A-CGA-O2A-C1
20	A	1139	CLA	O1A-CGA-O2A-C1
20	B	1237	CLA	O1A-CGA-O2A-C1
20	B	1203	CLA	O1A-CGA-O2A-C1
20	B	1216	CLA	O1A-CGA-O2A-C1
20	B	1227	CLA	O1A-CGA-O2A-C1
20	F	1301	CLA	O1A-CGA-O2A-C1
20	Z	606	CLA	O1A-CGA-O2A-C1
20	Z	607	CLA	O1A-CGA-O2A-C1
20	4	601	CLA	O1A-CGA-O2A-C1
20	4	602	CLA	O1A-CGA-O2A-C1
20	4	607	CLA	O1A-CGA-O2A-C1
20	5	601	CLA	O1A-CGA-O2A-C1
20	5	607	CLA	O1A-CGA-O2A-C1
20	5	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	5	618	CLA	O1A-CGA-O2A-C1
20	6	602	CLA	O1A-CGA-O2A-C1
25	A	5004	NKP	OAE-CAK-OAJ-CAI
20	8	606	CLA	O1D-CGD-O2D-CED
23	5	503	BCR	C9-C10-C11-C12
23	5	504	BCR	C9-C10-C11-C12
23	6	503	BCR	C9-C10-C11-C12
20	A	1110	CLA	CBD-CGD-O2D-CED
20	A	1120	CLA	CBD-CGD-O2D-CED
20	B	1236	CLA	CBD-CGD-O2D-CED
20	A	1130	CLA	O1D-CGD-O2D-CED
24	A	5001	LHG	O2-C2-C3-O3
24	B	5001	LHG	O2-C2-C3-O3
24	Z	801	LHG	O2-C2-C3-O3
24	4	801	LHG	O2-C2-C3-O3
24	6	801	LHG	O2-C2-C3-O3
25	8	802	NKP	OAF-CAG-CAH-OBC
20	A	1103	CLA	C3-C5-C6-C7
20	A	1122	CLA	C3-C5-C6-C7
20	A	1127	CLA	C3-C5-C6-C7
20	A	1134	CLA	C3-C5-C6-C7
20	B	1204	CLA	C3-C5-C6-C7
20	B	1228	CLA	C3-C5-C6-C7
20	B	1229	CLA	C3-C5-C6-C7
20	B	1240	CLA	C3-C5-C6-C7
20	L	1502	CLA	C3-C5-C6-C7
20	3	612	CLA	C3-C5-C6-C7
20	A	1119	CLA	CBA-CGA-O2A-C1
20	B	1210	CLA	CBA-CGA-O2A-C1
20	B	1217	CLA	CBA-CGA-O2A-C1
20	1	601	CLA	CBA-CGA-O2A-C1
20	Z	603	CLA	CBA-CGA-O2A-C1
20	Z	606	CLA	CBA-CGA-O2A-C1
20	8	607	CLA	CBA-CGA-O2A-C1
20	4	606	CLA	CBA-CGA-O2A-C1
20	4	607	CLA	CBA-CGA-O2A-C1
20	5	618	CLA	CBA-CGA-O2A-C1
20	6	602	CLA	CBA-CGA-O2A-C1
20	6	607	CLA	CBA-CGA-O2A-C1
20	A	1123	CLA	O1A-CGA-O2A-C1
20	A	1130	CLA	O1A-CGA-O2A-C1
20	B	1230	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	5	606	CLA	O1A-CGA-O2A-C1
26	A	5006	LMT	O5B-C5B-C6B-O6B
20	B	1209	CLA	O1D-CGD-O2D-CED
20	Z	606	CLA	O1D-CGD-O2D-CED
20	6	612	CLA	O1D-CGD-O2D-CED
25	A	5004	NKP	OBC-CAH-CAI-OAJ
30	A	5005	DGA	CB2-CB1-OG2-CG2
20	3	602	CLA	CBA-CGA-O2A-C1
20	5	622	CLA	CBA-CGA-O2A-C1
20	A	1125	CLA	CBD-CGD-O2D-CED
20	B	1221	CLA	CBD-CGD-O2D-CED
20	B	1240	CLA	CBD-CGD-O2D-CED
20	3	601	CLA	CBD-CGD-O2D-CED
20	5	612	CLA	CBD-CGD-O2D-CED
26	F	5001	LMT	O5B-C5B-C6B-O6B
20	8	607	CLA	O1A-CGA-O2A-C1
20	B	1212	CLA	O1D-CGD-O2D-CED
20	B	1222	CLA	O1D-CGD-O2D-CED
20	3	612	CLA	O1D-CGD-O2D-CED
20	B	1220	CLA	CBD-CGD-O2D-CED
20	8	609	CLA	C3-C5-C6-C7
20	A	1117	CLA	CBA-CGA-O2A-C1
20	A	1124	CLA	CBA-CGA-O2A-C1
20	B	1211	CLA	CBA-CGA-O2A-C1
20	F	1301	CLA	CBA-CGA-O2A-C1
20	1	615	CLA	CBA-CGA-O2A-C1
20	Z	607	CLA	CBA-CGA-O2A-C1
20	6	606	CLA	CBA-CGA-O2A-C1
25	A	5004	NKP	CAL-CAK-OAJ-CAI
30	A	5005	DGA	OB1-CB1-OG2-CG2
26	B	6101	LMT	C4B-C5B-C6B-O6B
26	8	805	LMT	C4'-C5'-C6'-O6'
24	7	801	LHG	C2-C3-O3-P
20	1	601	CLA	O1A-CGA-O2A-C1
20	Z	603	CLA	O1A-CGA-O2A-C1
20	8	601	CLA	O1A-CGA-O2A-C1
20	4	606	CLA	O1A-CGA-O2A-C1
20	A	1115	CLA	C4-C3-C5-C6
20	B	1234	CLA	C4-C3-C5-C6
20	A	1115	CLA	C2-C3-C5-C6
20	B	1237	CLA	C2-C3-C5-C6
20	B	1234	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	1105	CLA	C2A-CAA-CBA-CGA
20	A	1106	CLA	C2A-CAA-CBA-CGA
20	A	1122	CLA	C2A-CAA-CBA-CGA
20	A	1141	CLA	C2A-CAA-CBA-CGA
20	B	1207	CLA	C2A-CAA-CBA-CGA
20	B	1211	CLA	C2A-CAA-CBA-CGA
20	B	1214	CLA	C2A-CAA-CBA-CGA
20	F	1302	CLA	C2A-CAA-CBA-CGA
20	A	1133	CLA	O1D-CGD-O2D-CED
20	B	1223	CLA	O1D-CGD-O2D-CED
26	4	803	LMT	O5'-C5'-C6'-O6'
20	B	1210	CLA	O1A-CGA-O2A-C1
20	B	1211	CLA	O1A-CGA-O2A-C1
20	B	1217	CLA	O1A-CGA-O2A-C1
20	3	613	CLA	O1A-CGA-O2A-C1
20	6	607	CLA	O1A-CGA-O2A-C1
20	1	606	CLA	O1D-CGD-O2D-CED
20	5	602	CLA	C3-C5-C6-C7
20	A	1106	CLA	CBA-CGA-O2A-C1
20	A	1120	CLA	CBA-CGA-O2A-C1
20	7	606	CLA	CBA-CGA-O2A-C1
20	8	606	CLA	CBA-CGA-O2A-C1
20	8	611	CLA	CBA-CGA-O2A-C1
20	5	615	CLA	CBA-CGA-O2A-C1
20	G	1602	CLA	O1D-CGD-O2D-CED
26	A	5006	LMT	C4'-C5'-C6'-O6'
20	F	1301	CLA	O1D-CGD-O2D-CED
20	A	1120	CLA	O1A-CGA-O2A-C1
26	A	5006	LMT	C4B-C5B-C6B-O6B
20	A	1103	CLA	O1D-CGD-O2D-CED
20	A	1112	CLA	O1D-CGD-O2D-CED
20	6	607	CLA	O1D-CGD-O2D-CED
24	B	5001	LHG	C1-C2-C3-O3
24	Z	801	LHG	C1-C2-C3-O3
24	3	801	LHG	C1-C2-C3-O3
24	7	801	LHG	C1-C2-C3-O3
24	5	801	LHG	C1-C2-C3-O3
25	8	802	NKP	OAF-CAG-CAH-CAI
20	A	1106	CLA	O1A-CGA-O2A-C1
20	A	1117	CLA	O1A-CGA-O2A-C1
20	B	1239	CLA	O1A-CGA-O2A-C1
20	7	606	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	8	606	CLA	O1A-CGA-O2A-C1
20	6	606	CLA	O1A-CGA-O2A-C1
20	A	1112	CLA	C3-C5-C6-C7
20	4	607	CLA	C3-C5-C6-C7
20	6	615	CLA	C3-C5-C6-C7
20	B	1230	CLA	O1D-CGD-O2D-CED
20	7	608	CLA	O1D-CGD-O2D-CED
20	8	605	CLA	O1D-CGD-O2D-CED
20	A	1105	CLA	CBA-CGA-O2A-C1
20	A	1108	CLA	CBA-CGA-O2A-C1
20	A	1112	CLA	CBA-CGA-O2A-C1
20	A	1116	CLA	CBA-CGA-O2A-C1
20	A	1121	CLA	CBA-CGA-O2A-C1
20	A	1131	CLA	CBA-CGA-O2A-C1
20	A	1137	CLA	CBA-CGA-O2A-C1
20	B	1023	CLA	CBA-CGA-O2A-C1
20	B	1214	CLA	CBA-CGA-O2A-C1
20	B	1219	CLA	CBA-CGA-O2A-C1
20	B	1224	CLA	CBA-CGA-O2A-C1
20	B	1231	CLA	CBA-CGA-O2A-C1
20	B	1236	CLA	CBA-CGA-O2A-C1
20	B	1239	CLA	CBA-CGA-O2A-C1
20	K	1402	CLA	CBA-CGA-O2A-C1
20	K	1403	CLA	CBA-CGA-O2A-C1
20	L	1502	CLA	CBA-CGA-O2A-C1
20	1	607	CLA	CBA-CGA-O2A-C1
20	Z	608	CLA	CBA-CGA-O2A-C1
20	3	606	CLA	CBA-CGA-O2A-C1
20	3	607	CLA	CBA-CGA-O2A-C1
20	3	610	CLA	CBA-CGA-O2A-C1
20	7	615	CLA	CBA-CGA-O2A-C1
20	8	608	CLA	CBA-CGA-O2A-C1
20	5	609	CLA	CBA-CGA-O2A-C1
20	5	612	CLA	CBA-CGA-O2A-C1
20	6	608	CLA	CBA-CGA-O2A-C1
20	6	605	CLA	CBA-CGA-O2A-C1
30	A	5005	DGA	CA2-CA1-OG1-CG1
20	A	1134	CLA	CBD-CGD-O2D-CED
20	Z	608	CLA	CBD-CGD-O2D-CED
20	5	618	CLA	CBD-CGD-O2D-CED
23	7	504	BCR	C9-C10-C11-C12
34	5	505	C7Z	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	Z	503	LUT	C29-C30-C31-C32
25	8	802	NKP	CAK-CAL-CAM-CAN
20	A	1117	CLA	C13-C15-C16-C17
20	B	1210	CLA	C13-C15-C16-C17
20	B	1223	CLA	C13-C15-C16-C17
20	1	615	CLA	C15-C16-C17-C18
20	7	607	CLA	C15-C16-C17-C18
26	F	5001	LMT	O5'-C5'-C6'-O6'
26	B	5005	LMT	C4'-C5'-C6'-O6'
20	B	1218	CLA	O1D-CGD-O2D-CED
20	3	602	CLA	O1A-CGA-O2A-C1
20	A	1107	CLA	C8-C10-C11-C12
20	A	1111	CLA	C15-C16-C17-C18
20	B	1204	CLA	C5-C6-C7-C8
20	B	1228	CLA	C5-C6-C7-C8
20	3	603	CLA	C5-C6-C7-C8
20	3	610	CLA	C10-C11-C12-C13
20	3	612	CLA	C8-C10-C11-C12
20	7	601	CLA	C8-C10-C11-C12
24	B	5002	LHG	O2-C2-C3-O3
24	B	5006	LHG	O2-C2-C3-O3
24	7	801	LHG	O2-C2-C3-O3
24	8	801	LHG	O2-C2-C3-O3
20	A	1105	CLA	O1A-CGA-O2A-C1
20	B	1231	CLA	O1A-CGA-O2A-C1
20	B	1236	CLA	O1A-CGA-O2A-C1
20	L	1502	CLA	O1A-CGA-O2A-C1
20	3	607	CLA	O1A-CGA-O2A-C1
20	3	610	CLA	O1A-CGA-O2A-C1
20	8	611	CLA	O1A-CGA-O2A-C1
20	5	612	CLA	O1A-CGA-O2A-C1
20	6	605	CLA	O1A-CGA-O2A-C1
20	B	1206	CLA	C4-C3-C5-C6
20	A	1104	CLA	C6-C7-C8-C9
20	A	1107	CLA	C6-C7-C8-C9
20	A	1121	CLA	C11-C10-C8-C9
20	A	1136	CLA	C14-C13-C15-C16
20	B	1203	CLA	C6-C7-C8-C9
20	B	1205	CLA	C14-C13-C15-C16
20	B	1226	CLA	C11-C10-C8-C9
20	B	1239	CLA	C11-C10-C8-C9
20	1	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	Z	610	CHL	C14-C13-C15-C16
20	A	1105	CLA	O1D-CGD-O2D-CED
20	A	1113	CLA	O1D-CGD-O2D-CED
20	A	1127	CLA	O1D-CGD-O2D-CED
20	8	609	CLA	CBD-CGD-O2D-CED
20	B	1210	CLA	C10-C11-C12-C13
20	3	612	CLA	C5-C6-C7-C8
20	5	605	CLA	C5-C6-C7-C8
20	A	1133	CLA	C2A-CAA-CBA-CGA
20	L	1503	CLA	C2A-CAA-CBA-CGA
20	3	616	CLA	C2A-CAA-CBA-CGA
20	8	606	CLA	C2A-CAA-CBA-CGA
23	A	4004	BCR	C37-C22-C23-C24
23	B	4001	BCR	C7-C8-C9-C34
23	B	4001	BCR	C36-C18-C19-C20
23	B	4007	BCR	C7-C8-C9-C34
23	G	4001	BCR	C7-C8-C9-C34
23	G	4001	BCR	C37-C22-C23-C24
23	L	4001	BCR	C37-C22-C23-C24
23	L	4002	BCR	C36-C18-C19-C20
23	3	504	BCR	C36-C18-C19-C20
23	8	503	BCR	C7-C8-C9-C34
23	5	503	BCR	C37-C22-C23-C24
23	5	504	BCR	C37-C22-C23-C24
23	6	504	BCR	C37-C22-C23-C24
23	6	503	BCR	C7-C8-C9-C34
33	F	4001	RRX	C37-C22-C23-C24
34	J	4002	C7Z	C7-C8-C9-C19
34	J	4002	C7Z	C11-C12-C13-C20
34	5	505	C7Z	C11-C12-C13-C20
23	B	4001	BCR	C17-C18-C19-C20
23	G	4001	BCR	C21-C22-C23-C24
23	K	4001	BCR	C7-C8-C9-C10
23	L	4001	BCR	C21-C22-C23-C24
23	8	503	BCR	C7-C8-C9-C10
23	5	504	BCR	C21-C22-C23-C24
23	6	504	BCR	C21-C22-C23-C24
33	F	4001	RRX	C21-C22-C23-C24
34	J	4002	C7Z	C7-C8-C9-C10
34	J	4002	C7Z	C11-C12-C13-C14
34	J	4002	C7Z	C31-C32-C33-C34
34	5	505	C7Z	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	B	5005	LMT	O5'-C5'-C6'-O6'
24	8	801	LHG	C23-C24-C25-C26
20	A	1108	CLA	O1A-CGA-O2A-C1
20	A	1116	CLA	O1A-CGA-O2A-C1
20	A	1121	CLA	O1A-CGA-O2A-C1
20	B	1214	CLA	O1A-CGA-O2A-C1
20	8	608	CLA	O1A-CGA-O2A-C1
20	5	609	CLA	O1A-CGA-O2A-C1
30	A	5005	DGA	OA1-CA1-OG1-CG1
20	A	1102	CLA	C5-C6-C7-C8
20	A	1104	CLA	C8-C10-C11-C12
20	A	1101	CLA	C13-C15-C16-C17
20	B	1204	CLA	C15-C16-C17-C18
20	B	1216	CLA	C8-C10-C11-C12
20	B	1224	CLA	C13-C15-C16-C17
20	B	1240	CLA	C15-C16-C17-C18
20	B	1230	CLA	C5-C6-C7-C8
20	L	1502	CLA	C5-C6-C7-C8
20	8	605	CLA	C8-C10-C11-C12
20	B	1203	CLA	O1D-CGD-O2D-CED
20	4	601	CLA	O1D-CGD-O2D-CED
20	1	613	CLA	CBA-CGA-O2A-C1
26	4	803	LMT	C4'-C5'-C6'-O6'
20	3	607	CLA	O1D-CGD-O2D-CED
20	B	1212	CLA	CBA-CGA-O2A-C1
20	B	1229	CLA	CBA-CGA-O2A-C1
20	L	1503	CLA	CBA-CGA-O2A-C1
20	3	616	CLA	CBA-CGA-O2A-C1
20	A	1110	CLA	C8-C10-C11-C12
20	A	1111	CLA	C13-C15-C16-C17
20	B	1202	CLA	C15-C16-C17-C18
20	B	1216	CLA	C10-C11-C12-C13
20	B	1220	CLA	C8-C10-C11-C12
20	B	1222	CLA	C13-C15-C16-C17
20	L	1502	CLA	C15-C16-C17-C18
20	1	601	CLA	C10-C11-C12-C13
20	1	606	CLA	C5-C6-C7-C8
20	Z	612	CLA	C5-C6-C7-C8
20	Z	612	CLA	C8-C10-C11-C12
20	3	601	CLA	C13-C15-C16-C17
20	3	606	CLA	C15-C16-C17-C18
20	3	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	7	603	CLA	C5-C6-C7-C8
20	7	607	CLA	C5-C6-C7-C8
20	7	616	CLA	C5-C6-C7-C8
20	8	603	CLA	C5-C6-C7-C8
20	8	606	CLA	C8-C10-C11-C12
24	4	801	LHG	C7-C8-C9-C10
20	A	1013	CLA	O1D-CGD-O2D-CED
20	7	612	CLA	CBD-CGD-O2D-CED
20	A	1012	CLA	C5-C6-C7-C8
20	A	1109	CLA	C13-C15-C16-C17
20	A	1122	CLA	C15-C16-C17-C18
20	A	1131	CLA	C5-C6-C7-C8
20	A	1137	CLA	C10-C11-C12-C13
20	A	1013	CLA	C15-C16-C17-C18
20	A	1130	CLA	C10-C11-C12-C13
20	B	1202	CLA	C13-C15-C16-C17
20	B	1213	CLA	C5-C6-C7-C8
20	B	1229	CLA	C5-C6-C7-C8
20	B	1229	CLA	C13-C15-C16-C17
20	B	1236	CLA	C15-C16-C17-C18
20	Z	612	CLA	C10-C11-C12-C13
20	7	603	CLA	C10-C11-C12-C13
20	8	609	CLA	C13-C15-C16-C17
20	8	605	CLA	C10-C11-C12-C13
20	8	605	CLA	C15-C16-C17-C18
20	5	618	CLA	C8-C10-C11-C12
20	6	609	CLA	C8-C10-C11-C12
20	6	619	CLA	C10-C11-C12-C13
37	Z	609	CHL	C5-C6-C7-C8
20	B	1227	CLA	O1D-CGD-O2D-CED
24	3	801	LHG	O1-C1-C2-O2
20	B	1224	CLA	O1A-CGA-O2A-C1
24	A	5001	LHG	C23-C24-C25-C26
24	A	5002	LHG	C7-C8-C9-C10
24	6	801	LHG	C23-C24-C25-C26
30	A	5005	DGA	CB1-CB2-CB3-CB4
40	7	802	3PH	C31-C32-C33-C34
26	B	6101	LMT	O1'-C1-C2-C3
20	3	604	CLA	CBD-CGD-O2D-CED
20	L	1502	CLA	O1D-CGD-O2D-CED
20	A	1133	CLA	C15-C16-C17-C18
20	A	1130	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	B	1203	CLA	C10-C11-C12-C13
20	B	1221	CLA	C13-C15-C16-C17
20	B	1239	CLA	C15-C16-C17-C18
20	B	1241	CLA	C5-C6-C7-C8
20	1	611	CLA	C15-C16-C17-C18
20	Z	611	CLA	C5-C6-C7-C8
20	5	601	CLA	C10-C11-C12-C13
20	Z	605	CLA	CBA-CGA-O2A-C1
20	6	601	CLA	CBA-CGA-O2A-C1
20	5	622	CLA	O1A-CGA-O2A-C1
20	6	609	CLA	O1D-CGD-O2D-CED
19	A	1011	CL0	C2-C1-O2A-CGA
20	A	1012	CLA	C2-C1-O2A-CGA
20	A	1112	CLA	C2-C1-O2A-CGA
20	A	1126	CLA	C2-C1-O2A-CGA
20	A	1129	CLA	C2-C1-O2A-CGA
20	B	1022	CLA	C2-C1-O2A-CGA
20	B	1212	CLA	C2-C1-O2A-CGA
20	B	1213	CLA	C2-C1-O2A-CGA
20	B	1226	CLA	C2-C1-O2A-CGA
20	B	1228	CLA	C2-C1-O2A-CGA
20	B	1235	CLA	C2-C1-O2A-CGA
20	B	1241	CLA	C2-C1-O2A-CGA
20	B	1230	CLA	C2-C1-O2A-CGA
20	K	1403	CLA	C2-C1-O2A-CGA
20	L	1503	CLA	C2-C1-O2A-CGA
20	Z	612	CLA	C2-C1-O2A-CGA
20	3	601	CLA	C2-C1-O2A-CGA
20	7	602	CLA	C2-C1-O2A-CGA
20	7	604	CLA	C2-C1-O2A-CGA
20	7	606	CLA	C2-C1-O2A-CGA
20	8	609	CLA	C2-C1-O2A-CGA
20	8	602	CLA	C2-C1-O2A-CGA
20	8	608	CLA	C2-C1-O2A-CGA
20	4	608	CLA	C2-C1-O2A-CGA
20	4	609	CLA	C2-C1-O2A-CGA
20	5	602	CLA	C2-C1-O2A-CGA
20	5	604	CLA	C2-C1-O2A-CGA
20	5	613	CLA	C2-C1-O2A-CGA
20	6	608	CLA	C2-C1-O2A-CGA
20	6	601	CLA	C2-C1-O2A-CGA
20	6	603	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
26	1	803	LMT	C4'-C5'-C6'-O6'
20	A	1104	CLA	C13-C15-C16-C17
20	A	1120	CLA	C5-C6-C7-C8
20	A	1132	CLA	C15-C16-C17-C18
20	B	1203	CLA	C15-C16-C17-C18
20	B	1209	CLA	C5-C6-C7-C8
20	B	1218	CLA	C10-C11-C12-C13
20	B	1240	CLA	C10-C11-C12-C13
20	1	611	CLA	C5-C6-C7-C8
20	7	609	CLA	C5-C6-C7-C8
20	7	603	CLA	C15-C16-C17-C18
24	4	802	LHG	C7-C8-C9-C10
37	1	609	CHL	C8-C10-C11-C12
29	A	5003	LMG	C11-C10-O7-C8
20	A	1109	CLA	C15-C16-C17-C18
20	A	1123	CLA	C15-C16-C17-C18
20	B	1207	CLA	C15-C16-C17-C18
20	B	1225	CLA	C5-C6-C7-C8
20	Z	612	CLA	C15-C16-C17-C18
20	7	601	CLA	C10-C11-C12-C13
20	A	1101	CLA	O1D-CGD-O2D-CED
20	7	609	CLA	O1D-CGD-O2D-CED
20	A	1110	CLA	C12-C13-C15-C16
20	A	1117	CLA	C6-C7-C8-C10
20	B	1203	CLA	C11-C10-C8-C7
20	B	1206	CLA	C11-C12-C13-C15
20	B	1238	CLA	C6-C7-C8-C10
20	1	604	CLA	C11-C10-C8-C7
20	1	615	CLA	C12-C13-C15-C16
20	7	604	CLA	C11-C12-C13-C15
20	5	607	CLA	C6-C7-C8-C10
20	6	603	CLA	C6-C7-C8-C10
20	A	1137	CLA	O1A-CGA-O2A-C1
20	B	1219	CLA	O1A-CGA-O2A-C1
20	K	1403	CLA	O1A-CGA-O2A-C1
20	Z	608	CLA	O1A-CGA-O2A-C1
23	A	4001	BCR	C9-C10-C11-C12
23	B	4007	BCR	C13-C14-C15-C16
23	3	506	BCR	C19-C20-C21-C22
23	7	504	BCR	C13-C14-C15-C16
23	6	504	BCR	C13-C14-C15-C16
34	J	4002	C7Z	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
34	1	503	C7Z	C29-C30-C31-C32
20	A	1125	CLA	C2A-CAA-CBA-CGA
20	B	1240	CLA	C2A-CAA-CBA-CGA
20	8	609	CLA	C2A-CAA-CBA-CGA
20	6	615	CLA	C2A-CAA-CBA-CGA
20	A	1106	CLA	O1D-CGD-O2D-CED
20	A	1118	CLA	O1D-CGD-O2D-CED
20	B	1211	CLA	O1D-CGD-O2D-CED
20	3	603	CLA	O1D-CGD-O2D-CED
20	7	601	CLA	O1D-CGD-O2D-CED
20	5	606	CLA	O1D-CGD-O2D-CED
20	6	601	CLA	O1D-CGD-O2D-CED
20	A	1121	CLA	C15-C16-C17-C18
20	A	1101	CLA	C8-C10-C11-C12
20	B	1203	CLA	C5-C6-C7-C8
20	B	1210	CLA	C8-C10-C11-C12
20	B	1213	CLA	C10-C11-C12-C13
20	B	1222	CLA	C10-C11-C12-C13
20	B	1225	CLA	C15-C16-C17-C18
20	1	601	CLA	C15-C16-C17-C18
20	Z	604	CLA	C10-C11-C12-C13
20	3	603	CLA	C15-C16-C17-C18
20	3	606	CLA	C10-C11-C12-C13
20	4	609	CLA	C5-C6-C7-C8
20	6	606	CLA	C13-C15-C16-C17
26	1	803	LMT	O1'-C1-C2-C3
20	A	1131	CLA	O1A-CGA-O2A-C1
20	B	1023	CLA	O1A-CGA-O2A-C1
20	K	1402	CLA	O1A-CGA-O2A-C1
20	7	615	CLA	O1A-CGA-O2A-C1
26	1	803	LMT	O5'-C1'-O1'-C1
20	A	1107	CLA	C5-C6-C7-C8
20	A	1112	CLA	C5-C6-C7-C8
20	A	1013	CLA	C10-C11-C12-C13
20	B	1229	CLA	C10-C11-C12-C13
20	B	1241	CLA	C10-C11-C12-C13
20	F	1301	CLA	C5-C6-C7-C8
20	K	1404	CLA	C5-C6-C7-C8
20	Z	601	CLA	C10-C11-C12-C13
20	8	601	CLA	C8-C10-C11-C12
20	6	619	CLA	C5-C6-C7-C8
23	A	4003	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	A	4005	BCR	C10-C11-C12-C13
23	B	4004	BCR	C10-C11-C12-C13
23	B	4006	BCR	C10-C11-C12-C13
23	K	4002	BCR	C10-C11-C12-C13
26	8	805	LMT	O5'-C5'-C6'-O6'
24	3	801	LHG	O2-C2-C3-O3
20	B	1216	CLA	C3-C5-C6-C7
20	A	1113	CLA	C13-C15-C16-C17
20	A	1115	CLA	C10-C11-C12-C13
20	A	1128	CLA	C10-C11-C12-C13
20	A	1132	CLA	C10-C11-C12-C13
20	B	1226	CLA	C10-C11-C12-C13
20	1	604	CLA	C5-C6-C7-C8
20	1	611	CLA	C10-C11-C12-C13
20	Z	605	CLA	C8-C10-C11-C12
20	3	605	CLA	C8-C10-C11-C12
20	4	601	CLA	C5-C6-C7-C8
20	6	608	CLA	C5-C6-C7-C8
20	6	603	CLA	C15-C16-C17-C18
21	A	2001	PQN	C25-C26-C27-C28
37	Z	610	CHL	C10-C11-C12-C13
20	7	601	CLA	CBA-CGA-O2A-C1
20	4	609	CLA	CBA-CGA-O2A-C1
20	A	1112	CLA	O1A-CGA-O2A-C1
20	B	1229	CLA	O1A-CGA-O2A-C1
20	1	607	CLA	O1A-CGA-O2A-C1
20	Z	605	CLA	O1A-CGA-O2A-C1
20	3	606	CLA	O1A-CGA-O2A-C1
20	5	615	CLA	O1A-CGA-O2A-C1
20	6	608	CLA	O1A-CGA-O2A-C1
24	B	5006	LHG	C7-C8-C9-C10
24	8	801	LHG	C7-C8-C9-C10
20	A	1104	CLA	C5-C6-C7-C8
20	A	1119	CLA	C13-C15-C16-C17
20	A	1138	CLA	C13-C15-C16-C17
20	B	1021	CLA	C13-C15-C16-C17
20	B	1207	CLA	C10-C11-C12-C13
20	B	1209	CLA	C10-C11-C12-C13
20	B	1209	CLA	C13-C15-C16-C17
20	B	1223	CLA	C10-C11-C12-C13
20	B	1226	CLA	C13-C15-C16-C17
20	B	1229	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	F	1301	CLA	C10-C11-C12-C13
20	L	1502	CLA	C13-C15-C16-C17
20	7	607	CLA	C13-C15-C16-C17
20	4	603	CLA	C10-C11-C12-C13
20	5	602	CLA	C5-C6-C7-C8
20	6	619	CLA	C8-C10-C11-C12
20	B	1212	CLA	O1A-CGA-O2A-C1
20	3	616	CLA	O1A-CGA-O2A-C1
20	6	601	CLA	O1A-CGA-O2A-C1
24	A	5002	LHG	C8-C7-O7-C5
20	B	1238	CLA	O1D-CGD-O2D-CED
20	A	1012	CLA	C8-C10-C11-C12
20	A	1012	CLA	C13-C15-C16-C17
20	A	1108	CLA	C15-C16-C17-C18
20	A	1118	CLA	C10-C11-C12-C13
20	A	1125	CLA	C8-C10-C11-C12
20	A	1132	CLA	C5-C6-C7-C8
20	B	1205	CLA	C10-C11-C12-C13
20	B	1206	CLA	C5-C6-C7-C8
20	F	1301	CLA	C13-C15-C16-C17
20	1	603	CLA	C10-C11-C12-C13
20	1	607	CLA	C5-C6-C7-C8
20	1	612	CLA	C5-C6-C7-C8
20	1	612	CLA	C13-C15-C16-C17
20	3	603	CLA	C8-C10-C11-C12
20	3	606	CLA	C8-C10-C11-C12
20	7	616	CLA	C8-C10-C11-C12
20	8	603	CLA	C15-C16-C17-C18
20	5	609	CLA	C15-C16-C17-C18
20	6	603	CLA	C13-C15-C16-C17
24	A	5001	LHG	C4-O6-P-O3
24	A	5002	LHG	C3-O3-P-O6
24	B	5006	LHG	C4-O6-P-O3
24	1	801	LHG	C4-O6-P-O3
24	7	801	LHG	C4-O6-P-O3
24	4	802	LHG	C3-O3-P-O6
24	5	801	LHG	C4-O6-P-O3
20	A	1012	CLA	C3-C5-C6-C7
20	B	1241	CLA	C3-C5-C6-C7
20	A	1115	CLA	CBA-CGA-O2A-C1
20	G	1601	CLA	CBA-CGA-O2A-C1
20	A	1136	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	8	605	CLA	C5-C6-C7-C8
24	7	801	LHG	C23-C24-C25-C26
40	7	802	3PH	C21-C22-C23-C24
24	B	5002	LHG	C1-C2-C3-O3
42	8	803	LPX	O1-C3-C4-C5
29	A	5003	LMG	O9-C10-O7-C8
20	8	608	CLA	C4-C3-C5-C6
20	B	1206	CLA	C2-C3-C5-C6
19	A	1011	CL0	C5-C6-C7-C8
20	A	1121	CLA	C8-C10-C11-C12
20	A	1013	CLA	C5-C6-C7-C8
20	B	1224	CLA	C10-C11-C12-C13
20	7	601	CLA	C5-C6-C7-C8
20	A	1132	CLA	CBD-CGD-O2D-CED
20	A	1128	CLA	C2A-CAA-CBA-CGA
20	B	1023	CLA	C2A-CAA-CBA-CGA
20	B	1226	CLA	C2A-CAA-CBA-CGA
20	8	602	CLA	C2A-CAA-CBA-CGA
37	8	613	CHL	C2A-CAA-CBA-CGA
20	A	1102	CLA	C6-C7-C8-C9
20	B	1223	CLA	C16-C17-C18-C19
20	5	604	CLA	C16-C17-C18-C19
20	B	1238	CLA	CBA-CGA-O2A-C1
20	8	604	CLA	CBA-CGA-O2A-C1
20	5	604	CLA	CBA-CGA-O2A-C1
20	F	1301	CLA	C8-C10-C11-C12
20	1	611	CLA	C8-C10-C11-C12
23	B	4005	BCR	C19-C20-C21-C22
23	I	4001	BCR	C9-C10-C11-C12
23	I	4001	BCR	C15-C16-C17-C18
23	3	506	BCR	C9-C10-C11-C12
33	F	4001	RRX	C19-C20-C21-C22
24	7	801	LHG	C7-C8-C9-C10
20	A	1126	CLA	C15-C16-C17-C18
23	B	4003	BCR	C11-C10-C9-C34
23	L	4002	BCR	C11-C10-C9-C34
23	3	503	BCR	C11-C10-C9-C34
23	5	504	BCR	C11-C10-C9-C34
26	1	803	LMT	O5'-C5'-C6'-O6'
20	A	1110	CLA	C3-C5-C6-C7
20	3	603	CLA	C3-C5-C6-C7
24	Z	801	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	4	802	LHG	C13-C14-C15-C16
25	A	5004	NKP	CAX-CAY-CAZ-CBA
35	K	5001	SPH	C12-C13-C14-C15
20	A	1129	CLA	O1D-CGD-O2D-CED
20	A	1117	CLA	C16-C17-C18-C19
20	A	1118	CLA	C11-C12-C13-C14
20	A	1119	CLA	C16-C17-C18-C20
20	6	619	CLA	C16-C17-C18-C20
37	6	613	CHL	C6-C7-C8-C10
19	A	1011	CL0	CBA-CGA-O2A-C1
25	8	802	NKP	CAL-CAK-OAJ-CAI
25	8	802	NKP	CAG-CAH-CAI-OAJ
24	A	5002	LHG	C25-C26-C27-C28
24	1	801	LHG	C11-C10-C9-C8
24	6	801	LHG	C11-C10-C9-C8
30	A	5005	DGA	CB4-CB5-CB6-CB7
35	K	5001	SPH	C7-C8-C9-C10
35	7	804	SPH	C12-C13-C14-C15
35	K	5001	SPH	O3-C3-C4-C5
24	A	5002	LHG	O9-C7-O7-C5
20	A	1110	CLA	C10-C11-C12-C13
20	B	1023	CLA	C13-C15-C16-C17
24	A	5002	LHG	C23-C24-C25-C26
26	A	5006	LMT	C3-C4-C5-C6
35	K	5001	SPH	C9-C10-C11-C12
40	5	802	3PH	C22-C23-C24-C25
20	A	1115	CLA	O1A-CGA-O2A-C1
24	A	5001	LHG	C11-C10-C9-C8
24	Z	801	LHG	C30-C31-C32-C33
26	F	5001	LMT	C2-C3-C4-C5
26	1	803	LMT	C11-C10-C9-C8
38	1	802	SQD	C10-C11-C12-C13
28	A	5007	DAO	C4-C5-C6-C7
40	7	802	3PH	C22-C23-C24-C25
24	4	801	LHG	C23-C24-C25-C26
23	B	4003	BCR	C11-C10-C9-C8
23	L	4002	BCR	C11-C10-C9-C8
23	3	503	BCR	C11-C10-C9-C8
23	5	504	BCR	C11-C10-C9-C8
20	A	1013	CLA	CBA-CGA-O2A-C1
24	6	801	LHG	C12-C13-C14-C15
20	L	1503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1126	CLA	C16-C17-C18-C19
20	7	607	CLA	C16-C17-C18-C20
20	6	608	CLA	C6-C7-C8-C10
20	6	609	CLA	C16-C17-C18-C20
37	8	610	CHL	C6-C7-C8-C9
20	A	1123	CLA	C4-C3-C5-C6
24	Z	801	LHG	C28-C29-C30-C31
24	7	801	LHG	C11-C12-C13-C14
24	4	801	LHG	C28-C29-C30-C31
38	1	802	SQD	C17-C18-C19-C20
20	A	1105	CLA	C11-C12-C13-C14
20	A	1128	CLA	C14-C13-C15-C16
20	B	1021	CLA	C14-C13-C15-C16
20	B	1231	CLA	C11-C12-C13-C14
20	B	1236	CLA	C6-C7-C8-C9
20	1	606	CLA	C11-C10-C8-C9
20	Z	607	CLA	C6-C7-C8-C9
20	8	604	CLA	C11-C10-C8-C9
20	6	615	CLA	C11-C10-C8-C9
20	3	601	CLA	O1D-CGD-O2D-CED
30	A	5005	DGA	CA1-CA2-CA3-CA4
24	7	801	LHG	C11-C10-C9-C8
24	7	801	LHG	C29-C30-C31-C32
24	8	801	LHG	C11-C10-C9-C8
30	A	5005	DGA	CCA-CDA-CEA-CFA
35	7	804	SPH	C6-C7-C8-C9
35	7	803	SPH	C7-C8-C9-C10
26	A	5006	LMT	O5'-C5'-C6'-O6'
20	B	1227	CLA	C2A-CAA-CBA-CGA
20	B	1239	CLA	C2A-CAA-CBA-CGA
20	3	607	CLA	C2A-CAA-CBA-CGA
20	3	612	CLA	C2A-CAA-CBA-CGA
20	3	618	CLA	C2A-CAA-CBA-CGA
20	6	612	CLA	C2A-CAA-CBA-CGA
23	B	4005	BCR	C36-C18-C19-C20
34	J	4002	C7Z	C27-C28-C29-C39
20	B	1219	CLA	C10-C11-C12-C13
24	A	5002	LHG	C13-C14-C15-C16
24	A	5001	LHG	O1-C1-C2-C3
24	1	801	LHG	O1-C1-C2-C3
24	3	801	LHG	O1-C1-C2-C3
24	8	801	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	4	801	LHG	O1-C1-C2-C3
24	6	801	LHG	O1-C1-C2-C3
23	B	4001	BCR	C7-C8-C9-C10
23	B	4005	BCR	C11-C12-C13-C14
23	B	4005	BCR	C17-C18-C19-C20
23	J	4001	BCR	C11-C12-C13-C14
23	J	4001	BCR	C17-C18-C19-C20
34	J	4002	C7Z	C27-C28-C29-C30
36	5	501	LUT	C27-C28-C29-C30
20	B	1219	CLA	C3-C5-C6-C7
20	1	615	CLA	C3-C5-C6-C7
20	6	603	CLA	C3-C5-C6-C7
20	A	1106	CLA	C15-C16-C17-C18
20	A	1121	CLA	C5-C6-C7-C8
20	B	1230	CLA	C8-C10-C11-C12
20	3	603	CLA	C13-C15-C16-C17
26	4	803	LMT	O1'-C1-C2-C3
38	1	802	SQD	C9-C10-C11-C12
24	4	802	LHG	C11-C12-C13-C14
35	7	804	SPH	C10-C11-C12-C13
26	4	803	LMT	C1-C2-C3-C4
20	A	1116	CLA	C4B-C3B-CAB-CBB
20	A	1129	CLA	C4B-C3B-CAB-CBB
20	B	1219	CLA	C4B-C3B-CAB-CBB
20	B	1227	CLA	C4B-C3B-CAB-CBB
20	B	1231	CLA	C4B-C3B-CAB-CBB
20	B	1241	CLA	C4B-C3B-CAB-CBB
20	K	1403	CLA	C4B-C3B-CAB-CBB
20	1	601	CLA	C4B-C3B-CAB-CBB
20	1	605	CLA	C4B-C3B-CAB-CBB
20	1	611	CLA	C4B-C3B-CAB-CBB
20	Z	603	CLA	C4B-C3B-CAB-CBB
20	Z	607	CLA	C4B-C3B-CAB-CBB
20	Z	612	CLA	C4B-C3B-CAB-CBB
20	3	603	CLA	C4B-C3B-CAB-CBB
20	3	608	CLA	C4B-C3B-CAB-CBB
20	3	612	CLA	C4B-C3B-CAB-CBB
20	3	613	CLA	C4B-C3B-CAB-CBB
20	7	609	CLA	C4B-C3B-CAB-CBB
20	7	604	CLA	C4B-C3B-CAB-CBB
20	7	605	CLA	C4B-C3B-CAB-CBB
20	7	615	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	7	616	CLA	C4B-C3B-CAB-CBB
20	8	604	CLA	C4B-C3B-CAB-CBB
20	8	607	CLA	C4B-C3B-CAB-CBB
20	8	608	CLA	C4B-C3B-CAB-CBB
20	4	602	CLA	C4B-C3B-CAB-CBB
20	4	608	CLA	C4B-C3B-CAB-CBB
20	5	602	CLA	C4B-C3B-CAB-CBB
20	5	606	CLA	C4B-C3B-CAB-CBB
20	5	607	CLA	C4B-C3B-CAB-CBB
20	5	609	CLA	C4B-C3B-CAB-CBB
20	5	613	CLA	C4B-C3B-CAB-CBB
20	5	622	CLA	C4B-C3B-CAB-CBB
20	6	608	CLA	C4B-C3B-CAB-CBB
20	6	618	CLA	C4B-C3B-CAB-CBB
20	A	1102	CLA	C6-C7-C8-C10
20	A	1103	CLA	C16-C17-C18-C20
20	A	1115	CLA	C11-C12-C13-C14
20	A	1116	CLA	C11-C12-C13-C14
20	A	1116	CLA	C11-C12-C13-C15
20	A	1118	CLA	C11-C12-C13-C15
20	B	1223	CLA	C16-C17-C18-C20
20	5	604	CLA	C16-C17-C18-C20
20	5	613	CLA	C6-C7-C8-C10
20	5	618	CLA	C16-C17-C18-C19
20	5	618	CLA	C16-C17-C18-C20
20	6	619	CLA	C16-C17-C18-C19
37	6	613	CHL	C6-C7-C8-C9
26	B	5005	LMT	O5'-C1'-O1'-C1
20	A	1103	CLA	C5-C6-C7-C8
20	A	1119	CLA	C8-C10-C11-C12
20	B	1206	CLA	C8-C10-C11-C12
20	1	612	CLA	C8-C10-C11-C12
20	A	1110	CLA	O1D-CGD-O2D-CED
24	A	5001	LHG	C13-C14-C15-C16
24	8	801	LHG	C28-C29-C30-C31
24	6	801	LHG	C28-C29-C30-C31
26	4	803	LMT	C4-C5-C6-C7
35	K	5001	SPH	C6-C7-C8-C9
20	A	1137	CLA	CBD-CGD-O2D-CED
20	A	1120	CLA	O1D-CGD-O2D-CED
24	A	5001	LHG	C14-C15-C16-C17
24	4	802	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	5	801	LHG	C26-C27-C28-C29
26	B	6101	LMT	C2-C3-C4-C5
38	1	802	SQD	C11-C12-C13-C14
20	A	1125	CLA	C15-C16-C17-C18
20	7	604	CLA	C10-C11-C12-C13
20	6	603	CLA	C5-C6-C7-C8
20	8	604	CLA	O1A-CGA-O2A-C1
20	4	609	CLA	O1A-CGA-O2A-C1
24	5	801	LHG	C11-C12-C13-C14
35	K	5001	SPH	C11-C12-C13-C14
42	8	803	LPX	C17-C18-C19-C20
20	B	1241	CLA	CBA-CGA-O2A-C1
20	5	602	CLA	CBA-CGA-O2A-C1
20	6	604	CLA	CBA-CGA-O2A-C1
24	5	801	LHG	C25-C26-C27-C28
20	B	1236	CLA	O1D-CGD-O2D-CED
20	5	612	CLA	O1D-CGD-O2D-CED
20	A	1104	CLA	C3A-C2A-CAA-CBA
20	A	1108	CLA	C3A-C2A-CAA-CBA
20	A	1109	CLA	C3A-C2A-CAA-CBA
20	A	1122	CLA	C3A-C2A-CAA-CBA
20	A	1131	CLA	C3A-C2A-CAA-CBA
20	A	1130	CLA	C3A-C2A-CAA-CBA
20	A	1140	CLA	C3A-C2A-CAA-CBA
20	A	1101	CLA	C3A-C2A-CAA-CBA
20	B	1204	CLA	C3A-C2A-CAA-CBA
20	B	1207	CLA	C3A-C2A-CAA-CBA
20	B	1219	CLA	C3A-C2A-CAA-CBA
20	B	1222	CLA	C3A-C2A-CAA-CBA
20	B	1223	CLA	C3A-C2A-CAA-CBA
20	B	1226	CLA	C3A-C2A-CAA-CBA
20	B	1234	CLA	C3A-C2A-CAA-CBA
20	B	1236	CLA	C3A-C2A-CAA-CBA
20	1	613	CLA	C3A-C2A-CAA-CBA
20	3	608	CLA	C3A-C2A-CAA-CBA
20	7	601	CLA	C3A-C2A-CAA-CBA
20	7	603	CLA	C3A-C2A-CAA-CBA
20	7	604	CLA	C3A-C2A-CAA-CBA
20	8	603	CLA	C3A-C2A-CAA-CBA
20	8	604	CLA	C3A-C2A-CAA-CBA
20	4	603	CLA	C3A-C2A-CAA-CBA
20	5	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	6	608	CLA	C3A-C2A-CAA-CBA
20	6	601	CLA	C3A-C2A-CAA-CBA
20	6	618	CLA	C3A-C2A-CAA-CBA
37	Z	613	CHL	C3A-C2A-CAA-CBA
37	Z	609	CHL	C3A-C2A-CAA-CBA
37	8	613	CHL	C3A-C2A-CAA-CBA
37	4	613	CHL	C3A-C2A-CAA-CBA
20	A	1112	CLA	C10-C11-C12-C13
20	A	1013	CLA	C8-C10-C11-C12
20	L	1502	CLA	C10-C11-C12-C13
20	7	615	CLA	C5-C6-C7-C8
23	B	4003	BCR	C19-C20-C21-C22
36	4	502	LUT	C29-C30-C31-C32
26	A	5006	LMT	C2-C1-O1'-C1'
24	6	801	LHG	C13-C14-C15-C16
20	A	1125	CLA	O1D-CGD-O2D-CED
20	B	1238	CLA	O1A-CGA-O2A-C1
20	G	1601	CLA	O1A-CGA-O2A-C1
20	7	601	CLA	O1A-CGA-O2A-C1
20	A	1103	CLA	C16-C17-C18-C19
20	A	1115	CLA	C11-C12-C13-C15
20	B	1207	CLA	C16-C17-C18-C19
20	B	1207	CLA	C16-C17-C18-C20
20	B	1213	CLA	C16-C17-C18-C19
20	B	1213	CLA	C16-C17-C18-C20
20	B	1218	CLA	C16-C17-C18-C19
20	7	616	CLA	C11-C12-C13-C14
20	7	616	CLA	C11-C12-C13-C15
20	8	605	CLA	C16-C17-C18-C20
20	6	603	CLA	C16-C17-C18-C19
20	6	603	CLA	C16-C17-C18-C20
37	8	610	CHL	C6-C7-C8-C10
24	7	801	LHG	C28-C29-C30-C31
24	6	801	LHG	C16-C17-C18-C19
35	7	804	SPH	C7-C8-C9-C10
40	7	802	3PH	C25-C26-C27-C28
20	A	1013	CLA	C3-C5-C6-C7
20	Z	604	CLA	C15-C16-C17-C18
20	A	1125	CLA	C4-C3-C5-C6
20	B	1229	CLA	C4-C3-C5-C6
20	A	1122	CLA	C2-C3-C5-C6
20	A	1123	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	8	605	CLA	C2-C3-C5-C6
24	5	801	LHG	C8-C7-O7-C5
24	B	5001	LHG	O1-C1-C2-O2
24	B	5006	LHG	O1-C1-C2-O2
24	Z	801	LHG	O1-C1-C2-O2
24	4	801	LHG	O1-C1-C2-O2
24	4	802	LHG	O1-C1-C2-O2
24	5	801	LHG	O1-C1-C2-O2
24	A	5001	LHG	C15-C16-C17-C18
24	A	5002	LHG	C11-C12-C13-C14
24	5	801	LHG	C28-C29-C30-C31
24	B	5001	LHG	C7-C8-C9-C10
24	4	802	LHG	C23-C24-C25-C26
25	8	802	NKP	CAT-CAU-CAV-CAW
20	3	610	CLA	C11-C12-C13-C15
20	6	609	CLA	C16-C17-C18-C19
24	4	801	LHG	C11-C12-C13-C14
20	A	1104	CLA	C2B-C3B-CAB-CBB
20	A	1116	CLA	C2B-C3B-CAB-CBB
20	A	1129	CLA	C2B-C3B-CAB-CBB
20	A	1130	CLA	C2B-C3B-CAB-CBB
20	B	1219	CLA	C2B-C3B-CAB-CBB
20	B	1227	CLA	C2B-C3B-CAB-CBB
20	B	1231	CLA	C2B-C3B-CAB-CBB
20	B	1232	CLA	C2B-C3B-CAB-CBB
20	B	1241	CLA	C2B-C3B-CAB-CBB
20	K	1403	CLA	C2B-C3B-CAB-CBB
20	1	601	CLA	C2B-C3B-CAB-CBB
20	1	605	CLA	C2B-C3B-CAB-CBB
20	1	608	CLA	C2B-C3B-CAB-CBB
20	1	611	CLA	C2B-C3B-CAB-CBB
20	Z	603	CLA	C2B-C3B-CAB-CBB
20	Z	607	CLA	C2B-C3B-CAB-CBB
20	Z	611	CLA	C2B-C3B-CAB-CBB
20	Z	612	CLA	C2B-C3B-CAB-CBB
20	3	602	CLA	C2B-C3B-CAB-CBB
20	3	603	CLA	C2B-C3B-CAB-CBB
20	3	607	CLA	C2B-C3B-CAB-CBB
20	3	608	CLA	C2B-C3B-CAB-CBB
20	3	612	CLA	C2B-C3B-CAB-CBB
20	3	613	CLA	C2B-C3B-CAB-CBB
20	7	609	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	7	603	CLA	C2B-C3B-CAB-CBB
20	7	604	CLA	C2B-C3B-CAB-CBB
20	7	605	CLA	C2B-C3B-CAB-CBB
20	7	615	CLA	C2B-C3B-CAB-CBB
20	7	616	CLA	C2B-C3B-CAB-CBB
20	8	604	CLA	C2B-C3B-CAB-CBB
20	8	607	CLA	C2B-C3B-CAB-CBB
20	8	608	CLA	C2B-C3B-CAB-CBB
20	4	602	CLA	C2B-C3B-CAB-CBB
20	4	608	CLA	C2B-C3B-CAB-CBB
20	5	602	CLA	C2B-C3B-CAB-CBB
20	5	606	CLA	C2B-C3B-CAB-CBB
20	5	607	CLA	C2B-C3B-CAB-CBB
20	5	609	CLA	C2B-C3B-CAB-CBB
20	5	613	CLA	C2B-C3B-CAB-CBB
20	5	622	CLA	C2B-C3B-CAB-CBB
20	6	608	CLA	C2B-C3B-CAB-CBB
20	6	618	CLA	C2B-C3B-CAB-CBB
20	B	1236	CLA	C13-C15-C16-C17
24	6	801	LHG	C11-C12-C13-C14
20	B	1224	CLA	C3-C5-C6-C7
20	4	603	CLA	C3-C5-C6-C7
26	B	5005	LMT	C4B-C5B-C6B-O6B
25	8	802	NKP	OAE-CAK-OAJ-CAI
20	B	1214	CLA	C10-C11-C12-C13
24	5	801	LHG	O9-C7-O7-C5
20	A	1103	CLA	C2-C1-O2A-CGA
20	A	1111	CLA	C2-C1-O2A-CGA
20	A	1120	CLA	C2-C1-O2A-CGA
20	A	1127	CLA	C2-C1-O2A-CGA
20	A	1134	CLA	C2-C1-O2A-CGA
20	A	1141	CLA	C2-C1-O2A-CGA
20	A	1130	CLA	C2-C1-O2A-CGA
20	B	1204	CLA	C2-C1-O2A-CGA
20	B	1209	CLA	C2-C1-O2A-CGA
20	B	1216	CLA	C2-C1-O2A-CGA
20	B	1217	CLA	C2-C1-O2A-CGA
20	B	1218	CLA	C2-C1-O2A-CGA
20	B	1219	CLA	C2-C1-O2A-CGA
20	B	1220	CLA	C2-C1-O2A-CGA
20	B	1223	CLA	C2-C1-O2A-CGA
20	B	1225	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	B	1227	CLA	C2-C1-O2A-CGA
20	K	1404	CLA	C2-C1-O2A-CGA
20	L	1502	CLA	C2-C1-O2A-CGA
20	1	601	CLA	C2-C1-O2A-CGA
20	1	611	CLA	C2-C1-O2A-CGA
20	Z	605	CLA	C2-C1-O2A-CGA
20	Z	611	CLA	C2-C1-O2A-CGA
20	3	604	CLA	C2-C1-O2A-CGA
20	3	606	CLA	C2-C1-O2A-CGA
20	7	601	CLA	C2-C1-O2A-CGA
20	8	601	CLA	C2-C1-O2A-CGA
20	8	604	CLA	C2-C1-O2A-CGA
20	5	603	CLA	C2-C1-O2A-CGA
20	6	606	CLA	C2-C1-O2A-CGA
20	6	619	CLA	C2-C1-O2A-CGA
24	4	801	LHG	C13-C14-C15-C16
20	A	1106	CLA	C8-C10-C11-C12
20	A	1127	CLA	C15-C16-C17-C18
20	B	1211	CLA	C5-C6-C7-C8
20	B	1215	CLA	C8-C10-C11-C12
20	B	1221	CLA	C8-C10-C11-C12
20	6	609	CLA	C5-C6-C7-C8
19	A	1011	CL0	O1A-CGA-O2A-C1
20	A	1013	CLA	O1A-CGA-O2A-C1
20	5	604	CLA	O1A-CGA-O2A-C1
24	6	801	LHG	C34-C35-C36-C37
40	7	802	3PH	C26-C27-C28-C29
40	6	802	3PH	C22-C23-C24-C25
20	A	1140	CLA	C16-C17-C18-C19
41	7	805	PLM	C1-C2-C3-C4
23	A	4003	BCR	C1-C6-C7-C8
23	A	4003	BCR	C23-C24-C25-C26
23	A	4004	BCR	C1-C6-C7-C8
23	A	4004	BCR	C5-C6-C7-C8
23	A	4005	BCR	C5-C6-C7-C8
23	B	4001	BCR	C5-C6-C7-C8
23	B	4002	BCR	C5-C6-C7-C8
23	B	4005	BCR	C23-C24-C25-C26
23	B	4005	BCR	C23-C24-C25-C30
23	B	4006	BCR	C23-C24-C25-C26
23	B	4006	BCR	C23-C24-C25-C30
23	G	4001	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	G	4001	BCR	C5-C6-C7-C8
23	G	4001	BCR	C23-C24-C25-C26
23	G	4001	BCR	C23-C24-C25-C30
23	I	4001	BCR	C1-C6-C7-C8
23	I	4001	BCR	C5-C6-C7-C8
23	K	4001	BCR	C5-C6-C7-C8
23	K	4001	BCR	C23-C24-C25-C30
23	K	4002	BCR	C23-C24-C25-C26
23	K	4002	BCR	C23-C24-C25-C30
23	L	4001	BCR	C1-C6-C7-C8
23	L	4001	BCR	C5-C6-C7-C8
23	L	4002	BCR	C1-C6-C7-C8
23	L	4002	BCR	C5-C6-C7-C8
23	L	4002	BCR	C23-C24-C25-C26
23	3	503	BCR	C1-C6-C7-C8
23	3	503	BCR	C23-C24-C25-C26
23	3	505	BCR	C23-C24-C25-C26
23	3	505	BCR	C23-C24-C25-C30
23	3	506	BCR	C1-C6-C7-C8
23	3	506	BCR	C5-C6-C7-C8
23	8	503	BCR	C1-C6-C7-C8
23	4	503	BCR	C1-C6-C7-C8
23	4	503	BCR	C5-C6-C7-C8
23	5	503	BCR	C23-C24-C25-C26
23	5	503	BCR	C23-C24-C25-C30
23	5	504	BCR	C23-C24-C25-C26
23	5	504	BCR	C23-C24-C25-C30
23	6	504	BCR	C23-C24-C25-C30
34	1	503	C7Z	C25-C26-C27-C28
34	5	505	C7Z	C21-C26-C27-C28
20	8	604	CLA	C13-C15-C16-C17
20	5	618	CLA	O1D-CGD-O2D-CED
20	A	1109	CLA	CBA-CGA-O2A-C1
20	8	605	CLA	CBA-CGA-O2A-C1
20	A	1126	CLA	C5-C6-C7-C8
20	A	1127	CLA	C10-C11-C12-C13
20	B	1223	CLA	C15-C16-C17-C18
20	4	604	CLA	C8-C10-C11-C12
20	5	602	CLA	O1A-CGA-O2A-C1
20	A	1122	CLA	C10-C11-C12-C13
20	A	1136	CLA	C13-C15-C16-C17
20	7	605	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	8	604	CLA	C5-C6-C7-C8
37	Z	609	CHL	C13-C15-C16-C17
20	A	1119	CLA	C4-C3-C5-C6
20	A	1139	CLA	C4-C3-C5-C6
20	B	1241	CLA	C4-C3-C5-C6
20	3	607	CLA	C4-C3-C5-C6
20	8	605	CLA	C4-C3-C5-C6
20	5	605	CLA	C4-C3-C5-C6
20	B	1221	CLA	O1D-CGD-O2D-CED
20	A	1103	CLA	C11-C12-C13-C15
20	A	1105	CLA	C11-C12-C13-C15
20	A	1105	CLA	C12-C13-C15-C16
20	A	1119	CLA	C2-C3-C5-C6
20	A	1125	CLA	C2-C3-C5-C6
20	A	1128	CLA	C12-C13-C15-C16
20	B	1021	CLA	C12-C13-C15-C16
20	B	1202	CLA	C6-C7-C8-C10
20	B	1213	CLA	C6-C7-C8-C10
20	B	1229	CLA	C2-C3-C5-C6
20	B	1231	CLA	C11-C12-C13-C15
20	B	1236	CLA	C6-C7-C8-C10
20	B	1241	CLA	C2-C3-C5-C6
20	1	611	CLA	C6-C7-C8-C10
20	Z	607	CLA	C6-C7-C8-C10
20	7	609	CLA	C12-C13-C15-C16
20	7	605	CLA	C6-C7-C8-C10
20	8	602	CLA	C11-C10-C8-C7
20	8	606	CLA	C11-C10-C8-C7
20	4	603	CLA	C11-C12-C13-C15
20	6	615	CLA	C11-C10-C8-C7
37	5	610	CHL	C11-C12-C13-C15
20	B	1241	CLA	O1A-CGA-O2A-C1
20	8	605	CLA	O1A-CGA-O2A-C1
40	7	802	3PH	C39-C3A-C3B-C3C
20	A	1110	CLA	C15-C16-C17-C18
20	4	605	CLA	C10-C11-C12-C13
20	4	605	CLA	C15-C16-C17-C18
23	I	4001	BCR	C13-C14-C15-C16
23	3	504	BCR	C13-C14-C15-C16
23	5	503	BCR	C15-C16-C17-C18
20	A	1125	CLA	C16-C17-C18-C20
20	6	608	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	A	5001	LHG	C7-C8-C9-C10
29	A	5003	LMG	C10-C11-C12-C13
40	5	802	3PH	C21-C22-C23-C24
20	1	613	CLA	O1A-CGA-O2A-C1
20	7	604	CLA	CBA-CGA-O2A-C1
20	8	609	CLA	CBA-CGA-O2A-C1
20	A	1012	CLA	C2A-CAA-CBA-CGA
20	A	1109	CLA	C2A-CAA-CBA-CGA
20	A	1013	CLA	C2A-CAA-CBA-CGA
20	B	1216	CLA	C2A-CAA-CBA-CGA
20	B	1225	CLA	C2A-CAA-CBA-CGA
20	B	1236	CLA	C2A-CAA-CBA-CGA
20	7	609	CLA	C2A-CAA-CBA-CGA
37	Z	613	CHL	C2A-CAA-CBA-CGA
20	B	1209	CLA	C15-C16-C17-C18
20	B	1218	CLA	C5-C6-C7-C8
20	8	602	CLA	C15-C16-C17-C18
24	4	801	LHG	C10-C11-C12-C13
26	4	803	LMT	C11-C10-C9-C8
20	7	612	CLA	O1D-CGD-O2D-CED
24	Z	801	LHG	C7-C8-C9-C10
24	5	801	LHG	C7-C8-C9-C10
20	6	606	CLA	C5-C6-C7-C8
24	A	5002	LHG	C31-C32-C33-C34
20	K	1402	CLA	C6-C7-C8-C9
20	4	603	CLA	C16-C17-C18-C19
20	A	1133	CLA	C5-C6-C7-C8
20	B	1021	CLA	C15-C16-C17-C18
20	B	1022	CLA	C10-C11-C12-C13
20	5	604	CLA	C15-C16-C17-C18
24	1	801	LHG	O6-C4-C5-O7
24	6	801	LHG	O6-C4-C5-O7
24	B	5006	LHG	C9-C10-C11-C12
40	7	802	3PH	C23-C24-C25-C26
26	F	5001	LMT	C4'-C5'-C6'-O6'
20	A	1107	CLA	C15-C16-C17-C18
20	8	609	CLA	C15-C16-C17-C18
20	A	1108	CLA	C3-C5-C6-C7
20	B	1217	CLA	C3-C5-C6-C7
24	A	5001	LHG	C9-C10-C11-C12
24	6	801	LHG	C31-C32-C33-C34
26	B	5005	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	3	604	CLA	O1D-CGD-O2D-CED
20	A	1119	CLA	C16-C17-C18-C19
20	A	1126	CLA	C16-C17-C18-C20
20	A	1131	CLA	C16-C17-C18-C19
24	1	801	LHG	C29-C30-C31-C32
20	A	1139	CLA	C10-C11-C12-C13
20	B	1213	CLA	C8-C10-C11-C12
20	B	1239	CLA	C13-C15-C16-C17
20	B	1241	CLA	C8-C10-C11-C12
20	3	605	CLA	C5-C6-C7-C8
20	6	605	CLA	C4-C3-C5-C6
20	8	608	CLA	C2-C3-C5-C6
20	5	605	CLA	C2-C3-C5-C6
20	A	1103	CLA	C6-C7-C8-C9
20	A	1103	CLA	C11-C12-C13-C14
20	A	1105	CLA	C14-C13-C15-C16
20	A	1117	CLA	C6-C7-C8-C9
20	B	1206	CLA	C11-C12-C13-C14
20	B	1207	CLA	C14-C13-C15-C16
20	B	1210	CLA	C11-C12-C13-C14
20	B	1213	CLA	C6-C7-C8-C9
20	B	1222	CLA	C6-C7-C8-C9
20	B	1223	CLA	C6-C7-C8-C9
20	B	1223	CLA	C11-C12-C13-C14
20	B	1231	CLA	C14-C13-C15-C16
20	B	1236	CLA	C11-C10-C8-C9
20	B	1238	CLA	C6-C7-C8-C9
20	B	1239	CLA	C6-C7-C8-C9
20	1	604	CLA	C11-C10-C8-C9
20	1	606	CLA	C6-C7-C8-C9
20	1	615	CLA	C14-C13-C15-C16
20	Z	604	CLA	C6-C7-C8-C9
20	7	609	CLA	C14-C13-C15-C16
20	7	603	CLA	C14-C13-C15-C16
20	7	604	CLA	C11-C12-C13-C14
20	8	602	CLA	C11-C10-C8-C9
20	8	605	CLA	C11-C12-C13-C14
20	8	606	CLA	C11-C10-C8-C9
20	4	603	CLA	C11-C12-C13-C14
20	4	604	CLA	C11-C10-C8-C9
20	4	609	CLA	C11-C10-C8-C9
20	6	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
40	7	802	3PH	C34-C35-C36-C37
20	A	1104	CLA	C2A-CAA-CBA-CGA
20	B	1022	CLA	C2A-CAA-CBA-CGA
20	1	604	CLA	C2A-CAA-CBA-CGA
20	1	606	CLA	C2A-CAA-CBA-CGA
20	1	608	CLA	C2A-CAA-CBA-CGA
20	3	606	CLA	C2A-CAA-CBA-CGA
20	8	612	CLA	C2A-CAA-CBA-CGA
20	4	612	CLA	C2A-CAA-CBA-CGA
37	8	610	CHL	C2A-CAA-CBA-CGA
23	A	4001	BCR	C36-C18-C19-C20
20	3	607	CLA	C10-C11-C12-C13
34	5	505	C7Z	C31-C32-C33-C34
20	6	604	CLA	O1A-CGA-O2A-C1
20	A	1102	CLA	C1A-C2A-CAA-CBA
20	A	1103	CLA	C1A-C2A-CAA-CBA
20	A	1106	CLA	C1A-C2A-CAA-CBA
20	A	1107	CLA	C1A-C2A-CAA-CBA
20	A	1121	CLA	C1A-C2A-CAA-CBA
20	A	1131	CLA	C1A-C2A-CAA-CBA
20	A	1132	CLA	C1A-C2A-CAA-CBA
20	A	1101	CLA	C1A-C2A-CAA-CBA
20	B	1207	CLA	C1A-C2A-CAA-CBA
20	B	1217	CLA	C1A-C2A-CAA-CBA
20	B	1220	CLA	C1A-C2A-CAA-CBA
20	B	1223	CLA	C1A-C2A-CAA-CBA
20	B	1227	CLA	C1A-C2A-CAA-CBA
20	B	1229	CLA	C1A-C2A-CAA-CBA
20	B	1234	CLA	C1A-C2A-CAA-CBA
20	B	1240	CLA	C1A-C2A-CAA-CBA
20	B	1241	CLA	C1A-C2A-CAA-CBA
20	K	1402	CLA	C1A-C2A-CAA-CBA
20	1	604	CLA	C1A-C2A-CAA-CBA
20	1	608	CLA	C1A-C2A-CAA-CBA
20	1	613	CLA	C1A-C2A-CAA-CBA
20	Z	601	CLA	C1A-C2A-CAA-CBA
20	Z	606	CLA	C1A-C2A-CAA-CBA
20	Z	607	CLA	C1A-C2A-CAA-CBA
20	3	606	CLA	C1A-C2A-CAA-CBA
20	3	608	CLA	C1A-C2A-CAA-CBA
20	3	610	CLA	C1A-C2A-CAA-CBA
20	3	612	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	3	616	CLA	C1A-C2A-CAA-CBA
20	7	609	CLA	C1A-C2A-CAA-CBA
20	7	607	CLA	C1A-C2A-CAA-CBA
20	7	608	CLA	C1A-C2A-CAA-CBA
20	7	612	CLA	C1A-C2A-CAA-CBA
20	7	615	CLA	C1A-C2A-CAA-CBA
20	8	608	CLA	C1A-C2A-CAA-CBA
20	8	615	CLA	C1A-C2A-CAA-CBA
20	5	601	CLA	C1A-C2A-CAA-CBA
20	5	607	CLA	C1A-C2A-CAA-CBA
20	5	608	CLA	C1A-C2A-CAA-CBA
20	5	612	CLA	C1A-C2A-CAA-CBA
20	5	618	CLA	C1A-C2A-CAA-CBA
20	6	607	CLA	C1A-C2A-CAA-CBA
20	6	618	CLA	C1A-C2A-CAA-CBA
37	Z	610	CHL	C1A-C2A-CAA-CBA
37	8	610	CHL	C1A-C2A-CAA-CBA
37	4	611	CHL	C1A-C2A-CAA-CBA
37	4	613	CHL	C1A-C2A-CAA-CBA
20	A	1108	CLA	C16-C17-C18-C19
20	A	1117	CLA	C16-C17-C18-C20
20	8	607	CLA	C6-C7-C8-C10
20	5	613	CLA	C6-C7-C8-C9
26	F	5001	LMT	C3-C4-C5-C6
31	B	5003	DGD	CAA-CBA-CCA-CDA
23	B	4002	BCR	C9-C10-C11-C12
23	L	4002	BCR	C13-C14-C15-C16
23	3	503	BCR	C13-C14-C15-C16
36	3	502	LUT	C29-C30-C31-C32
20	B	1240	CLA	O1D-CGD-O2D-CED
20	8	609	CLA	O1D-CGD-O2D-CED
20	A	1140	CLA	C15-C16-C17-C18
20	B	1206	CLA	C15-C16-C17-C18
20	8	607	CLA	C5-C6-C7-C8
30	A	5005	DGA	CA2-CA3-CA4-CA5
24	B	5006	LHG	C23-C24-C25-C26
24	4	802	LHG	C9-C10-C11-C12
20	1	603	CLA	C5-C6-C7-C8
20	7	602	CLA	CBA-CGA-O2A-C1
24	A	5001	LHG	O6-C4-C5-C6
24	7	801	LHG	O6-C4-C5-C6
24	4	801	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
24	4	802	LHG	O6-C4-C5-C6
24	5	801	LHG	O6-C4-C5-C6
24	5	801	LHG	C11-C10-C9-C8
20	A	1134	CLA	O1D-CGD-O2D-CED
20	A	1108	CLA	C10-C11-C12-C13
20	3	610	CLA	C11-C12-C13-C14
20	7	607	CLA	C16-C17-C18-C19
24	A	5002	LHG	C24-C25-C26-C27
24	6	801	LHG	C7-C8-C9-C10
20	1	603	CLA	CBA-CGA-O2A-C1
24	A	5002	LHG	C24-C23-O8-C6
20	B	1220	CLA	O1D-CGD-O2D-CED
20	8	601	CLA	C4-C3-C5-C6
20	A	1139	CLA	C2-C3-C5-C6
20	J	1901	CLA	C3A-C2A-CAA-CBA
20	7	613	CLA	C3A-C2A-CAA-CBA
25	8	802	NKP	CAN-CAO-CAP-CAQ
20	8	602	CLA	C8-C10-C11-C12
24	A	5001	LHG	C11-C12-C13-C14
38	1	802	SQD	C15-C16-C17-C18
40	6	802	3PH	C27-C28-C29-C2A
24	Z	801	LHG	C23-C24-C25-C26
24	7	801	LHG	C8-C7-O7-C5
20	A	1109	CLA	O1A-CGA-O2A-C1
20	1	603	CLA	O1A-CGA-O2A-C1
24	4	801	LHG	C29-C30-C31-C32
20	A	1133	CLA	C16-C17-C18-C20
20	B	1222	CLA	C16-C17-C18-C20
20	B	1238	CLA	C16-C17-C18-C19
26	B	6101	LMT	O5'-C5'-C6'-O6'
24	Z	801	LHG	C4-C5-C6-O8
24	3	801	LHG	C4-C5-C6-O8
24	4	801	LHG	C4-C5-C6-O8
20	1	612	CLA	CBA-CGA-O2A-C1
20	A	1103	CLA	C8-C10-C11-C12
20	A	1108	CLA	C5-C6-C7-C8
24	4	802	LHG	C10-C11-C12-C13
20	A	1137	CLA	C8-C10-C11-C12
20	B	1228	CLA	C15-C16-C17-C18
26	8	805	LMT	C11-C10-C9-C8
24	5	801	LHG	C13-C14-C15-C16
26	4	803	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	6	618	CLA	CBA-CGA-O2A-C1
20	K	1402	CLA	C6-C7-C8-C10
20	B	1226	CLA	CBA-CGA-O2A-C1
24	A	5002	LHG	C35-C36-C37-C38
35	K	5001	SPH	C11-C10-C9-C8
25	8	802	NKP	CAP-CAQ-CAR-CAS
20	B	1235	CLA	C13-C15-C16-C17
41	7	805	PLM	CA-CB-CC-CD
20	A	1139	CLA	C13-C15-C16-C17
20	1	612	CLA	C10-C11-C12-C13
20	A	1132	CLA	C4-C3-C5-C6
20	B	1224	CLA	C4-C3-C5-C6
20	B	1228	CLA	C4-C3-C5-C6
30	A	5005	DGA	CDB-CEB-CFB-CGB
20	B	1228	CLA	C2-C3-C5-C6
20	A	1106	CLA	C16-C17-C18-C19
20	4	603	CLA	C16-C17-C18-C20
20	3	601	CLA	CBA-CGA-O2A-C1
20	3	604	CLA	CBA-CGA-O2A-C1
20	B	1204	CLA	CBD-CGD-O2D-CED
20	A	1124	CLA	C15-C16-C17-C18
20	B	1021	CLA	C8-C10-C11-C12
20	B	1219	CLA	C5-C6-C7-C8
20	B	1226	CLA	C8-C10-C11-C12
20	6	601	CLA	C10-C11-C12-C13
29	J	5001	LMG	C7-C8-O7-C10
40	7	802	3PH	C3-C2-O21-C21
20	Z	608	CLA	O1D-CGD-O2D-CED
20	B	1236	CLA	C10-C11-C12-C13
20	A	1106	CLA	C2-C1-O2A-CGA
20	A	1110	CLA	C2-C1-O2A-CGA
20	B	1210	CLA	C2-C1-O2A-CGA
20	B	1215	CLA	C2-C1-O2A-CGA
20	3	613	CLA	C2-C1-O2A-CGA
20	8	607	CLA	C2-C1-O2A-CGA
20	6	604	CLA	C2-C1-O2A-CGA
20	A	1132	CLA	O1D-CGD-O2D-CED
20	A	1117	CLA	C3-C5-C6-C7
25	A	5004	NKP	CAS-CAT-CAU-CAV
25	8	802	NKP	CAG-OAF-PAC-OAD
40	6	802	3PH	C1-O11-P-O12
35	7	803	SPH	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	8	806	3PH	C3A-C3B-C3C-C3D
20	A	1132	CLA	CBA-CGA-O2A-C1
20	7	612	CLA	CBA-CGA-O2A-C1
20	7	604	CLA	O1A-CGA-O2A-C1
20	8	609	CLA	O1A-CGA-O2A-C1
24	B	5002	LHG	O6-C4-C5-O7
24	3	801	LHG	O6-C4-C5-O7
20	A	1125	CLA	C16-C17-C18-C19
24	Z	801	LHG	C11-C12-C13-C14
20	4	604	CLA	C10-C11-C12-C13
24	6	801	LHG	C19-C20-C21-C22
20	A	1137	CLA	O1D-CGD-O2D-CED
20	7	602	CLA	O1A-CGA-O2A-C1
24	4	801	LHG	C16-C17-C18-C19
20	Z	604	CLA	C5-C6-C7-C8
20	4	601	CLA	C8-C10-C11-C12
20	A	1138	CLA	CAA-CBA-CGA-O2A
24	B	5006	LHG	O7-C5-C6-O8
24	7	801	LHG	O7-C5-C6-O8
24	4	802	LHG	O7-C5-C6-O8
31	B	5003	DGD	O2G-C2G-C3G-O3G
20	A	1132	CLA	O1A-CGA-O2A-C1
20	1	612	CLA	O1A-CGA-O2A-C1
24	8	801	LHG	C13-C14-C15-C16
31	B	5003	DGD	C7A-C8A-C9A-CAA
41	7	805	PLM	C7-C8-C9-CA
20	A	1108	CLA	C4-C3-C5-C6
20	A	1138	CLA	C4-C3-C5-C6
20	A	1012	CLA	C11-C12-C13-C15
20	A	1103	CLA	C6-C7-C8-C10
20	A	1107	CLA	C6-C7-C8-C10
20	A	1111	CLA	C6-C7-C8-C10
20	A	1113	CLA	C11-C12-C13-C15
20	A	1122	CLA	C12-C13-C15-C16
20	A	1126	CLA	C6-C7-C8-C10
20	A	1126	CLA	C11-C12-C13-C15
20	A	1132	CLA	C2-C3-C5-C6
20	A	1136	CLA	C12-C13-C15-C16
20	A	1138	CLA	C11-C10-C8-C7
20	A	1101	CLA	C11-C10-C8-C7
20	A	1101	CLA	C11-C12-C13-C15
20	B	1021	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	1023	CLA	C11-C10-C8-C7
20	B	1203	CLA	C6-C7-C8-C10
20	B	1203	CLA	C11-C12-C13-C15
20	B	1206	CLA	C6-C7-C8-C10
20	B	1207	CLA	C12-C13-C15-C16
20	B	1209	CLA	C11-C10-C8-C7
20	B	1209	CLA	C11-C12-C13-C15
20	B	1216	CLA	C6-C7-C8-C10
20	B	1218	CLA	C6-C7-C8-C10
20	B	1221	CLA	C11-C12-C13-C15
20	B	1222	CLA	C6-C7-C8-C10
20	B	1223	CLA	C6-C7-C8-C10
20	B	1223	CLA	C11-C12-C13-C15
20	B	1224	CLA	C2-C3-C5-C6
20	B	1225	CLA	C12-C13-C15-C16
20	B	1231	CLA	C12-C13-C15-C16
20	B	1234	CLA	C6-C7-C8-C10
20	B	1234	CLA	C11-C10-C8-C7
20	B	1236	CLA	C11-C12-C13-C15
20	B	1239	CLA	C6-C7-C8-C10
20	B	1240	CLA	C11-C12-C13-C15
20	B	1241	CLA	C11-C10-C8-C7
20	1	603	CLA	C11-C10-C8-C7
20	1	606	CLA	C6-C7-C8-C10
20	Z	604	CLA	C6-C7-C8-C10
20	Z	605	CLA	C6-C7-C8-C10
20	3	603	CLA	C11-C10-C8-C7
20	3	610	CLA	C11-C10-C8-C7
20	7	609	CLA	C6-C7-C8-C10
20	7	603	CLA	C12-C13-C15-C16
20	7	607	CLA	C11-C12-C13-C15
20	8	604	CLA	C11-C10-C8-C7
20	8	605	CLA	C11-C12-C13-C15
20	4	604	CLA	C11-C10-C8-C7
20	4	605	CLA	C11-C10-C8-C7
20	4	609	CLA	C11-C10-C8-C7
20	5	601	CLA	C6-C7-C8-C10
20	5	602	CLA	C6-C7-C8-C10
20	6	603	CLA	C12-C13-C15-C16
20	6	619	CLA	C11-C10-C8-C7
21	B	2002	PQN	C17-C18-C20-C21
21	B	2002	PQN	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
37	Z	610	CHL	C12-C13-C15-C16
37	8	613	CHL	C11-C12-C13-C15
20	A	1012	CLA	C11-C12-C13-C14
20	A	1106	CLA	C11-C12-C13-C14
20	A	1108	CLA	C6-C7-C8-C9
20	A	1113	CLA	C11-C12-C13-C14
20	A	1115	CLA	C6-C7-C8-C9
20	A	1116	CLA	C11-C10-C8-C9
20	A	1117	CLA	C11-C10-C8-C9
20	A	1117	CLA	C11-C12-C13-C14
20	A	1121	CLA	C14-C13-C15-C16
20	A	1122	CLA	C14-C13-C15-C16
20	A	1126	CLA	C11-C12-C13-C14
20	A	1132	CLA	C11-C12-C13-C14
20	A	1136	CLA	C6-C7-C8-C9
20	A	1130	CLA	C11-C10-C8-C9
20	A	1101	CLA	C11-C12-C13-C14
20	B	1023	CLA	C11-C12-C13-C14
20	B	1203	CLA	C11-C10-C8-C9
20	B	1203	CLA	C11-C12-C13-C14
20	B	1205	CLA	C11-C10-C8-C9
20	B	1206	CLA	C6-C7-C8-C9
20	B	1209	CLA	C11-C10-C8-C9
20	B	1210	CLA	C14-C13-C15-C16
20	B	1212	CLA	C6-C7-C8-C9
20	B	1216	CLA	C6-C7-C8-C9
20	B	1221	CLA	C11-C12-C13-C14
20	B	1234	CLA	C6-C7-C8-C9
20	B	1234	CLA	C11-C10-C8-C9
20	B	1235	CLA	C11-C12-C13-C14
20	B	1236	CLA	C11-C12-C13-C14
20	B	1241	CLA	C11-C10-C8-C9
20	L	1502	CLA	C11-C10-C8-C9
20	1	603	CLA	C11-C10-C8-C9
20	1	607	CLA	C6-C7-C8-C9
20	1	612	CLA	C11-C12-C13-C14
20	1	612	CLA	C14-C13-C15-C16
20	Z	605	CLA	C6-C7-C8-C9
20	7	605	CLA	C6-C7-C8-C9
20	7	607	CLA	C11-C10-C8-C9
20	7	607	CLA	C11-C12-C13-C14
20	4	605	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	5	601	CLA	C6-C7-C8-C9
20	5	602	CLA	C6-C7-C8-C9
20	6	603	CLA	C14-C13-C15-C16
21	B	2002	PQN	C21-C22-C23-C24
37	Z	609	CHL	C11-C10-C8-C9
37	8	613	CHL	C11-C12-C13-C14
20	7	608	CLA	C2A-CAA-CBA-CGA
26	A	5006	LMT	C2-C3-C4-C5
24	B	5006	LHG	C24-C23-O8-C6
20	B	1202	CLA	C8-C10-C11-C12
20	5	609	CLA	C10-C11-C12-C13
21	B	2002	PQN	C15-C16-C17-C18
20	A	1107	CLA	C2A-CAA-CBA-CGA
20	Z	601	CLA	C2A-CAA-CBA-CGA
24	A	5002	LHG	O10-C23-O8-C6
23	A	4003	BCR	C37-C22-C23-C24
36	Z	503	LUT	C7-C8-C9-C19
36	4	501	LUT	C27-C28-C29-C39
20	A	1110	CLA	C16-C17-C18-C20
20	A	1133	CLA	C16-C17-C18-C19
24	4	801	LHG	C33-C34-C35-C36
23	7	503	BCR	C21-C22-C23-C24
23	7	504	BCR	C11-C12-C13-C14
23	6	503	BCR	C7-C8-C9-C10
41	7	805	PLM	C2-C3-C4-C5
20	B	1228	CLA	C8-C10-C11-C12
20	B	1226	CLA	O1A-CGA-O2A-C1
24	4	801	LHG	C26-C27-C28-C29
40	6	802	3PH	C29-C2A-C2B-C2C
20	B	1215	CLA	C5-C6-C7-C8
20	B	1216	CLA	C15-C16-C17-C18
20	7	604	CLA	C8-C10-C11-C12
24	Z	801	LHG	C16-C17-C18-C19
26	B	6101	LMT	C1-C2-C3-C4
20	A	1012	CLA	C4B-C3B-CAB-CBB
20	A	1108	CLA	C4B-C3B-CAB-CBB
20	A	1109	CLA	C4B-C3B-CAB-CBB
20	A	1118	CLA	C4B-C3B-CAB-CBB
20	A	1119	CLA	C4B-C3B-CAB-CBB
20	A	1121	CLA	C4B-C3B-CAB-CBB
20	A	1124	CLA	C4B-C3B-CAB-CBB
20	A	1126	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	1134	CLA	C4B-C3B-CAB-CBB
20	B	1237	CLA	C4B-C3B-CAB-CBB
20	B	1023	CLA	C4B-C3B-CAB-CBB
20	B	1203	CLA	C4B-C3B-CAB-CBB
20	B	1204	CLA	C4B-C3B-CAB-CBB
20	B	1205	CLA	C4B-C3B-CAB-CBB
20	B	1220	CLA	C4B-C3B-CAB-CBB
20	B	1224	CLA	C4B-C3B-CAB-CBB
20	B	1235	CLA	C4B-C3B-CAB-CBB
20	G	1601	CLA	C4B-C3B-CAB-CBB
20	K	1402	CLA	C4B-C3B-CAB-CBB
20	K	1404	CLA	C4B-C3B-CAB-CBB
20	1	603	CLA	C4B-C3B-CAB-CBB
20	1	604	CLA	C4B-C3B-CAB-CBB
20	1	606	CLA	C4B-C3B-CAB-CBB
20	1	608	CLA	C4B-C3B-CAB-CBB
20	Z	601	CLA	C4B-C3B-CAB-CBB
20	Z	605	CLA	C4B-C3B-CAB-CBB
20	Z	608	CLA	C4B-C3B-CAB-CBB
20	Z	611	CLA	C4B-C3B-CAB-CBB
20	Z	615	CLA	C4B-C3B-CAB-CBB
20	3	606	CLA	C4B-C3B-CAB-CBB
20	3	618	CLA	C4B-C3B-CAB-CBB
20	7	601	CLA	C4B-C3B-CAB-CBB
20	7	602	CLA	C4B-C3B-CAB-CBB
20	7	606	CLA	C4B-C3B-CAB-CBB
20	8	605	CLA	C4B-C3B-CAB-CBB
20	8	615	CLA	C4B-C3B-CAB-CBB
20	4	603	CLA	C4B-C3B-CAB-CBB
20	4	606	CLA	C4B-C3B-CAB-CBB
20	6	606	CLA	C4B-C3B-CAB-CBB
20	6	607	CLA	C4B-C3B-CAB-CBB
20	A	1106	CLA	C16-C17-C18-C20
20	A	1108	CLA	C16-C17-C18-C20
20	B	1238	CLA	C16-C17-C18-C20
24	1	801	LHG	O6-C4-C5-C6
24	6	801	LHG	O6-C4-C5-C6
40	5	802	3PH	O11-C1-C2-C3
40	6	802	3PH	O11-C1-C2-C3
24	4	801	LHG	C18-C19-C20-C21
25	A	5004	NKP	CAO-CAP-CAQ-CAR
35	K	5001	SPH	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	1	801	LHG	C23-C24-C25-C26
20	A	1125	CLA	CBA-CGA-O2A-C1
21	A	2001	PQN	C15-C16-C17-C18
24	4	801	LHG	C31-C32-C33-C34
20	A	1108	CLA	C2-C3-C5-C6
20	A	1138	CLA	C2-C3-C5-C6
20	6	605	CLA	C2-C3-C5-C6
20	B	1240	CLA	C8-C10-C11-C12
20	1	601	CLA	C5-C6-C7-C8
20	8	601	CLA	C10-C11-C12-C13
20	7	605	CLA	C14-C13-C15-C16
20	A	1140	CLA	C3-C5-C6-C7
20	B	1220	CLA	C10-C11-C12-C13
20	A	1140	CLA	CBA-CGA-O2A-C1
20	8	602	CLA	CBA-CGA-O2A-C1
20	B	1205	CLA	CAA-CBA-CGA-O2A
20	B	1209	CLA	CAA-CBA-CGA-O2A
20	A	1102	CLA	C3A-C2A-CAA-CBA
20	A	1103	CLA	C3A-C2A-CAA-CBA
20	A	1110	CLA	C3A-C2A-CAA-CBA
20	A	1126	CLA	C3A-C2A-CAA-CBA
20	B	1213	CLA	C3A-C2A-CAA-CBA
20	3	616	CLA	C3A-C2A-CAA-CBA
20	7	616	CLA	C3A-C2A-CAA-CBA
20	5	603	CLA	C3A-C2A-CAA-CBA
20	5	606	CLA	C3A-C2A-CAA-CBA
20	6	605	CLA	C3A-C2A-CAA-CBA
37	7	610	CHL	C3A-C2A-CAA-CBA
37	6	610	CHL	C3A-C2A-CAA-CBA
23	A	4002	BCR	C9-C10-C11-C12
23	A	4004	BCR	C13-C14-C15-C16
23	A	4005	BCR	C19-C20-C21-C22
23	B	4005	BCR	C9-C10-C11-C12
23	I	4001	BCR	C19-C20-C21-C22
23	7	503	BCR	C9-C10-C11-C12
23	4	503	BCR	C9-C10-C11-C12
34	1	503	C7Z	C13-C14-C15-C35
36	5	501	LUT	C29-C30-C31-C32
26	F	5001	LMT	C2-C1-O1'-C1'
24	B	5006	LHG	C25-C26-C27-C28
20	A	1119	CLA	C15-C16-C17-C18
20	B	1220	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	6	801	LHG	C24-C25-C26-C27
20	A	1110	CLA	C16-C17-C18-C19
20	A	1131	CLA	C16-C17-C18-C20
20	B	1214	CLA	C8-C10-C11-C12
20	5	613	CLA	C5-C6-C7-C8
20	B	1204	CLA	O1D-CGD-O2D-CED
24	B	5001	LHG	C4-C5-C6-O8
24	7	801	LHG	C4-C5-C6-O8
24	8	801	LHG	C4-C5-C6-O8
24	4	802	LHG	C4-C5-C6-O8
29	J	5001	LMG	O1-C7-C8-C9
30	A	5005	DGA	OG1-CG1-CG2-CG3
38	1	802	SQD	C44-C45-C46-O48
24	A	5002	LHG	C17-C18-C19-C20
35	7	804	SPH	C15-C16-C17-C18
24	6	801	LHG	C30-C31-C32-C33
20	A	1121	CLA	C13-C15-C16-C17
20	A	1140	CLA	C16-C17-C18-C20
20	7	615	CLA	C10-C11-C12-C13
24	A	5002	LHG	C28-C29-C30-C31
26	A	5006	LMT	C7-C8-C9-C10
30	A	5005	DGA	CCB-CDB-CEB-CFB
25	8	802	NKP	CAO-CAP-CAQ-CAR
20	A	1133	CLA	C10-C11-C12-C13
24	B	5002	LHG	C3-O3-P-O6
20	3	601	CLA	O1A-CGA-O2A-C1
24	4	801	LHG	C9-C10-C11-C12
30	A	5005	DGA	CFB-CGB-CHB-CIB
20	5	608	CLA	C2A-CAA-CBA-CGA
20	6	608	CLA	C2A-CAA-CBA-CGA
24	6	801	LHG	O1-C1-C2-O2
24	Z	801	LHG	O6-C4-C5-O7
24	4	802	LHG	O6-C4-C5-O7
24	6	801	LHG	C27-C28-C29-C30
20	7	612	CLA	O1A-CGA-O2A-C1
20	B	1222	CLA	C16-C17-C18-C19
20	8	605	CLA	C16-C17-C18-C19
20	B	1221	CLA	CAA-CBA-CGA-O2A
20	A	1108	CLA	C2B-C3B-CAB-CBB
20	A	1109	CLA	C2B-C3B-CAB-CBB
20	A	1118	CLA	C2B-C3B-CAB-CBB
20	A	1124	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	1134	CLA	C2B-C3B-CAB-CBB
20	B	1237	CLA	C2B-C3B-CAB-CBB
20	B	1203	CLA	C2B-C3B-CAB-CBB
20	B	1205	CLA	C2B-C3B-CAB-CBB
20	B	1220	CLA	C2B-C3B-CAB-CBB
20	B	1224	CLA	C2B-C3B-CAB-CBB
20	B	1235	CLA	C2B-C3B-CAB-CBB
20	G	1601	CLA	C2B-C3B-CAB-CBB
20	K	1402	CLA	C2B-C3B-CAB-CBB
20	K	1404	CLA	C2B-C3B-CAB-CBB
20	1	603	CLA	C2B-C3B-CAB-CBB
20	1	606	CLA	C2B-C3B-CAB-CBB
20	Z	605	CLA	C2B-C3B-CAB-CBB
20	Z	615	CLA	C2B-C3B-CAB-CBB
20	3	606	CLA	C2B-C3B-CAB-CBB
20	3	618	CLA	C2B-C3B-CAB-CBB
20	7	601	CLA	C2B-C3B-CAB-CBB
20	7	606	CLA	C2B-C3B-CAB-CBB
20	8	605	CLA	C2B-C3B-CAB-CBB
20	8	615	CLA	C2B-C3B-CAB-CBB
35	K	5001	SPH	C14-C15-C16-C17
24	B	5006	LHG	O10-C23-O8-C6
26	B	5005	LMT	C3-C4-C5-C6
26	B	6101	LMT	C7-C8-C9-C10
24	A	5002	LHG	O7-C5-C6-O8
24	B	5002	LHG	O7-C5-C6-O8
24	Z	801	LHG	O7-C5-C6-O8
24	8	801	LHG	O7-C5-C6-O8
24	4	801	LHG	O7-C5-C6-O8
24	6	801	LHG	O7-C5-C6-O8
38	1	802	SQD	O47-C45-C46-O48
20	8	607	CLA	C6-C7-C8-C9
20	A	1110	CLA	C13-C15-C16-C17
20	A	1128	CLA	C15-C16-C17-C18
20	B	1209	CLA	C4-C3-C5-C6
37	5	610	CHL	C2-C1-O2A-CGA
24	1	801	LHG	C11-C12-C13-C14
20	A	1109	CLA	C14-C13-C15-C16
20	A	1111	CLA	C6-C7-C8-C9
20	A	1114	CLA	C6-C7-C8-C9
20	A	1119	CLA	C14-C13-C15-C16
20	A	1124	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1124	CLA	C11-C12-C13-C14
20	A	1140	CLA	C11-C12-C13-C14
20	B	1021	CLA	C11-C10-C8-C9
20	B	1203	CLA	C14-C13-C15-C16
20	B	1211	CLA	C6-C7-C8-C9
20	B	1215	CLA	C6-C7-C8-C9
20	B	1226	CLA	C14-C13-C15-C16
20	B	1240	CLA	C11-C12-C13-C14
20	3	607	CLA	C6-C7-C8-C9
20	3	610	CLA	C11-C10-C8-C9
20	3	612	CLA	C6-C7-C8-C9
20	8	609	CLA	C11-C10-C8-C9
20	5	602	CLA	C11-C10-C8-C9
20	5	602	CLA	C11-C12-C13-C14
20	5	618	CLA	C11-C10-C8-C9
20	6	619	CLA	C11-C10-C8-C9
37	5	610	CHL	C11-C10-C8-C9
37	5	610	CHL	C14-C13-C15-C16
24	A	5002	LHG	C16-C17-C18-C19
40	6	802	3PH	C32-C33-C34-C35
20	A	1107	CLA	CBD-CGD-O2D-CED
20	A	1113	CLA	C5-C6-C7-C8
20	B	1234	CLA	C8-C10-C11-C12
20	7	605	CLA	C5-C6-C7-C8
24	B	5001	LHG	C2-C3-O3-P
24	8	801	LHG	C2-C3-O3-P
24	6	801	LHG	C2-C3-O3-P
42	8	803	LPX	C4-C3-O1-P1
24	1	801	LHG	C9-C10-C11-C12
26	1	803	LMT	C5-C6-C7-C8
41	7	805	PLM	C6-C7-C8-C9
20	8	608	CLA	C6-C7-C8-C10
20	4	605	CLA	C3-C5-C6-C7
23	B	4001	BCR	C23-C24-C25-C26
23	B	4003	BCR	C23-C24-C25-C26
23	B	4004	BCR	C23-C24-C25-C26
23	B	4007	BCR	C5-C6-C7-C8
23	K	4002	BCR	C1-C6-C7-C8
23	K	4002	BCR	C5-C6-C7-C8
23	6	503	BCR	C23-C24-C25-C26
23	6	503	BCR	C23-C24-C25-C30
36	1	501	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	4	501	LUT	C1-C6-C7-C8
36	4	501	LUT	C5-C6-C7-C8
36	4	502	LUT	C5-C6-C7-C8
37	6	610	CHL	C3-C5-C6-C7
20	1	611	CLA	C13-C15-C16-C17
20	5	607	CLA	C8-C10-C11-C12
20	B	1219	CLA	C11-C12-C13-C14
24	1	801	LHG	C31-C32-C33-C34
40	8	806	3PH	C3C-C3D-C3E-C3F
23	7	503	BCR	C37-C22-C23-C24
26	B	5005	LMT	O5B-C5B-C6B-O6B
23	B	4007	BCR	C7-C8-C9-C10
23	G	4001	BCR	C7-C8-C9-C10
23	I	4001	BCR	C17-C18-C19-C20
23	6	503	BCR	C17-C18-C19-C20
36	Z	503	LUT	C7-C8-C9-C10
20	A	1139	CLA	C8-C10-C11-C12
20	B	1223	CLA	C8-C10-C11-C12
24	7	801	LHG	O9-C7-O7-C5
30	A	5005	DGA	CA5-CA6-CA7-CA8
20	B	1218	CLA	C15-C16-C17-C18
20	B	1236	CLA	C5-C6-C7-C8
20	B	1238	CLA	C4-C3-C5-C6
20	A	1104	CLA	C6-C7-C8-C10
20	A	1106	CLA	C11-C12-C13-C15
20	A	1107	CLA	C11-C10-C8-C7
20	A	1107	CLA	C12-C13-C15-C16
20	A	1108	CLA	C6-C7-C8-C10
20	A	1109	CLA	C12-C13-C15-C16
20	A	1114	CLA	C6-C7-C8-C10
20	A	1115	CLA	C6-C7-C8-C10
20	A	1117	CLA	C11-C10-C8-C7
20	A	1117	CLA	C11-C12-C13-C15
20	A	1119	CLA	C12-C13-C15-C16
20	A	1121	CLA	C12-C13-C15-C16
20	A	1122	CLA	C6-C7-C8-C10
20	A	1124	CLA	C11-C12-C13-C15
20	A	1125	CLA	C12-C13-C15-C16
20	A	1132	CLA	C11-C10-C8-C7
20	A	1132	CLA	C11-C12-C13-C15
20	A	1136	CLA	C6-C7-C8-C10
20	A	1130	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	A	1140	CLA	C11-C12-C13-C15
20	B	1023	CLA	C11-C12-C13-C15
20	B	1203	CLA	C12-C13-C15-C16
20	B	1205	CLA	C11-C10-C8-C7
20	B	1210	CLA	C12-C13-C15-C16
20	B	1211	CLA	C6-C7-C8-C10
20	B	1211	CLA	C11-C10-C8-C7
20	B	1212	CLA	C6-C7-C8-C10
20	B	1217	CLA	C6-C7-C8-C10
20	B	1219	CLA	C6-C7-C8-C10
20	B	1222	CLA	C12-C13-C15-C16
20	B	1223	CLA	C12-C13-C15-C16
20	B	1228	CLA	C11-C10-C8-C7
20	B	1235	CLA	C11-C12-C13-C15
20	B	1235	CLA	C12-C13-C15-C16
20	L	1502	CLA	C11-C10-C8-C7
20	1	607	CLA	C6-C7-C8-C10
20	1	612	CLA	C6-C7-C8-C10
20	1	612	CLA	C11-C12-C13-C15
20	1	612	CLA	C12-C13-C15-C16
20	Z	612	CLA	C11-C10-C8-C7
20	3	601	CLA	C11-C12-C13-C15
20	3	606	CLA	C6-C7-C8-C10
20	3	607	CLA	C6-C7-C8-C10
20	7	601	CLA	C6-C7-C8-C10
20	7	607	CLA	C11-C10-C8-C7
20	8	609	CLA	C11-C10-C8-C7
20	8	602	CLA	C12-C13-C15-C16
20	5	602	CLA	C11-C10-C8-C7
20	5	602	CLA	C11-C12-C13-C15
20	5	604	CLA	C12-C13-C15-C16
20	6	604	CLA	C11-C12-C13-C15
37	Z	609	CHL	C11-C10-C8-C7
37	Z	609	CHL	C12-C13-C15-C16
37	8	613	CHL	C11-C10-C8-C7
37	5	610	CHL	C11-C10-C8-C7
37	5	610	CHL	C12-C13-C15-C16
23	G	4001	BCR	C9-C10-C11-C12
23	L	4001	BCR	C9-C10-C11-C12
23	L	4001	BCR	C13-C14-C15-C16
23	3	503	BCR	C19-C20-C21-C22
23	3	505	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	8	503	BCR	C9-C10-C11-C12
23	8	503	BCR	C19-C20-C21-C22
23	6	504	BCR	C9-C10-C11-C12
23	6	503	BCR	C19-C20-C21-C22
34	5	505	C7Z	C29-C30-C31-C32
36	1	501	LUT	C29-C30-C31-C32
36	Z	502	LUT	C29-C30-C31-C32
36	7	502	LUT	C29-C30-C31-C32
36	4	501	LUT	C29-C30-C31-C32
36	6	501	LUT	C29-C30-C31-C32
20	B	1218	CLA	C16-C17-C18-C20
20	5	609	CLA	C8-C10-C11-C12
20	K	1402	CLA	CAA-CBA-CGA-O2A
20	3	604	CLA	O1A-CGA-O2A-C1
20	A	1118	CLA	C2A-CAA-CBA-CGA
24	8	801	LHG	C30-C31-C32-C33
40	7	802	3PH	C3A-C3B-C3C-C3D
24	Z	801	LHG	C9-C10-C11-C12
20	A	1128	CLA	C3-C5-C6-C7
40	7	802	3PH	C27-C28-C29-C2A
20	1	603	CLA	C15-C16-C17-C18
20	B	1205	CLA	CBA-CGA-O2A-C1
20	B	1221	CLA	CBA-CGA-O2A-C1
20	Z	601	CLA	CBA-CGA-O2A-C1
24	4	801	LHG	C35-C36-C37-C38
30	A	5005	DGA	CA6-CA7-CA8-CA9
20	A	1122	CLA	C8-C10-C11-C12
20	A	1124	CLA	CAD-CBD-CGD-O2D
20	A	1138	CLA	CAD-CBD-CGD-O2D
20	B	1205	CLA	CAD-CBD-CGD-O2D
20	B	1218	CLA	CAD-CBD-CGD-O2D
20	Z	604	CLA	CAD-CBD-CGD-O2D
20	4	606	CLA	CAD-CBD-CGD-O2D
20	6	609	CLA	CAD-CBD-CGD-O2D
37	1	609	CHL	CAD-CBD-CGD-O2D
37	Z	609	CHL	CAD-CBD-CGD-O2D
37	4	617	CHL	CAD-CBD-CGD-O2D
20	A	1140	CLA	C8-C10-C11-C12
20	B	1224	CLA	C15-C16-C17-C18
20	8	601	CLA	C5-C6-C7-C8
20	8	602	CLA	O1A-CGA-O2A-C1
20	A	1122	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1110	CLA	C4-C3-C5-C6
20	6	603	CLA	C4-C3-C5-C6
20	B	1238	CLA	C2-C3-C5-C6
20	Z	612	CLA	C2-C3-C5-C6
24	A	5002	LHG	C4-C5-C6-O8
24	Z	801	LHG	C2-C3-O3-P
24	4	802	LHG	C2-C3-O3-P
24	5	801	LHG	C4-C5-C6-O8
24	6	801	LHG	C4-C5-C6-O8
40	7	802	3PH	C1-C2-C3-O31
40	6	802	3PH	C1-C2-C3-O31
20	B	1205	CLA	O1A-CGA-O2A-C1
24	7	801	LHG	O6-C4-C5-O7
20	A	1124	CLA	C8-C10-C11-C12
20	1	615	CLA	C8-C10-C11-C12
20	7	604	CLA	C5-C6-C7-C8
20	7	606	CLA	C3-C5-C6-C7
20	A	1127	CLA	CAA-CBA-CGA-O2A
20	B	1208	CLA	C2A-CAA-CBA-CGA
20	B	1210	CLA	C2A-CAA-CBA-CGA
20	5	615	CLA	C2A-CAA-CBA-CGA
20	6	602	CLA	C2A-CAA-CBA-CGA
20	A	1116	CLA	C10-C11-C12-C13
40	7	802	3PH	C24-C25-C26-C27
20	A	1107	CLA	O1D-CGD-O2D-CED
20	A	1012	CLA	CHA-CBD-CGD-O2D
20	A	1103	CLA	CHA-CBD-CGD-O1D
20	A	1103	CLA	CHA-CBD-CGD-O2D
20	A	1106	CLA	CHA-CBD-CGD-O1D
20	A	1106	CLA	CHA-CBD-CGD-O2D
20	A	1111	CLA	CHA-CBD-CGD-O1D
20	A	1111	CLA	CHA-CBD-CGD-O2D
20	A	1121	CLA	CHA-CBD-CGD-O1D
20	A	1121	CLA	CHA-CBD-CGD-O2D
20	A	1134	CLA	CHA-CBD-CGD-O1D
20	A	1134	CLA	CHA-CBD-CGD-O2D
20	A	1137	CLA	CHA-CBD-CGD-O1D
20	A	1137	CLA	CHA-CBD-CGD-O2D
20	A	1141	CLA	CHA-CBD-CGD-O1D
20	A	1141	CLA	CHA-CBD-CGD-O2D
20	A	1013	CLA	CHA-CBD-CGD-O2D
20	B	1021	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	B	1210	CLA	CHA-CBD-CGD-O1D
20	B	1210	CLA	CHA-CBD-CGD-O2D
20	B	1227	CLA	CHA-CBD-CGD-O1D
20	B	1227	CLA	CHA-CBD-CGD-O2D
20	B	1228	CLA	CHA-CBD-CGD-O2D
20	B	1230	CLA	CHA-CBD-CGD-O1D
20	B	1230	CLA	CHA-CBD-CGD-O2D
20	G	1602	CLA	CHA-CBD-CGD-O1D
20	G	1602	CLA	CHA-CBD-CGD-O2D
20	1	605	CLA	CHA-CBD-CGD-O1D
20	1	605	CLA	CHA-CBD-CGD-O2D
20	1	612	CLA	CHA-CBD-CGD-O1D
20	1	612	CLA	CHA-CBD-CGD-O2D
20	Z	601	CLA	CHA-CBD-CGD-O1D
20	Z	606	CLA	CHA-CBD-CGD-O1D
20	Z	608	CLA	CHA-CBD-CGD-O1D
20	Z	608	CLA	CHA-CBD-CGD-O2D
20	Z	611	CLA	CHA-CBD-CGD-O2D
20	Z	615	CLA	CHA-CBD-CGD-O2D
20	7	603	CLA	CHA-CBD-CGD-O1D
20	7	608	CLA	CHA-CBD-CGD-O1D
20	7	608	CLA	CHA-CBD-CGD-O2D
20	7	612	CLA	CHA-CBD-CGD-O1D
20	7	612	CLA	CHA-CBD-CGD-O2D
20	8	609	CLA	CHA-CBD-CGD-O1D
20	8	609	CLA	CHA-CBD-CGD-O2D
20	8	605	CLA	CHA-CBD-CGD-O1D
20	8	605	CLA	CHA-CBD-CGD-O2D
20	4	606	CLA	CHA-CBD-CGD-O1D
20	6	606	CLA	CHA-CBD-CGD-O2D
20	6	619	CLA	CHA-CBD-CGD-O1D
20	6	619	CLA	CHA-CBD-CGD-O2D
37	1	610	CHL	CHA-CBD-CGD-O1D
37	4	610	CHL	CHA-CBD-CGD-O2D
20	A	1128	CLA	C5-C6-C7-C8
20	A	1125	CLA	O1A-CGA-O2A-C1
20	A	1140	CLA	O1A-CGA-O2A-C1
26	B	5005	LMT	C2'-C1'-O1'-C1
24	B	5001	LHG	O7-C5-C6-O8
30	A	5005	DGA	OG1-CG1-CG2-OG2
40	6	802	3PH	O21-C2-C3-O31
20	A	1127	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	4	605	CLA	C8-C10-C11-C12
20	B	1234	CLA	C11-C12-C13-C14
24	7	801	LHG	O1-C1-C2-O2
20	B	1213	CLA	C4-C3-C5-C6
20	B	1236	CLA	C4-C3-C5-C6
20	1	603	CLA	C4-C3-C5-C6
20	Z	612	CLA	C4-C3-C5-C6
20	8	602	CLA	C4-C3-C5-C6
25	8	802	NKP	CAL-CAM-CAN-CAO
20	Z	601	CLA	O1A-CGA-O2A-C1
20	B	1209	CLA	C2-C3-C5-C6
20	1	603	CLA	C2-C3-C5-C6
40	8	806	3PH	C3B-C3C-C3D-C3E
20	A	1107	CLA	C11-C10-C8-C9
20	A	1125	CLA	C14-C13-C15-C16
20	A	1128	CLA	C11-C10-C8-C9
20	B	1219	CLA	C6-C7-C8-C9
20	B	1223	CLA	C14-C13-C15-C16
20	3	601	CLA	C11-C12-C13-C14
20	3	603	CLA	C11-C12-C13-C14
20	7	603	CLA	C11-C10-C8-C9
20	7	605	CLA	C11-C10-C8-C9
20	B	1221	CLA	O1A-CGA-O2A-C1
30	A	5005	DGA	CDA-CEA-CFA-CGA
20	B	1241	CLA	C2A-CAA-CBA-CGA
20	1	612	CLA	C2A-CAA-CBA-CGA
37	4	610	CHL	C2A-CAA-CBA-CGA
24	A	5002	LHG	C9-C10-C11-C12
24	B	5006	LHG	C11-C12-C13-C14
24	7	801	LHG	C30-C31-C32-C33
24	6	801	LHG	C26-C27-C28-C29
23	A	4003	BCR	C36-C18-C19-C20
23	B	4002	BCR	C36-C18-C19-C20
20	Z	604	CLA	C13-C15-C16-C17
23	A	4003	BCR	C21-C22-C23-C24
23	L	4002	BCR	C17-C18-C19-C20
36	4	501	LUT	C27-C28-C29-C30
20	B	1230	CLA	C1A-C2A-CAA-CBA
20	1	611	CLA	C1A-C2A-CAA-CBA
20	Z	608	CLA	C1A-C2A-CAA-CBA
20	Z	611	CLA	C1A-C2A-CAA-CBA
20	4	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	1122	CLA	C16-C17-C18-C20
20	8	608	CLA	C6-C7-C8-C9
21	A	2001	PQN	C26-C27-C28-C30
20	A	1118	CLA	C2-C1-O2A-CGA
20	K	1402	CLA	C2-C1-O2A-CGA
20	3	605	CLA	C2-C1-O2A-CGA
20	4	606	CLA	C2-C1-O2A-CGA
20	3	605	CLA	CBA-CGA-O2A-C1
26	B	5005	LMT	C5-C6-C7-C8
20	A	1101	CLA	C15-C16-C17-C18
24	A	5001	LHG	C3-O3-P-O6
24	B	5001	LHG	C3-O3-P-O6
24	B	5001	LHG	C4-O6-P-O3
24	1	801	LHG	C3-O3-P-O6
24	5	801	LHG	C3-O3-P-O6
25	8	802	NKP	CAM-CAN-CAO-CAP
20	B	1214	CLA	C11-C12-C13-C14
20	B	1211	CLA	C4-C3-C5-C6
20	Z	608	CLA	C5-C6-C7-C8
20	3	606	CLA	C13-C15-C16-C17
20	B	1220	CLA	C3-C5-C6-C7
24	1	801	LHG	C2-C3-O3-P
20	3	607	CLA	C2-C3-C5-C6
24	A	5002	LHG	C19-C20-C21-C22
20	A	1135	CLA	C4B-C3B-CAB-CBB
20	A	1139	CLA	C4B-C3B-CAB-CBB
20	A	1101	CLA	C4B-C3B-CAB-CBB
20	B	1239	CLA	C4B-C3B-CAB-CBB
20	7	608	CLA	C4B-C3B-CAB-CBB
20	8	603	CLA	C4B-C3B-CAB-CBB
20	4	609	CLA	C4B-C3B-CAB-CBB
20	5	603	CLA	C4B-C3B-CAB-CBB
20	5	615	CLA	C4B-C3B-CAB-CBB
20	6	603	CLA	C4B-C3B-CAB-CBB
24	A	5001	LHG	C4-O6-P-O5
24	B	5001	LHG	C3-O3-P-O4
24	1	801	LHG	C4-O6-P-O5
24	8	801	LHG	C4-O6-P-O4
24	4	802	LHG	C3-O3-P-O5
42	8	803	LPX	C3-O1-P1-O3
35	7	803	SPH	C10-C11-C12-C13
20	B	1237	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	1	606	CLA	C8-C10-C11-C12
24	B	5001	LHG	O6-C4-C5-C6
24	B	5002	LHG	O6-C4-C5-C6
24	B	5006	LHG	O6-C4-C5-C6
42	8	803	LPX	O2-C1-C2-N1
20	3	605	CLA	O1A-CGA-O2A-C1
20	8	612	CLA	O1D-CGD-O2D-CED
20	5	618	CLA	C3-C5-C6-C7
20	B	1236	CLA	C16-C17-C18-C20
20	B	1230	CLA	C10-C11-C12-C13
24	4	801	LHG	C27-C28-C29-C30
24	4	801	LHG	C30-C31-C32-C33
20	Z	606	CLA	CAD-CBD-CGD-O1D
20	7	609	CLA	CAD-CBD-CGD-O1D
20	8	609	CLA	CAD-CBD-CGD-O1D
20	6	615	CLA	CAD-CBD-CGD-O1D
37	1	610	CHL	CAD-CBD-CGD-O1D
38	1	802	SQD	C5-C6-S-O7
20	A	1111	CLA	C3-C5-C6-C7
31	B	5003	DGD	CFA-CGA-CHA-CIA
20	A	1013	CLA	C4-C3-C5-C6
20	B	1221	CLA	C4-C3-C5-C6
20	7	616	CLA	C4-C3-C5-C6
19	A	1011	CL0	C11-C10-C8-C7
20	A	1012	CLA	C11-C10-C8-C7
20	A	1108	CLA	C12-C13-C15-C16
20	A	1110	CLA	C6-C7-C8-C10
20	A	1110	CLA	C11-C12-C13-C15
20	A	1121	CLA	C6-C7-C8-C10
20	A	1128	CLA	C11-C10-C8-C7
20	A	1137	CLA	C11-C10-C8-C7
20	A	1140	CLA	C6-C7-C8-C10
20	B	1205	CLA	C12-C13-C15-C16
20	B	1209	CLA	C12-C13-C15-C16
20	B	1213	CLA	C11-C12-C13-C15
20	B	1226	CLA	C11-C10-C8-C7
20	B	1238	CLA	C11-C10-C8-C7
20	B	1230	CLA	C3A-C2A-CAA-CBA
20	1	612	CLA	C11-C10-C8-C7
20	3	603	CLA	C11-C12-C13-C15
20	7	603	CLA	C11-C10-C8-C7
21	B	2002	PQN	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	A	5002	LHG	O6-C4-C5-O7
24	B	5006	LHG	O6-C4-C5-O7
36	Z	503	LUT	C25-C26-C27-C28
36	7	502	LUT	C25-C26-C27-C28
36	8	502	LUT	C25-C26-C27-C28
36	4	502	LUT	C25-C26-C27-C28
36	5	502	LUT	C25-C26-C27-C28
36	6	501	LUT	C25-C26-C27-C28
40	6	802	3PH	O11-C1-C2-O21
23	K	4002	BCR	C19-C20-C21-C22
23	7	503	BCR	C15-C16-C17-C18
23	4	503	BCR	C19-C20-C21-C22
36	3	501	LUT	C29-C30-C31-C32
36	5	502	LUT	C29-C30-C31-C32
37	8	610	CHL	CAA-CBA-CGA-O2A
40	8	806	3PH	C34-C35-C36-C37
40	8	806	3PH	C31-C32-C33-C34
24	Z	801	LHG	C11-C10-C9-C8
20	A	1127	CLA	O1A-CGA-O2A-C1
24	A	5001	LHG	C10-C11-C12-C13
20	B	1209	CLA	C2A-CAA-CBA-CGA
20	K	1404	CLA	C2A-CAA-CBA-CGA
20	6	609	CLA	C10-C11-C12-C13
24	B	5006	LHG	C4-C5-C6-O8
24	B	5006	LHG	C26-C27-C28-C29
31	B	5003	DGD	O1G-C1G-C2G-C3G
31	B	5003	DGD	C1G-C2G-C3G-O3G
40	8	806	3PH	C1-C2-C3-O31
31	B	5003	DGD	O1G-C1G-C2G-O2G
40	7	802	3PH	O21-C2-C3-O31
40	8	806	3PH	O21-C2-C3-O31
24	8	801	LHG	C25-C26-C27-C28
29	J	5001	LMG	C8-C7-O1-C1
20	A	1107	CLA	C10-C11-C12-C13
20	6	606	CLA	C10-C11-C12-C13
20	A	1122	CLA	O1A-CGA-O2A-C1
20	A	1114	CLA	C14-C13-C15-C16
20	6	603	CLA	C2-C3-C5-C6
20	A	1105	CLA	C13-C15-C16-C17
20	B	1220	CLA	C15-C16-C17-C18
20	A	1107	CLA	C14-C13-C15-C16
20	A	1111	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1122	CLA	C6-C7-C8-C9
20	B	1023	CLA	C11-C10-C8-C9
20	B	1211	CLA	C11-C10-C8-C9
20	B	1217	CLA	C6-C7-C8-C9
20	B	1222	CLA	C14-C13-C15-C16
20	B	1228	CLA	C11-C10-C8-C9
20	B	1235	CLA	C14-C13-C15-C16
20	F	1301	CLA	C11-C12-C13-C14
20	1	612	CLA	C6-C7-C8-C9
20	Z	612	CLA	C11-C10-C8-C9
20	3	606	CLA	C6-C7-C8-C9
20	8	609	CLA	C6-C7-C8-C9
20	8	602	CLA	C14-C13-C15-C16
20	5	604	CLA	C14-C13-C15-C16
20	6	604	CLA	C11-C12-C13-C14
20	6	619	CLA	C6-C7-C8-C9
37	8	613	CHL	C11-C10-C8-C9
20	B	1234	CLA	C11-C12-C13-C15
20	B	1021	CLA	O1A-CGA-O2A-C1
24	1	801	LHG	O1-C1-C2-O2
24	8	801	LHG	O1-C1-C2-O2
20	7	615	CLA	C8-C10-C11-C12
23	B	4005	BCR	C18-C19-C20-C21
23	3	506	BCR	C18-C19-C20-C21
23	5	504	BCR	C18-C19-C20-C21
23	6	504	BCR	C18-C19-C20-C21
23	6	503	BCR	C15-C16-C17-C18
36	6	502	LUT	C29-C30-C31-C32
23	B	4004	BCR	C7-C8-C9-C34
23	4	503	BCR	C11-C12-C13-C35
24	A	5001	LHG	C12-C13-C14-C15
20	3	607	CLA	C11-C12-C13-C14
20	4	605	CLA	C16-C17-C18-C20
37	7	610	CHL	C5-C6-C7-C8
20	A	1012	CLA	C2B-C3B-CAB-CBB
20	A	1119	CLA	C2B-C3B-CAB-CBB
20	A	1120	CLA	C2B-C3B-CAB-CBB
20	A	1121	CLA	C2B-C3B-CAB-CBB
20	A	1126	CLA	C2B-C3B-CAB-CBB
20	B	1023	CLA	C2B-C3B-CAB-CBB
20	B	1204	CLA	C2B-C3B-CAB-CBB
20	B	1214	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	B	1215	CLA	C2B-C3B-CAB-CBB
20	B	1238	CLA	C2B-C3B-CAB-CBB
20	B	1239	CLA	C2B-C3B-CAB-CBB
20	1	604	CLA	C2B-C3B-CAB-CBB
20	1	612	CLA	C2B-C3B-CAB-CBB
20	Z	601	CLA	C2B-C3B-CAB-CBB
20	Z	608	CLA	C2B-C3B-CAB-CBB
20	7	602	CLA	C2B-C3B-CAB-CBB
20	8	602	CLA	C2B-C3B-CAB-CBB
20	8	603	CLA	C2B-C3B-CAB-CBB
20	4	601	CLA	C2B-C3B-CAB-CBB
20	4	603	CLA	C2B-C3B-CAB-CBB
20	4	606	CLA	C2B-C3B-CAB-CBB
20	4	609	CLA	C2B-C3B-CAB-CBB
20	5	601	CLA	C2B-C3B-CAB-CBB
20	5	603	CLA	C2B-C3B-CAB-CBB
20	5	612	CLA	C2B-C3B-CAB-CBB
20	6	601	CLA	C2B-C3B-CAB-CBB
20	6	604	CLA	C2B-C3B-CAB-CBB
20	6	606	CLA	C2B-C3B-CAB-CBB
20	6	607	CLA	C2B-C3B-CAB-CBB
20	6	612	CLA	C2B-C3B-CAB-CBB
20	A	1126	CLA	C8-C10-C11-C12
20	B	1240	CLA	C5-C6-C7-C8
24	4	802	LHG	C12-C13-C14-C15
20	B	1213	CLA	C2-C3-C5-C6
20	8	601	CLA	C2-C3-C5-C6
20	8	602	CLA	C2-C3-C5-C6
20	1	615	CLA	C13-C15-C16-C17
31	B	5003	DGD	C1A-C2A-C3A-C4A
20	A	1111	CLA	C16-C17-C18-C20
20	A	1124	CLA	C16-C17-C18-C19
20	L	1502	CLA	C16-C17-C18-C20
20	A	1127	CLA	C5-C6-C7-C8
35	K	5001	SPH	C2-C3-C4-C5
24	Z	801	LHG	C24-C25-C26-C27
24	A	5002	LHG	O6-C4-C5-C6
24	3	801	LHG	O6-C4-C5-C6
24	1	801	LHG	C1-C2-C3-O3
20	B	1203	CLA	C2A-CAA-CBA-CGA
20	B	1217	CLA	C2A-CAA-CBA-CGA
20	7	605	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	7	606	CLA	C2A-CAA-CBA-CGA
20	5	601	CLA	C2A-CAA-CBA-CGA
20	A	1102	CLA	C2-C1-O2A-CGA
20	A	1136	CLA	C2-C1-O2A-CGA
20	A	1139	CLA	C2-C1-O2A-CGA
20	Z	601	CLA	C2-C1-O2A-CGA
20	Z	607	CLA	C2-C1-O2A-CGA
20	7	607	CLA	C2-C1-O2A-CGA
37	4	610	CHL	C2-C1-O2A-CGA
38	1	802	SQD	C7-C8-C9-C10
30	A	5005	DGA	CB6-CB7-CB8-CB9
23	3	505	BCR	C19-C20-C21-C22
24	5	801	LHG	O6-C4-C5-O7
20	4	603	CLA	C4-C3-C5-C6
40	8	806	3PH	C36-C37-C38-C39
23	B	4001	BCR	C23-C24-C25-C30
23	B	4003	BCR	C23-C24-C25-C30
23	B	4004	BCR	C23-C24-C25-C30
23	3	504	BCR	C5-C6-C7-C8
34	J	4002	C7Z	C5-C6-C7-C8
36	1	501	LUT	C5-C6-C7-C8
36	8	501	LUT	C5-C6-C7-C8
36	4	502	LUT	C1-C6-C7-C8
36	6	501	LUT	C5-C6-C7-C8
20	B	1208	CLA	O1A-CGA-O2A-C1
24	5	801	LHG	C24-C25-C26-C27
20	A	1111	CLA	C8-C10-C11-C12
20	B	1240	CLA	C16-C17-C18-C19
20	1	601	CLA	C16-C17-C18-C20
24	3	801	LHG	O7-C5-C6-O8
24	7	801	LHG	C26-C27-C28-C29
26	A	5006	LMT	O1'-C1-C2-C3
20	B	1208	CLA	CBA-CGA-O2A-C1
24	B	5002	LHG	C4-O6-P-O3
24	B	5006	LHG	C3-O3-P-O6
24	Z	801	LHG	C3-O3-P-O6
24	3	801	LHG	C3-O3-P-O6
24	3	801	LHG	C4-O6-P-O3
24	8	801	LHG	C3-O3-P-O6
24	4	801	LHG	C3-O3-P-O6
24	4	801	LHG	C4-O6-P-O3
20	6	618	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	5002	LHG	C4-C5-C6-O8
20	A	1104	CLA	C4-C3-C5-C6
20	5	601	CLA	C4-C3-C5-C6
20	A	1124	CLA	C6-C7-C8-C10
20	A	1133	CLA	C12-C13-C15-C16
20	B	1210	CLA	C11-C12-C13-C15
20	B	1236	CLA	C11-C10-C8-C7
20	6	619	CLA	C6-C7-C8-C10
20	A	1113	CLA	C3-C5-C6-C7
20	A	1012	CLA	C11-C10-C8-C9
20	A	1126	CLA	C6-C7-C8-C9
20	A	1137	CLA	C11-C10-C8-C9
20	A	1138	CLA	C11-C10-C8-C9
20	A	1140	CLA	C6-C7-C8-C9
20	B	1218	CLA	C6-C7-C8-C9
20	B	1225	CLA	C14-C13-C15-C16
20	1	612	CLA	C11-C10-C8-C9
20	3	603	CLA	C11-C10-C8-C9
20	7	609	CLA	C6-C7-C8-C9
21	B	2002	PQN	C16-C17-C18-C19
23	A	4004	BCR	C9-C10-C11-C12
23	B	4007	BCR	C19-C20-C21-C22
23	5	503	BCR	C13-C14-C15-C16
36	1	502	LUT	C29-C30-C31-C32
36	7	501	LUT	C29-C30-C31-C32
20	A	1132	CLA	C16-C17-C18-C20
20	Z	604	CLA	C16-C17-C18-C20
30	A	5005	DGA	CA8-CA9-CAA-CBA
26	B	5005	LMT	C9-C10-C11-C12
26	B	6101	LMT	C4'-C5'-C6'-O6'
23	A	4002	BCR	C36-C18-C19-C20
23	B	4003	BCR	C37-C22-C23-C24
20	A	1013	CLA	C16-C17-C18-C19
20	B	1236	CLA	C16-C17-C18-C19
24	4	801	LHG	C2-C3-O3-P
24	A	5002	LHG	C29-C30-C31-C32
20	A	1114	CLA	C12-C13-C15-C16
20	7	605	CLA	C12-C13-C15-C16
20	B	1221	CLA	C2-C3-C5-C6
20	7	609	CLA	C16-C17-C18-C19
20	5	604	CLA	C5-C6-C7-C8
24	1	801	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	1120	CLA	C4B-C3B-CAB-CBB
20	A	1133	CLA	C4B-C3B-CAB-CBB
20	B	1214	CLA	C4B-C3B-CAB-CBB
20	B	1215	CLA	C4B-C3B-CAB-CBB
20	B	1238	CLA	C4B-C3B-CAB-CBB
20	K	1401	CLA	C4B-C3B-CAB-CBB
20	1	612	CLA	C4B-C3B-CAB-CBB
20	1	613	CLA	C4B-C3B-CAB-CBB
20	3	604	CLA	C4B-C3B-CAB-CBB
20	8	602	CLA	C4B-C3B-CAB-CBB
20	8	606	CLA	C4B-C3B-CAB-CBB
20	4	601	CLA	C4B-C3B-CAB-CBB
20	5	601	CLA	C4B-C3B-CAB-CBB
20	5	612	CLA	C4B-C3B-CAB-CBB
20	6	601	CLA	C4B-C3B-CAB-CBB
20	6	604	CLA	C4B-C3B-CAB-CBB
20	6	612	CLA	C4B-C3B-CAB-CBB
31	B	5003	DGD	O6E-C1E-O5D-C6D
20	A	1131	CLA	C15-C16-C17-C18
23	A	4001	BCR	C15-C16-C17-C18
23	J	4001	BCR	C9-C10-C11-C12
23	K	4001	BCR	C9-C10-C11-C12
23	6	504	BCR	C19-C20-C21-C22
23	6	503	BCR	C13-C14-C15-C16
34	J	4002	C7Z	C13-C14-C15-C35
36	Z	501	LUT	C29-C30-C31-C32
36	8	502	LUT	C29-C30-C31-C32
20	A	1103	CLA	C15-C16-C17-C18
20	7	607	CLA	C8-C10-C11-C12
24	7	801	LHG	C27-C28-C29-C30
38	1	802	SQD	C14-C15-C16-C17
20	A	1136	CLA	CAA-CBA-CGA-O2A
24	5	801	LHG	O8-C23-C24-C25
20	A	1106	CLA	C3-C5-C6-C7
20	B	1217	CLA	C5-C6-C7-C8
31	B	5003	DGD	C2E-C1E-O5D-C6D
20	A	1135	CLA	C2A-CAA-CBA-CGA
20	6	609	CLA	C2A-CAA-CBA-CGA
29	A	5003	LMG	O1-C7-C8-O7
37	4	613	CHL	C2A-CAA-CBA-CGA
24	B	5006	LHG	C24-C25-C26-C27
20	B	1226	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	A	5004	NKP	CAH-CAG-OAF-PAC
20	A	1115	CLA	C3A-C2A-CAA-CBA
20	A	1125	CLA	C3A-C2A-CAA-CBA
20	B	1210	CLA	C3A-C2A-CAA-CBA
20	B	1221	CLA	C3A-C2A-CAA-CBA
20	3	603	CLA	C3A-C2A-CAA-CBA
20	3	607	CLA	C3A-C2A-CAA-CBA
20	6	604	CLA	C3A-C2A-CAA-CBA
20	4	609	CLA	O1D-CGD-O2D-CED
20	A	1132	CLA	C16-C17-C18-C19
35	7	803	SPH	C4-C5-C6-C7
26	B	6101	LMT	C5'-C4'-O1B-C1B
23	J	4001	BCR	C19-C20-C21-C22
20	B	1215	CLA	C4-C3-C5-C6
20	1	606	CLA	C4-C3-C5-C6
20	6	619	CLA	C4-C3-C5-C6
20	B	1211	CLA	C2-C3-C5-C6
20	A	1110	CLA	C6-C7-C8-C9
20	A	1119	CLA	C6-C7-C8-C9
20	B	1209	CLA	C6-C7-C8-C9
20	B	1213	CLA	C11-C10-C8-C9
20	3	605	CLA	C11-C12-C13-C14
20	7	604	CLA	C14-C13-C15-C16
20	7	607	CLA	C14-C13-C15-C16
20	6	619	CLA	C11-C12-C13-C14
37	3	611	CHL	C6-C7-C8-C9
24	1	801	LHG	C30-C31-C32-C33
20	B	1234	CLA	CBA-CGA-O2A-C1
24	5	801	LHG	C12-C13-C14-C15
20	A	1130	CLA	C8-C10-C11-C12
23	A	4005	BCR	C16-C17-C18-C36
23	B	4003	BCR	C20-C21-C22-C37
23	5	504	BCR	C16-C17-C18-C36
33	F	4001	RRX	C35-C13-C14-C15
37	5	610	CHL	C3-C5-C6-C7
20	4	609	CLA	CBD-CGD-O2D-CED
42	8	803	LPX	C10-C11-C12-C13
20	L	1502	CLA	C16-C17-C18-C19
23	A	4004	BCR	C36-C18-C19-C20
36	1	501	LUT	C27-C28-C29-C39
20	B	1207	CLA	C5-C6-C7-C8
40	6	802	3PH	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	A	4003	BCR	C17-C18-C19-C20
25	8	802	NKP	CAU-CAV-CAW-CAX
20	B	1220	CLA	C4-C3-C5-C6
20	A	1125	CLA	C1A-C2A-CAA-CBA
20	A	1140	CLA	C1A-C2A-CAA-CBA
20	B	1210	CLA	C1A-C2A-CAA-CBA
20	B	1213	CLA	C1A-C2A-CAA-CBA
20	B	1218	CLA	C1A-C2A-CAA-CBA
20	K	1403	CLA	C1A-C2A-CAA-CBA
20	3	603	CLA	C1A-C2A-CAA-CBA
20	4	607	CLA	C1A-C2A-CAA-CBA
20	6	609	CLA	C1A-C2A-CAA-CBA
20	6	605	CLA	C1A-C2A-CAA-CBA
37	5	611	CHL	C1A-C2A-CAA-CBA
26	8	805	LMT	C7-C8-C9-C10
20	A	1112	CLA	C11-C10-C8-C7
20	A	1118	CLA	C6-C7-C8-C10
20	A	1121	CLA	C11-C10-C8-C7
20	A	1125	CLA	C11-C10-C8-C7
20	A	1138	CLA	C12-C13-C15-C16
20	A	1013	CLA	C11-C10-C8-C7
20	B	1237	CLA	C6-C7-C8-C10
20	B	1215	CLA	C11-C10-C8-C7
20	L	1502	CLA	C11-C12-C13-C15
20	3	606	CLA	C11-C10-C8-C7
20	6	606	CLA	C11-C10-C8-C7
21	B	2002	PQN	C22-C23-C25-C26
37	3	611	CHL	C11-C12-C13-C15
31	B	5003	DGD	C7B-C8B-C9B-CAB
20	A	1130	CLA	C13-C15-C16-C17
20	B	1228	CLA	C13-C15-C16-C17
31	B	5003	DGD	C1B-C2B-C3B-C4B
24	6	801	LHG	C35-C36-C37-C38
20	B	1234	CLA	O1A-CGA-O2A-C1
24	Z	801	LHG	C29-C30-C31-C32
20	A	1115	CLA	C2A-CAA-CBA-CGA
20	5	605	CLA	C2A-CAA-CBA-CGA
20	B	1021	CLA	CBA-CGA-O2A-C1
20	B	1209	CLA	CBA-CGA-O2A-C1
26	B	5005	LMT	C4-C5-C6-C7
30	A	5005	DGA	CBB-CCB-CDB-CEB
38	1	802	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
41	7	805	PLM	C8-C9-CA-CB
20	A	1127	CLA	C8-C10-C11-C12
40	7	802	3PH	C38-C39-C3A-C3B
19	A	1011	CL0	C4-C3-C5-C6
20	5	607	CLA	C5-C6-C7-C8
20	B	1236	CLA	C2-C3-C5-C6
20	A	1135	CLA	C2B-C3B-CAB-CBB
20	A	1139	CLA	C2B-C3B-CAB-CBB
20	A	1101	CLA	C2B-C3B-CAB-CBB
20	B	1213	CLA	C2B-C3B-CAB-CBB
20	1	607	CLA	C2B-C3B-CAB-CBB
20	1	613	CLA	C2B-C3B-CAB-CBB
20	3	601	CLA	C2B-C3B-CAB-CBB
20	7	608	CLA	C2B-C3B-CAB-CBB
20	8	601	CLA	C2B-C3B-CAB-CBB
20	5	615	CLA	C2B-C3B-CAB-CBB
20	5	618	CLA	C2B-C3B-CAB-CBB
20	6	603	CLA	C2B-C3B-CAB-CBB
20	1	608	CLA	C5-C6-C7-C8
29	J	5001	LMG	C30-C31-C32-C33
23	A	4005	BCR	C16-C17-C18-C19
23	B	4003	BCR	C20-C21-C22-C23
23	5	504	BCR	C16-C17-C18-C19
33	F	4001	RRX	C12-C13-C14-C15
20	8	601	CLA	O1D-CGD-O2D-CED
20	B	1208	CLA	CAA-CBA-CGA-O2A
23	A	4003	BCR	C9-C10-C11-C12
23	B	4004	BCR	C9-C10-C11-C12
20	B	1023	CLA	C16-C17-C18-C19
20	3	607	CLA	C11-C12-C13-C15
24	5	801	LHG	C9-C10-C11-C12
20	B	1231	CLA	C8-C10-C11-C12
24	4	801	LHG	C19-C20-C21-C22
20	A	1141	CLA	C4-C3-C5-C6
20	B	1202	CLA	C4-C3-C5-C6
20	L	1502	CLA	C4-C3-C5-C6
20	6	609	CLA	C4-C3-C5-C6
37	3	611	CHL	C4-C3-C5-C6
20	A	1107	CLA	C2-C1-O2A-CGA
20	A	1138	CLA	C2-C1-O2A-CGA
20	1	606	CLA	C2-C1-O2A-CGA
20	A	1104	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1220	CLA	C2-C3-C5-C6
20	6	619	CLA	C2-C3-C5-C6
20	B	1209	CLA	O1A-CGA-O2A-C1
20	B	1220	CLA	C11-C10-C8-C9
20	Z	604	CLA	C14-C13-C15-C16
20	5	607	CLA	C6-C7-C8-C9
20	A	1141	CLA	C3-C5-C6-C7
20	6	615	CLA	C5-C6-C7-C8
20	A	1118	CLA	O1A-CGA-O2A-C1
20	7	615	CLA	CAA-CBA-CGA-O2A
31	B	5003	DGD	O1G-C1A-C2A-C3A
20	A	1113	CLA	C2A-CAA-CBA-CGA
20	A	1121	CLA	C2A-CAA-CBA-CGA
20	A	1138	CLA	CAA-CBA-CGA-O1A
23	A	4001	BCR	C1-C6-C7-C8
23	A	4005	BCR	C23-C24-C25-C30
23	B	4007	BCR	C1-C6-C7-C8
23	B	4007	BCR	C23-C24-C25-C30
23	J	4001	BCR	C1-C6-C7-C8
23	J	4001	BCR	C5-C6-C7-C8
23	8	503	BCR	C23-C24-C25-C30
36	7	501	LUT	C1-C6-C7-C8
36	8	501	LUT	C1-C6-C7-C8
36	6	501	LUT	C1-C6-C7-C8
35	7	804	SPH	C9-C10-C11-C12
20	B	1235	CLA	CAA-CBA-CGA-O2A
20	4	602	CLA	CAA-CBA-CGA-O2A
24	B	5002	LHG	O1-C1-C2-C3
23	B	4004	BCR	C19-C20-C21-C22
24	B	5006	LHG	C11-C10-C9-C8
20	A	1105	CLA	C4-C3-C5-C6
20	A	1117	CLA	C4-C3-C5-C6
20	B	1217	CLA	C4-C3-C5-C6
20	Z	608	CLA	C4-C3-C5-C6
21	B	2002	PQN	C14-C13-C15-C16
23	3	504	BCR	C17-C18-C19-C20
20	1	615	CLA	C2-C3-C5-C6
20	1	608	CLA	CAA-CBA-CGA-O2A
20	7	616	CLA	C3-C5-C6-C7
26	F	5001	LMT	C4-C5-C6-C7
20	3	608	CLA	CAA-CBA-CGA-O2A
20	B	1210	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	8	602	CLA	C16-C17-C18-C19
20	6	607	CLA	C3-C5-C6-C7
39	Z	504	QTB	C09-C10-C11-C12
20	7	604	CLA	C15-C16-C17-C18
20	A	1118	CLA	CBA-CGA-O2A-C1
20	A	1125	CLA	C3-C5-C6-C7
20	1	602	CLA	CAA-CBA-CGA-O2A
20	B	1213	CLA	C4B-C3B-CAB-CBB
20	L	1502	CLA	C4B-C3B-CAB-CBB
20	1	607	CLA	C4B-C3B-CAB-CBB
20	Z	604	CLA	C4B-C3B-CAB-CBB
20	3	601	CLA	C4B-C3B-CAB-CBB
20	8	601	CLA	C4B-C3B-CAB-CBB
20	8	612	CLA	C4B-C3B-CAB-CBB
20	4	612	CLA	C4B-C3B-CAB-CBB
20	5	618	CLA	C4B-C3B-CAB-CBB
24	Z	801	LHG	O6-C4-C5-C6
20	A	1107	CLA	C4-C3-C5-C6
20	B	1208	CLA	C4-C3-C5-C6
35	7	803	SPH	C12-C13-C14-C15
19	A	1011	CL0	C2-C3-C5-C6
20	A	1104	CLA	C11-C10-C8-C7
20	A	1013	CLA	C2-C3-C5-C6
20	B	1204	CLA	C11-C10-C8-C7
20	F	1301	CLA	C11-C12-C13-C15
20	Z	608	CLA	C2-C3-C5-C6
20	6	601	CLA	C6-C7-C8-C10
20	4	609	CLA	C8-C10-C11-C12
20	B	1209	CLA	CAA-CBA-CGA-O1A
20	B	1216	CLA	C16-C17-C18-C20
20	A	1135	CLA	CBA-CGA-O2A-C1
26	B	5005	LMT	C7-C8-C9-C10
20	B	1215	CLA	C10-C11-C12-C13
20	6	605	CLA	C5-C6-C7-C8
20	5	603	CLA	C3-C5-C6-C7
20	6	619	CLA	C3-C5-C6-C7
37	8	613	CHL	CAA-CBA-CGA-O2A
37	4	611	CHL	CAA-CBA-CGA-O2A
40	7	802	3PH	C37-C38-C39-C3A
20	A	1135	CLA	O1A-CGA-O2A-C1
20	1	601	CLA	C16-C17-C18-C19
20	4	605	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	6	605	CLA	C6-C7-C8-C9
20	1	605	CLA	O1D-CGD-O2D-CED
40	5	802	3PH	C1-O11-P-O14
20	B	1241	CLA	CAA-CBA-CGA-O2A
20	7	609	CLA	CAA-CBA-CGA-O2A
20	A	1102	CLA	C4-C3-C5-C6
20	5	612	CLA	C4-C3-C5-C6
37	7	610	CHL	C4-C3-C5-C6
20	3	607	CLA	C8-C10-C11-C12
20	1	602	CLA	CAA-CBA-CGA-O1A
20	A	1110	CLA	C2-C3-C5-C6
20	A	1141	CLA	C2-C3-C5-C6
20	L	1502	CLA	C2-C3-C5-C6
20	7	616	CLA	C2-C3-C5-C6
20	4	603	CLA	C2-C3-C5-C6
20	5	601	CLA	C2-C3-C5-C6
20	6	609	CLA	C2-C3-C5-C6
20	B	1240	CLA	C16-C17-C18-C20
20	K	1403	CLA	CAA-CBA-CGA-O2A
37	Z	609	CHL	CAA-CBA-CGA-O2A
20	B	1208	CLA	C11-C10-C8-C7
19	A	1011	CL0	C11-C10-C8-C9
20	A	1106	CLA	C11-C10-C8-C9
20	A	1108	CLA	C14-C13-C15-C16
20	A	1112	CLA	C11-C10-C8-C9
20	A	1133	CLA	C14-C13-C15-C16
20	B	1209	CLA	C14-C13-C15-C16
20	B	1213	CLA	C11-C12-C13-C14
20	B	1238	CLA	C11-C10-C8-C9
20	B	1241	CLA	C6-C7-C8-C9
20	L	1502	CLA	C11-C12-C13-C14
20	Z	604	CLA	C11-C12-C13-C14
20	7	601	CLA	C6-C7-C8-C9
20	5	609	CLA	C11-C10-C8-C9
20	6	601	CLA	C6-C7-C8-C9
20	6	606	CLA	C11-C10-C8-C9
21	B	2002	PQN	C24-C23-C25-C26
20	1	601	CLA	C3-C5-C6-C7
20	A	1133	CLA	C3A-C2A-CAA-CBA
20	3	601	CLA	C3A-C2A-CAA-CBA
20	3	618	CLA	C3A-C2A-CAA-CBA
20	6	609	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
37	4	611	CHL	C3A-C2A-CAA-CBA
37	5	611	CHL	C3A-C2A-CAA-CBA
20	A	1121	CLA	CAA-CBA-CGA-O2A
20	8	611	CLA	CAA-CBA-CGA-O2A
20	B	1212	CLA	CAD-CBD-CGD-O2D
20	1	602	CLA	CAD-CBD-CGD-O2D
20	1	604	CLA	CAD-CBD-CGD-O2D
20	A	1013	CLA	C16-C17-C18-C20
20	7	609	CLA	C16-C17-C18-C20
20	B	1225	CLA	C8-C10-C11-C12
23	6	504	BCR	C15-C16-C17-C18
20	B	1222	CLA	C2-C1-O2A-CGA
20	Z	603	CLA	C2-C1-O2A-CGA
20	A	1134	CLA	CAA-CBA-CGA-O2A
20	3	610	CLA	CAA-CBA-CGA-O2A
24	Z	801	LHG	O7-C7-C8-C9
25	A	5004	NKP	OAJ-CAK-CAL-CAM
20	A	1120	CLA	C4-C3-C5-C6
20	B	1226	CLA	C4-C3-C5-C6
20	1	612	CLA	C4-C3-C5-C6
20	1	615	CLA	C4-C3-C5-C6
20	5	609	CLA	C4-C3-C5-C6
20	3	608	CLA	CAA-CBA-CGA-O1A
20	A	1102	CLA	C2-C3-C5-C6
20	B	1202	CLA	C2-C3-C5-C6
20	A	1108	CLA	CAA-CBA-CGA-O2A
20	A	1112	CLA	CAA-CBA-CGA-O2A
20	3	607	CLA	CAA-CBA-CGA-O2A
20	4	605	CLA	CAA-CBA-CGA-O2A
26	A	5006	LMT	C5'-C4'-O1B-C1B
23	A	4001	BCR	C11-C12-C13-C14
23	A	4001	BCR	C17-C18-C19-C20
23	A	4004	BCR	C17-C18-C19-C20
23	B	4004	BCR	C7-C8-C9-C10
23	K	4001	BCR	C17-C18-C19-C20
23	3	506	BCR	C11-C12-C13-C14
23	4	503	BCR	C11-C12-C13-C14
36	1	501	LUT	C27-C28-C29-C30
24	Z	801	LHG	C26-C27-C28-C29
20	7	606	CLA	C5-C6-C7-C8
20	A	1128	CLA	CAA-CBA-CGA-O2A
20	A	1135	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	4	609	CLA	CAA-CBA-CGA-O2A
24	7	801	LHG	O8-C23-C24-C25
20	B	1205	CLA	CAA-CBA-CGA-O1A
20	1	605	CLA	CBD-CGD-O2D-CED
20	B	1214	CLA	O2A-C1-C2-C3
37	7	610	CHL	O2A-C1-C2-C3
20	Z	603	CLA	C2A-CAA-CBA-CGA
20	1	603	CLA	CAA-CBA-CGA-O2A
38	1	802	SQD	O48-C23-C24-C25
20	B	1221	CLA	CAA-CBA-CGA-O1A
19	A	1011	CL0	CBD-CGD-O2D-CED
20	A	1102	CLA	CHA-CBD-CGD-O1D
20	A	1102	CLA	CHA-CBD-CGD-O2D
20	A	1104	CLA	CHA-CBD-CGD-O1D
20	A	1119	CLA	CHA-CBD-CGD-O1D
20	A	1119	CLA	CHA-CBD-CGD-O2D
20	A	1120	CLA	CHA-CBD-CGD-O2D
20	A	1125	CLA	CHA-CBD-CGD-O1D
20	A	1125	CLA	CHA-CBD-CGD-O2D
20	A	1127	CLA	CHA-CBD-CGD-O1D
20	A	1127	CLA	CHA-CBD-CGD-O2D
20	A	1128	CLA	CHA-CBD-CGD-O1D
20	A	1128	CLA	CHA-CBD-CGD-O2D
20	A	1135	CLA	CHA-CBD-CGD-O1D
20	A	1135	CLA	CHA-CBD-CGD-O2D
20	A	1013	CLA	CHA-CBD-CGD-O1D
20	B	1022	CLA	CHA-CBD-CGD-O1D
20	B	1022	CLA	CHA-CBD-CGD-O2D
20	B	1201	CLA	CHA-CBD-CGD-O1D
20	B	1201	CLA	CHA-CBD-CGD-O2D
20	B	1228	CLA	CHA-CBD-CGD-O1D
20	B	1235	CLA	CHA-CBD-CGD-O1D
20	B	1235	CLA	CHA-CBD-CGD-O2D
20	B	1241	CLA	CHA-CBD-CGD-O1D
20	B	1241	CLA	CHA-CBD-CGD-O2D
20	K	1403	CLA	CHA-CBD-CGD-O1D
20	K	1403	CLA	CHA-CBD-CGD-O2D
20	1	601	CLA	CHA-CBD-CGD-O1D
20	1	601	CLA	CHA-CBD-CGD-O2D
20	Z	603	CLA	CHA-CBD-CGD-O1D
20	Z	603	CLA	CHA-CBD-CGD-O2D
20	Z	606	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	Z	612	CLA	CHA-CBD-CGD-O1D
20	Z	612	CLA	CHA-CBD-CGD-O2D
20	3	605	CLA	CHA-CBD-CGD-O1D
20	3	605	CLA	CHA-CBD-CGD-O2D
20	3	607	CLA	CHA-CBD-CGD-O2D
20	7	603	CLA	CHA-CBD-CGD-O2D
20	7	604	CLA	CHA-CBD-CGD-O2D
20	7	606	CLA	CHA-CBD-CGD-O1D
20	7	606	CLA	CHA-CBD-CGD-O2D
20	7	611	CLA	CHA-CBD-CGD-O1D
20	7	611	CLA	CHA-CBD-CGD-O2D
20	7	613	CLA	CHA-CBD-CGD-O1D
20	7	613	CLA	CHA-CBD-CGD-O2D
20	7	615	CLA	CHA-CBD-CGD-O1D
20	7	615	CLA	CHA-CBD-CGD-O2D
20	8	604	CLA	CHA-CBD-CGD-O2D
20	8	612	CLA	CHA-CBD-CGD-O2D
20	4	603	CLA	CHA-CBD-CGD-O2D
20	4	606	CLA	CHA-CBD-CGD-O2D
20	5	601	CLA	CHA-CBD-CGD-O2D
20	5	604	CLA	CHA-CBD-CGD-O1D
20	5	604	CLA	CHA-CBD-CGD-O2D
20	5	613	CLA	CHA-CBD-CGD-O1D
20	5	613	CLA	CHA-CBD-CGD-O2D
20	5	618	CLA	CHA-CBD-CGD-O1D
20	5	618	CLA	CHA-CBD-CGD-O2D
20	6	604	CLA	CHA-CBD-CGD-O1D
20	6	604	CLA	CHA-CBD-CGD-O2D
20	6	605	CLA	CHA-CBD-CGD-O1D
20	6	605	CLA	CHA-CBD-CGD-O2D
37	1	610	CHL	CHA-CBD-CGD-O2D
37	3	611	CHL	CHA-CBD-CGD-O1D
37	3	611	CHL	CHA-CBD-CGD-O2D
37	5	610	CHL	CHA-CBD-CGD-O1D
37	5	610	CHL	CHA-CBD-CGD-O2D
37	5	617	CHL	CHA-CBD-CGD-O1D
37	5	617	CHL	CHA-CBD-CGD-O2D
37	6	610	CHL	CHA-CBD-CGD-O1D
37	6	610	CHL	CHA-CBD-CGD-O2D
20	A	1104	CLA	CAA-CBA-CGA-O2A
20	A	1113	CLA	CAA-CBA-CGA-O2A
20	B	1216	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	L	1502	CLA	CAA-CBA-CGA-O2A
20	1	613	CLA	CAA-CBA-CGA-O2A
21	B	2002	PQN	C12-C13-C15-C16
20	A	1130	CLA	C16-C17-C18-C19
20	A	1126	CLA	C10-C11-C12-C13
20	6	615	CLA	CAA-CBA-CGA-O2A
24	1	801	LHG	O8-C23-C24-C25
37	6	611	CHL	CAA-CBA-CGA-O2A
24	A	5002	LHG	C11-C10-C9-C8
29	J	5001	LMG	O7-C8-C9-O8
26	4	803	LMT	C3-C4-C5-C6
20	A	1012	CLA	C15-C16-C17-C18
20	B	1228	CLA	C10-C11-C12-C13
20	B	1202	CLA	CAA-CBA-CGA-O2A
24	8	801	LHG	O7-C7-C8-C9
29	J	5001	LMG	O7-C10-C11-C12
20	A	1137	CLA	CAA-CBA-CGA-O2A
20	A	1141	CLA	CAA-CBA-CGA-O2A
20	B	1206	CLA	CAA-CBA-CGA-O2A
20	Z	603	CLA	CAA-CBA-CGA-O2A
27	A	5008	OCA	O1-C1-C2-C3
20	5	602	CLA	C4-C3-C5-C6
20	7	609	CLA	C15-C16-C17-C18
20	A	1104	CLA	C11-C12-C13-C15
20	A	1120	CLA	C2-C3-C5-C6
20	A	1140	CLA	C12-C13-C15-C16
20	B	1202	CLA	C11-C10-C8-C7
21	A	2001	PQN	C21-C22-C23-C25
26	B	5005	LMT	C2-C3-C4-C5
20	A	1110	CLA	C11-C12-C13-C14
20	A	1118	CLA	C6-C7-C8-C9
20	A	1121	CLA	C6-C7-C8-C9
20	A	1125	CLA	C11-C10-C8-C9
20	A	1132	CLA	C11-C10-C8-C9
20	A	1138	CLA	C14-C13-C15-C16
20	A	1013	CLA	C11-C10-C8-C9
20	B	1237	CLA	C6-C7-C8-C9
20	B	1202	CLA	C6-C7-C8-C9
20	B	1202	CLA	C11-C10-C8-C9
20	3	606	CLA	C11-C10-C8-C9
21	A	2001	PQN	C21-C22-C23-C24
21	B	2002	PQN	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
20	A	1122	CLA	O1D-CGD-O2D-CED
20	A	1112	CLA	CAA-CBA-CGA-O1A
20	B	1241	CLA	CAA-CBA-CGA-O1A
20	Z	604	CLA	C2B-C3B-CAB-CBB
20	4	612	CLA	C2B-C3B-CAB-CBB
37	8	610	CHL	C2B-C3B-CAB-CBB
37	4	610	CHL	C2B-C3B-CAB-CBB
37	4	611	CHL	C2B-C3B-CAB-CBB
37	5	611	CHL	C2B-C3B-CAB-CBB
37	6	610	CHL	C2B-C3B-CAB-CBB
37	6	611	CHL	C2B-C3B-CAB-CBB
37	6	613	CHL	C2B-C3B-CAB-CBB
20	A	1131	CLA	CAA-CBA-CGA-O2A
20	B	1237	CLA	CAA-CBA-CGA-O2A
20	1	605	CLA	CAA-CBA-CGA-O2A
38	1	802	SQD	C5-C6-S-O8
20	A	1116	CLA	C2A-CAA-CBA-CGA
20	Z	604	CLA	C2A-CAA-CBA-CGA
20	B	1208	CLA	C11-C10-C8-C9
20	B	1021	CLA	CAA-CBA-CGA-O2A
20	B	1207	CLA	CAA-CBA-CGA-O2A
35	7	803	SPH	C5-C6-C7-C8
20	4	605	CLA	CAA-CBA-CGA-O1A
37	4	611	CHL	CAA-CBA-CGA-O1A
20	B	1023	CLA	C16-C17-C18-C20
20	B	1210	CLA	C16-C17-C18-C20
37	3	611	CHL	C2-C3-C5-C6
20	A	1108	CLA	CAA-CBA-CGA-O1A
23	B	4005	BCR	C7-C8-C9-C10
35	7	803	SPH	C11-C12-C13-C14
20	A	1115	CLA	C1A-C2A-CAA-CBA
20	Z	615	CLA	C1A-C2A-CAA-CBA
20	3	607	CLA	C1A-C2A-CAA-CBA
20	7	616	CLA	C1A-C2A-CAA-CBA
20	5	622	CLA	C1A-C2A-CAA-CBA
20	6	603	CLA	C1A-C2A-CAA-CBA
24	A	5001	LHG	C24-C25-C26-C27
20	A	1128	CLA	CAA-CBA-CGA-O1A
20	A	1131	CLA	C10-C11-C12-C13
20	3	610	CLA	CAA-CBA-CGA-O1A
20	7	609	CLA	CAA-CBA-CGA-O1A
20	7	605	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	6	801	LHG	O8-C23-C24-C25
41	7	805	PLM	C3-C4-C5-C6
20	A	1123	CLA	C8-C10-C11-C12
20	A	1138	CLA	C2A-CAA-CBA-CGA
20	K	1402	CLA	C2A-CAA-CBA-CGA
20	A	1134	CLA	CAA-CBA-CGA-O1A
20	L	1502	CLA	CAA-CBA-CGA-O1A
20	1	613	CLA	CAA-CBA-CGA-O1A
37	8	613	CHL	CAA-CBA-CGA-O1A
37	6	611	CHL	CAA-CBA-CGA-O1A
20	5	606	CLA	CAA-CBA-CGA-O2A
20	6	601	CLA	CAA-CBA-CGA-O2A
20	6	604	CLA	C5-C6-C7-C8
24	A	5001	LHG	C16-C17-C18-C19
20	A	1113	CLA	CAA-CBA-CGA-O1A
20	B	1237	CLA	CAA-CBA-CGA-O1A
20	B	1207	CLA	CAA-CBA-CGA-O1A
25	A	5004	NKP	OAE-CAK-CAL-CAM
37	Z	609	CHL	CAA-CBA-CGA-O1A
20	B	1215	CLA	C2-C3-C5-C6
20	B	1234	CLA	C10-C11-C12-C13
20	B	1217	CLA	C4B-C3B-CAB-CBB
20	B	1230	CLA	C4B-C3B-CAB-CBB
20	6	602	CLA	C4B-C3B-CAB-CBB
24	B	5006	LHG	C3-O3-P-O5
24	1	801	LHG	C3-O3-P-O4
24	3	801	LHG	C4-O6-P-O5
24	8	801	LHG	C3-O3-P-O5
24	4	801	LHG	C4-O6-P-O5
20	4	609	CLA	C11-C12-C13-C15
24	Z	801	LHG	C31-C32-C33-C34
20	B	1216	CLA	CAA-CBA-CGA-O1A
20	K	1403	CLA	CAA-CBA-CGA-O1A
20	1	603	CLA	CAA-CBA-CGA-O1A
38	1	802	SQD	O10-C23-C24-C25
20	B	1211	CLA	CAA-CBA-CGA-O2A
20	B	1223	CLA	CAA-CBA-CGA-O2A
20	B	1236	CLA	CAA-CBA-CGA-O2A
20	L	1503	CLA	CAA-CBA-CGA-O2A
20	5	612	CLA	CAA-CBA-CGA-O2A
20	3	607	CLA	C5-C6-C7-C8
23	A	4001	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	1	503	C7Z	C5-C6-C7-C8
20	B	1210	CLA	C15-C16-C17-C18
20	6	603	CLA	C10-C11-C12-C13
20	A	1121	CLA	CAA-CBA-CGA-O1A
24	Z	801	LHG	O9-C7-C8-C9
24	7	801	LHG	O10-C23-C24-C25
20	A	1125	CLA	CAA-CBA-CGA-O2A
35	7	804	SPH	C11-C12-C13-C14
23	B	4001	BCR	C10-C11-C12-C13
20	A	1108	CLA	C2A-CAA-CBA-CGA
19	A	1011	CL0	O1D-CGD-O2D-CED
20	A	1104	CLA	CAA-CBA-CGA-O1A
20	3	607	CLA	CAA-CBA-CGA-O1A
20	4	609	CLA	CAA-CBA-CGA-O1A
20	1	606	CLA	C2-C3-C5-C6
40	6	802	3PH	C23-C24-C25-C26
20	A	1118	CLA	CAD-CBD-CGD-O1D
20	A	1128	CLA	CAD-CBD-CGD-O1D
20	B	1211	CLA	CAD-CBD-CGD-O1D
20	B	1214	CLA	CAD-CBD-CGD-O1D
20	B	1234	CLA	CAD-CBD-CGD-O1D
20	K	1402	CLA	CAD-CBD-CGD-O1D
20	K	1404	CLA	CAD-CBD-CGD-O1D
20	Z	605	CLA	CAD-CBD-CGD-O1D
20	7	606	CLA	CAD-CBD-CGD-O1D
20	8	604	CLA	CAD-CBD-CGD-O1D
20	8	611	CLA	CAD-CBD-CGD-O1D
20	4	604	CLA	CAD-CBD-CGD-O1D
20	5	601	CLA	CAD-CBD-CGD-O1D
37	3	611	CHL	CAD-CBD-CGD-O1D
37	8	613	CHL	CAD-CBD-CGD-O1D
37	5	617	CHL	CAD-CBD-CGD-O1D
37	6	610	CHL	CAD-CBD-CGD-O1D
37	6	611	CHL	CAD-CBD-CGD-O1D
20	A	1135	CLA	CAA-CBA-CGA-O1A
20	B	1202	CLA	CAA-CBA-CGA-O1A
24	1	801	LHG	O10-C23-C24-C25
20	5	605	CLA	CAA-CBA-CGA-O2A
20	A	1104	CLA	C11-C12-C13-C14
20	A	1121	CLA	C11-C12-C13-C14
20	A	1140	CLA	C14-C13-C15-C16
20	B	1237	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	1204	CLA	C11-C10-C8-C9
20	8	609	CLA	C14-C13-C15-C16
21	A	2001	PQN	C24-C23-C25-C26
26	B	6101	LMT	C3'-C4'-O1B-C1B
27	A	5008	OCA	O2-C1-C2-C3
20	1	608	CLA	C10-C11-C12-C13
40	7	802	3PH	C36-C37-C38-C39
20	B	1239	CLA	CAA-CBA-CGA-O2A
20	8	609	CLA	CAA-CBA-CGA-O2A
37	6	610	CHL	CAA-CBA-CGA-O2A
19	A	1011	CL0	C15-C16-C17-C18
20	B	1221	CLA	C15-C16-C17-C18
20	A	1131	CLA	CAA-CBA-CGA-O1A
20	A	1137	CLA	C15-C16-C17-C18
20	B	1205	CLA	C2A-CAA-CBA-CGA
20	F	1301	CLA	C2A-CAA-CBA-CGA
20	L	1502	CLA	C2A-CAA-CBA-CGA
24	1	801	LHG	C28-C29-C30-C31
20	B	1210	CLA	CAA-CBA-CGA-O2A
20	B	1219	CLA	CAA-CBA-CGA-O2A
20	Z	608	CLA	CAA-CBA-CGA-O2A
20	3	618	CLA	CAA-CBA-CGA-O2A
20	7	612	CLA	CAA-CBA-CGA-O2A
20	5	607	CLA	CAA-CBA-CGA-O2A
20	6	608	CLA	CAA-CBA-CGA-O2A
20	6	606	CLA	CAA-CBA-CGA-O2A
24	4	801	LHG	O8-C23-C24-C25
29	J	5001	LMG	O8-C28-C29-C30
20	A	1118	CLA	C5-C6-C7-C8
20	7	607	CLA	C10-C11-C12-C13
20	4	603	CLA	C15-C16-C17-C18
20	F	1302	CLA	CAA-CBA-CGA-O2A
20	5	608	CLA	CAA-CBA-CGA-O2A
20	B	1206	CLA	CAA-CBA-CGA-O1A
20	B	1239	CLA	CAA-CBA-CGA-O1A
20	B	1216	CLA	C4-C3-C5-C6
20	A	1111	CLA	C11-C10-C8-C7
20	B	1209	CLA	C6-C7-C8-C10
20	B	1217	CLA	C2-C3-C5-C6
20	B	1218	CLA	C12-C13-C15-C16
20	B	1236	CLA	C12-C13-C15-C16
20	B	1239	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	1241	CLA	C12-C13-C15-C16
20	F	1301	CLA	C3A-C2A-CAA-CBA
20	Z	612	CLA	C6-C7-C8-C10
20	3	605	CLA	C6-C7-C8-C10
20	7	609	CLA	C11-C10-C8-C7
20	8	609	CLA	C12-C13-C15-C16
20	5	618	CLA	C11-C12-C13-C15
20	A	1141	CLA	CAA-CBA-CGA-O1A
20	Z	603	CLA	CAA-CBA-CGA-O1A
20	5	605	CLA	CAA-CBA-CGA-O1A
24	8	801	LHG	O9-C7-C8-C9
38	1	802	SQD	C11-C10-C9-C8
20	B	1220	CLA	CAA-CBA-CGA-O2A
20	B	1234	CLA	CAA-CBA-CGA-O2A
20	4	608	CLA	CAA-CBA-CGA-O2A
24	5	801	LHG	O7-C7-C8-C9
40	8	806	3PH	O21-C21-C22-C23
23	A	4002	BCR	C17-C18-C19-C20
23	B	4002	BCR	C17-C18-C19-C20
23	B	4003	BCR	C21-C22-C23-C24
20	B	1210	CLA	CAA-CBA-CGA-O1A
20	8	609	CLA	CAA-CBA-CGA-O1A
20	5	606	CLA	CAA-CBA-CGA-O1A
29	J	5001	LMG	O9-C10-C11-C12
23	B	4007	BCR	C15-C16-C17-C18
23	G	4001	BCR	C19-C20-C21-C22
23	7	503	BCR	C13-C14-C15-C16
23	4	503	BCR	C13-C14-C15-C16
25	A	5004	NKP	CAL-CAM-CAN-CAO
20	6	605	CLA	C6-C7-C8-C10
20	B	1204	CLA	CAA-CBA-CGA-O2A
20	G	1601	CLA	CAA-CBA-CGA-O2A
20	B	1234	CLA	C5-C6-C7-C8
20	B	1240	CLA	C13-C15-C16-C17
21	A	2001	PQN	C23-C25-C26-C27
20	A	1125	CLA	CAA-CBA-CGA-O1A
20	B	1021	CLA	CAA-CBA-CGA-O1A
20	6	606	CLA	CAA-CBA-CGA-O1A
20	6	615	CLA	CAA-CBA-CGA-O1A
24	4	801	LHG	O10-C23-C24-C25
37	6	610	CHL	CAA-CBA-CGA-O1A
20	8	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1112	CLA	C8-C10-C11-C12
20	B	1237	CLA	C8-C10-C11-C12
20	Z	607	CLA	CAA-CBA-CGA-O2A
24	A	5001	LHG	O8-C23-C24-C25
24	A	5002	LHG	O8-C23-C24-C25
20	A	1108	CLA	C8-C10-C11-C12
20	1	605	CLA	CAA-CBA-CGA-O1A
20	3	618	CLA	CAA-CBA-CGA-O1A
20	7	605	CLA	CAA-CBA-CGA-O1A
20	B	1220	CLA	C2A-CAA-CBA-CGA
37	Z	609	CHL	C2A-CAA-CBA-CGA
20	A	1136	CLA	C15-C16-C17-C18
24	1	801	LHG	C16-C17-C18-C19
20	B	1219	CLA	CAA-CBA-CGA-O1A
20	B	1234	CLA	CAA-CBA-CGA-O1A
20	5	607	CLA	CAA-CBA-CGA-O1A
24	6	801	LHG	O10-C23-C24-C25
30	A	5005	DGA	CB3-CB4-CB5-CB6
20	6	605	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

264 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	7	609	CLA	1	0
23	6	504	BCR	2	0
24	7	801	LHG	2	0
20	6	609	CLA	9	0
36	5	501	LUT	3	0
20	8	606	CLA	1	0
36	6	502	LUT	1	0
20	1	605	CLA	2	0
26	A	5006	LMT	2	0
23	B	4003	BCR	1	0
20	B	1229	CLA	2	0
30	A	5005	DGA	5	0
23	3	506	BCR	2	0
20	3	607	CLA	2	0
23	5	504	BCR	1	0
20	A	1106	CLA	7	0
20	A	1128	CLA	3	0
23	3	503	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	6	801	LHG	4	0
20	A	1116	CLA	5	0
20	5	613	CLA	1	0
20	A	1118	CLA	2	0
20	A	1122	CLA	3	0
20	A	1012	CLA	7	0
20	B	1222	CLA	3	0
37	7	610	CHL	2	0
20	1	601	CLA	5	0
20	A	1113	CLA	4	0
20	1	613	CLA	3	0
20	7	601	CLA	4	0
20	A	1136	CLA	2	0
20	A	1107	CLA	4	0
23	B	4001	BCR	5	0
26	B	6101	LMT	1	0
20	B	1240	CLA	5	0
20	5	606	CLA	1	0
20	5	601	CLA	4	0
20	7	613	CLA	3	0
20	6	605	CLA	2	0
20	B	1221	CLA	4	0
20	1	608	CLA	2	0
20	1	611	CLA	3	0
36	3	501	LUT	6	0
20	4	608	CLA	1	0
36	Z	503	LUT	2	0
20	B	1206	CLA	2	0
20	6	608	CLA	6	0
20	8	608	CLA	1	0
20	B	1212	CLA	1	0
20	1	615	CLA	3	0
20	Z	604	CLA	4	0
20	7	611	CLA	1	0
20	B	1223	CLA	1	0
20	A	1127	CLA	5	0
20	3	604	CLA	3	0
24	8	801	LHG	2	0
20	A	1114	CLA	5	0
37	1	609	CHL	3	0
23	4	503	BCR	1	0
20	3	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	8	607	CLA	5	0
20	A	1111	CLA	6	0
20	B	1023	CLA	4	0
23	8	503	BCR	2	0
20	A	1115	CLA	2	0
20	K	1404	CLA	1	0
19	A	1011	CL0	3	0
37	Z	609	CHL	4	0
35	7	803	SPH	1	0
20	7	602	CLA	1	0
23	G	4001	BCR	3	0
20	4	602	CLA	2	0
20	B	1218	CLA	5	0
20	3	601	CLA	5	0
23	7	503	BCR	2	0
20	6	619	CLA	4	0
20	8	602	CLA	3	0
20	A	1125	CLA	4	0
20	B	1241	CLA	2	0
37	5	617	CHL	1	0
23	5	503	BCR	2	0
20	B	1205	CLA	3	0
20	8	611	CLA	1	0
20	4	601	CLA	5	0
20	A	1102	CLA	1	0
23	B	4005	BCR	2	0
20	1	603	CLA	2	0
24	A	5001	LHG	1	0
20	6	604	CLA	3	0
20	6	603	CLA	3	0
20	7	603	CLA	2	0
20	8	603	CLA	3	0
20	B	1213	CLA	2	0
22	C	3003	SF4	1	0
26	B	5005	LMT	1	0
20	B	1224	CLA	6	0
20	B	1232	CLA	1	0
20	7	604	CLA	1	0
20	B	1217	CLA	1	0
36	6	501	LUT	4	0
26	4	803	LMT	2	0
20	3	612	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	8	605	CLA	2	0
20	A	1138	CLA	3	0
36	Z	501	LUT	1	0
20	A	1126	CLA	12	0
20	4	609	CLA	4	0
20	A	1101	CLA	3	0
20	5	604	CLA	5	0
20	B	1225	CLA	7	0
20	B	1226	CLA	7	0
20	A	1120	CLA	3	0
20	4	604	CLA	3	0
20	5	609	CLA	3	0
20	B	1022	CLA	1	0
25	3	802	NKP	1	0
31	B	5003	DGD	5	0
37	8	610	CHL	1	0
20	B	1215	CLA	3	0
23	A	4002	BCR	4	0
33	F	4001	RRX	4	0
20	F	1302	CLA	5	0
26	1	803	LMT	1	0
36	1	502	LUT	2	0
20	6	601	CLA	6	0
36	4	502	LUT	4	0
20	8	609	CLA	2	0
24	5	801	LHG	1	0
38	1	802	SQD	1	0
37	4	613	CHL	1	0
37	5	610	CHL	5	0
36	7	502	LUT	1	0
20	A	1135	CLA	1	0
37	4	610	CHL	1	0
20	1	607	CLA	1	0
23	B	4007	BCR	1	0
20	Z	606	CLA	2	0
26	8	805	LMT	2	0
23	B	4004	BCR	3	0
20	7	607	CLA	3	0
20	A	1121	CLA	2	0
23	K	4002	BCR	3	0
20	Z	601	CLA	3	0
24	B	5006	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1130	CLA	2	0
21	B	2002	PQN	1	0
23	L	4002	BCR	2	0
23	6	503	BCR	4	0
20	B	1207	CLA	5	0
20	7	612	CLA	1	0
20	5	618	CLA	4	0
20	B	1227	CLA	4	0
20	5	615	CLA	1	0
20	7	615	CLA	5	0
20	B	1230	CLA	3	0
23	L	4001	BCR	4	0
20	Z	608	CLA	2	0
20	Z	611	CLA	1	0
20	6	602	CLA	1	0
36	8	502	LUT	1	0
24	A	5002	LHG	3	0
36	8	501	LUT	4	0
20	Z	615	CLA	2	0
20	K	1401	CLA	5	0
23	I	4001	BCR	2	0
20	B	1235	CLA	6	0
20	B	1239	CLA	3	0
36	3	502	LUT	5	0
20	4	603	CLA	4	0
20	G	1602	CLA	2	0
20	B	1208	CLA	1	0
23	B	4002	BCR	5	0
24	B	5001	LHG	1	0
24	4	802	LHG	1	0
20	A	1119	CLA	4	0
20	1	606	CLA	2	0
20	A	1112	CLA	5	0
20	B	1238	CLA	5	0
20	7	606	CLA	3	0
20	1	604	CLA	3	0
20	6	606	CLA	2	0
20	4	607	CLA	1	0
20	6	615	CLA	4	0
20	7	605	CLA	1	0
20	3	605	CLA	1	0
20	5	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	1	610	CHL	1	0
35	7	804	SPH	2	0
20	8	604	CLA	2	0
20	B	1209	CLA	3	0
36	5	502	LUT	8	0
23	A	4001	BCR	2	0
20	Z	603	CLA	1	0
20	7	608	CLA	1	0
20	4	612	CLA	1	0
23	A	4004	BCR	3	0
20	A	1123	CLA	3	0
20	A	1104	CLA	3	0
37	6	610	CHL	1	0
20	B	1216	CLA	3	0
20	A	1109	CLA	3	0
20	A	1140	CLA	3	0
20	8	612	CLA	1	0
20	8	601	CLA	5	0
37	3	611	CHL	4	0
20	B	1214	CLA	4	0
20	B	1236	CLA	4	0
20	A	1139	CLA	4	0
20	5	605	CLA	1	0
20	A	1129	CLA	2	0
23	B	4006	BCR	4	0
20	Z	605	CLA	5	0
35	K	5001	SPH	2	0
40	7	802	3PH	5	0
23	3	505	BCR	2	0
20	B	1203	CLA	6	0
20	A	1103	CLA	5	0
23	A	4003	BCR	4	0
20	L	1502	CLA	3	0
23	K	4001	BCR	2	0
37	4	617	CHL	1	0
20	A	1110	CLA	3	0
37	Z	610	CHL	3	0
20	A	1132	CLA	2	0
20	B	1234	CLA	3	0
20	B	1204	CLA	1	0
20	F	1301	CLA	4	0
24	4	801	LHG	3	0

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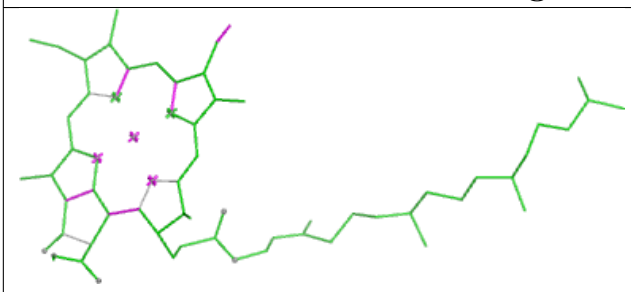
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1117	CLA	4	0
37	5	611	CHL	1	0
20	3	603	CLA	2	0
20	1	612	CLA	3	0
23	7	504	BCR	3	0
20	B	1237	CLA	1	0
20	7	616	CLA	5	0
20	A	1105	CLA	3	0
20	3	606	CLA	2	0
20	A	1013	CLA	7	0
37	6	617	CHL	1	0
20	B	1210	CLA	4	0
20	K	1402	CLA	2	0
20	B	1202	CLA	1	0
20	B	1021	CLA	5	0
36	Z	502	LUT	1	0
37	Z	613	CHL	3	0
36	1	501	LUT	2	0
36	4	501	LUT	5	0
20	5	622	CLA	1	0
20	6	612	CLA	2	0
20	A	1124	CLA	6	0
20	3	613	CLA	3	0
20	A	1137	CLA	2	0
20	3	610	CLA	3	0
37	6	613	CHL	3	0
37	8	613	CHL	4	0
24	1	801	LHG	2	0
20	A	1133	CLA	2	0
20	B	1211	CLA	1	0
23	A	4005	BCR	6	0
23	J	4001	BCR	3	0
20	5	612	CLA	2	0
20	B	1220	CLA	4	0
23	3	504	BCR	3	0
20	5	607	CLA	2	0

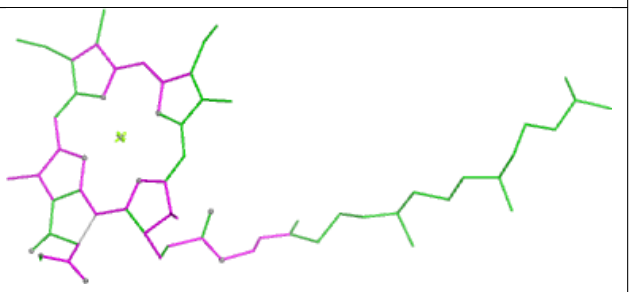
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

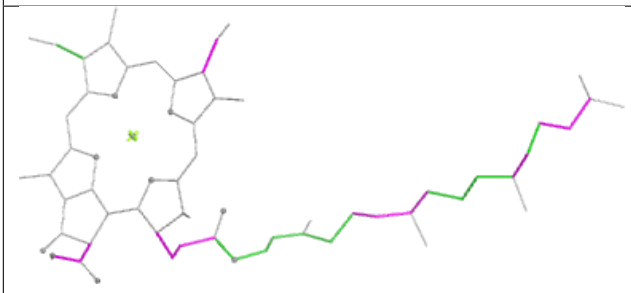
Ligand CLA 7 609



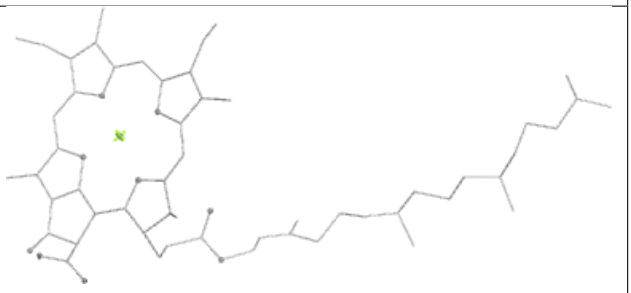
Bond lengths



Bond angles

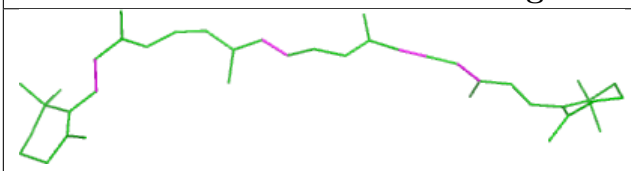


Torsions

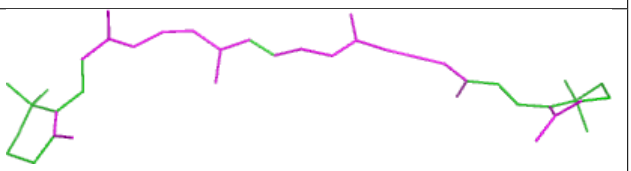


Rings

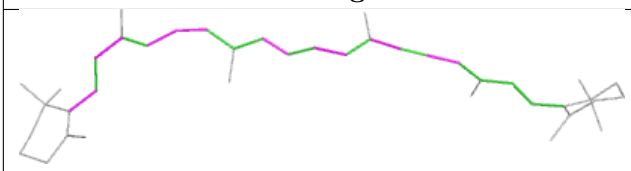
Ligand BCR 6 504



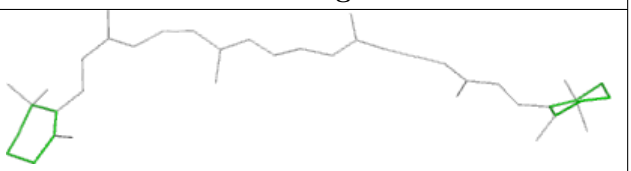
Bond lengths



Bond angles

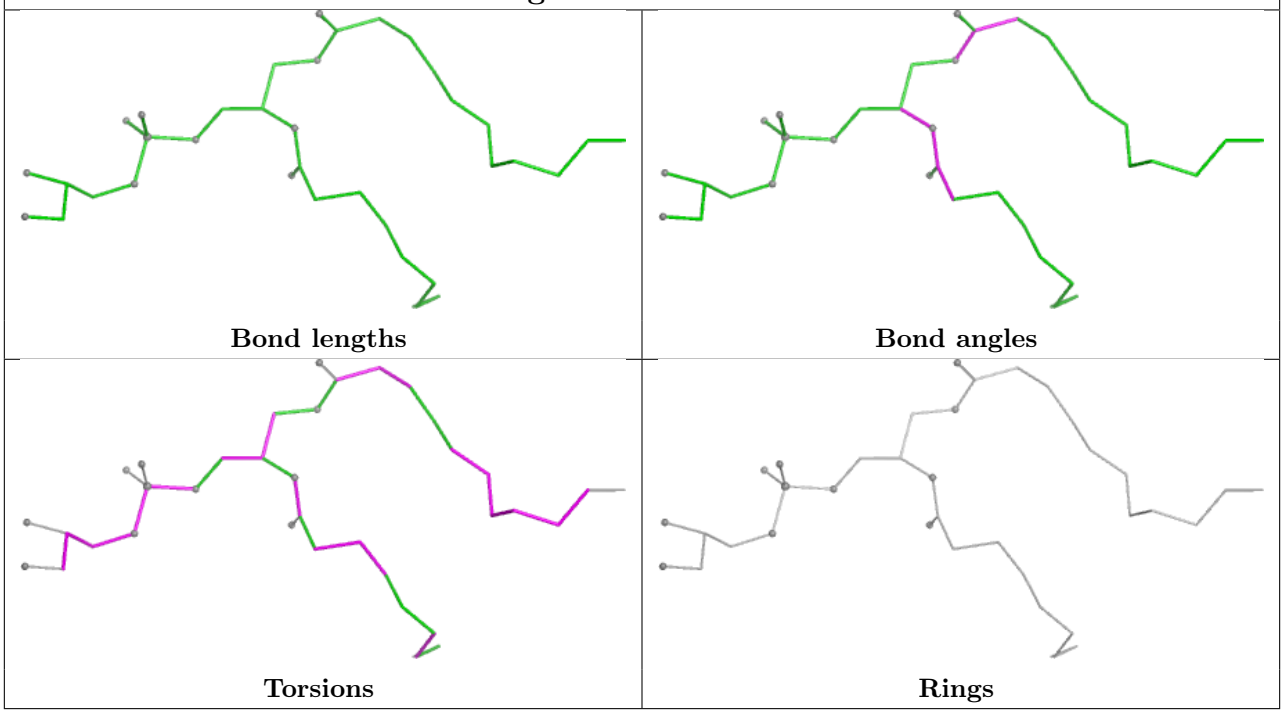


Torsions

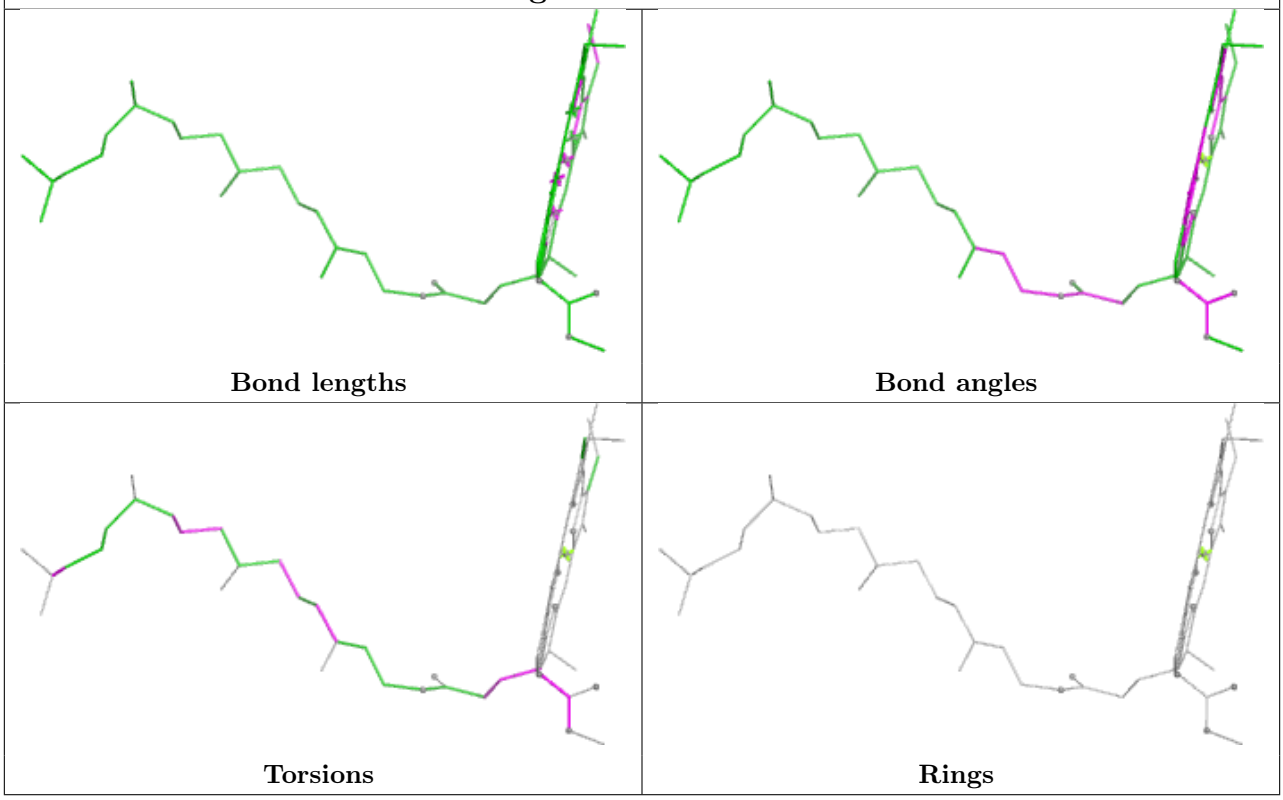


Rings

Ligand LHG 7 801



Ligand CLA 6 609



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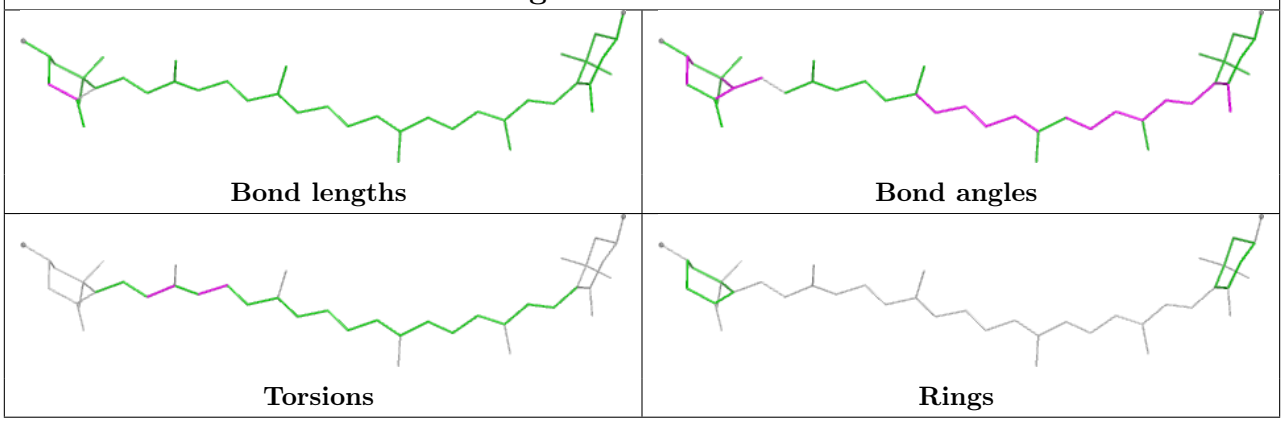
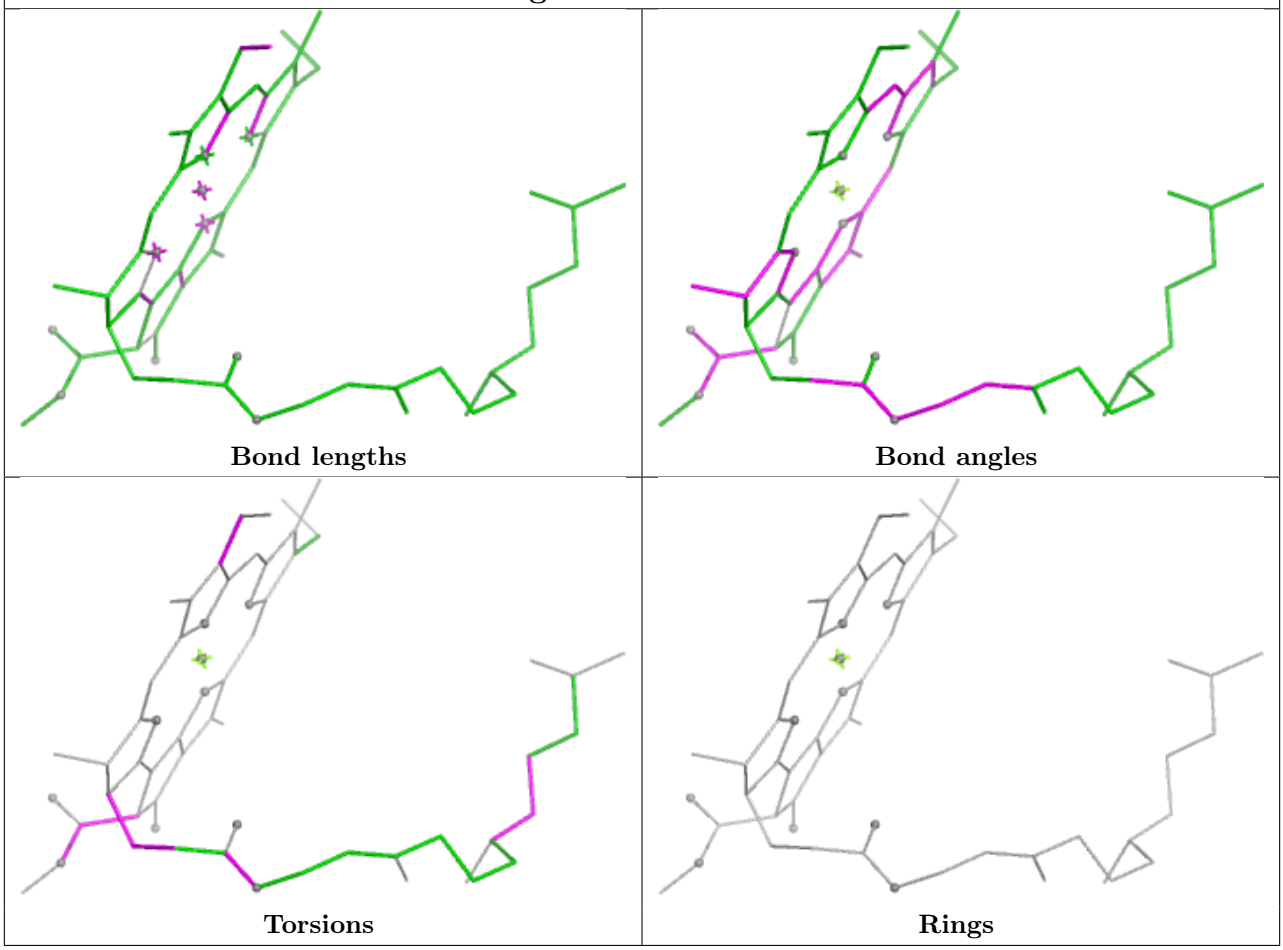


Ligand CLA 8 606



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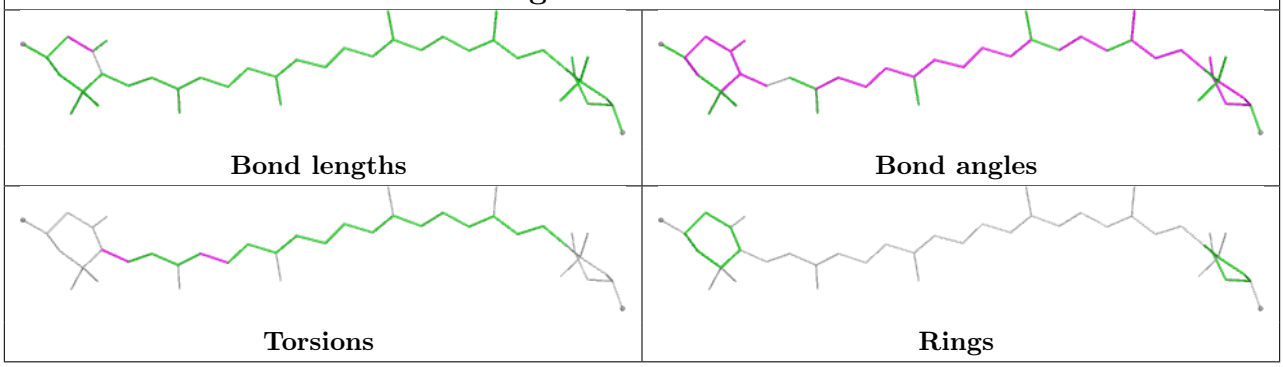
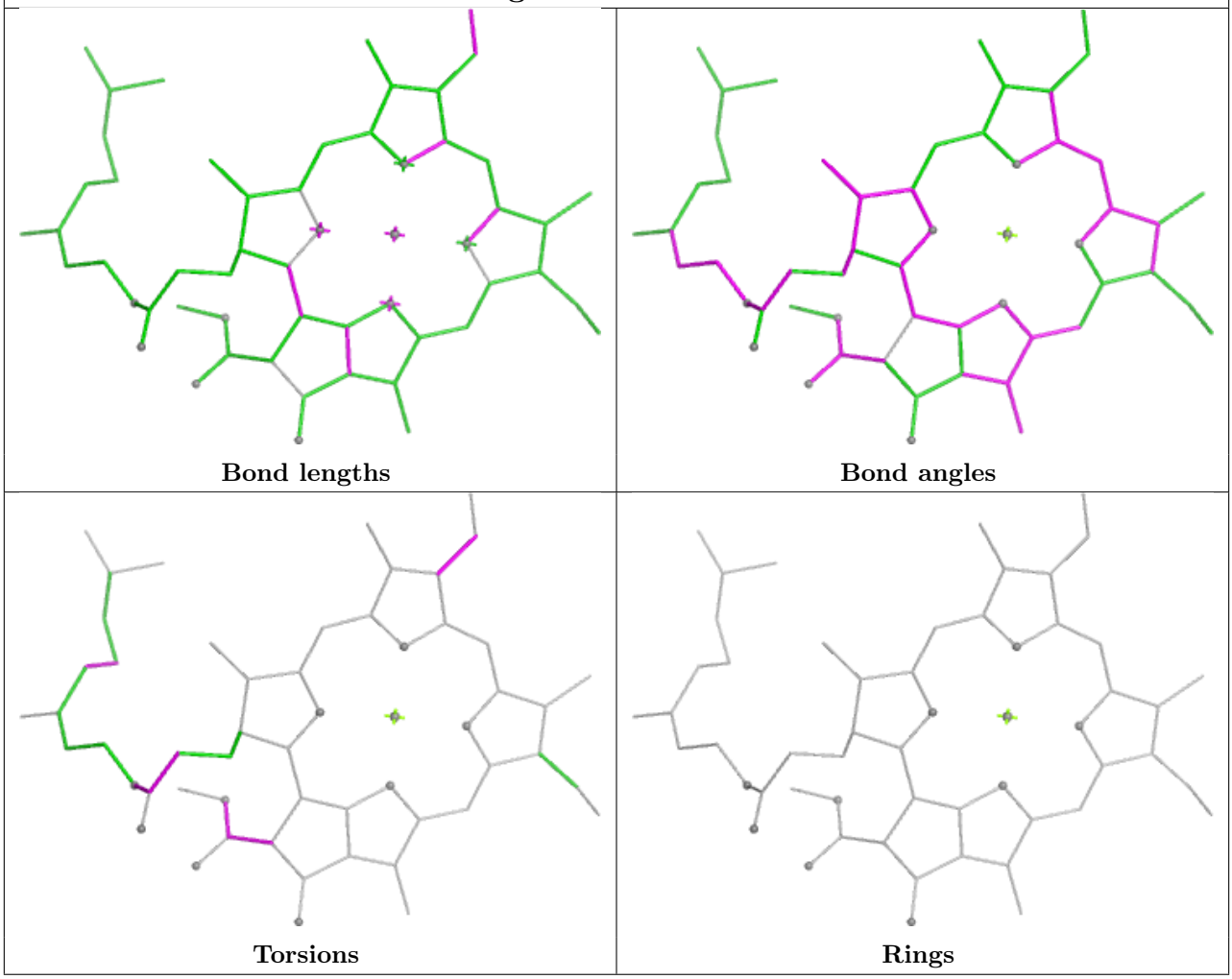
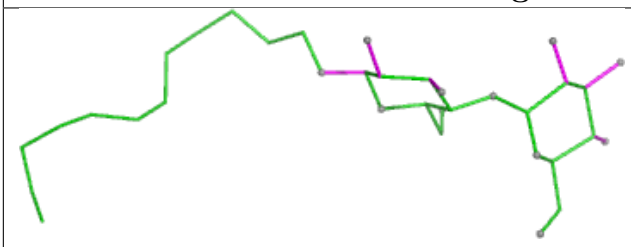
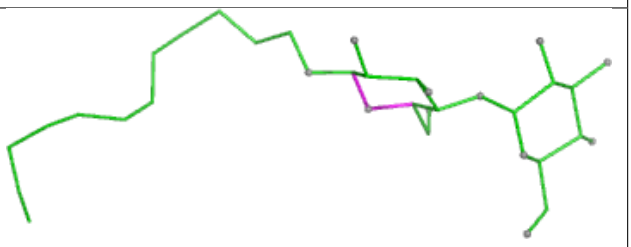
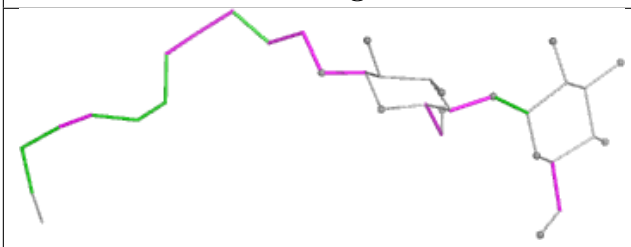
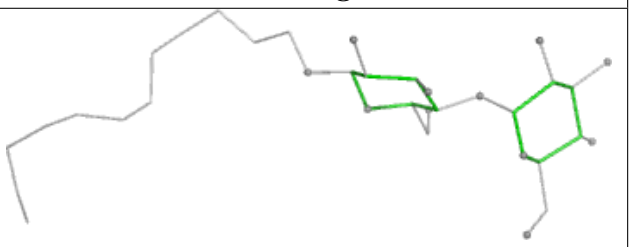
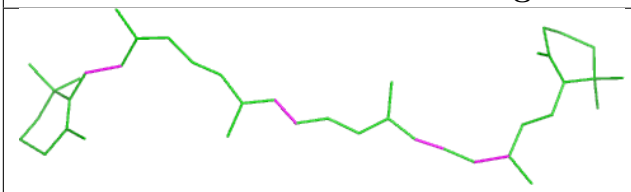
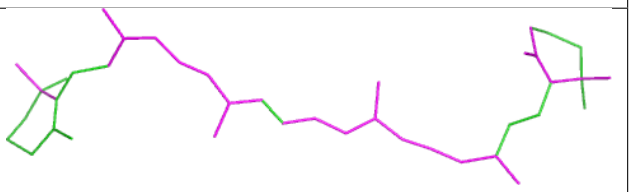
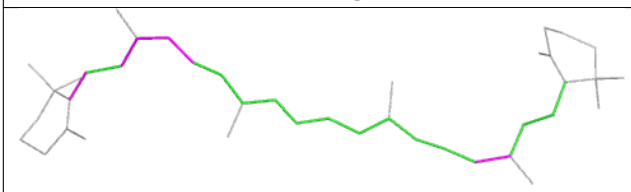
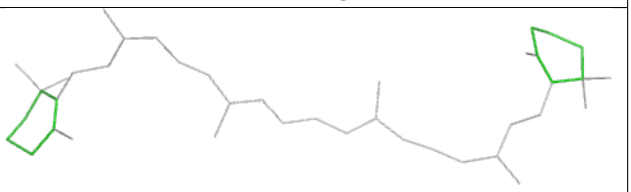


Ligand CLA 1 605



Ligand LMT A 5006	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 4003	
 Bond lengths	 Bond angles
 Torsions	 Rings

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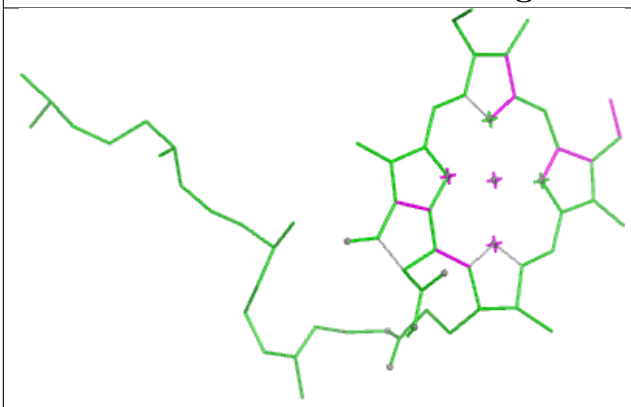
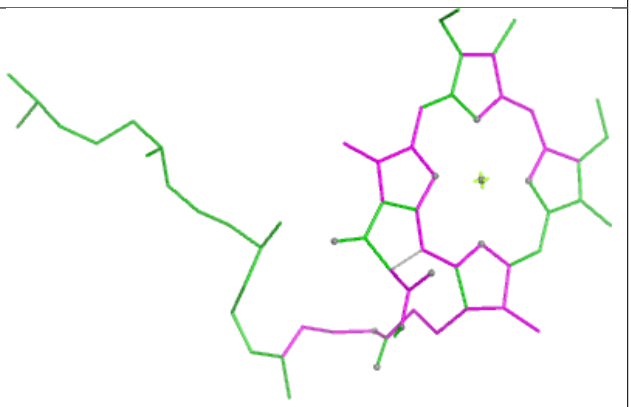
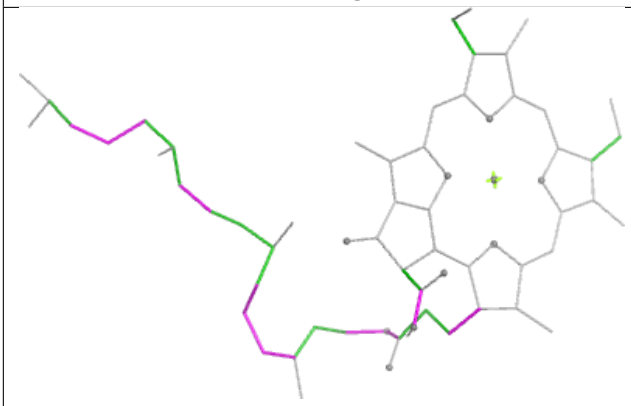
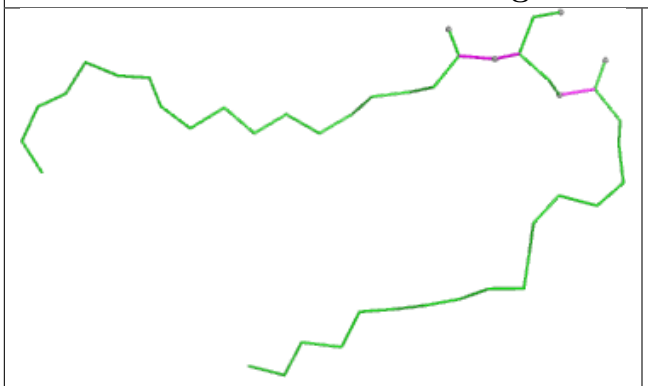
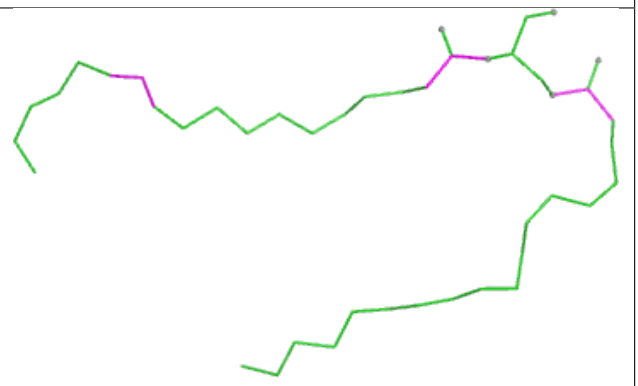
 Bond lengths	 Bond angles
 Torsions	Rings

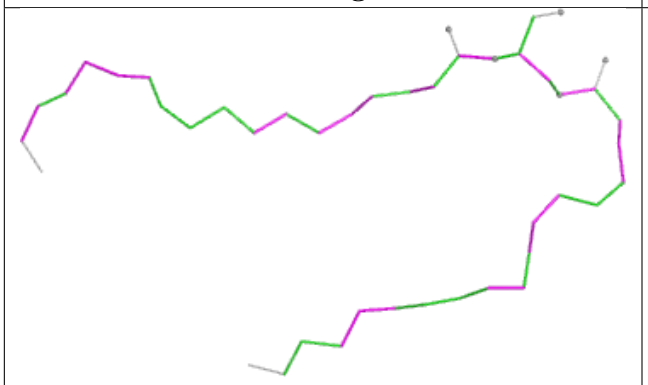
Ligand DGA A 5005



Bond lengths



Bond angles



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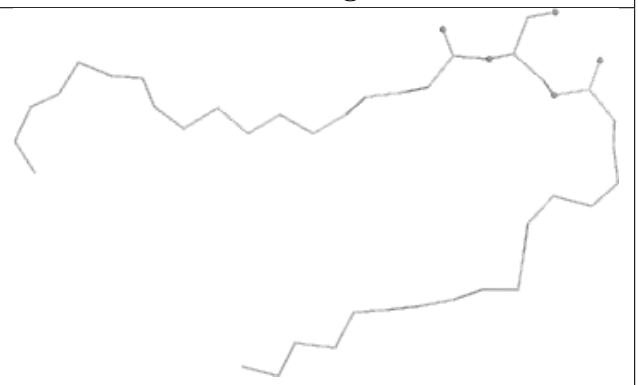
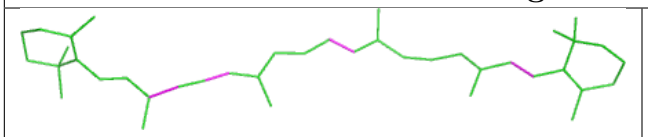


Rings

Ligand BCR 3 506



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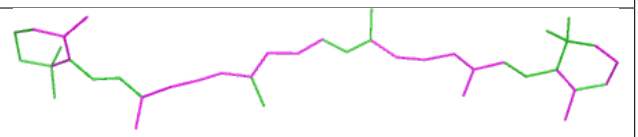

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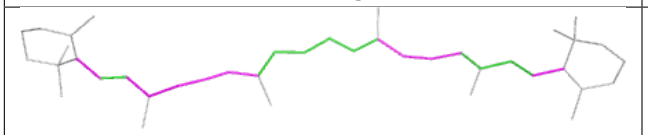

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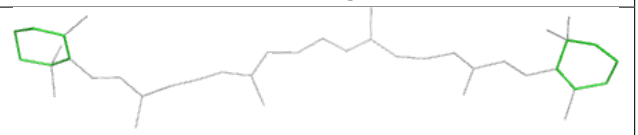
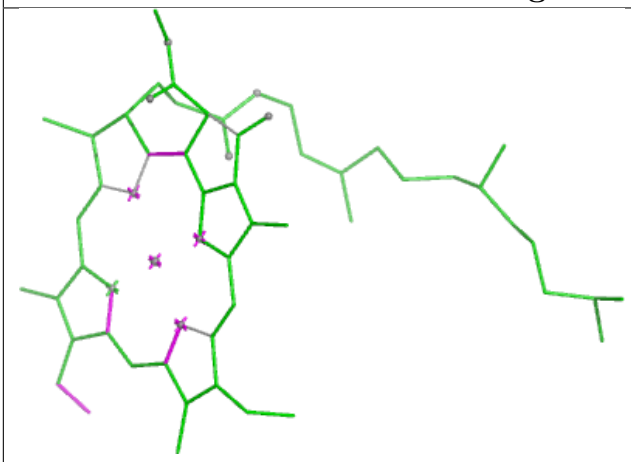


Rings

Ligand CLA 3 607



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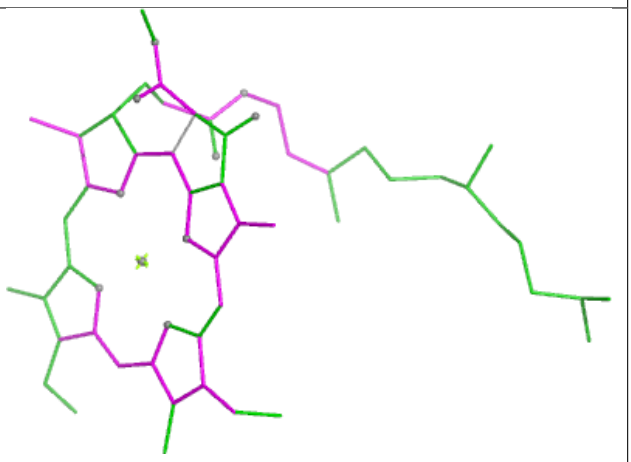
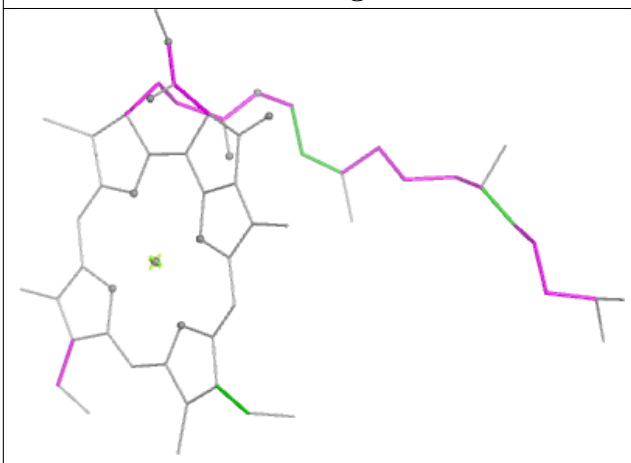


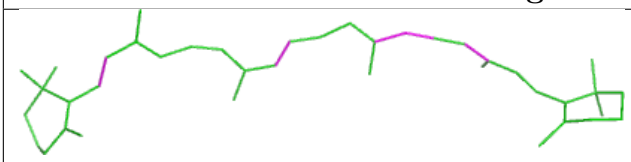
Bond angles



Torsions

Rings

Ligand BCR 5 504



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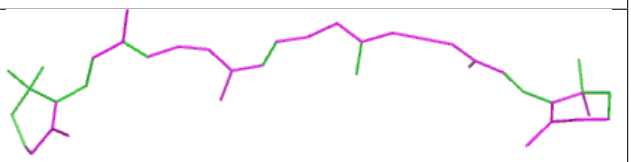
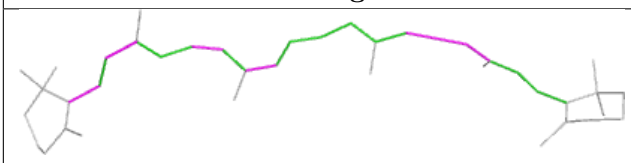


Bond angles



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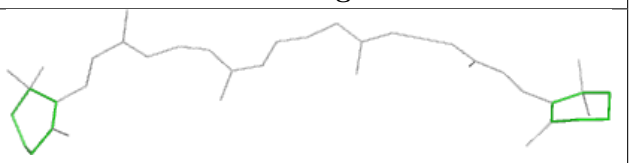
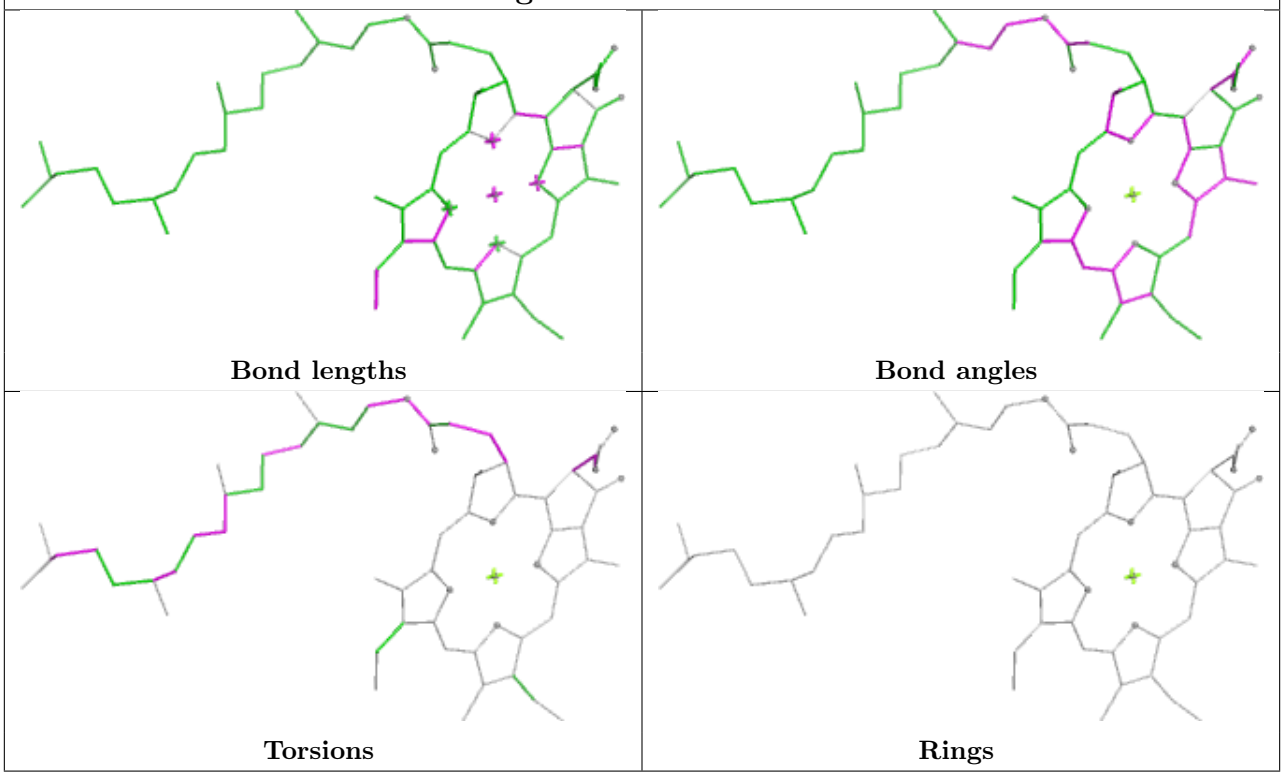
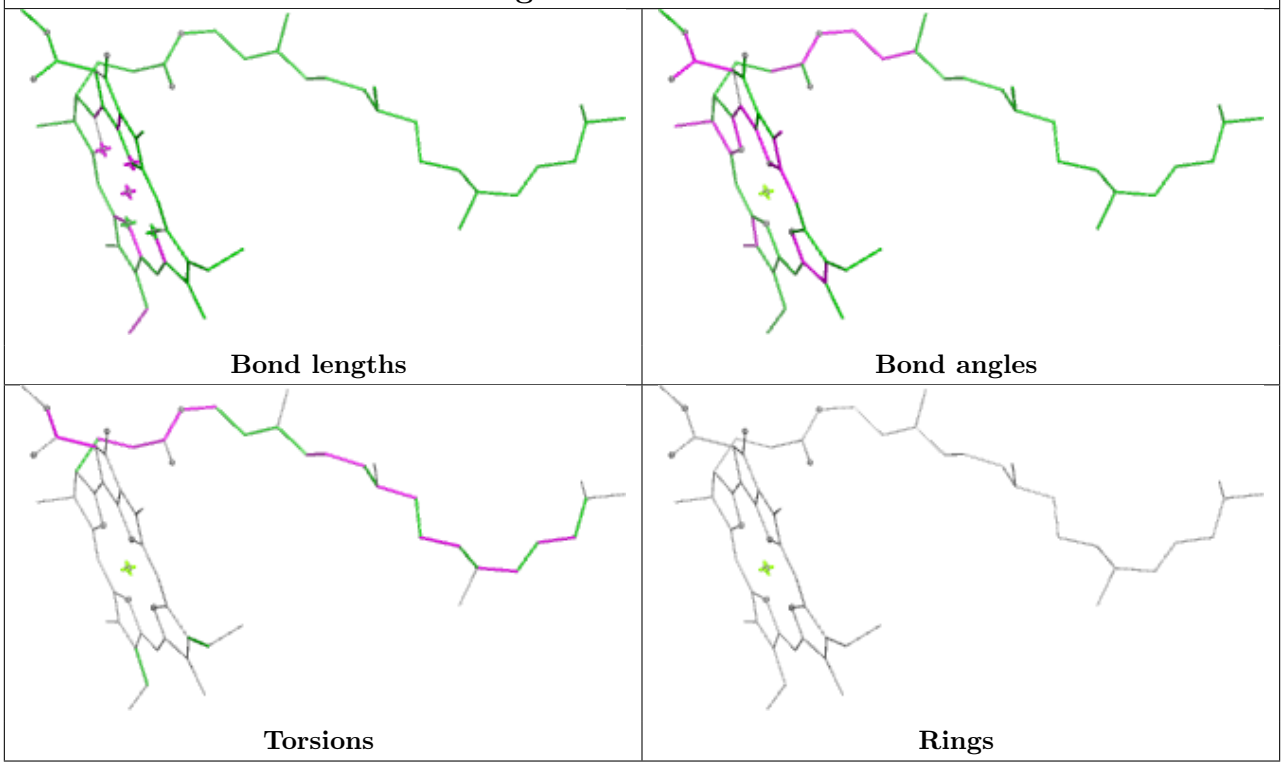


Rings

Ligand CLA A 1106



Ligand CLA A 1128



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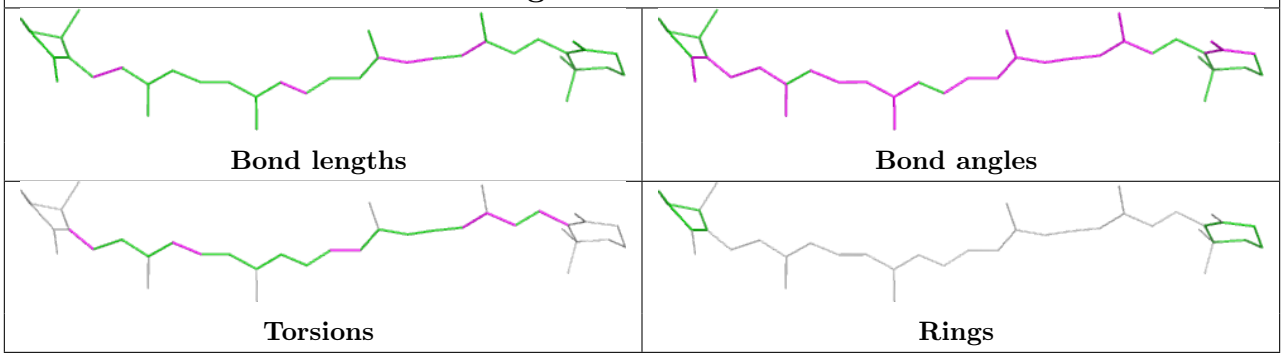
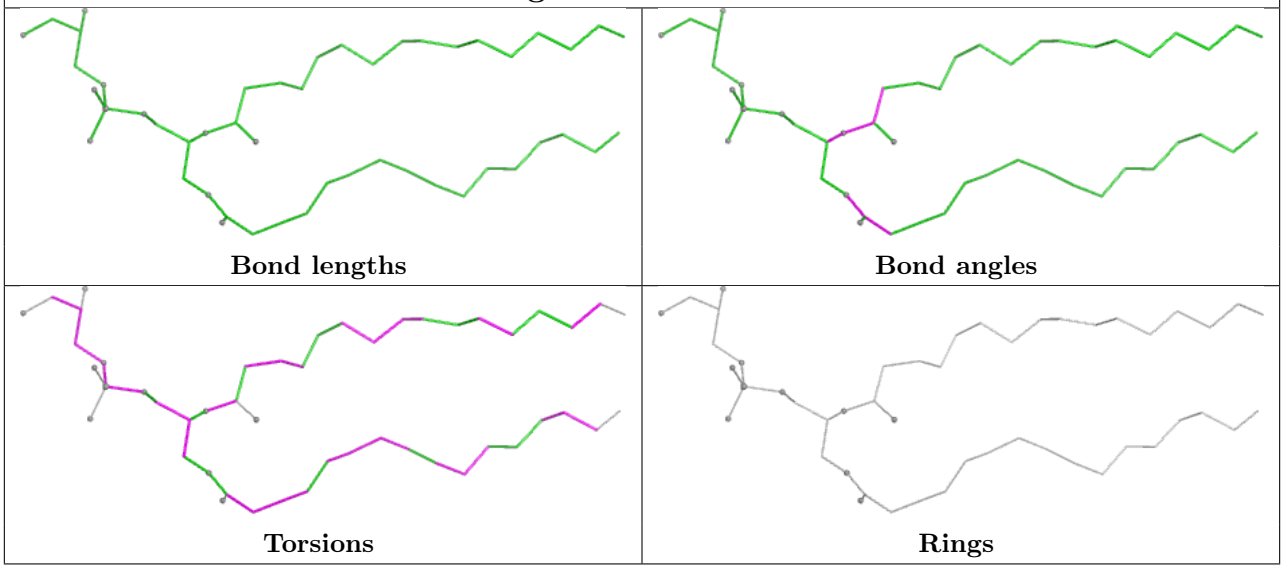
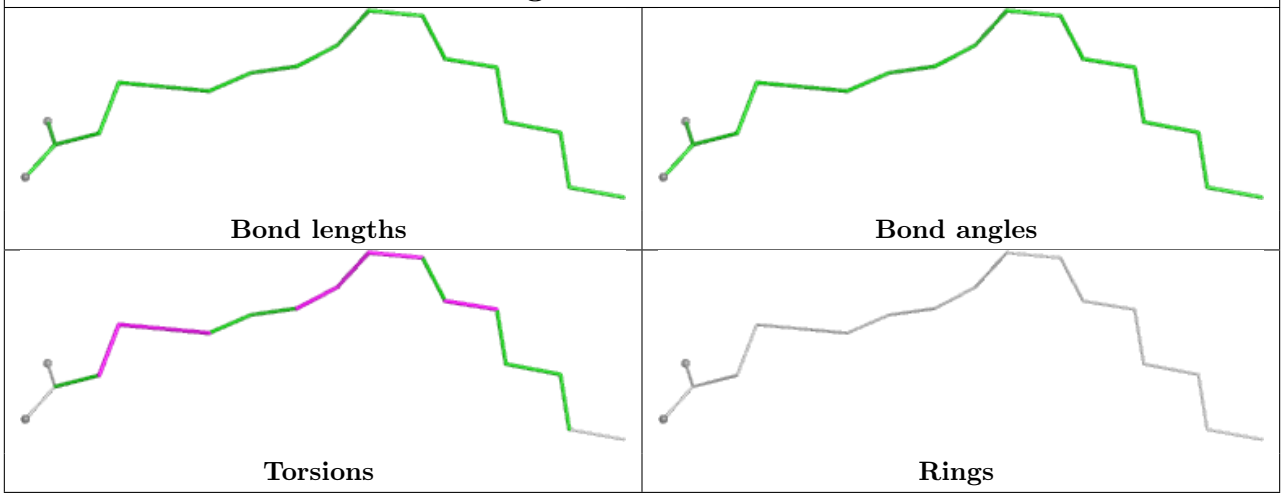


Ligand LHG 6 801



Ligand PLM 7 805



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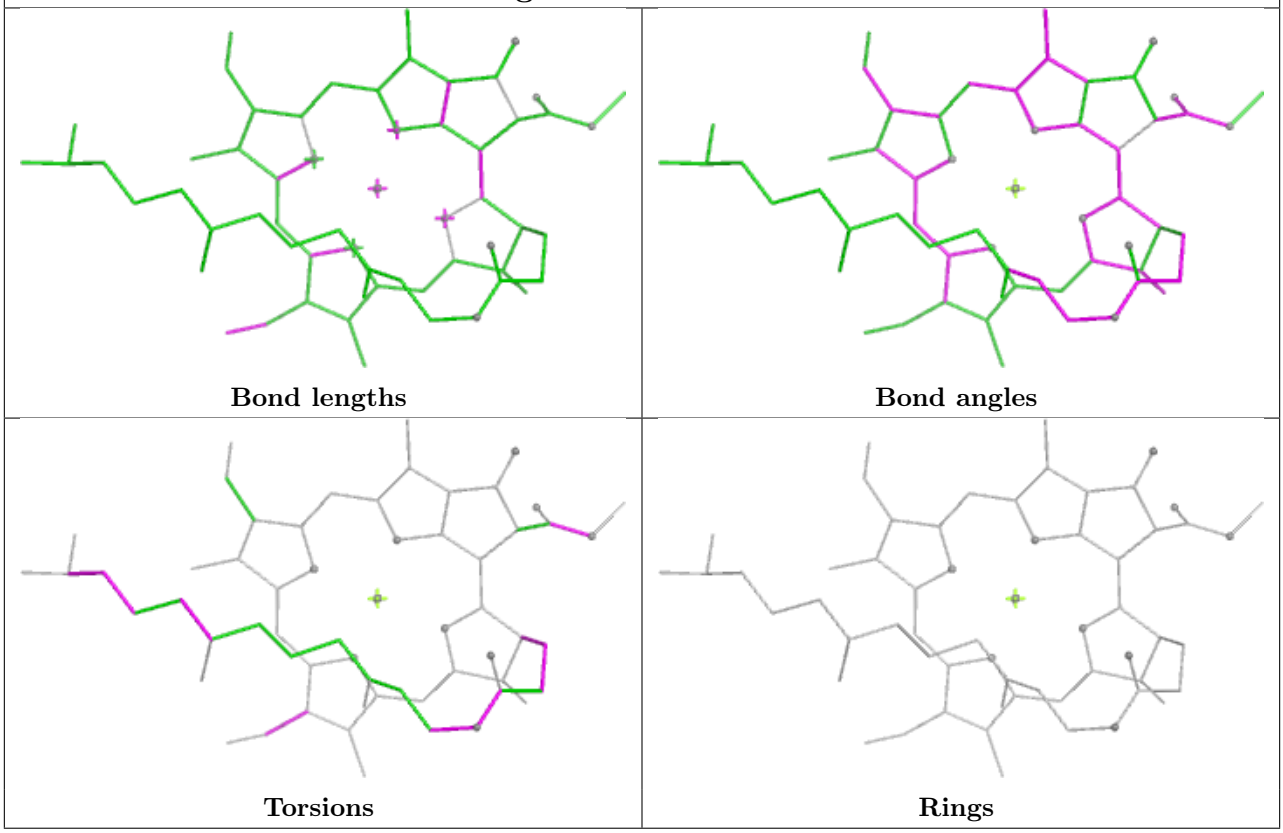
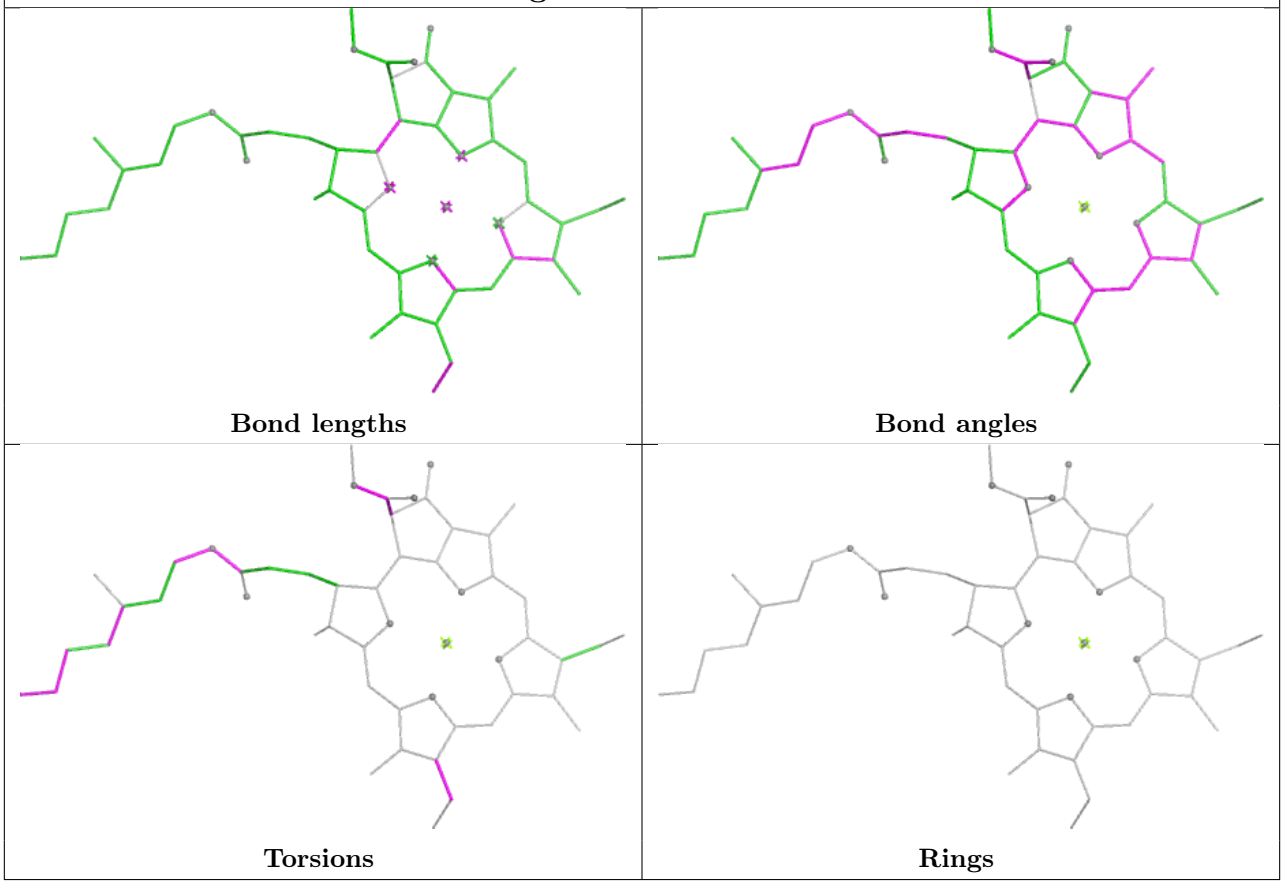


Ligand CLA 5 613



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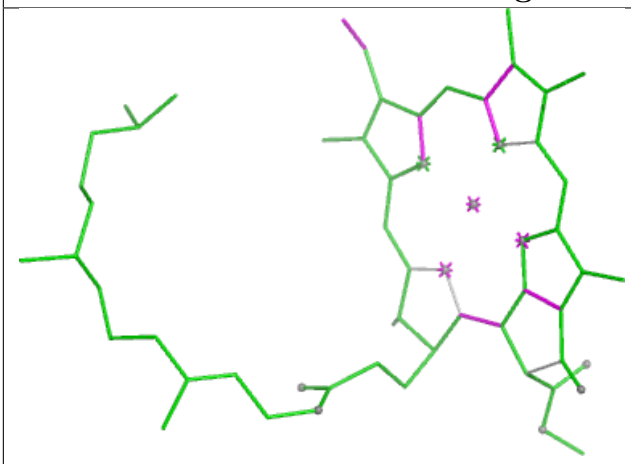
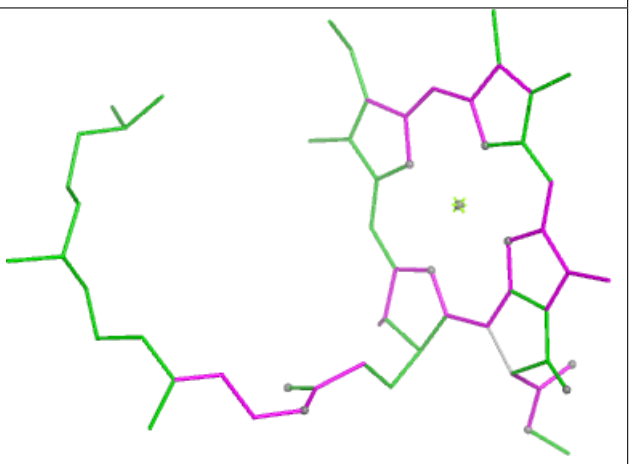
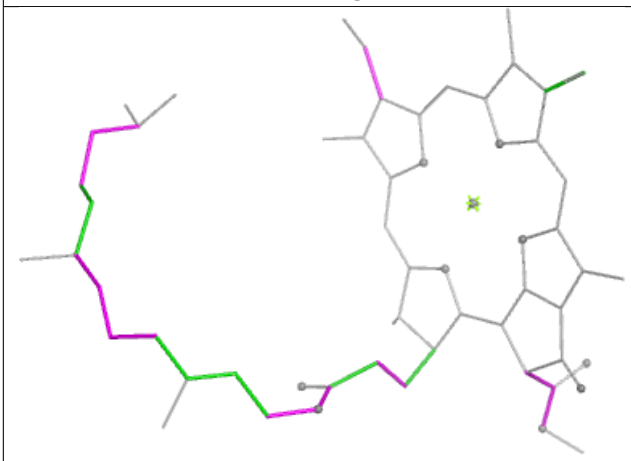
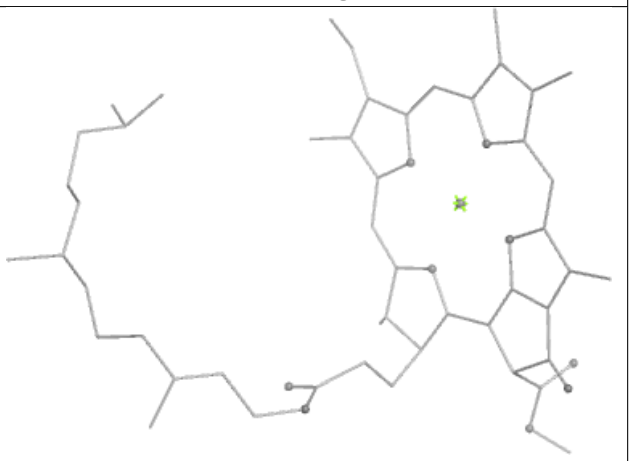
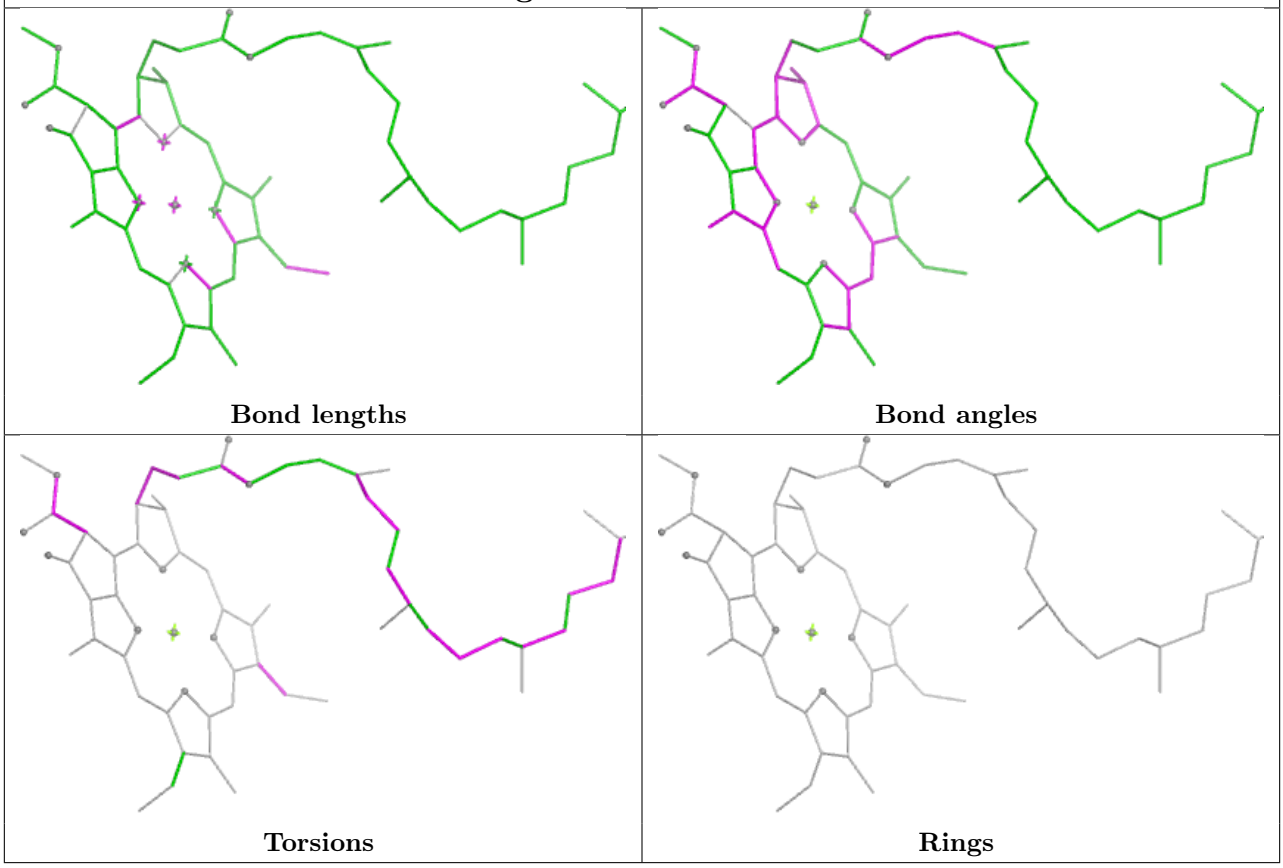
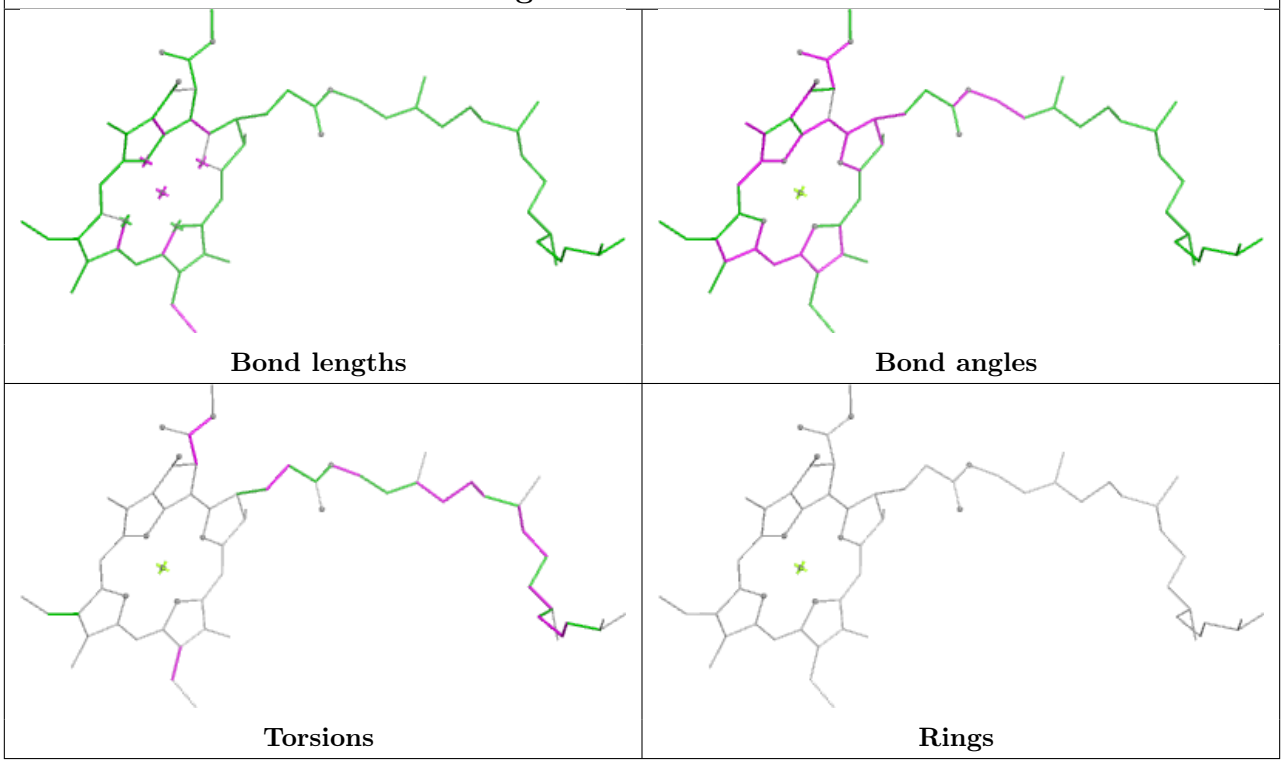
 Bond lengths	 Bond angles
 Torsions	 Rings

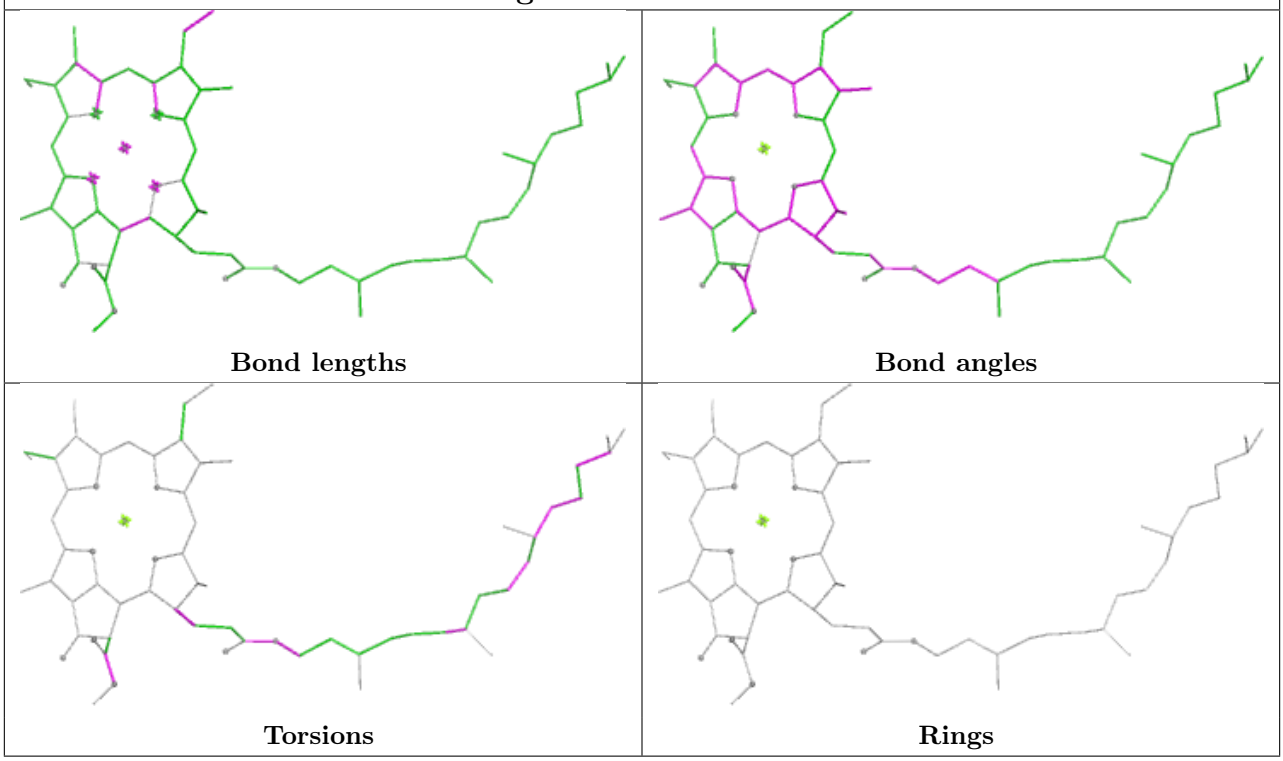
Ligand CLA A 1122



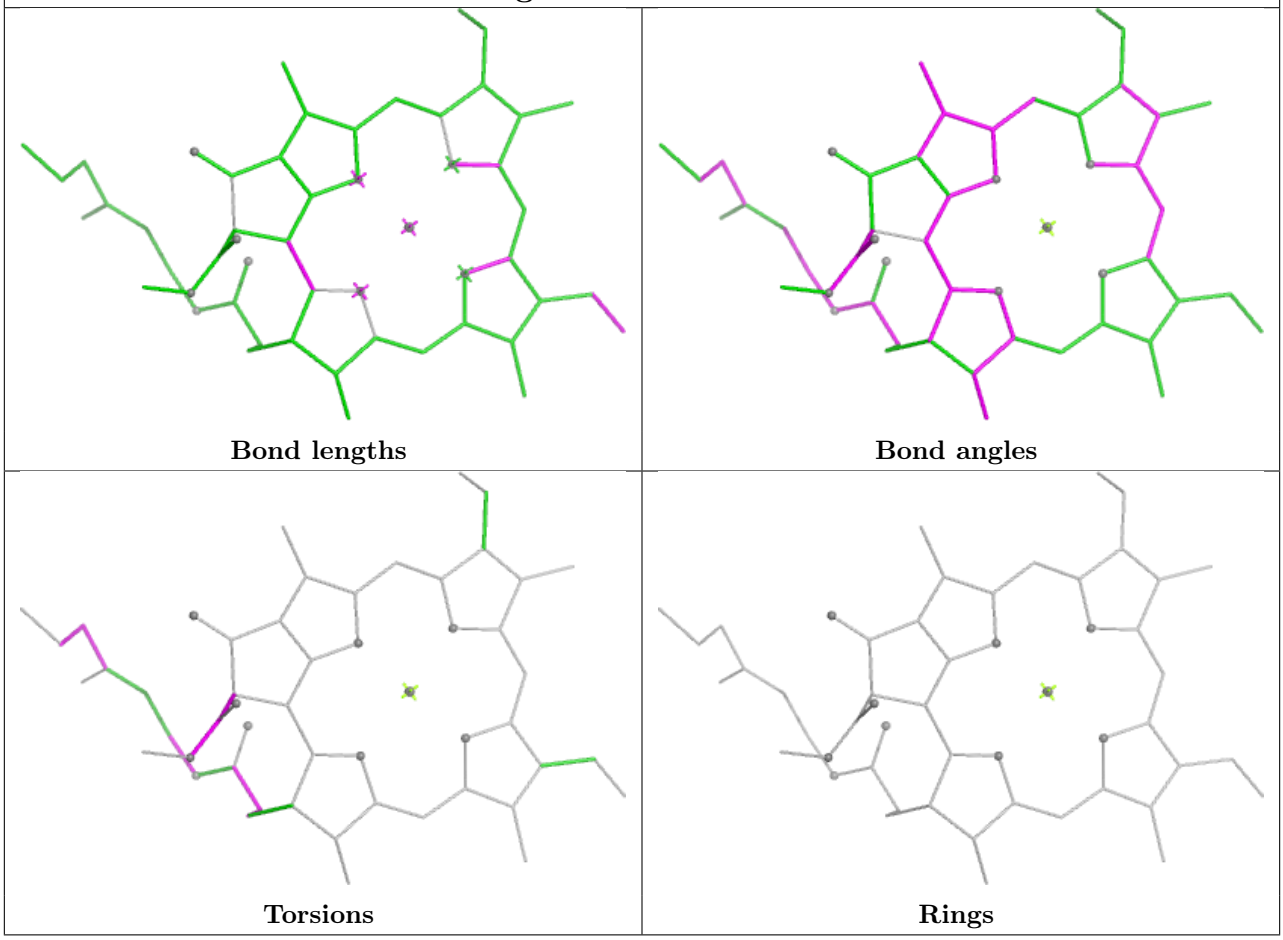
Ligand CLA A 1012

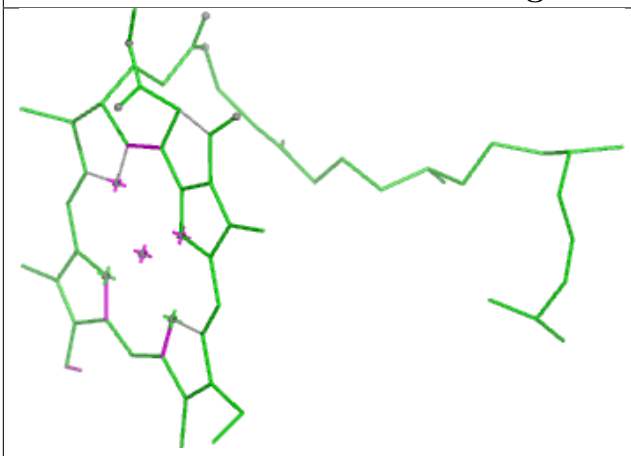
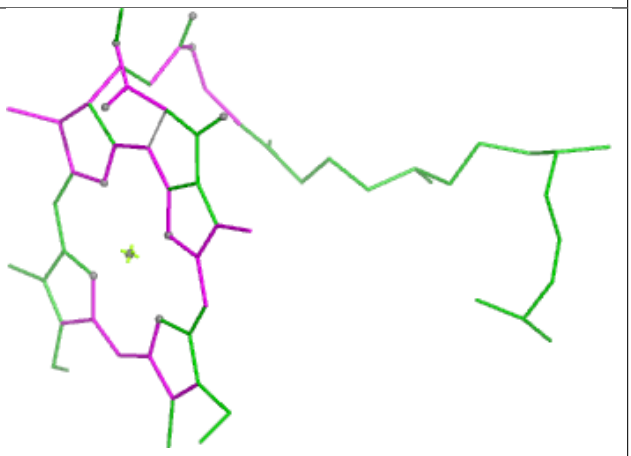


Ligand CLA B 1222



Ligand CLA A 1141



Ligand CLA Z 612	
	
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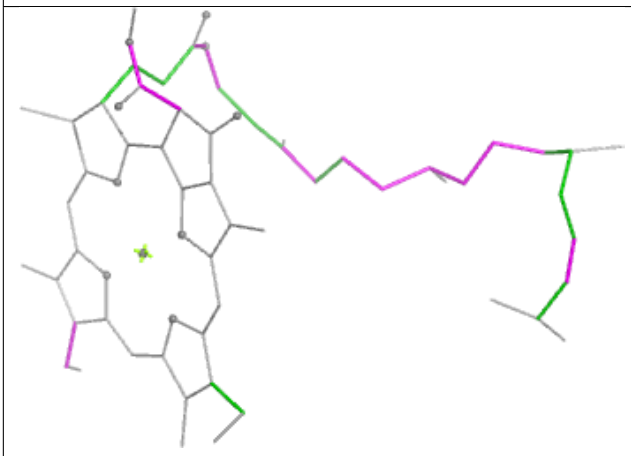
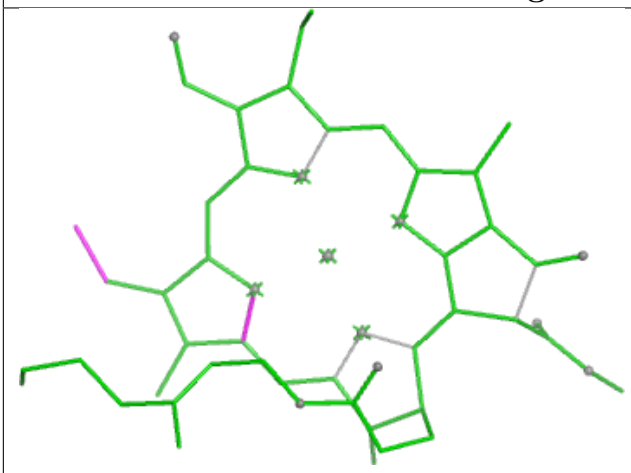
	
Torsions	**Rings**

Ligand CHL 7 610



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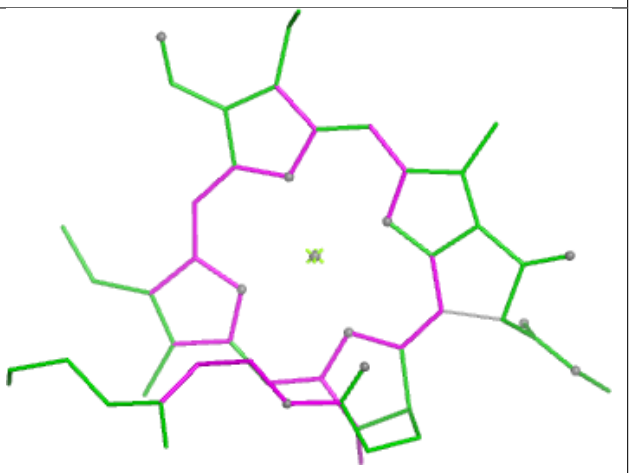

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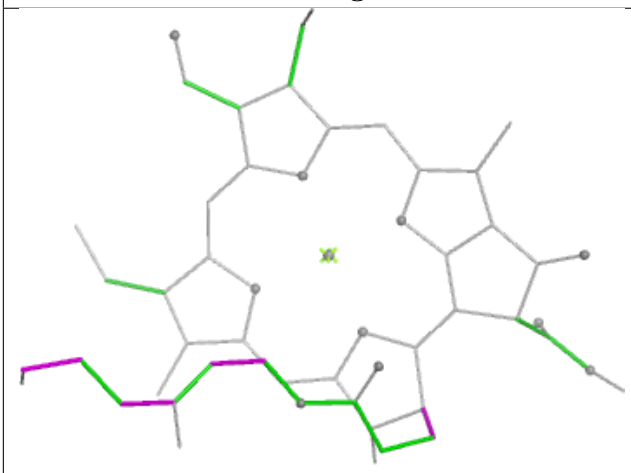
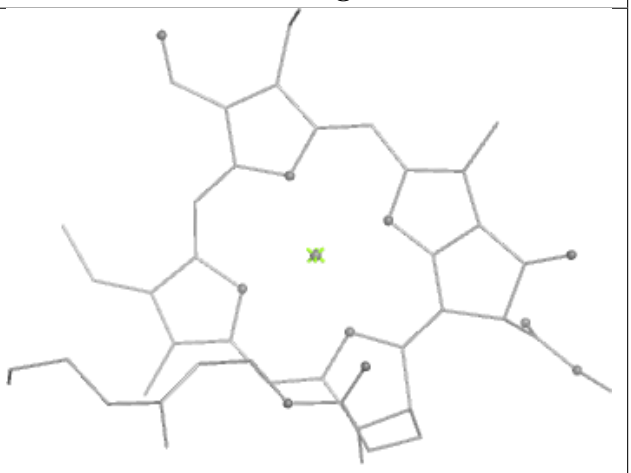
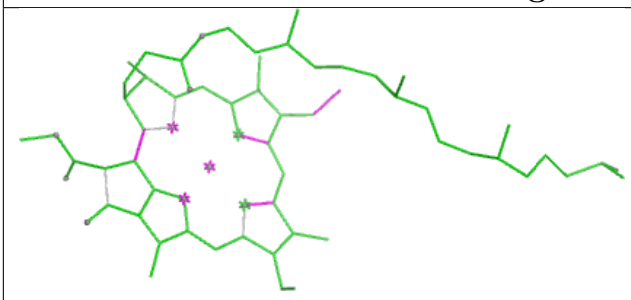


Torsions



Rings

Ligand CLA 1 601



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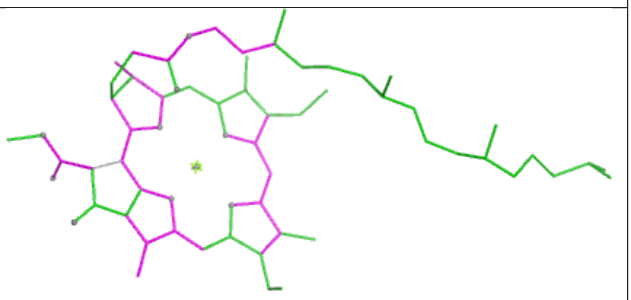

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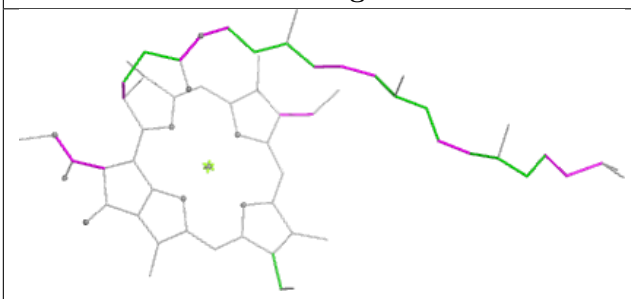

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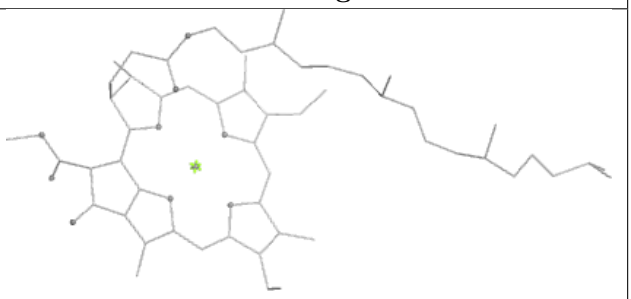
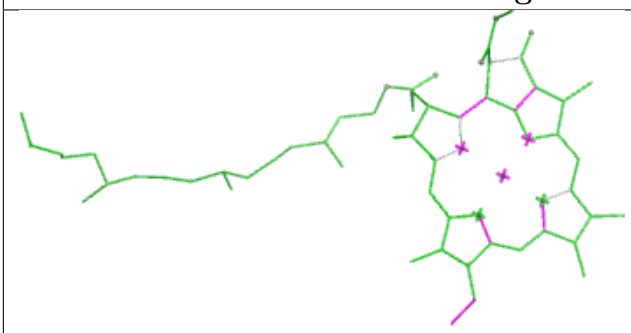
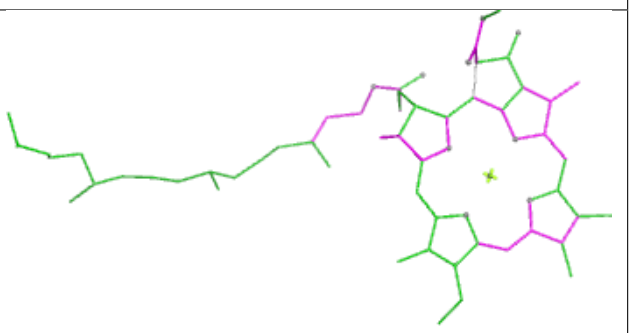
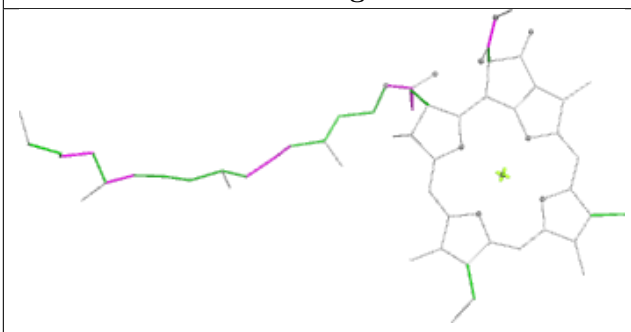
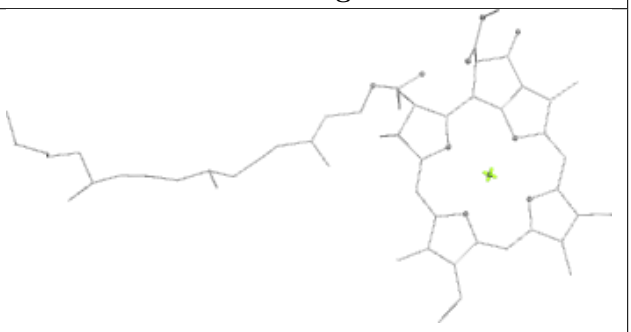


Rings

Ligand CLA A 1113	
 Bond lengths	 Bond angles
 Torsions	 Rings

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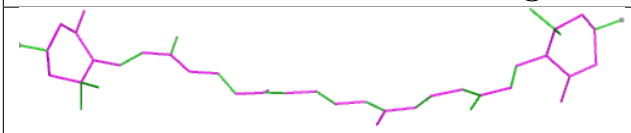
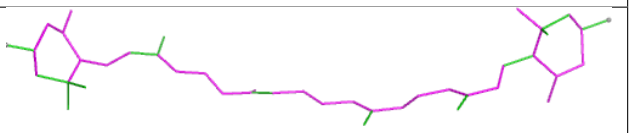
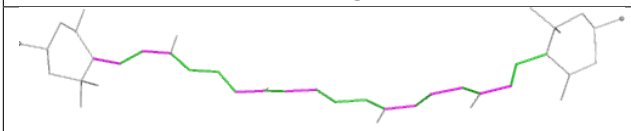
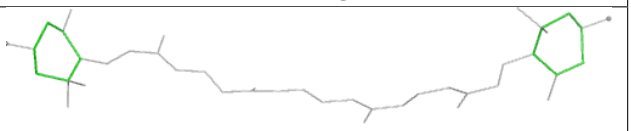
 Bond lengths	 Bond angles
 Torsions	 Rings

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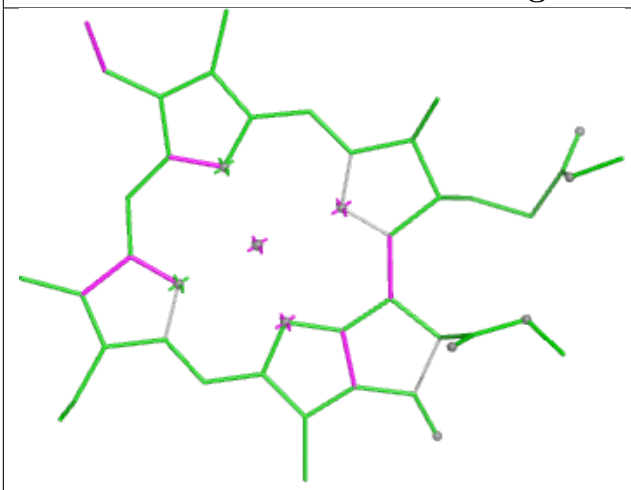
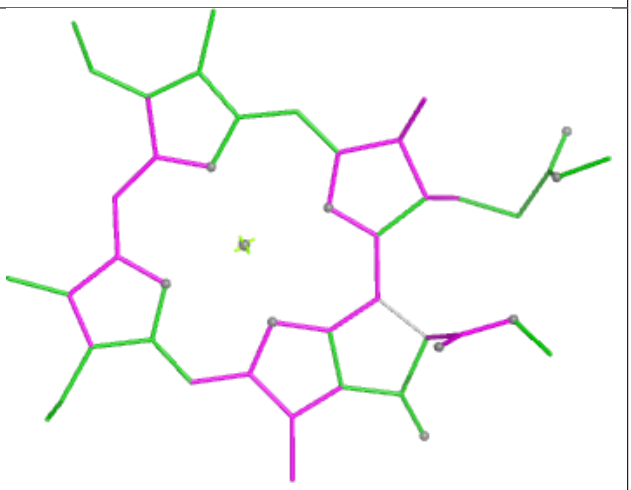
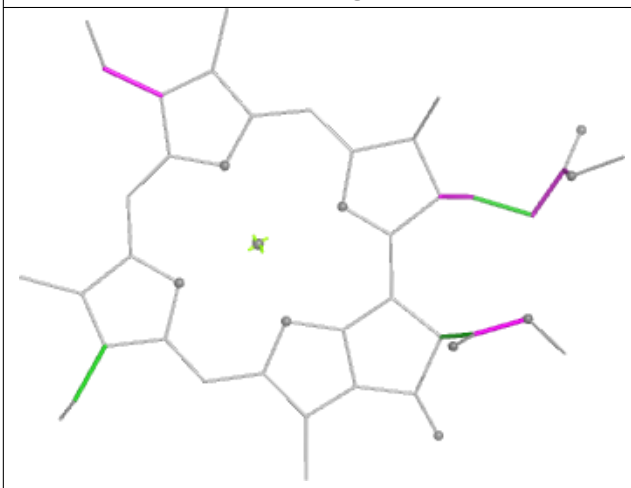
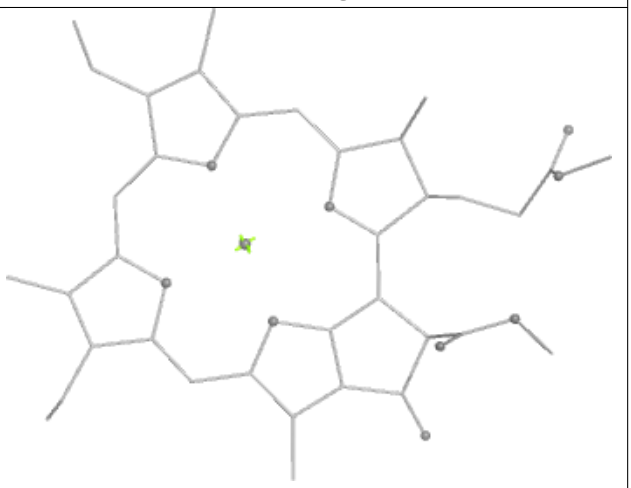
 Bond lengths	 Bond angles
 Torsions	 Rings

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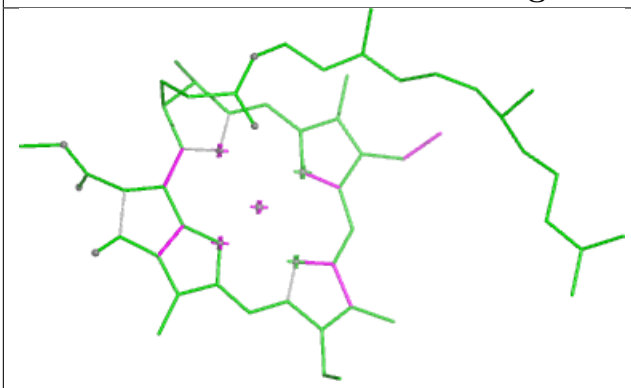
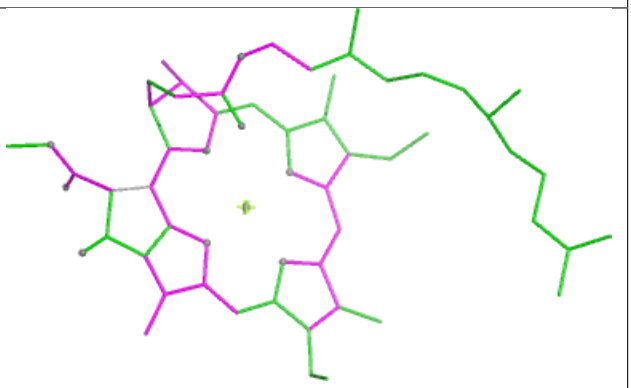
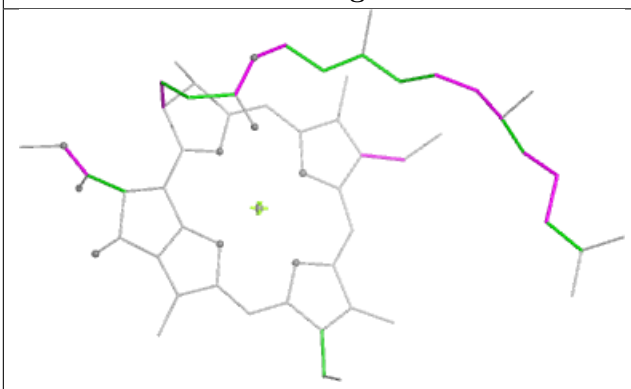
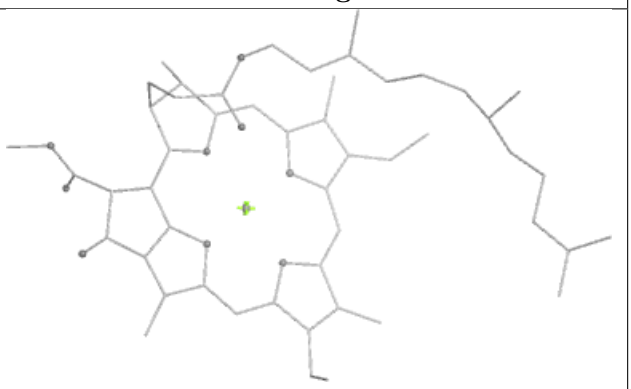
 Bond lengths	 Bond angles
 Torsions	 Rings

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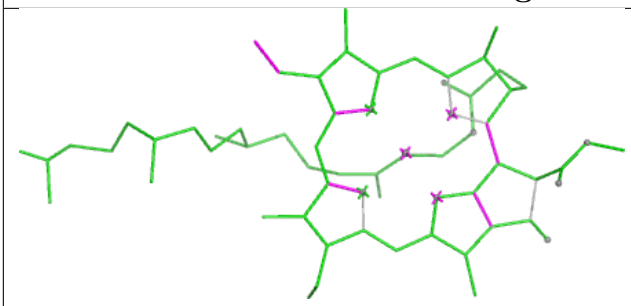
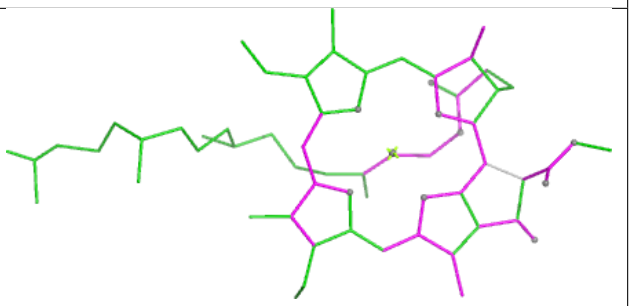
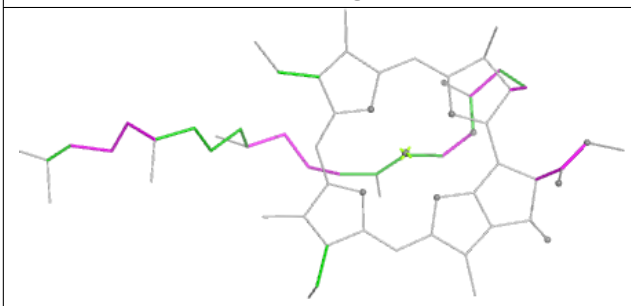
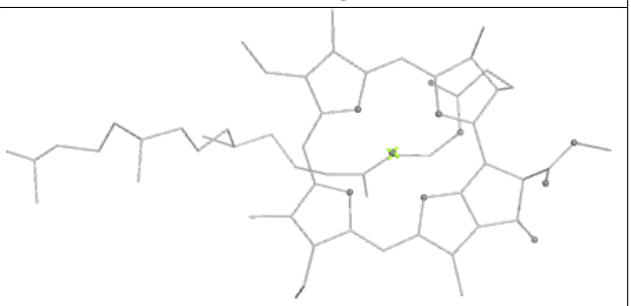
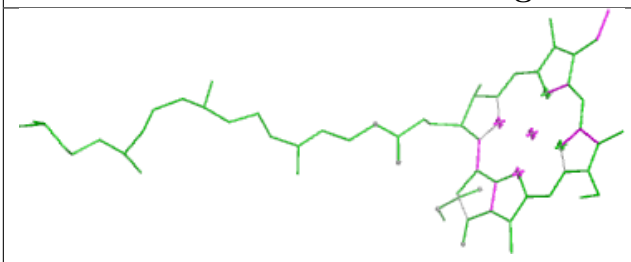
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1107



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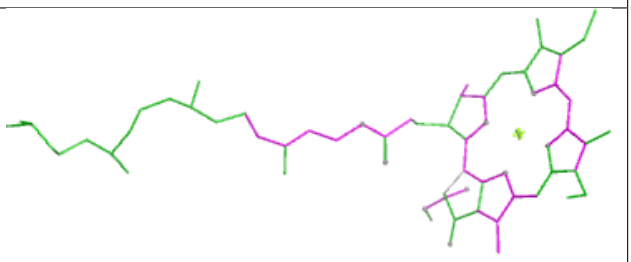

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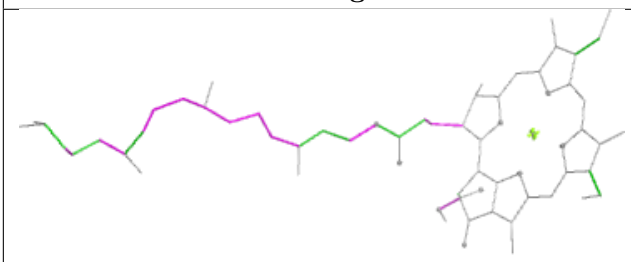

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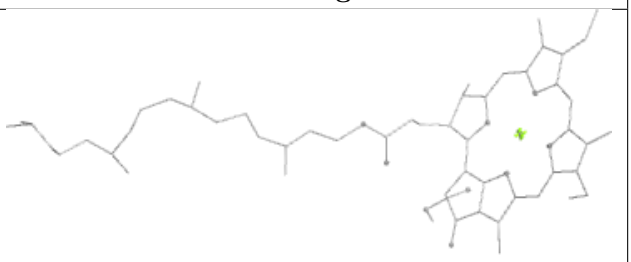
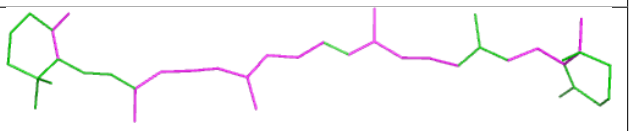


Rings

Ligand BCR B 4001

Bond lengths



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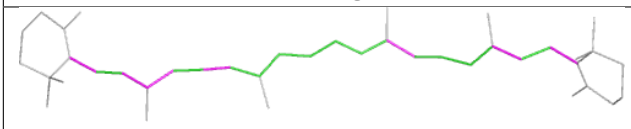

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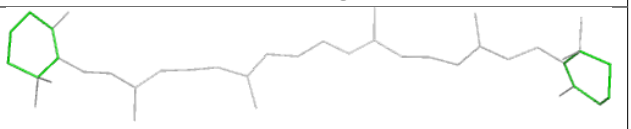
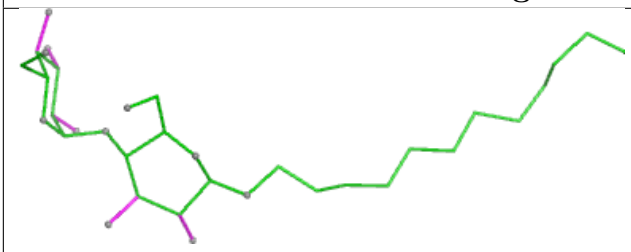


Rings

Ligand LMT B 6101



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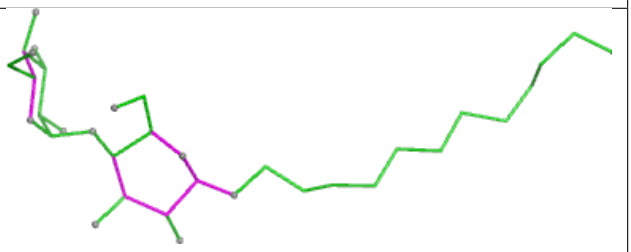

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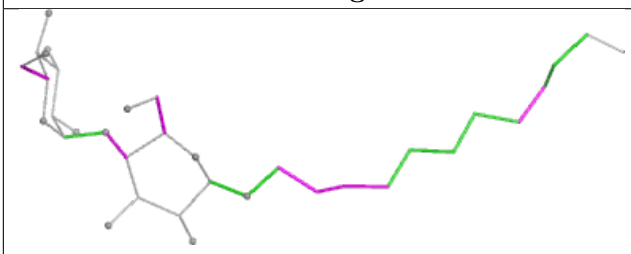

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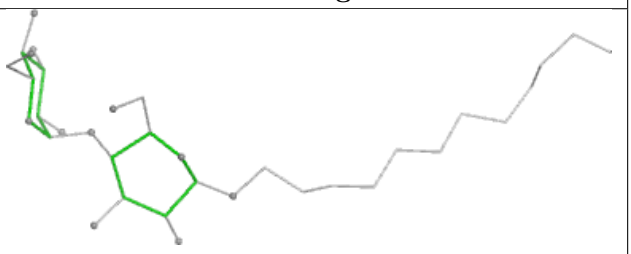
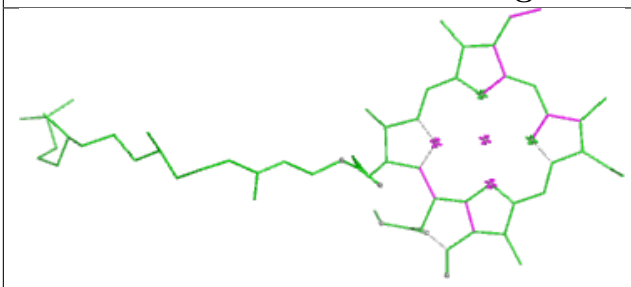
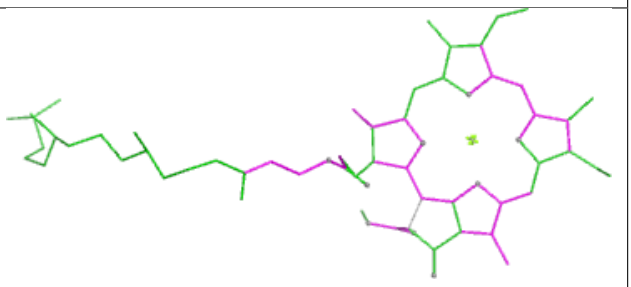
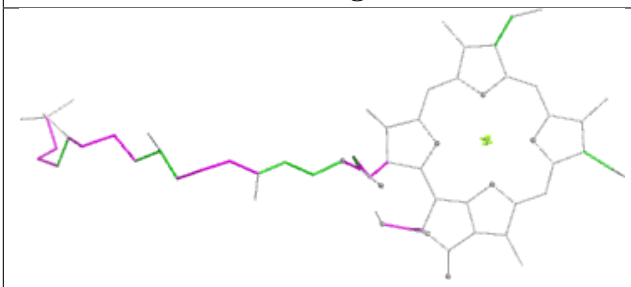
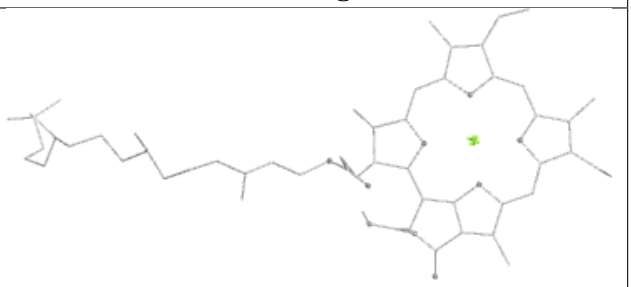
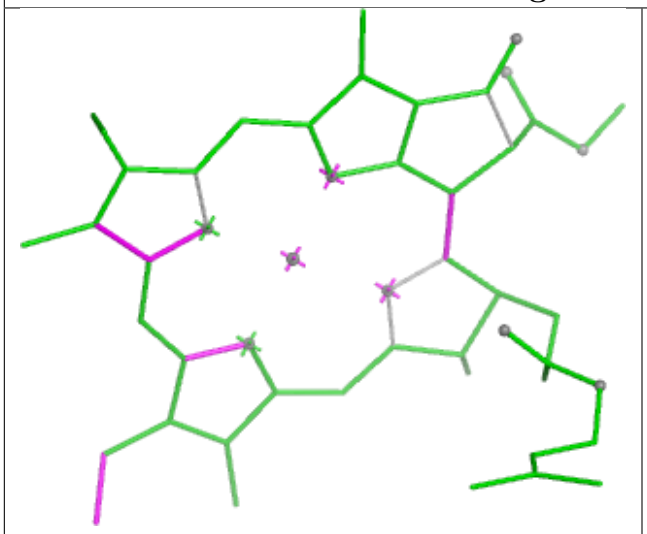


Rings

Ligand CLA B 1240	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 606



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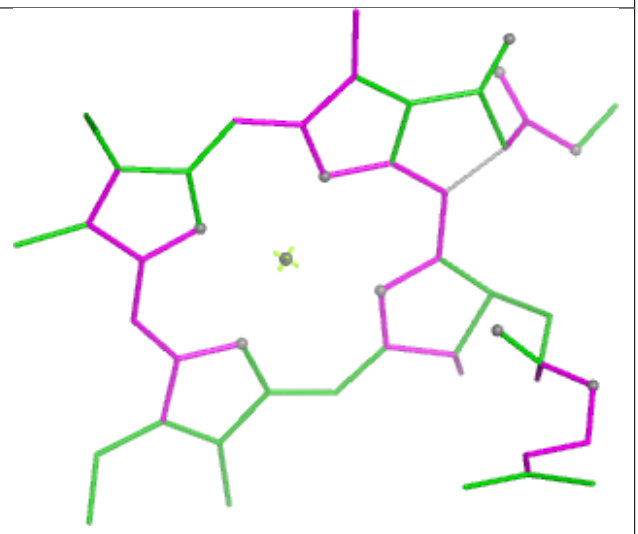
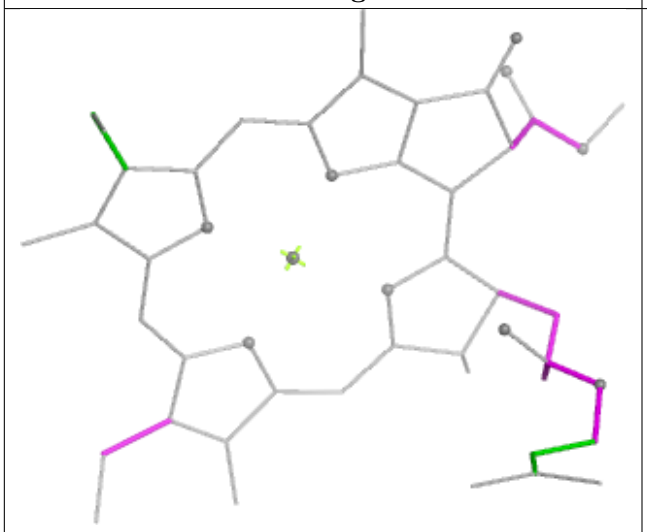


Bond angles



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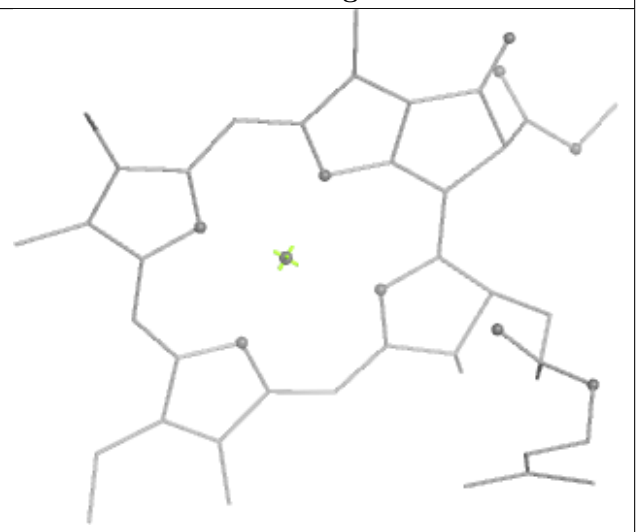

Rings

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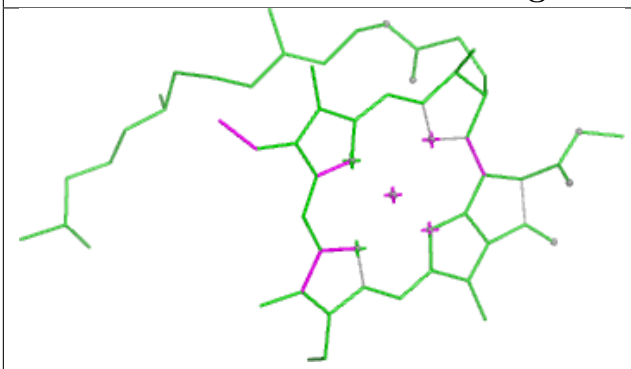
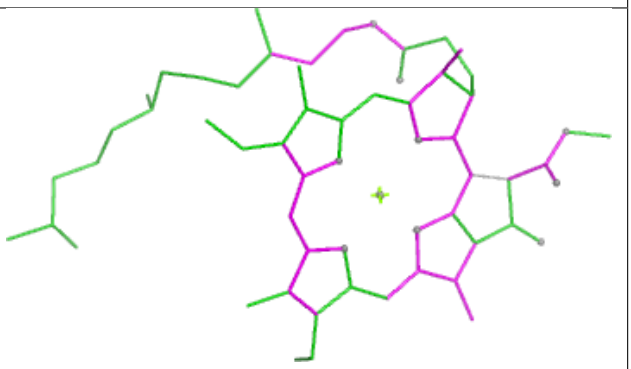
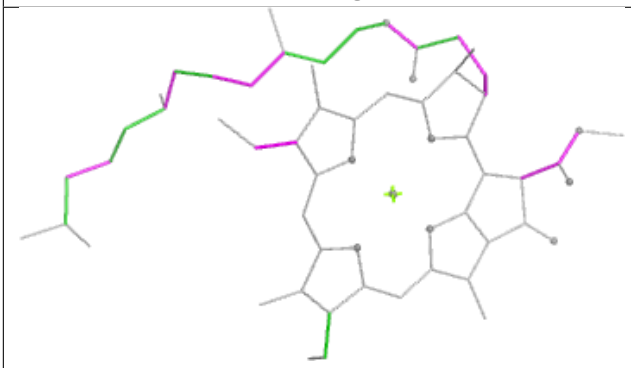
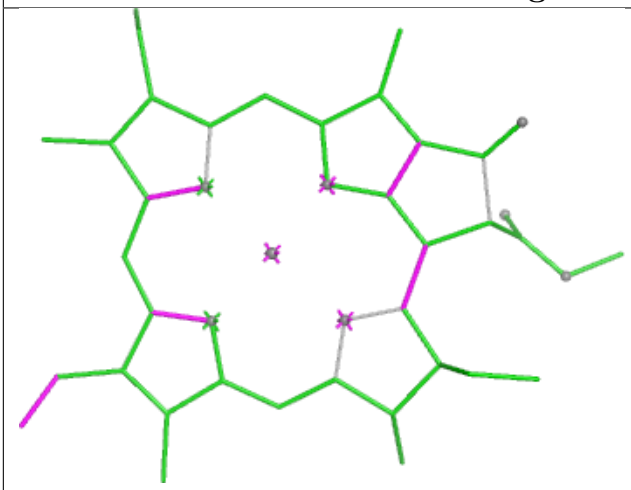
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 7 613



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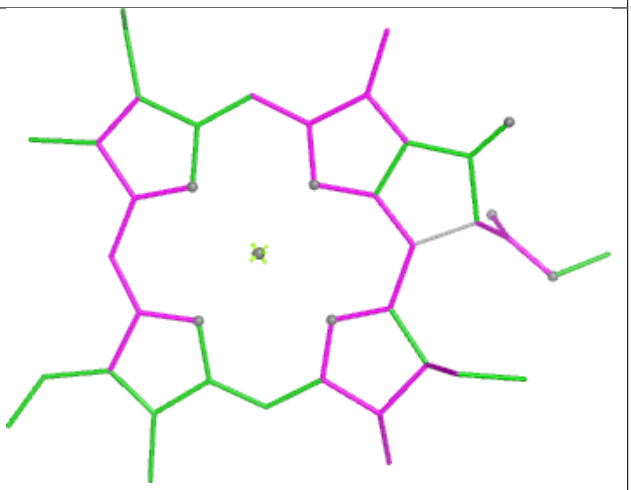
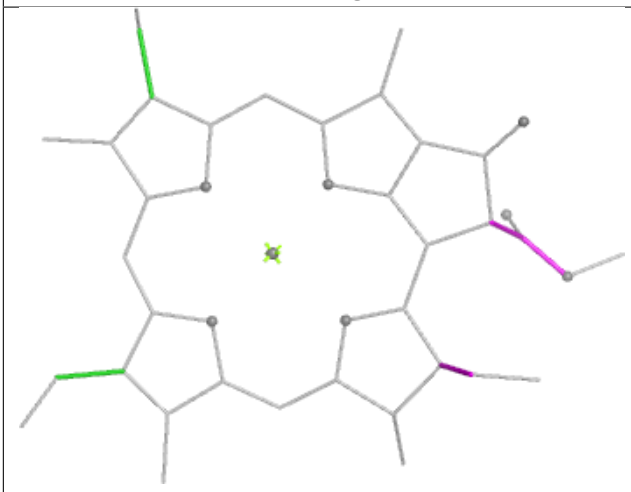
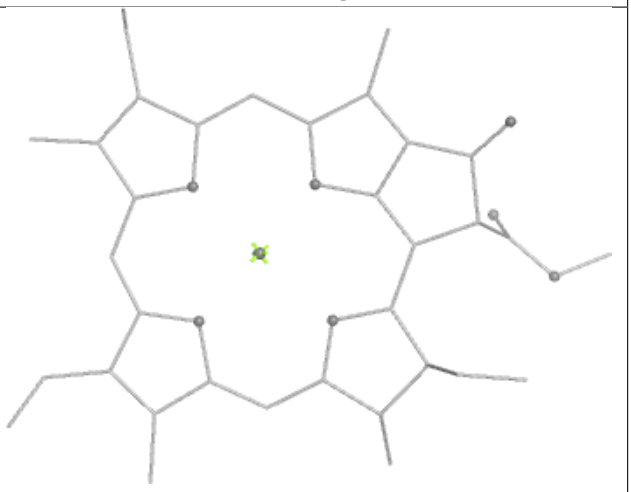


Bond angles

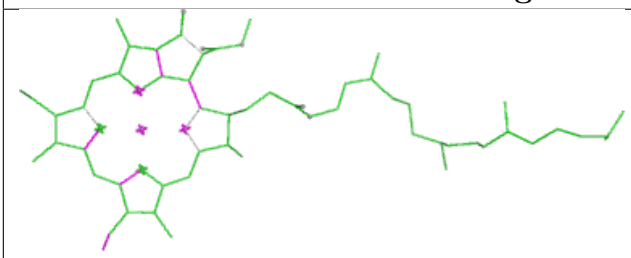


Torsions

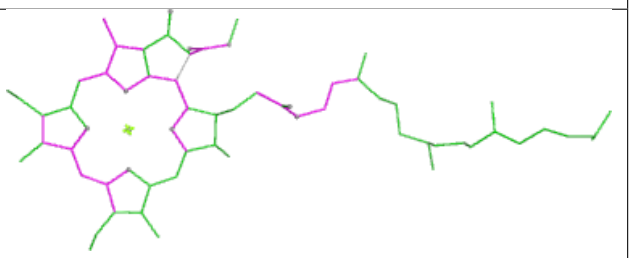


Rings

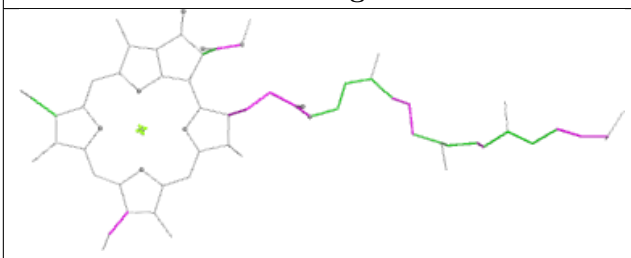
Ligand CLA A 1131



Bond lengths



Bond angles



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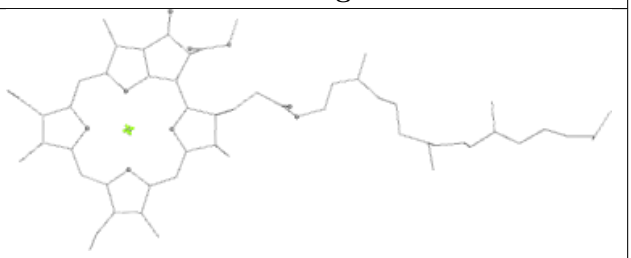
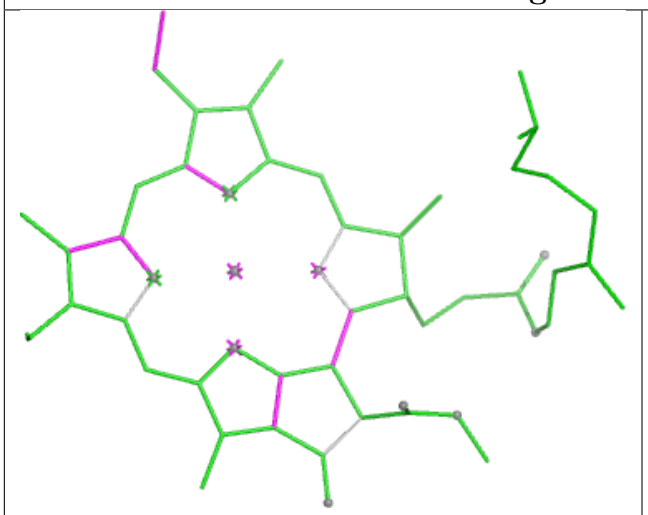


Rings

Ligand CLA 6 605



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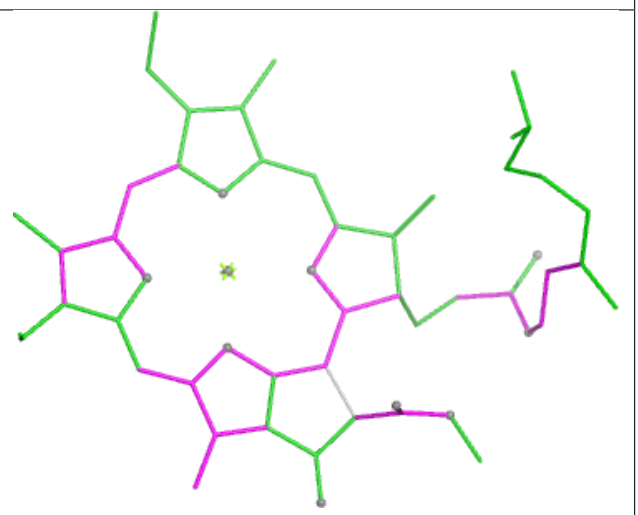
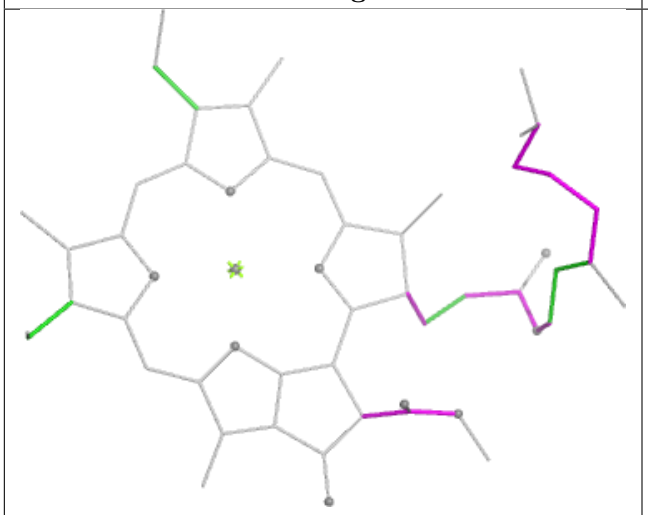


Bond angles



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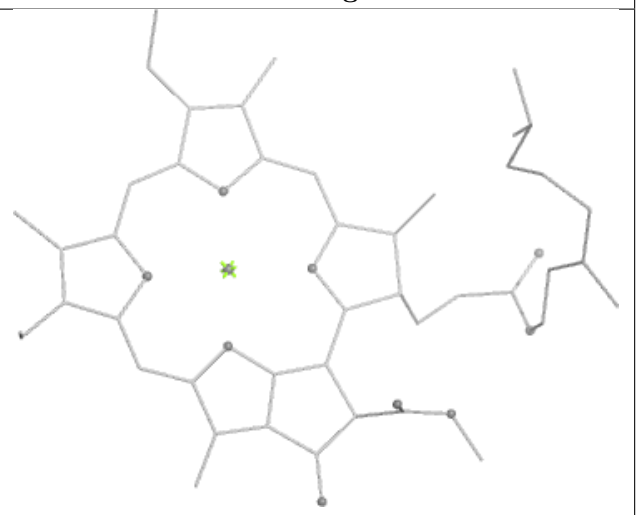
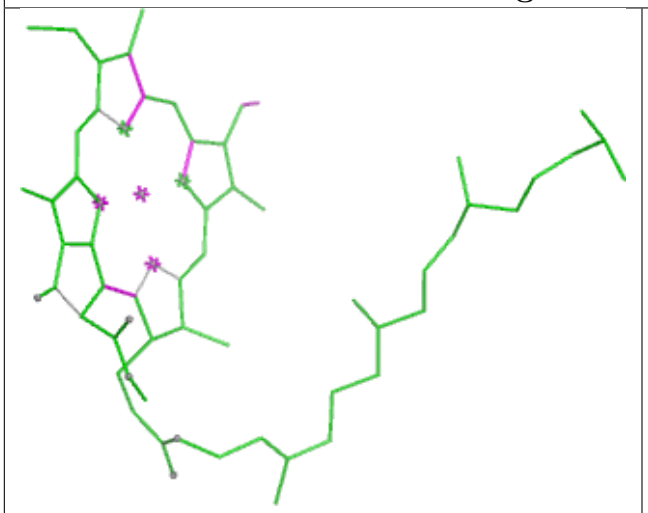


Rings

Ligand CLA B 1221



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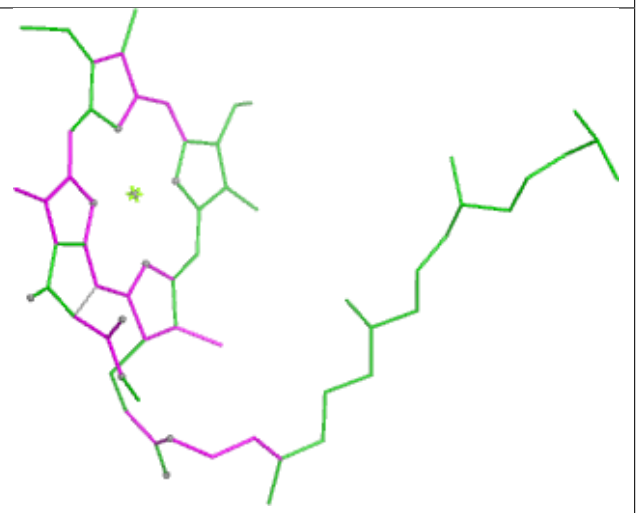

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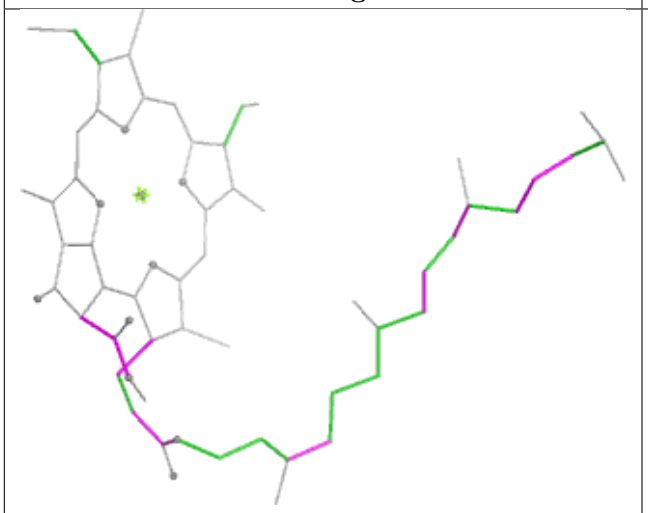

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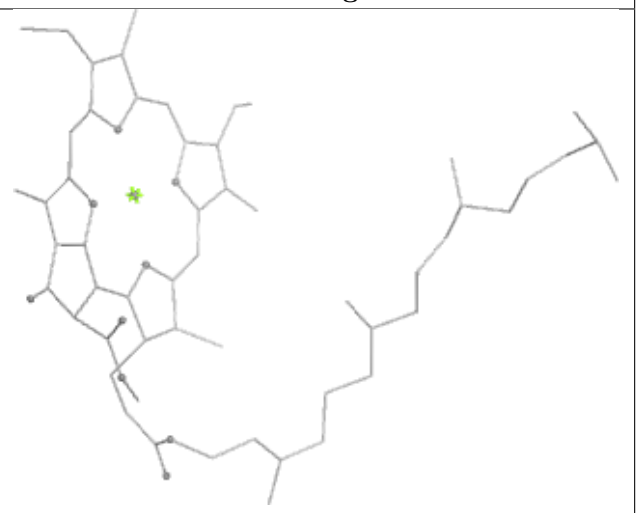
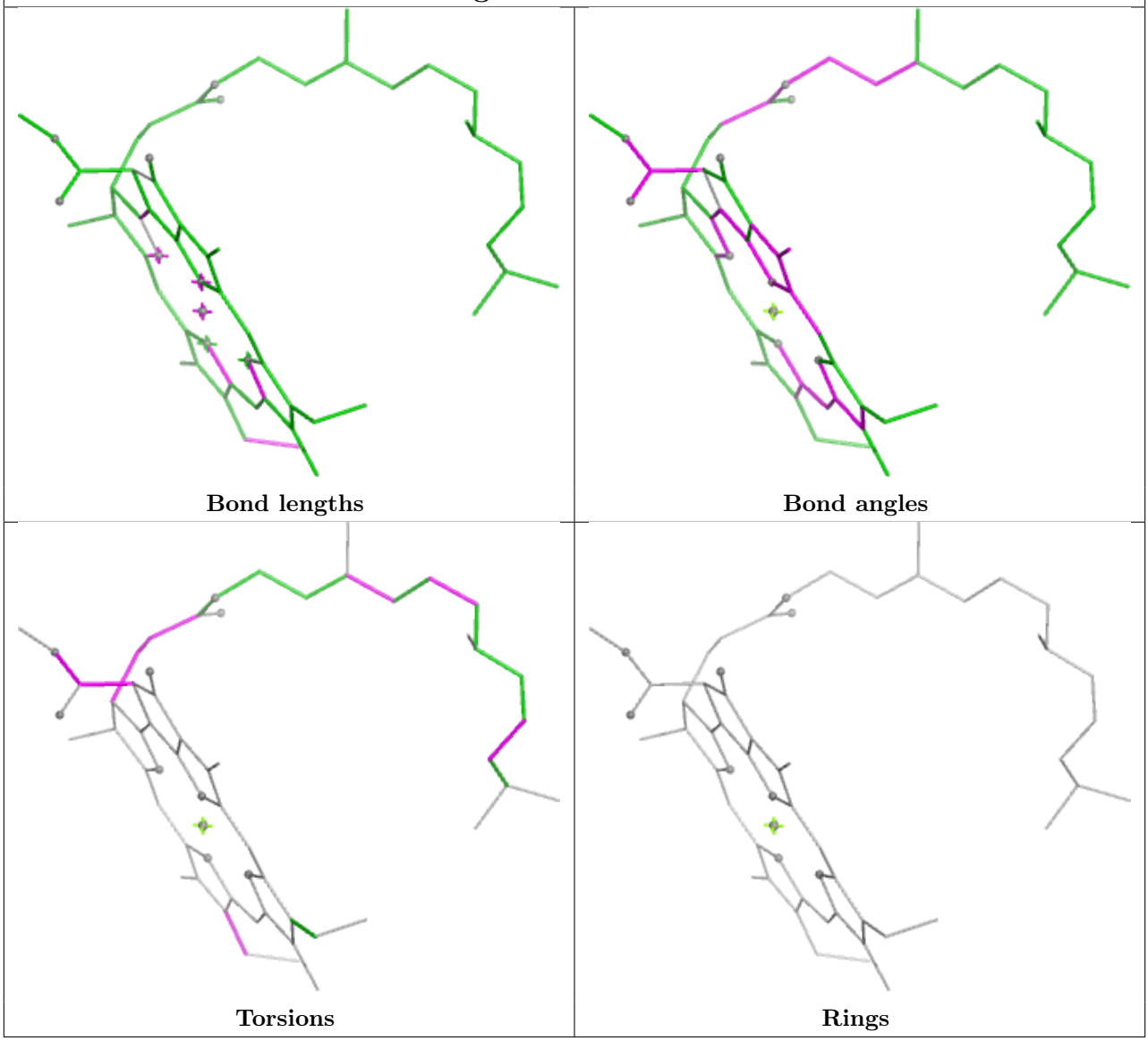
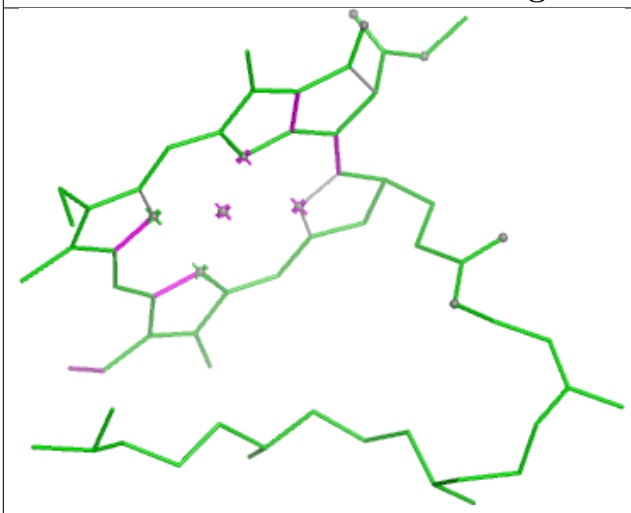


Rings

Ligand CLA 1 608



Ligand CLA 1 611



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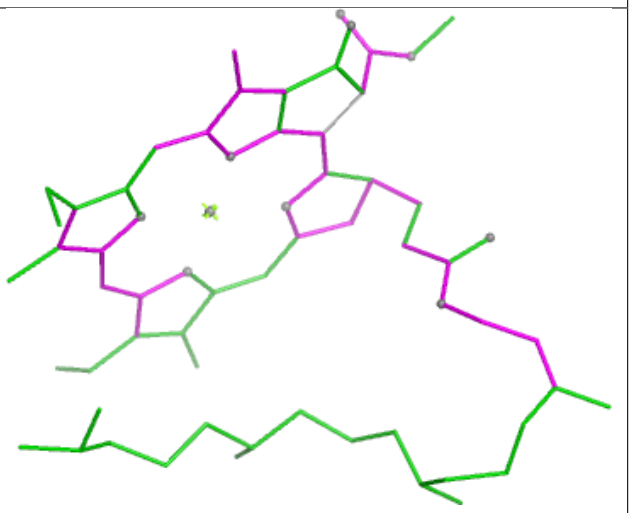
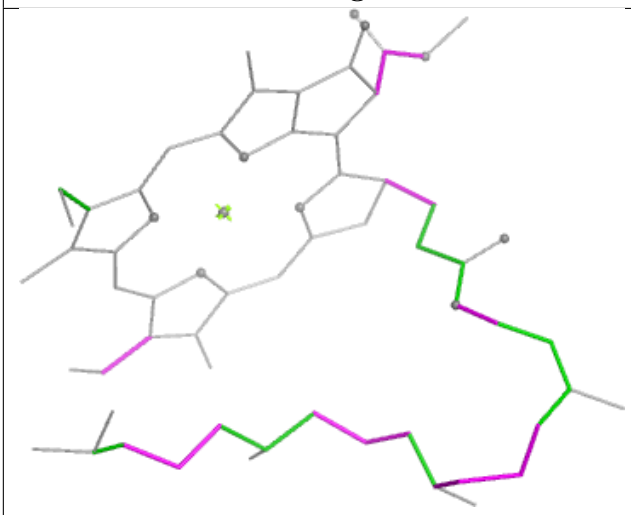


Bond angles



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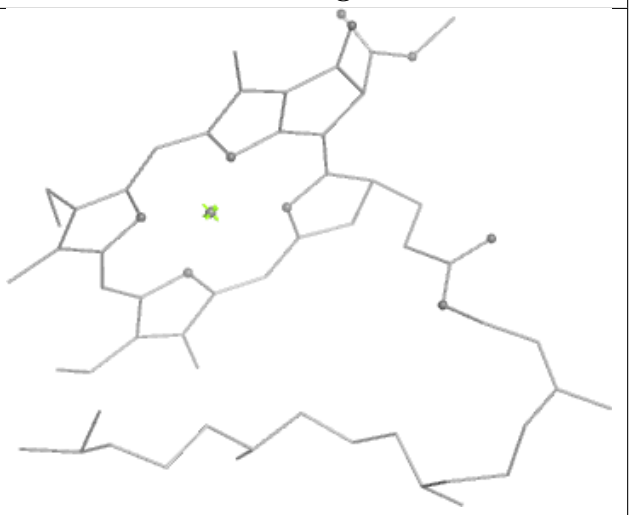
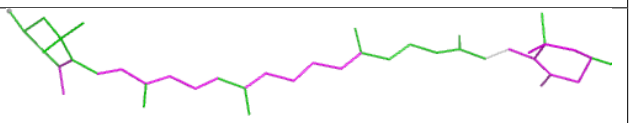


Rings

Ligand LUT 3 501

Bond lengths



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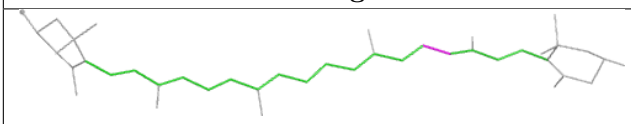

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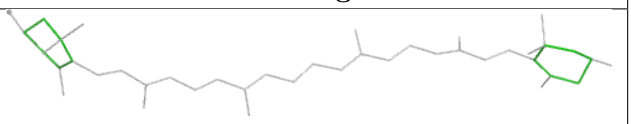
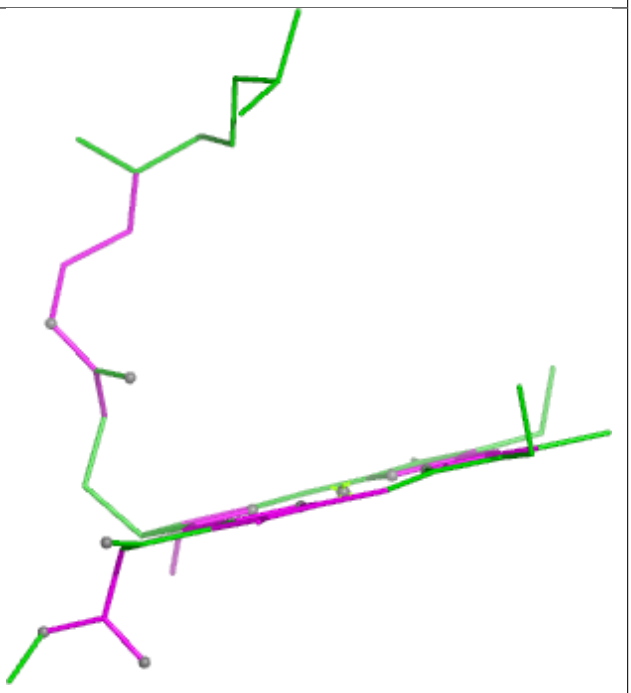


Rings

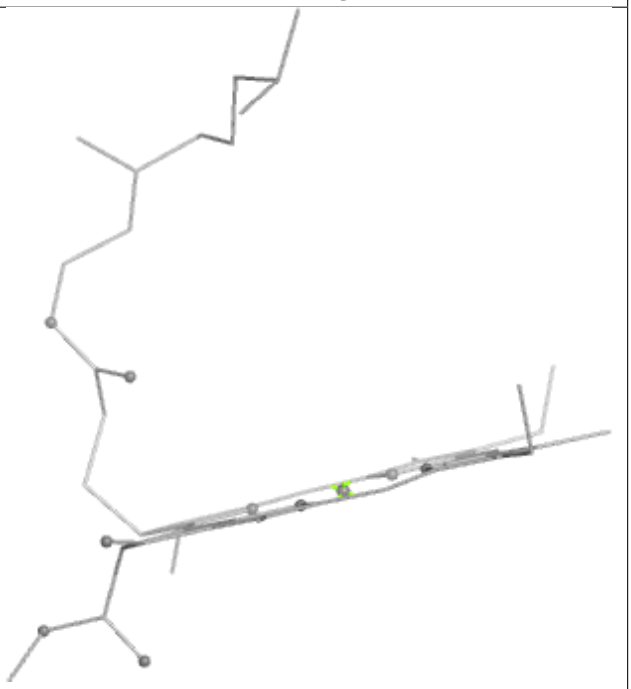
Ligand CLA 4 608

Bond lengths

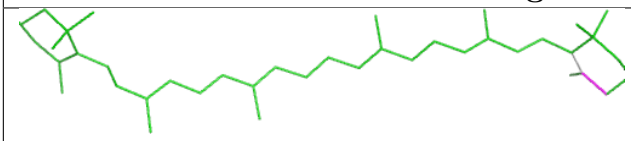
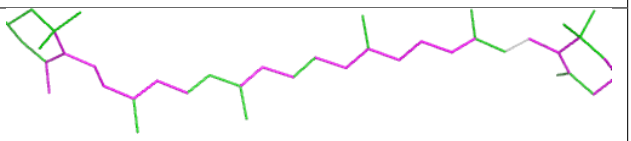
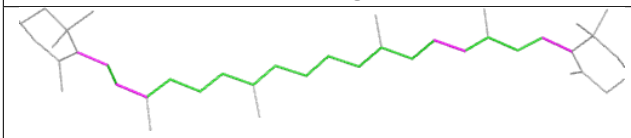
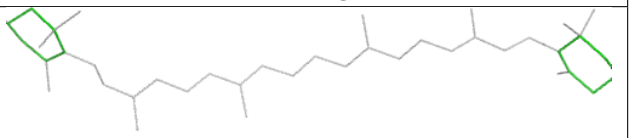


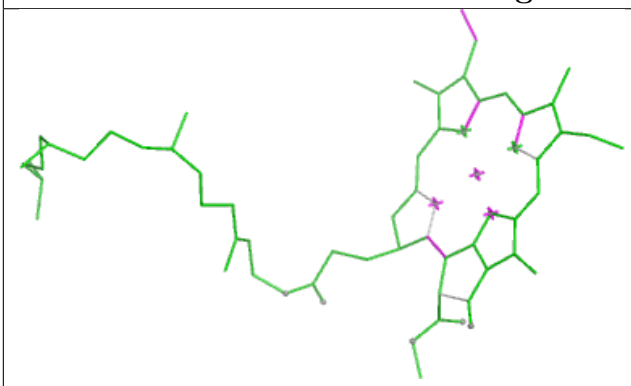
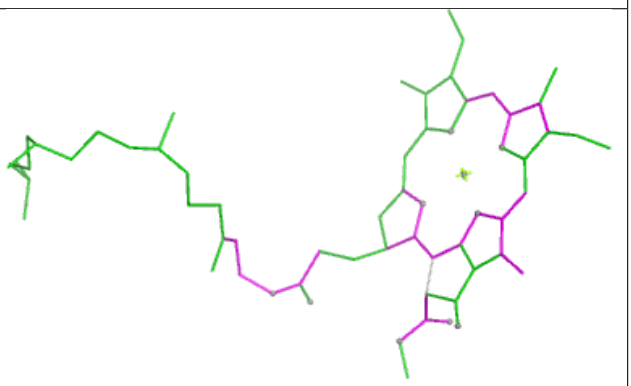
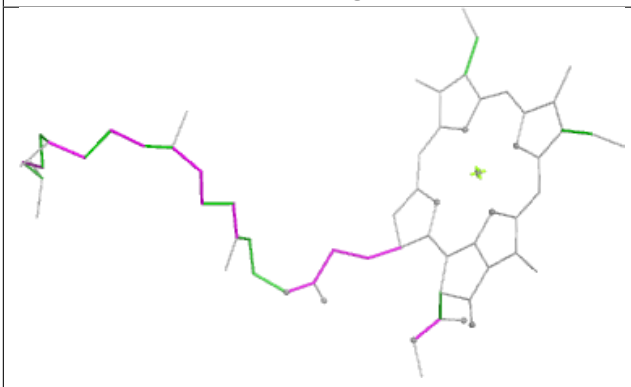
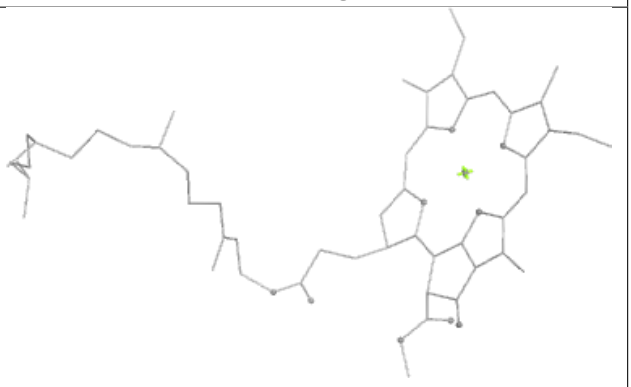
Bond angles

Torsions

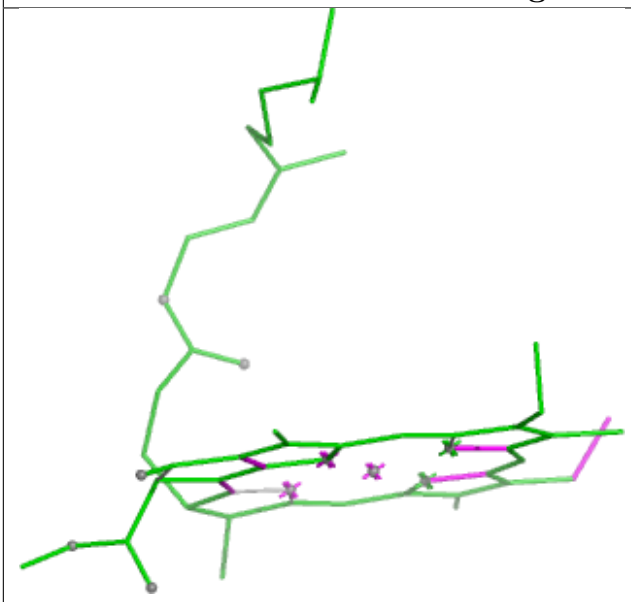


Rings

Ligand LUT Z 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1206	
 Bond lengths	 Bond angles
 Torsions	 Rings

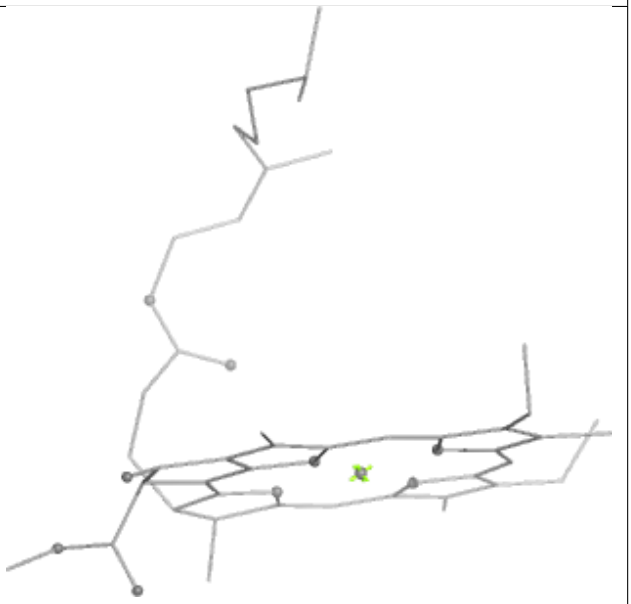
Ligand CLA 6 608



Bond lengths

Bond angles

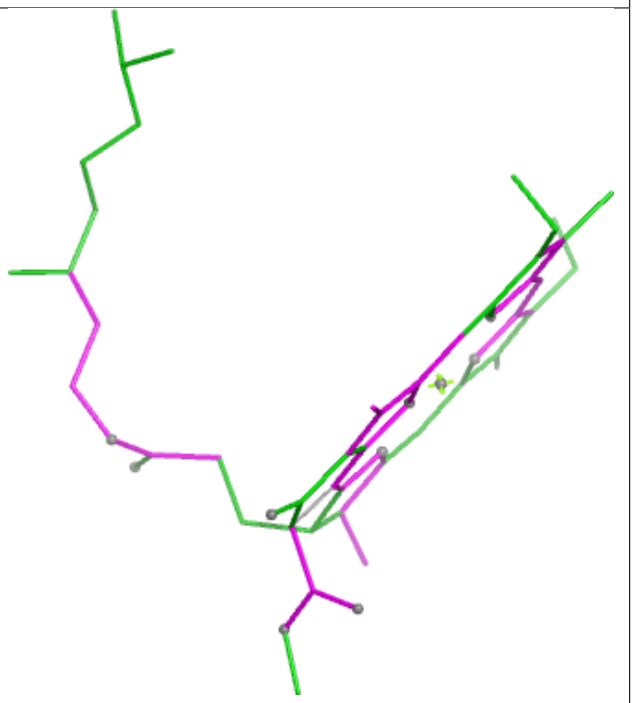
Torsions



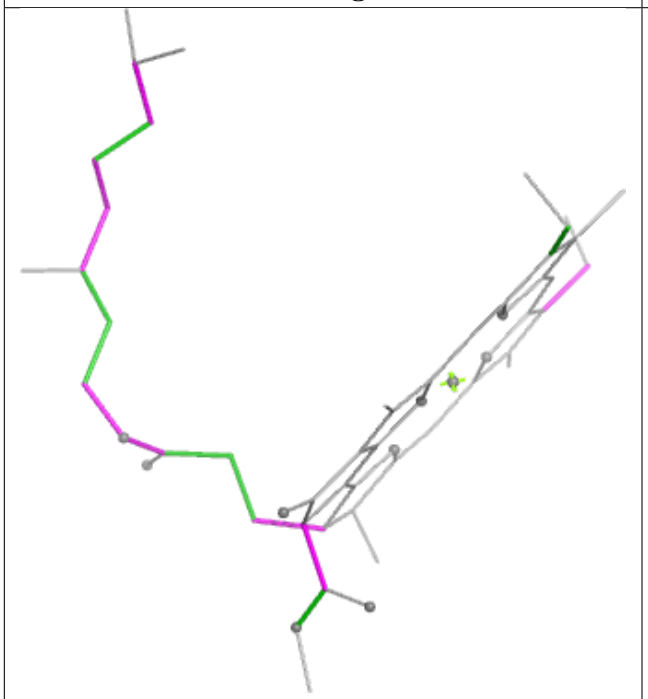
Rings

Ligand CLA 8 608

Bond lengths



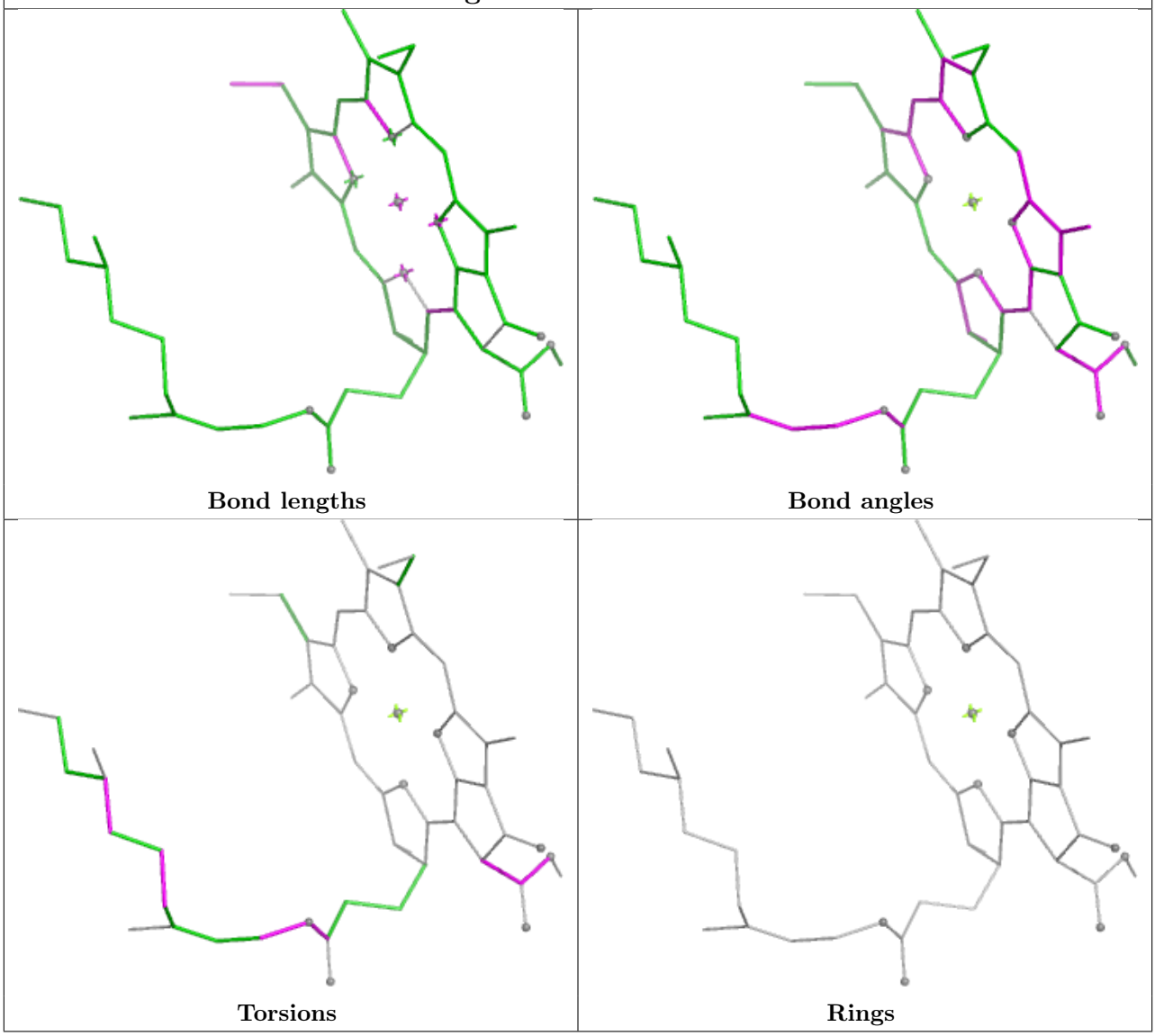
Bond angles



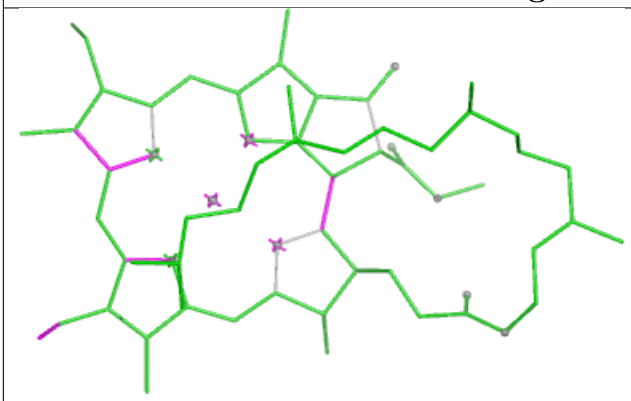
Torsions

Rings

Ligand CLA B 1212

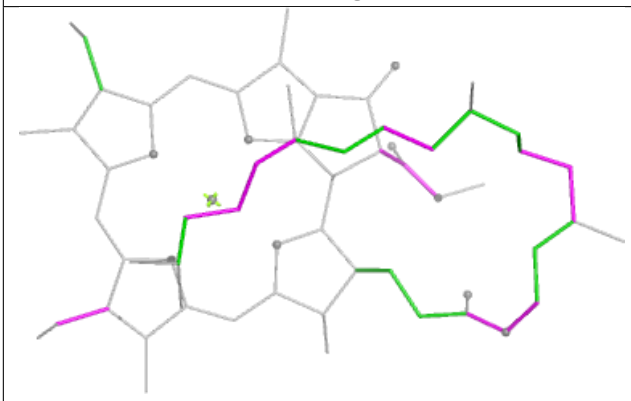


Ligand CLA 1 615



Bond lengths

Bond angles



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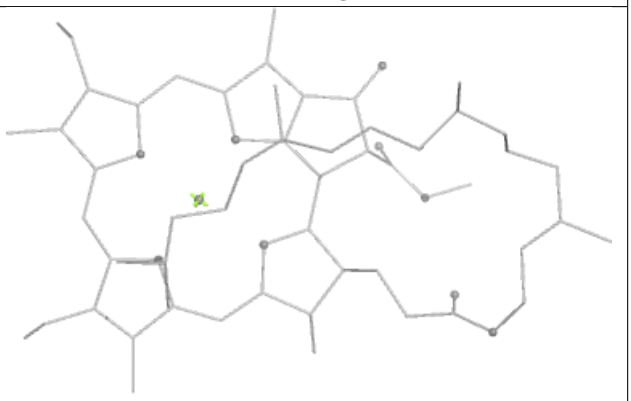
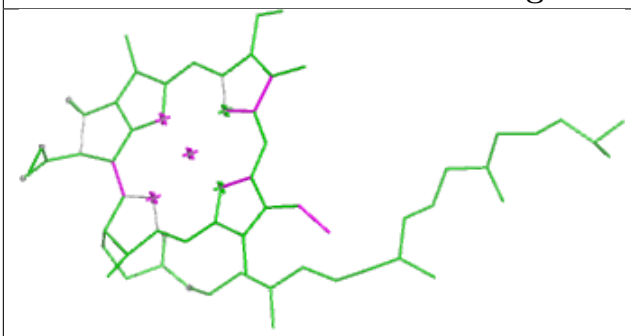
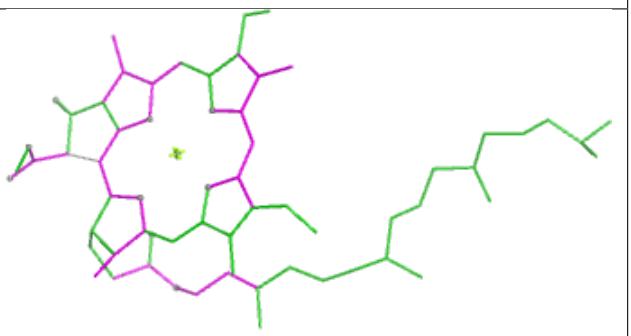


Rings

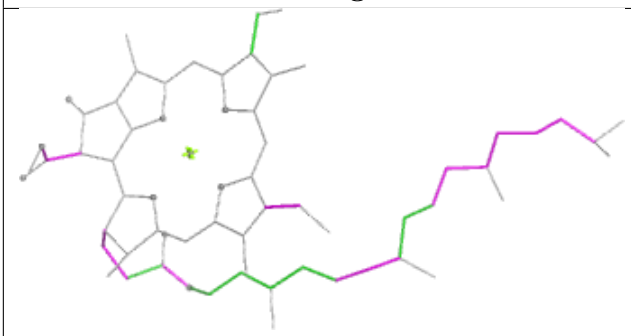
Ligand CLA Z 604



Bond lengths



Bond angles



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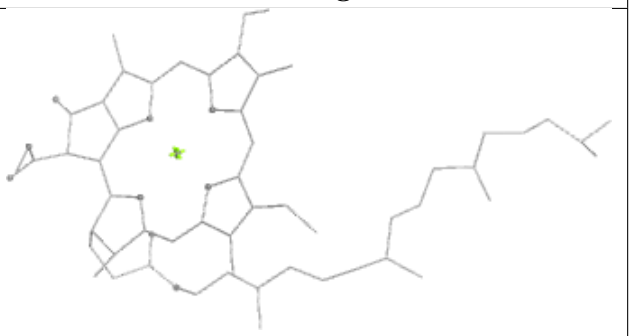
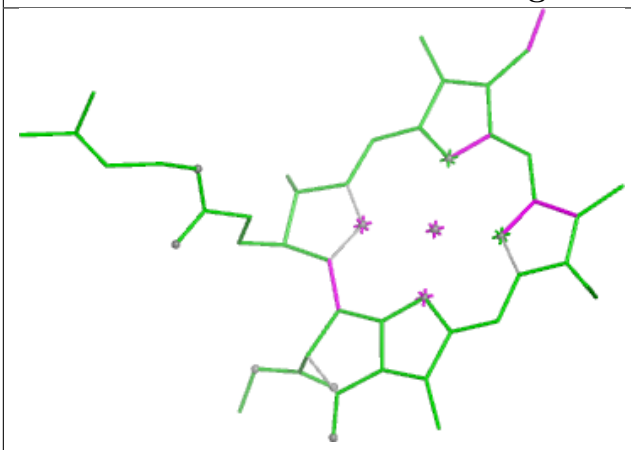


Rings

Ligand CLA 7 611



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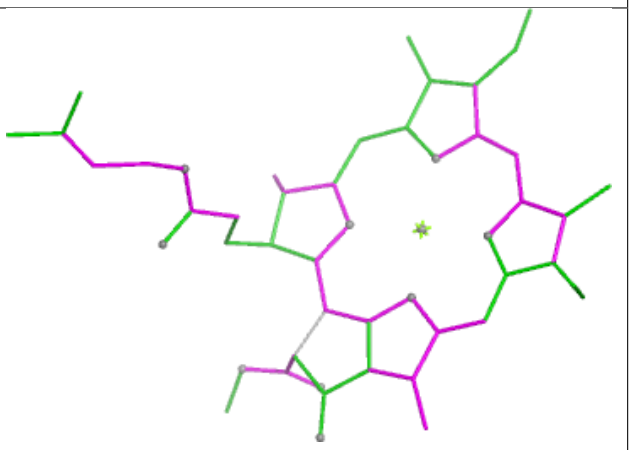
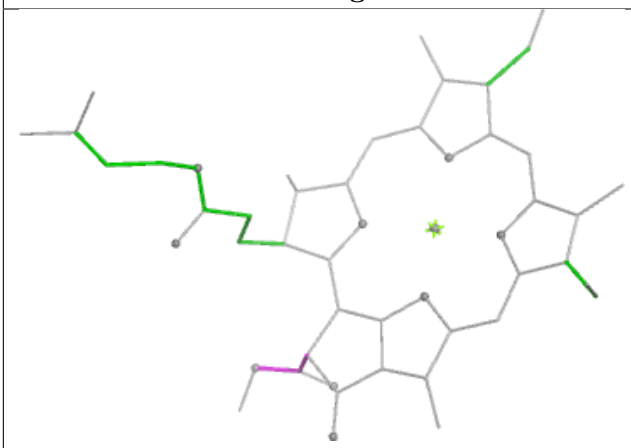


Bond angles



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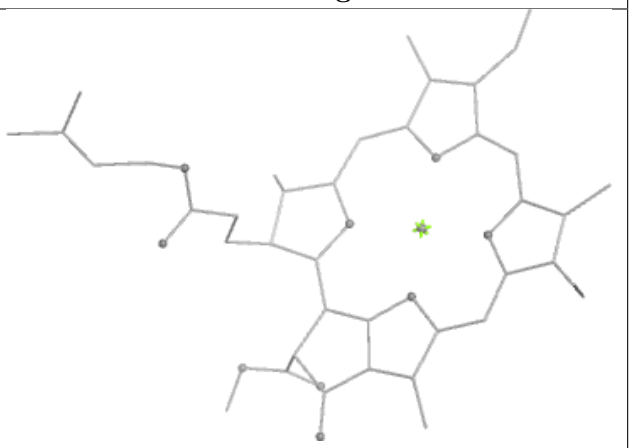
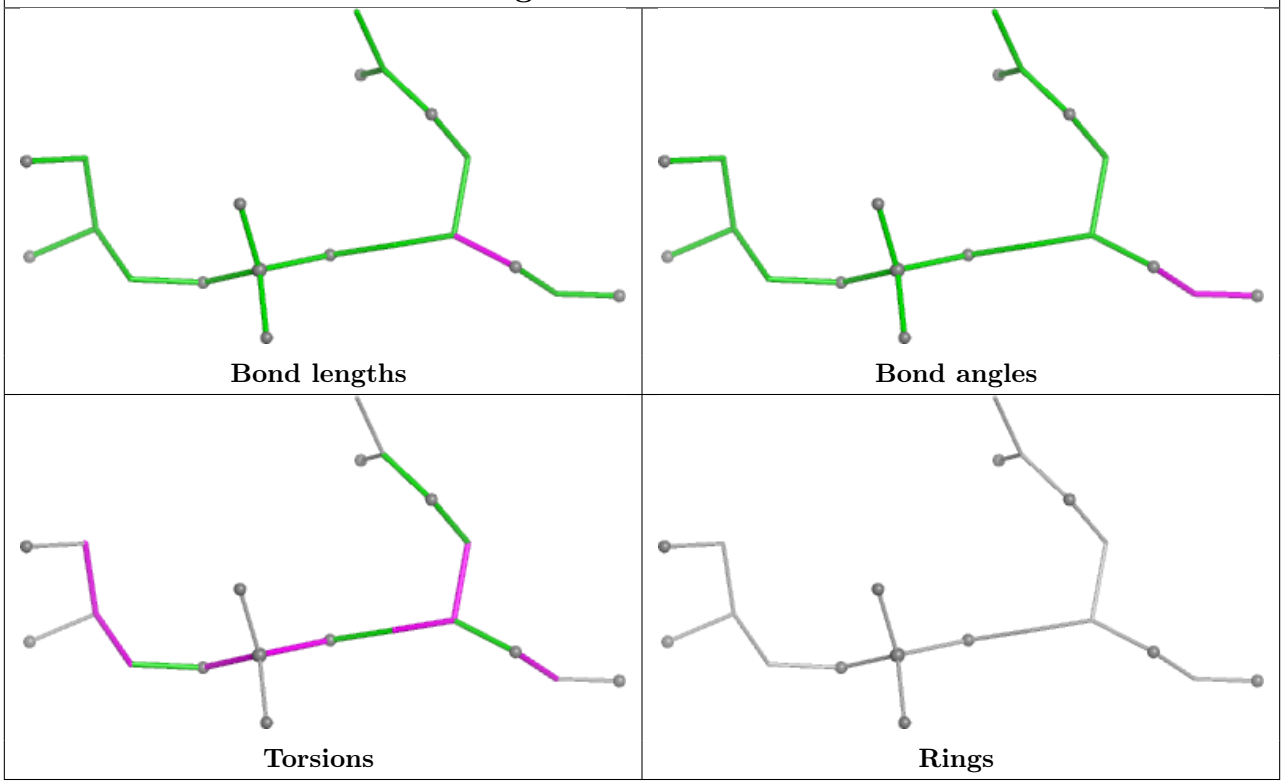
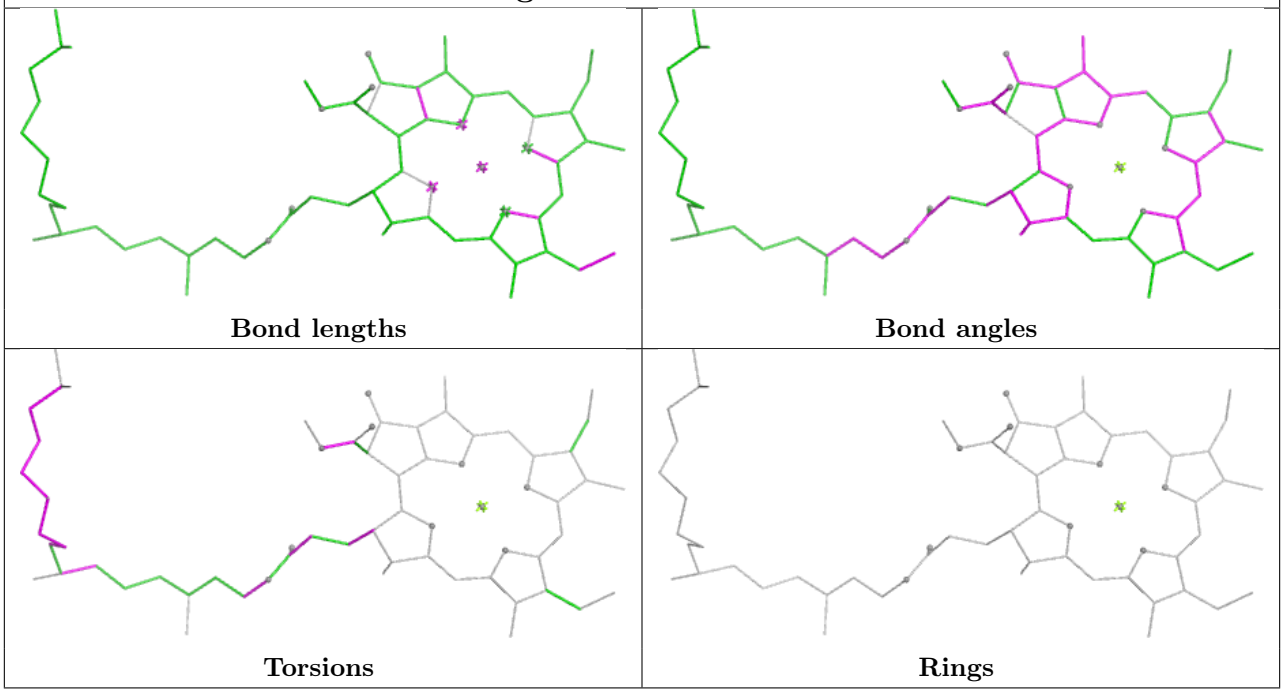


Rings

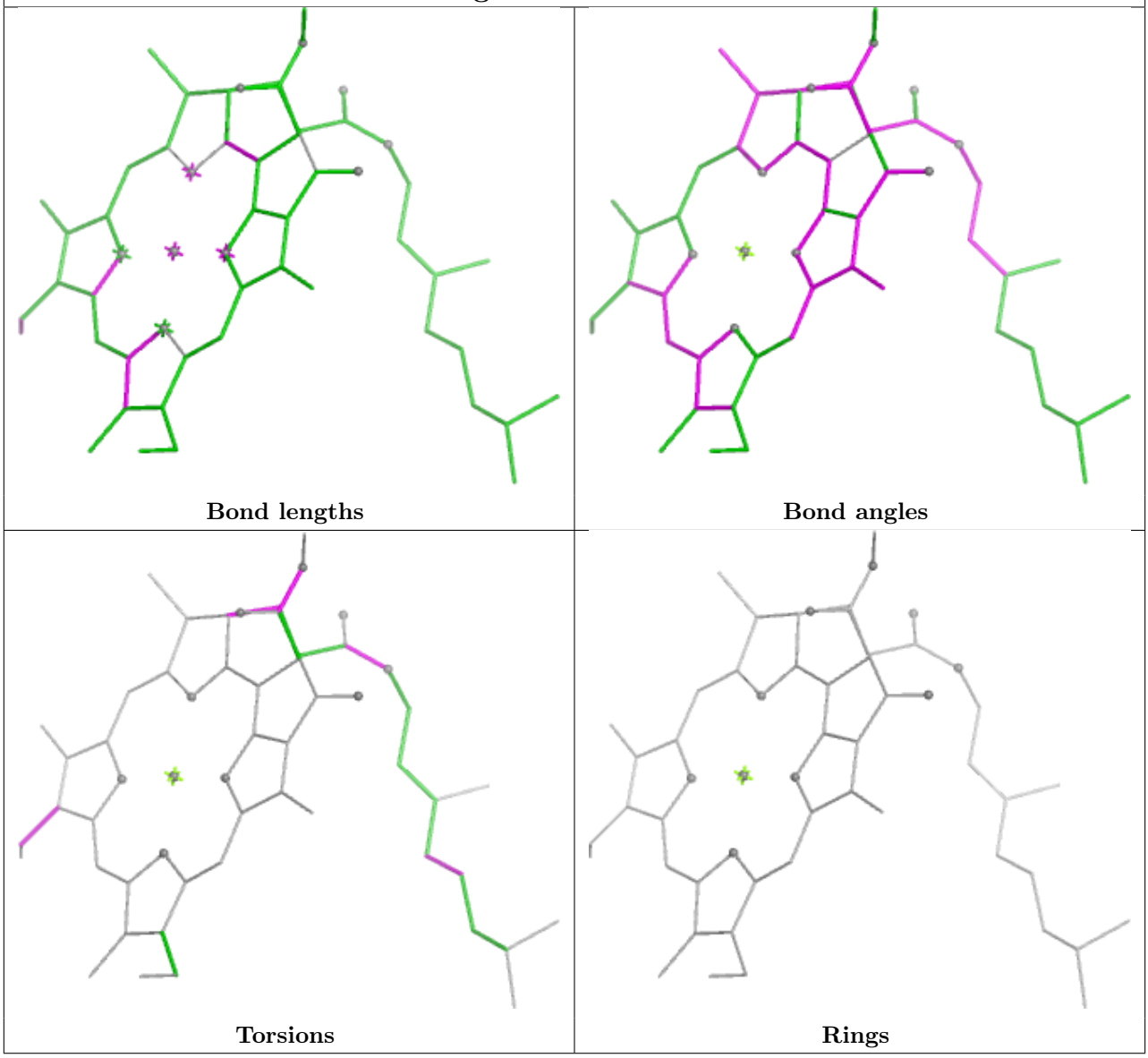
Ligand LHG B 5002

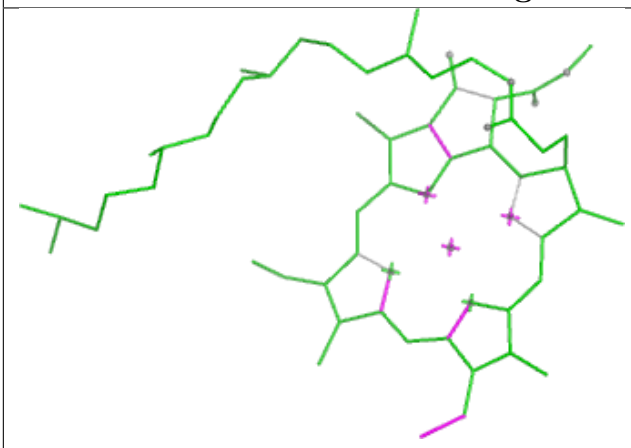
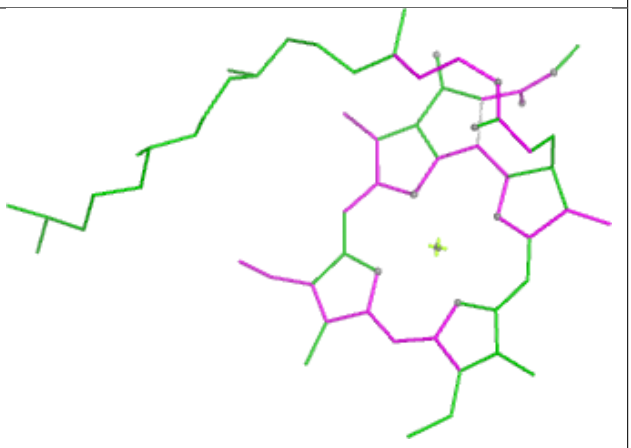
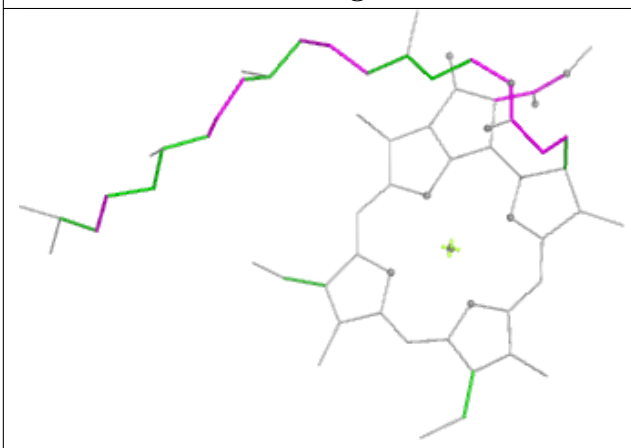


Ligand CLA B 1223

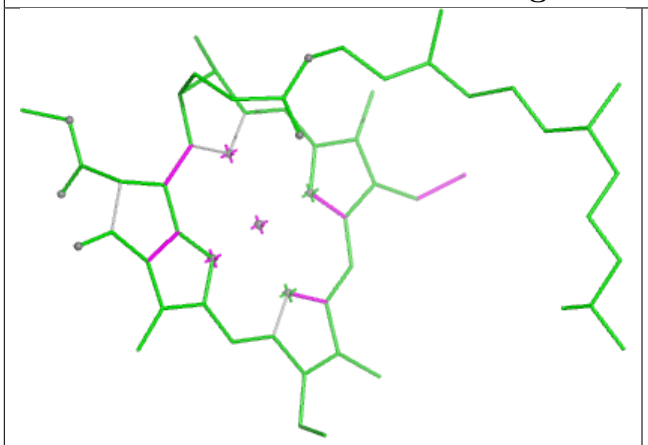


Ligand CLA 6 607

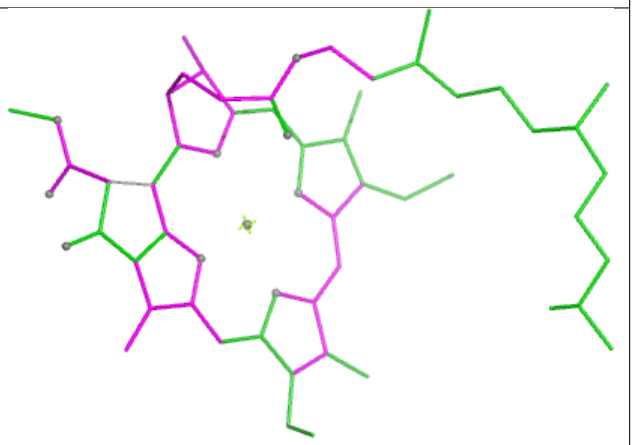


Ligand CLA A 1127	
 Bond lengths	 Bond angles
 Torsions	Rings

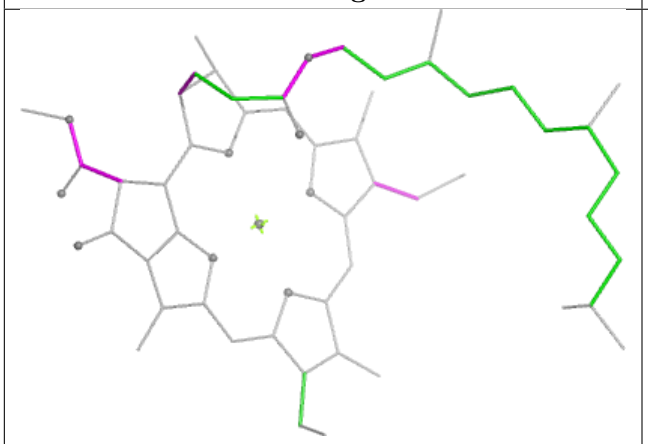
Ligand CLA 3 604



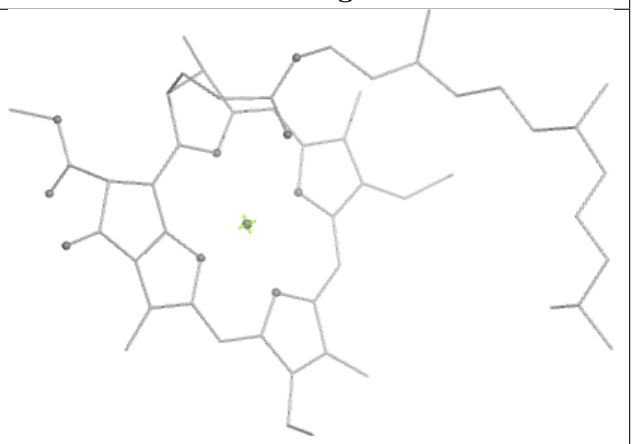
Bond lengths



Bond angles

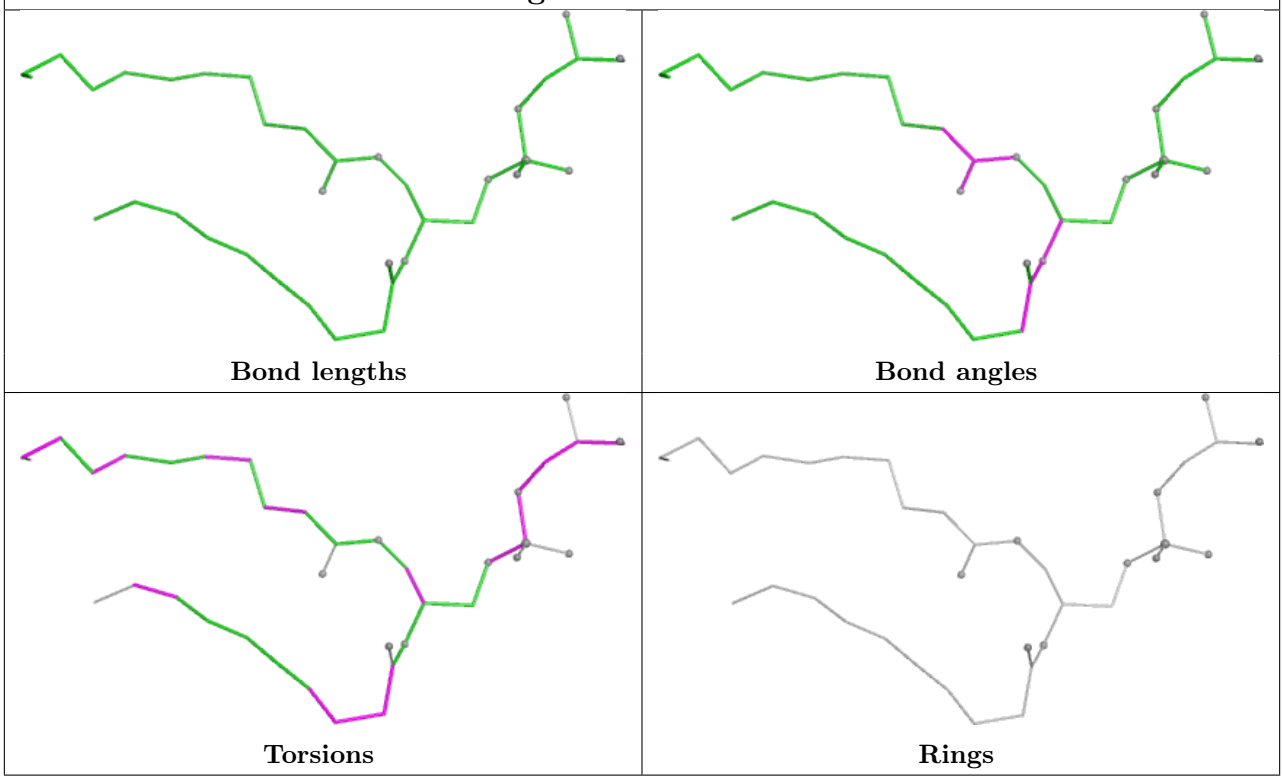


Torsions

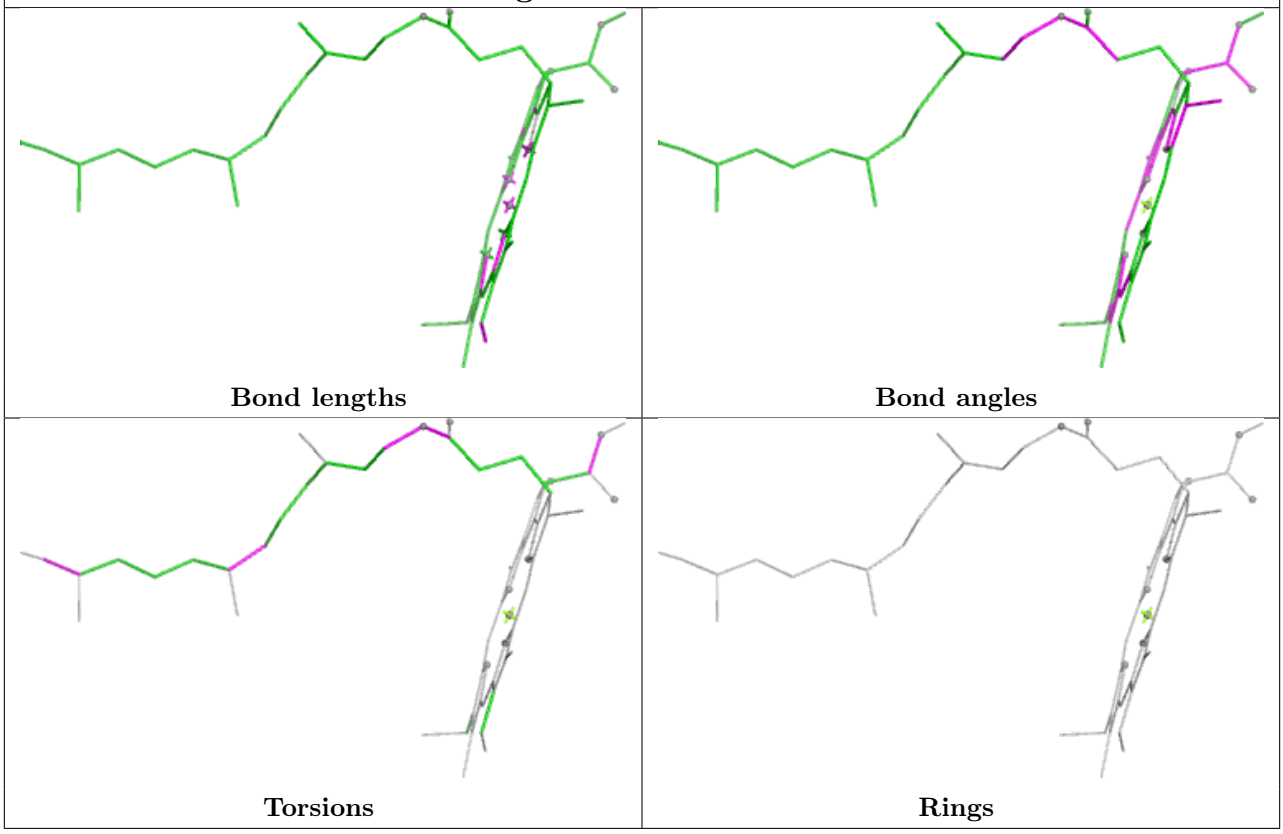


Rings

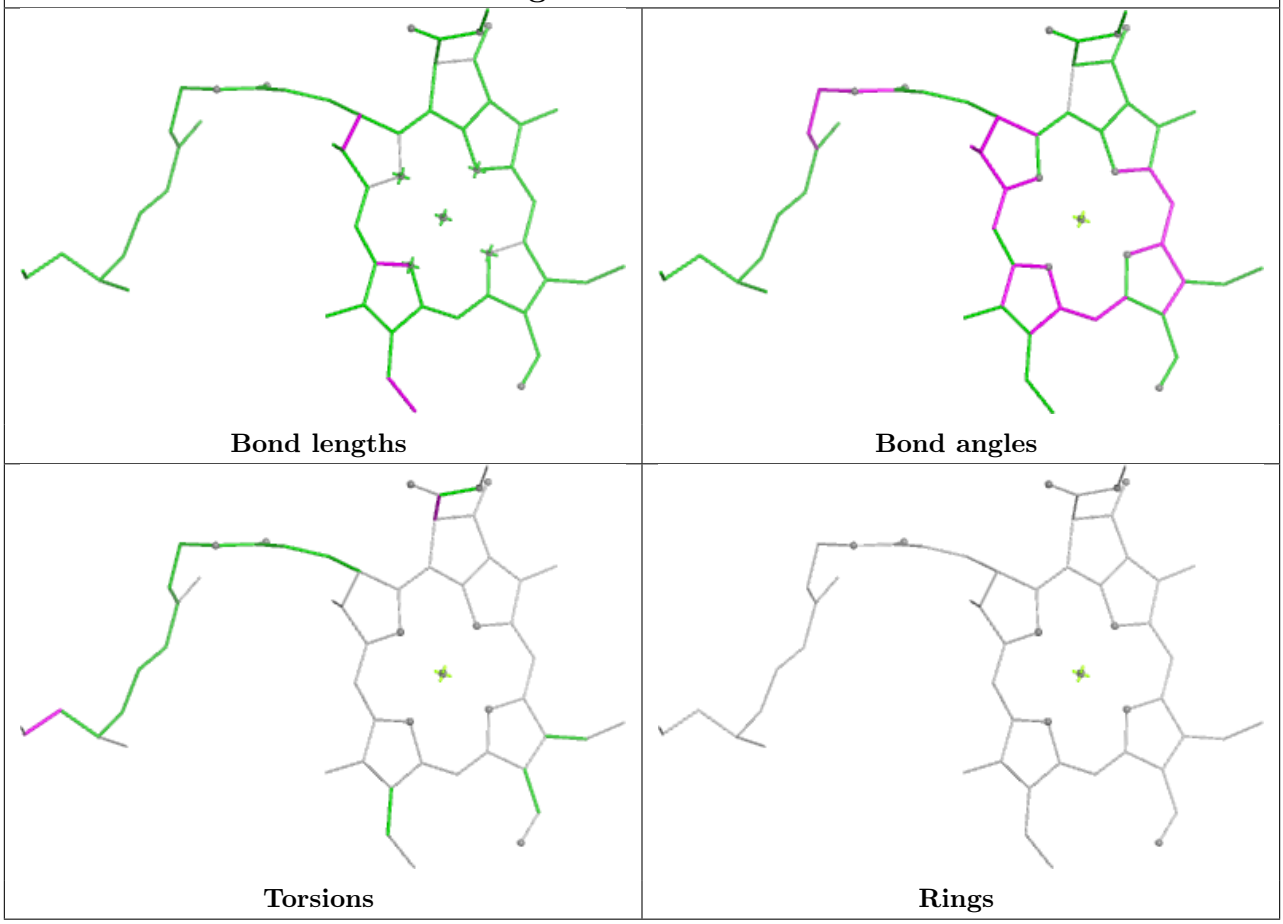
Ligand LHG 8 801



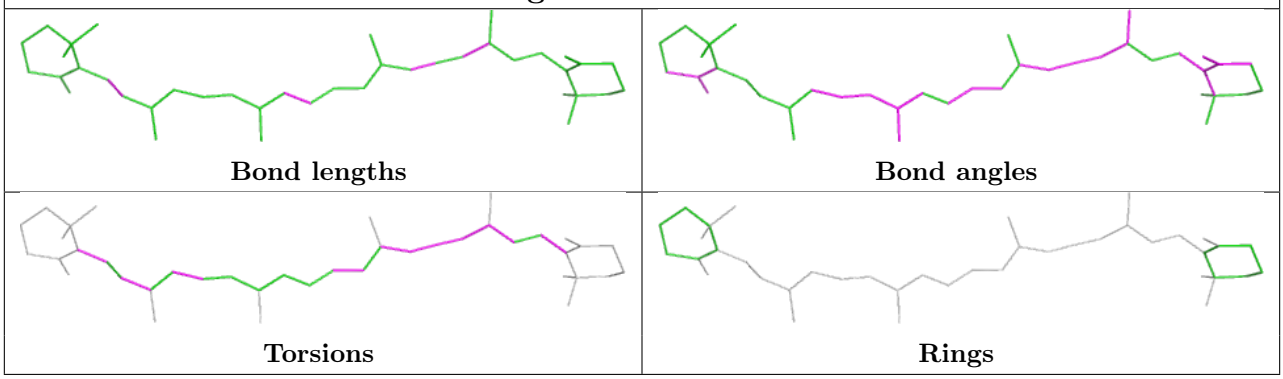
Ligand CLA A 1114



Ligand CHL 1 609



Ligand BCR 4 503



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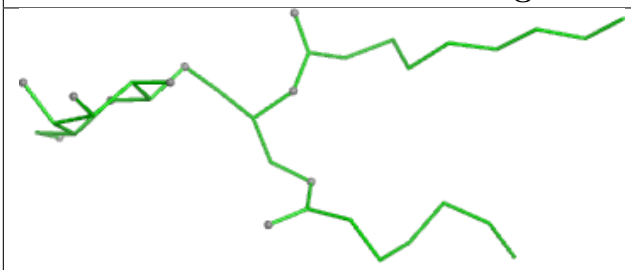
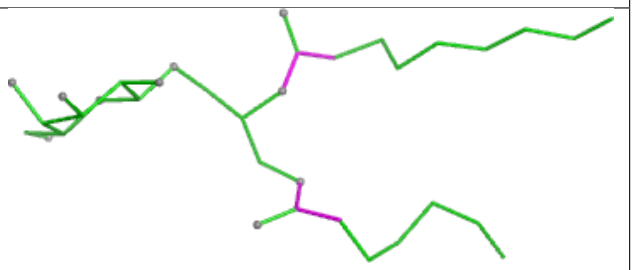
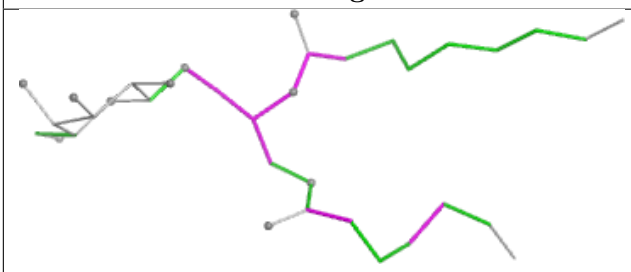
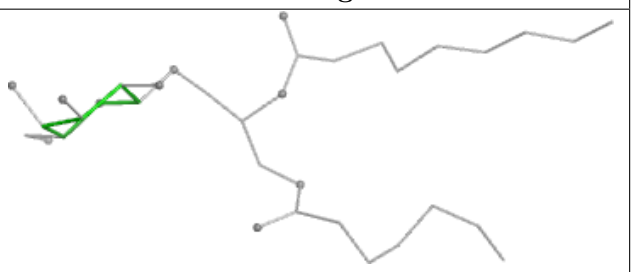
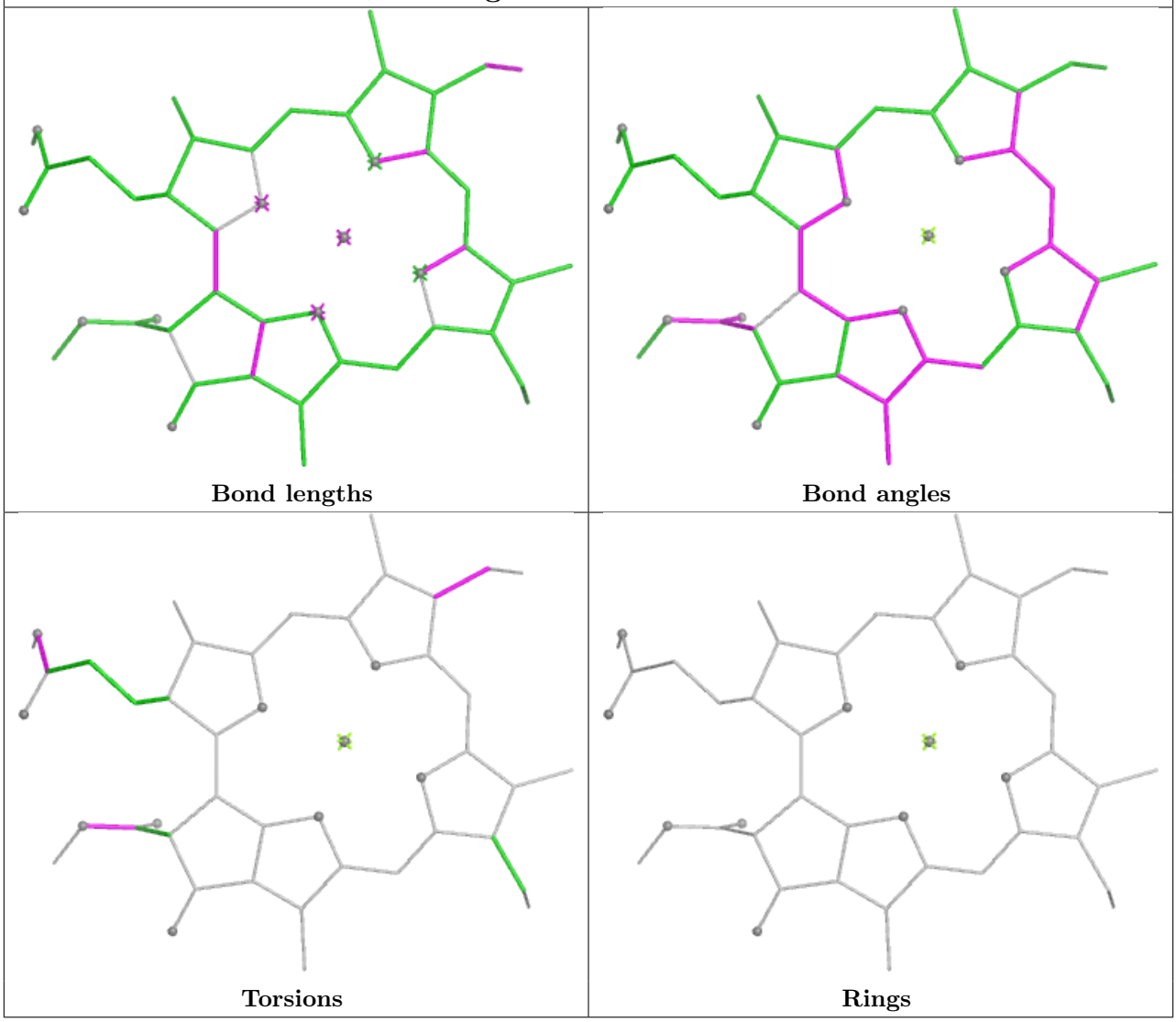
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 602



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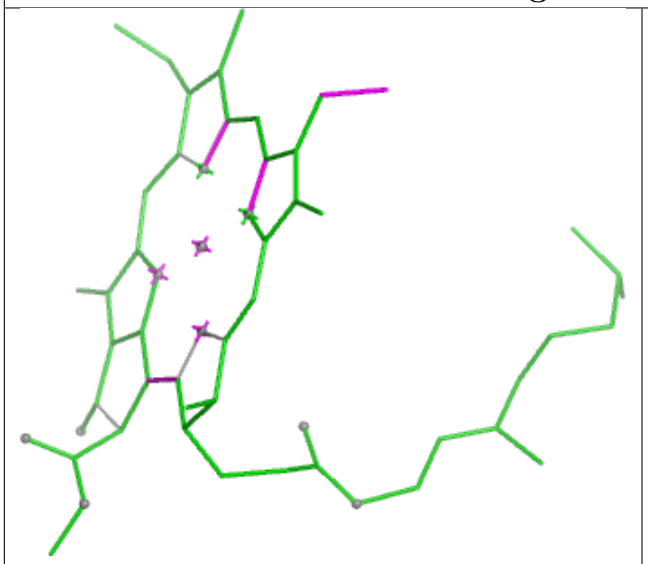
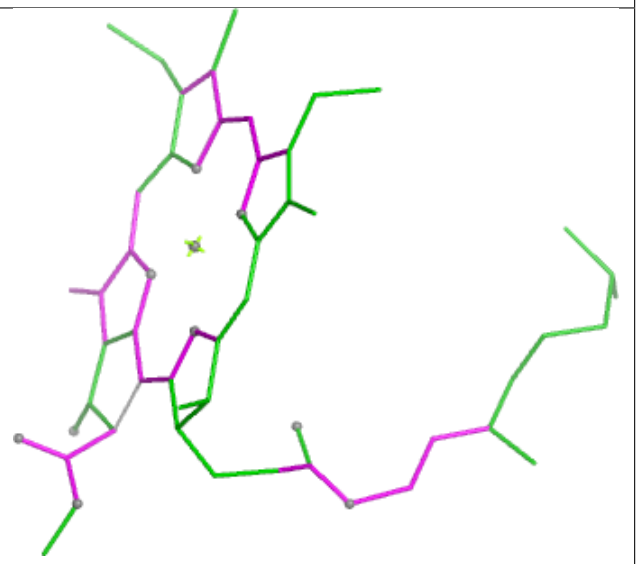
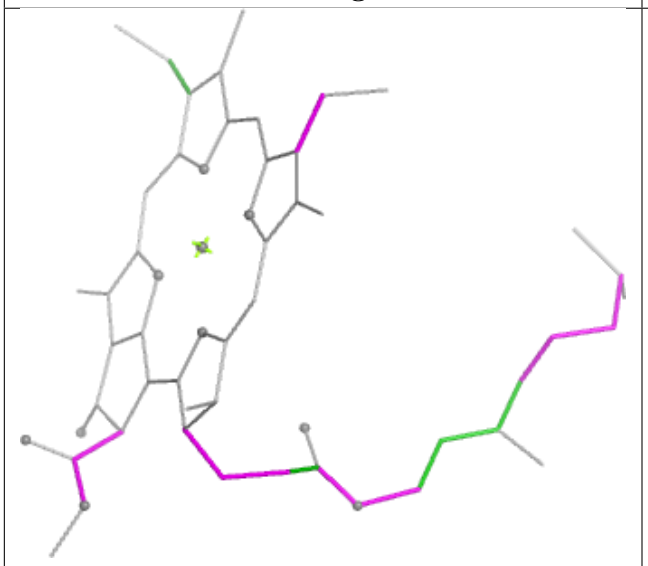


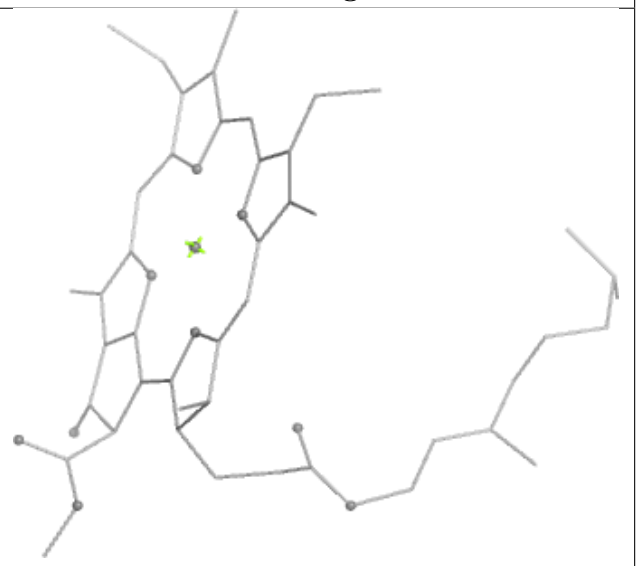
Bond lengths



Bond angles

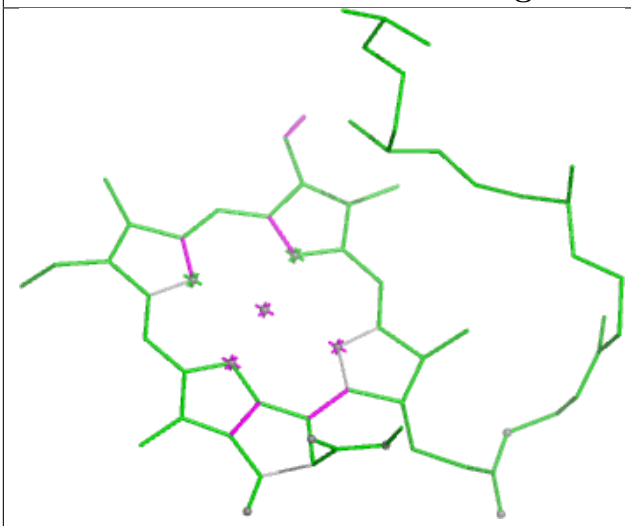


Torsions



Rings

Ligand CLA A 1111



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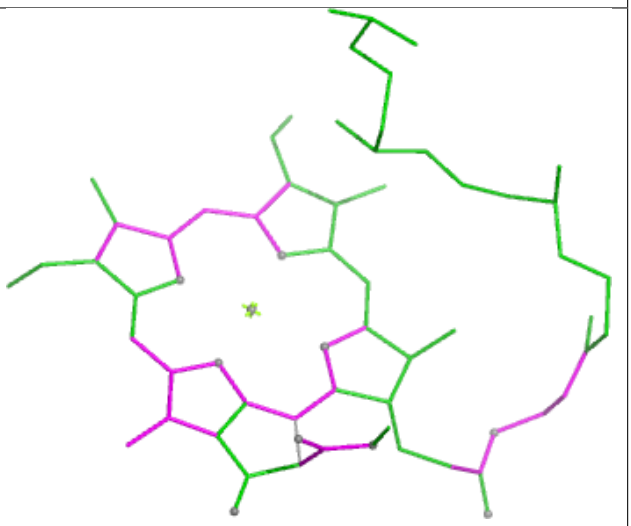
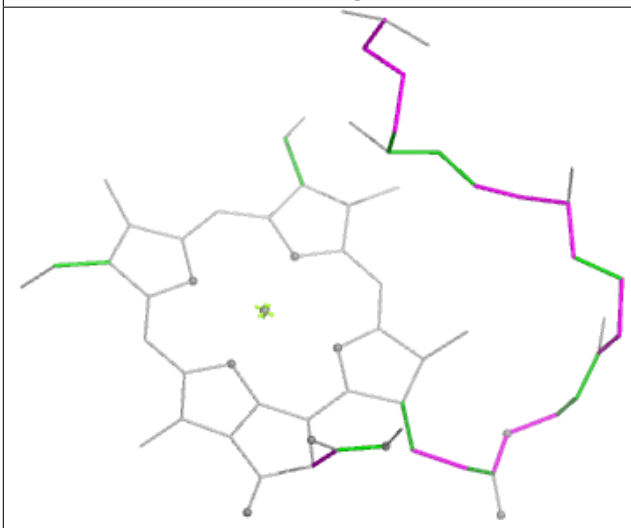


Bond angles



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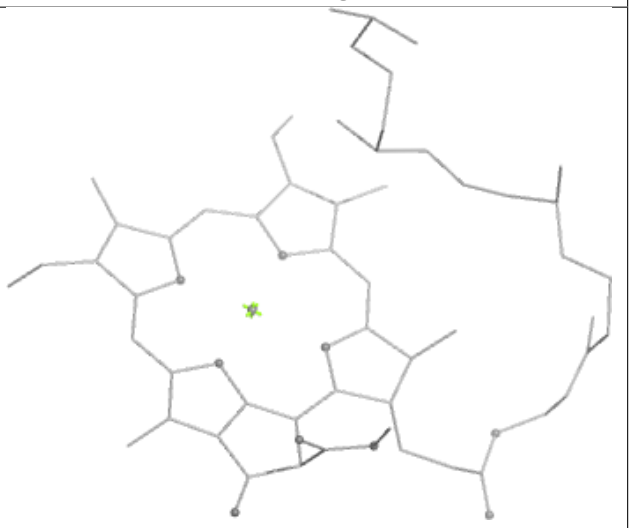
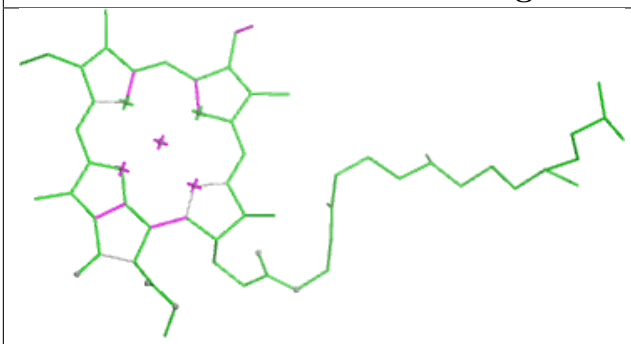


Rings

Ligand CLA B 1023



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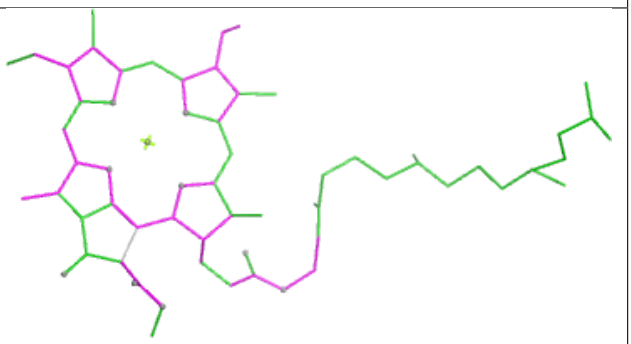

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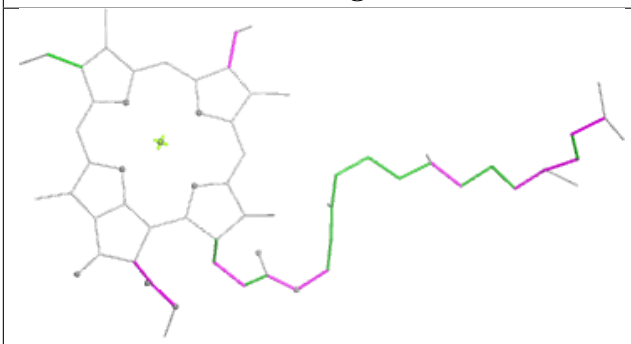

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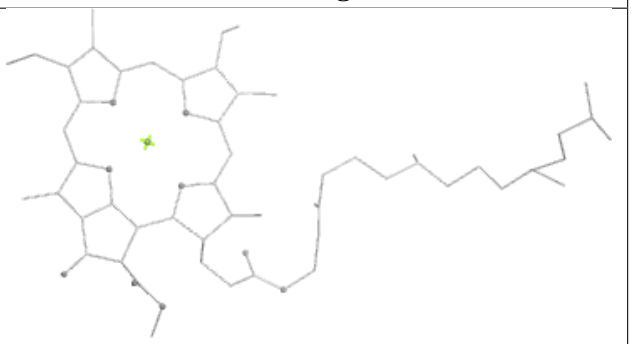
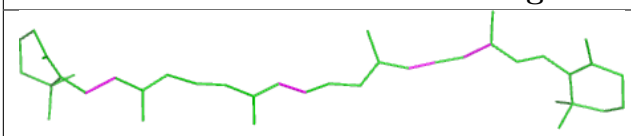


Rings

Ligand BCR 8 503



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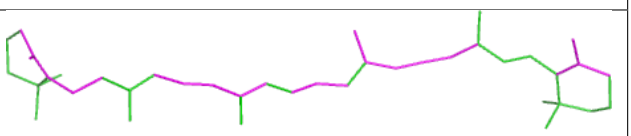

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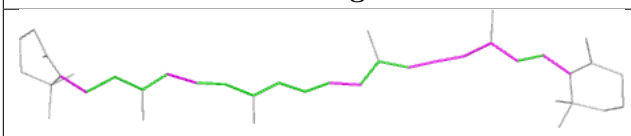
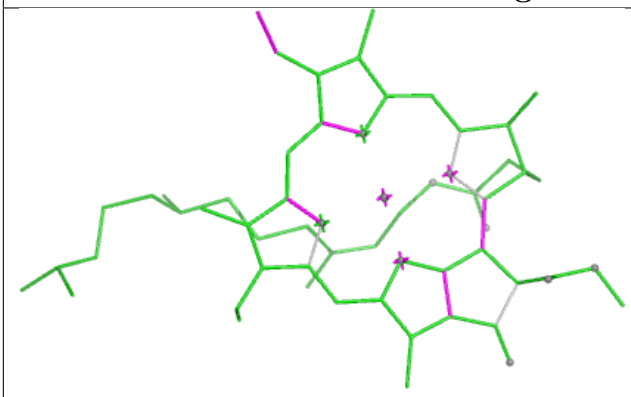


Torsions

Rings

Ligand CLA A 1115



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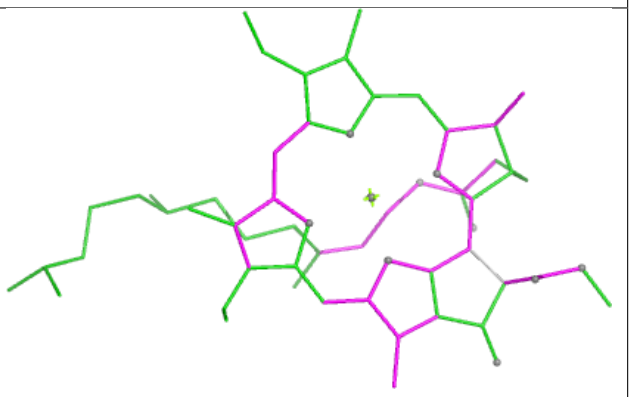

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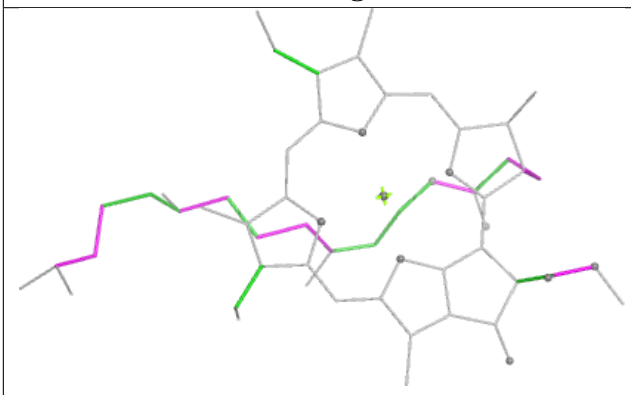

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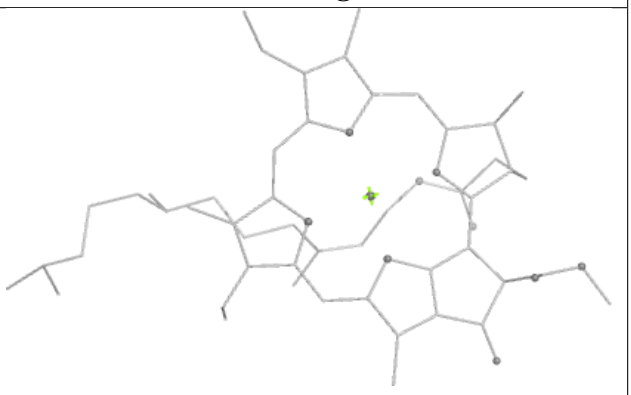
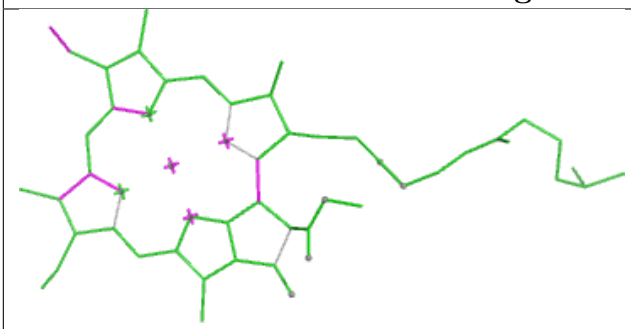


Rings

Ligand CLA K 1404



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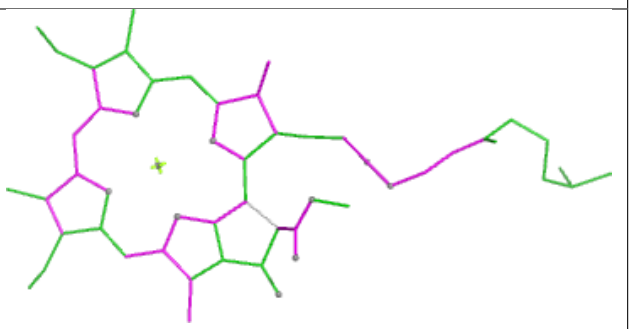

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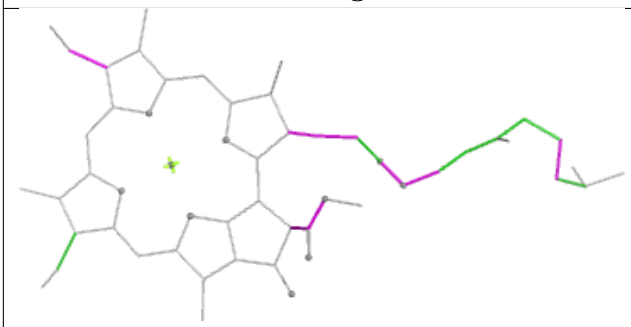

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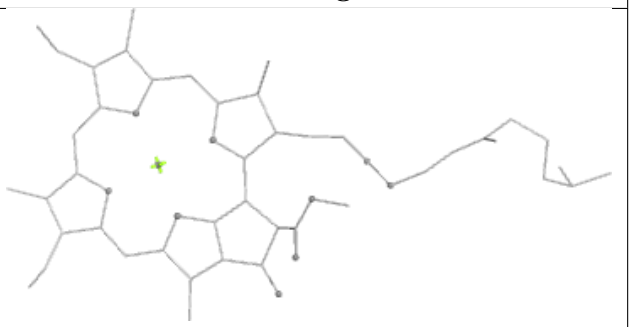
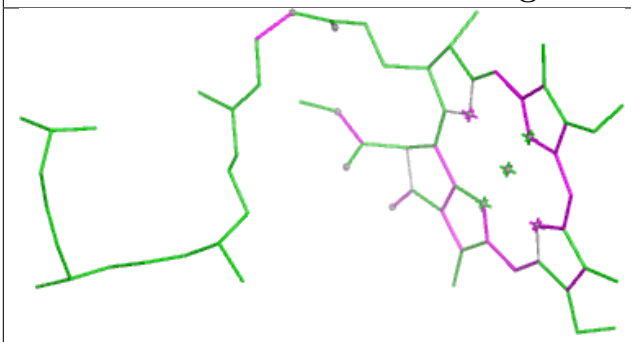
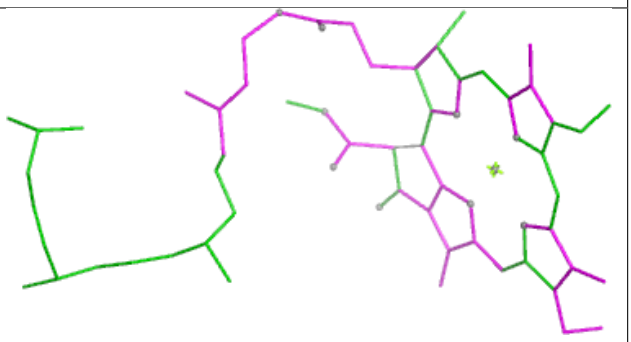
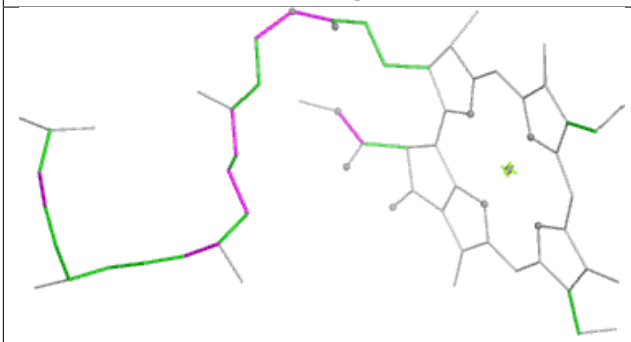
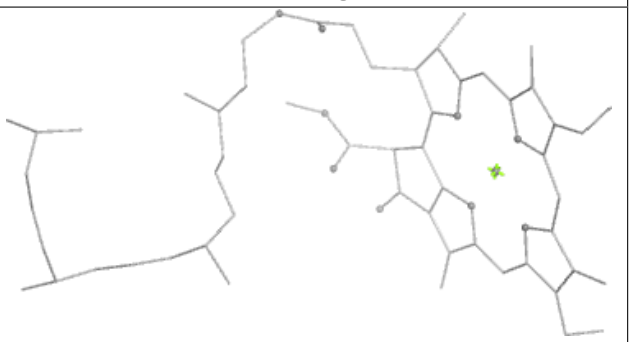


Rings

Ligand CL0 A 1011	
 Bond lengths	 Bond angles
 Torsions	 Rings

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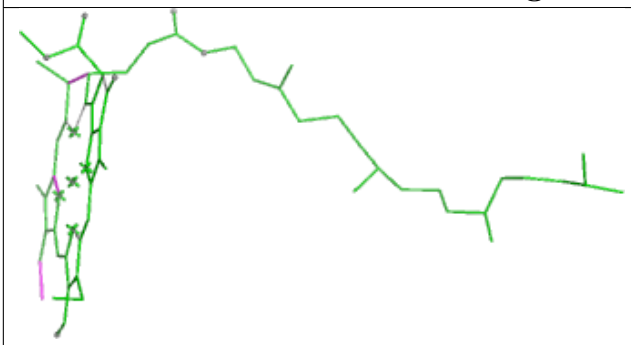
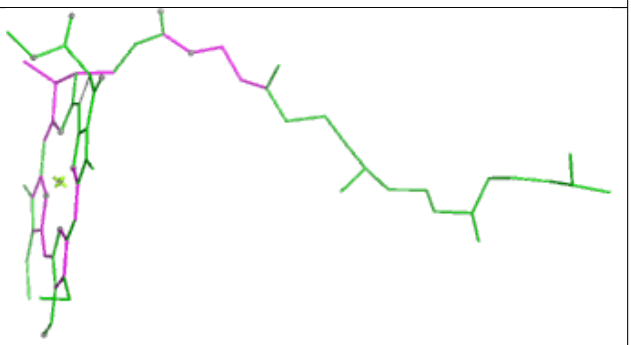
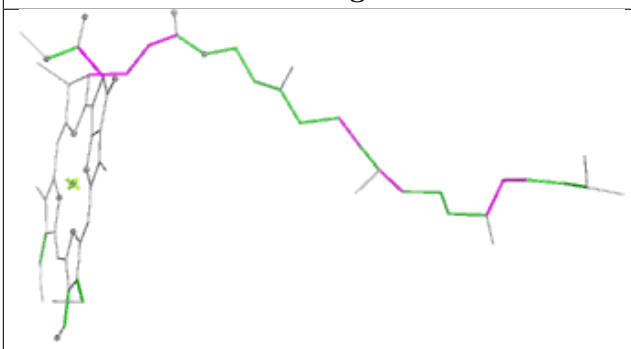
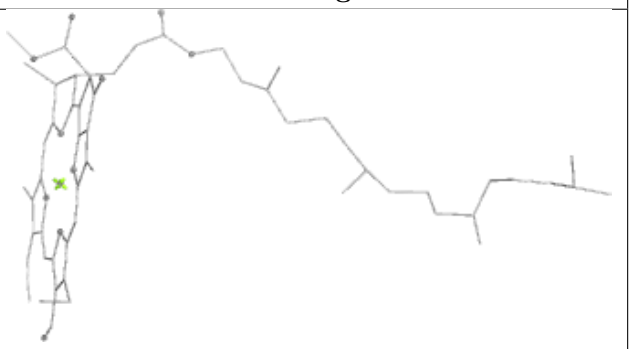
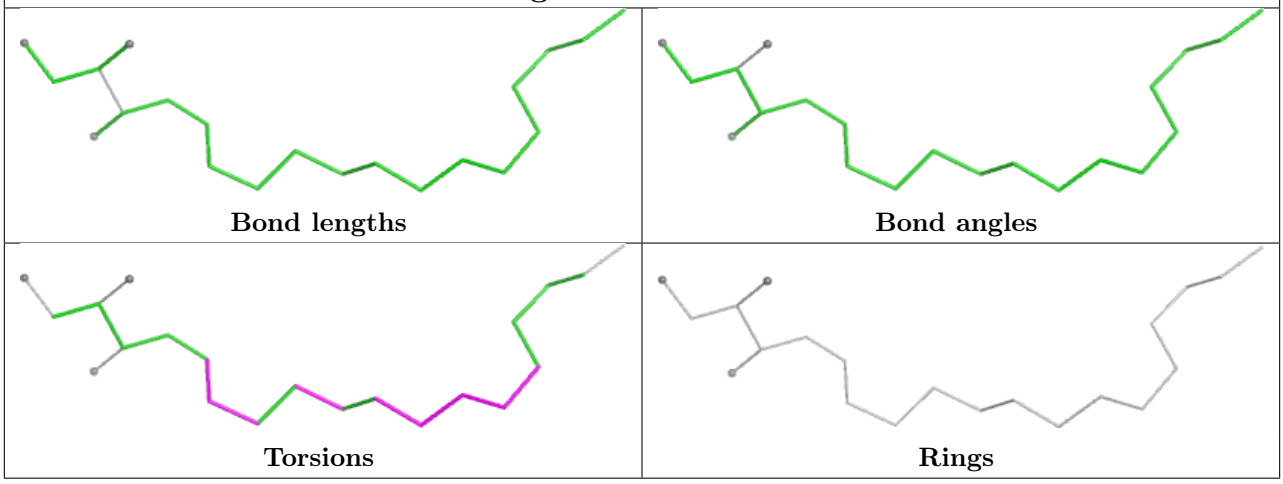
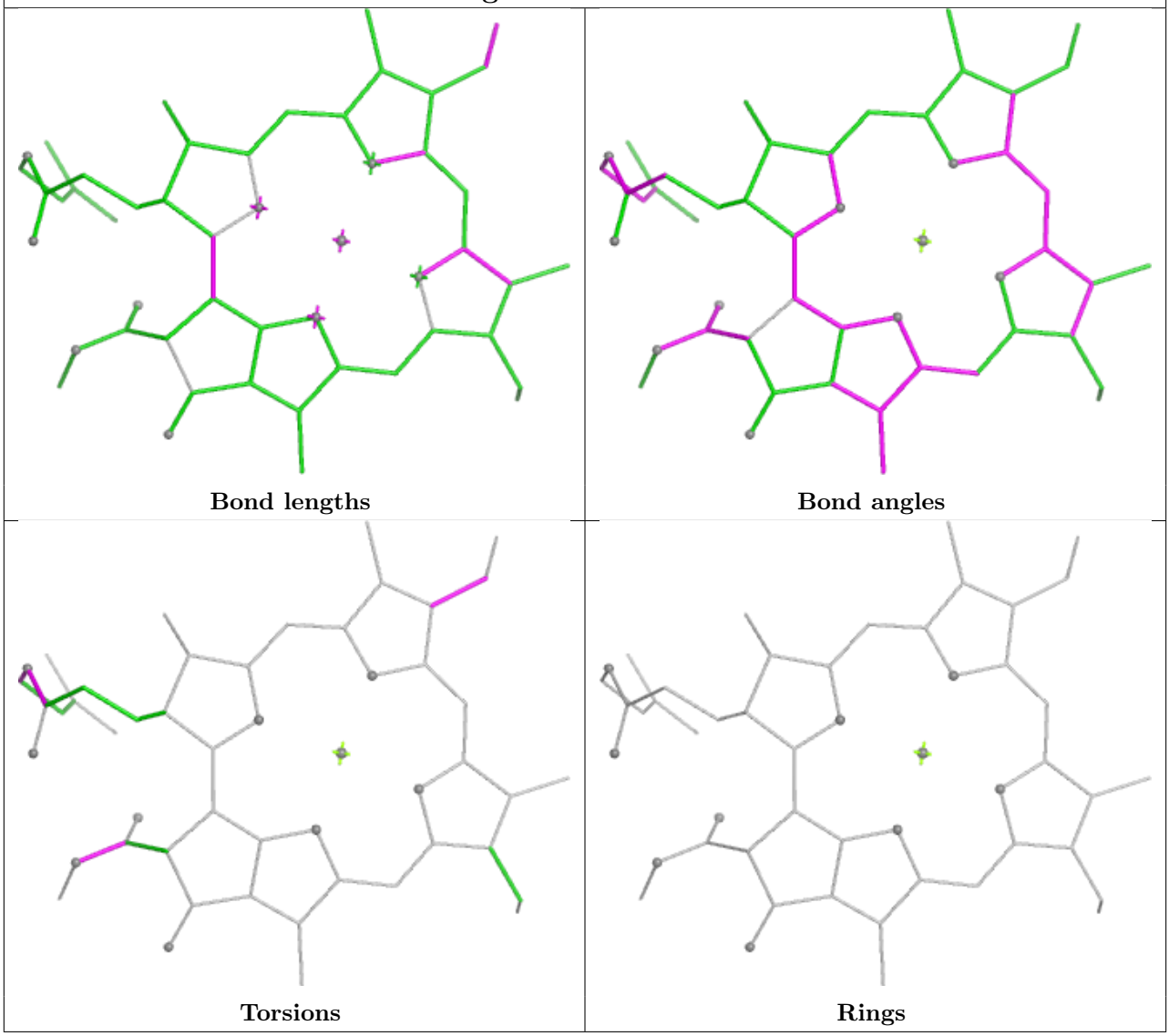
 Bond lengths	 Bond angles
 Torsions	 Rings

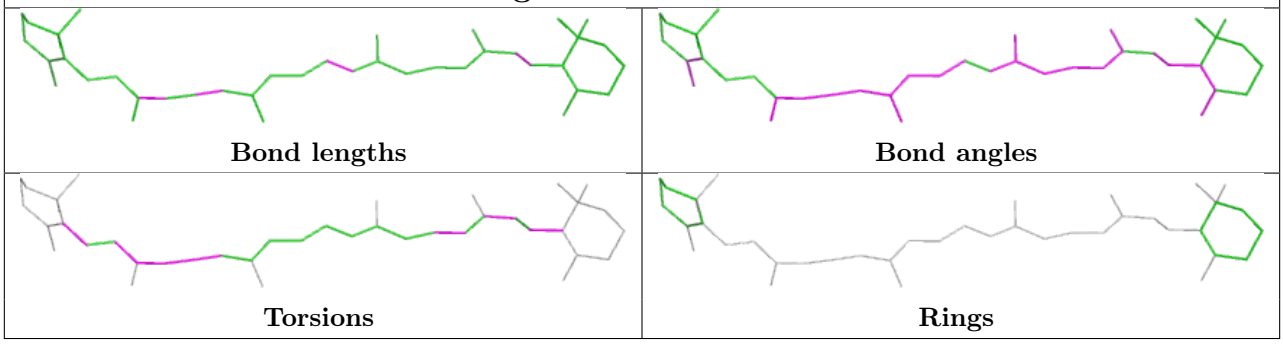
Ligand SPH 7 803



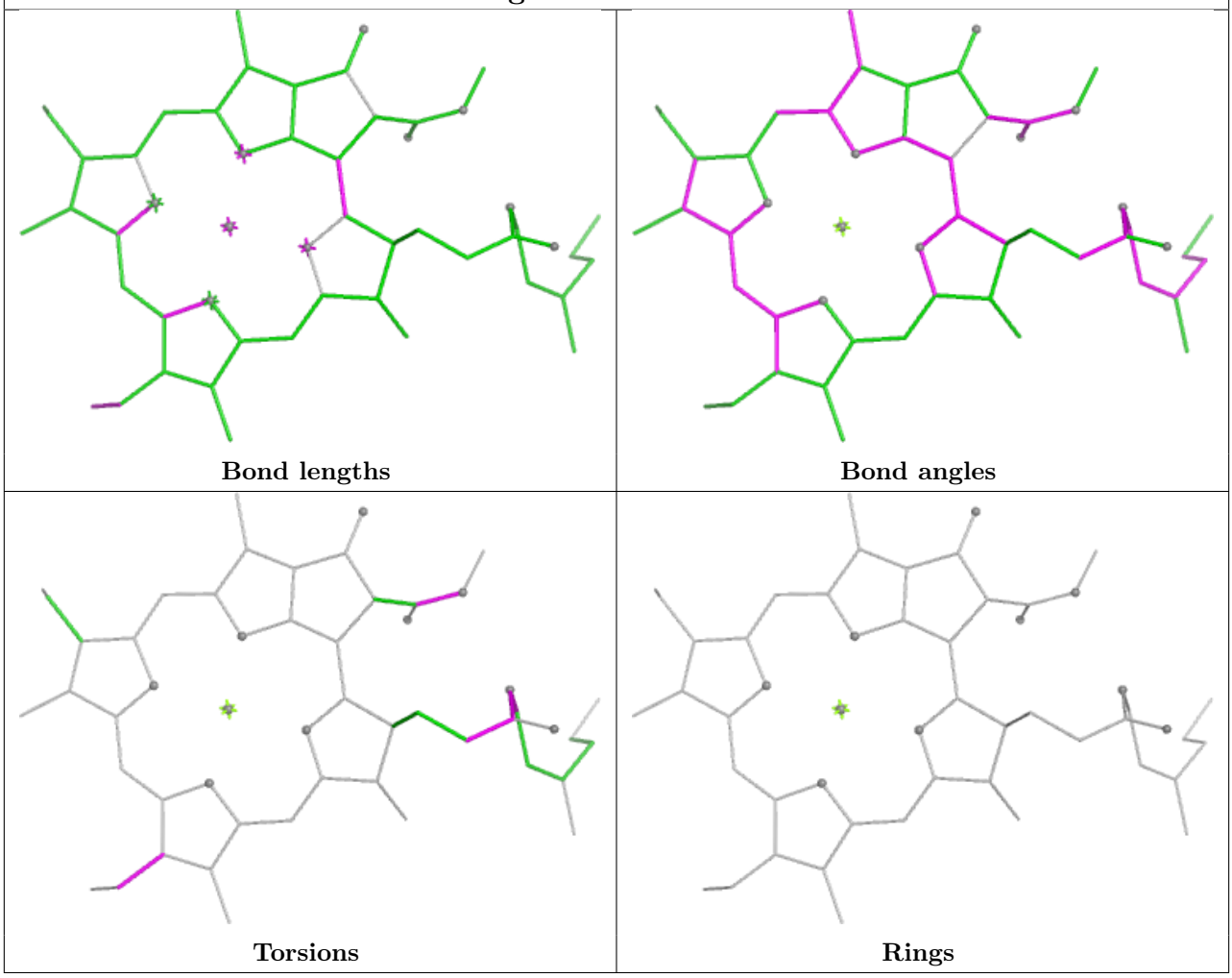
Ligand CLA 7 602



Ligand BCR G 4001



Ligand CLA 4 602



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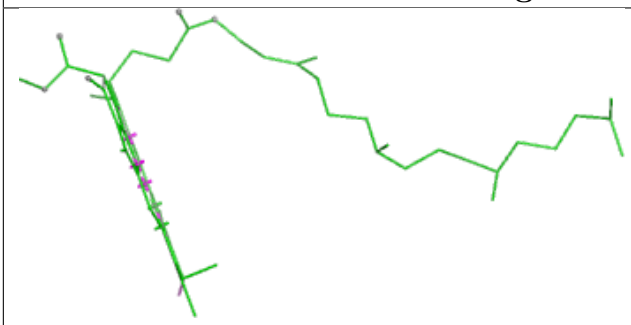
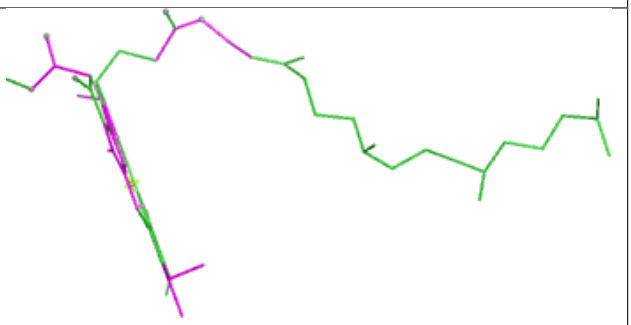
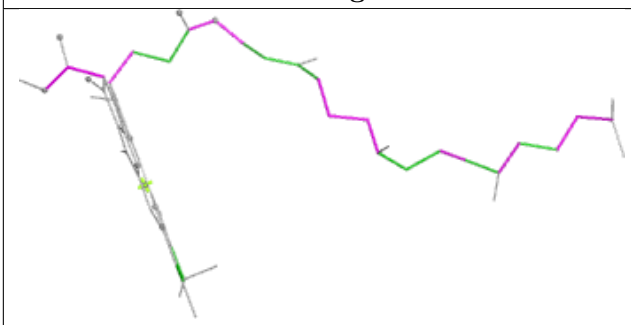
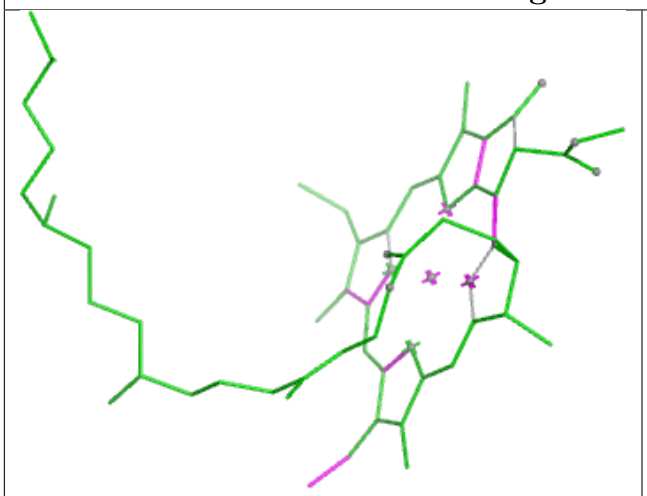
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 3 601



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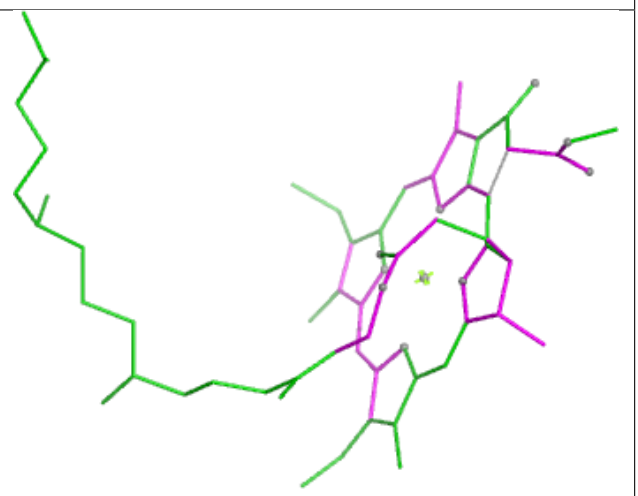

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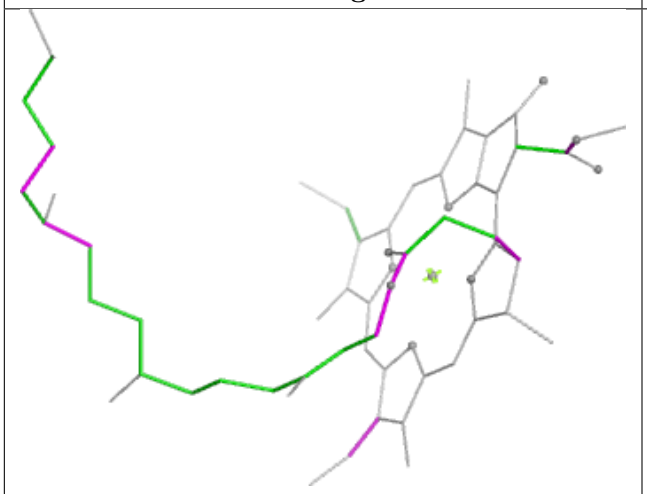

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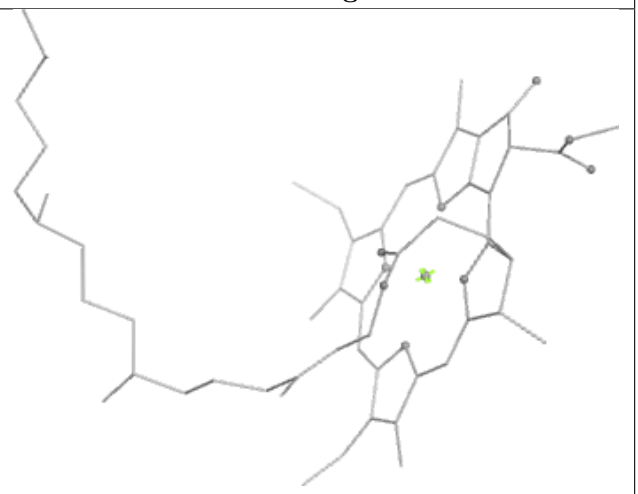
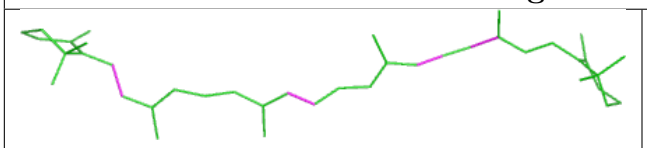


Rings

Ligand BCR 7 503



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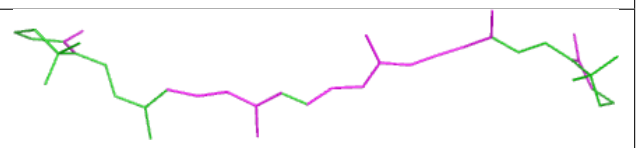
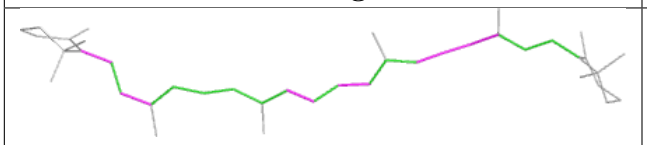


Bond angles



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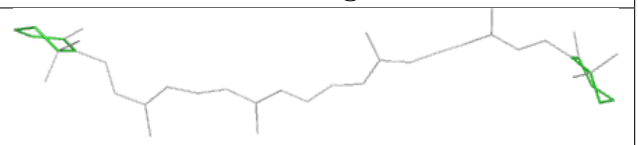
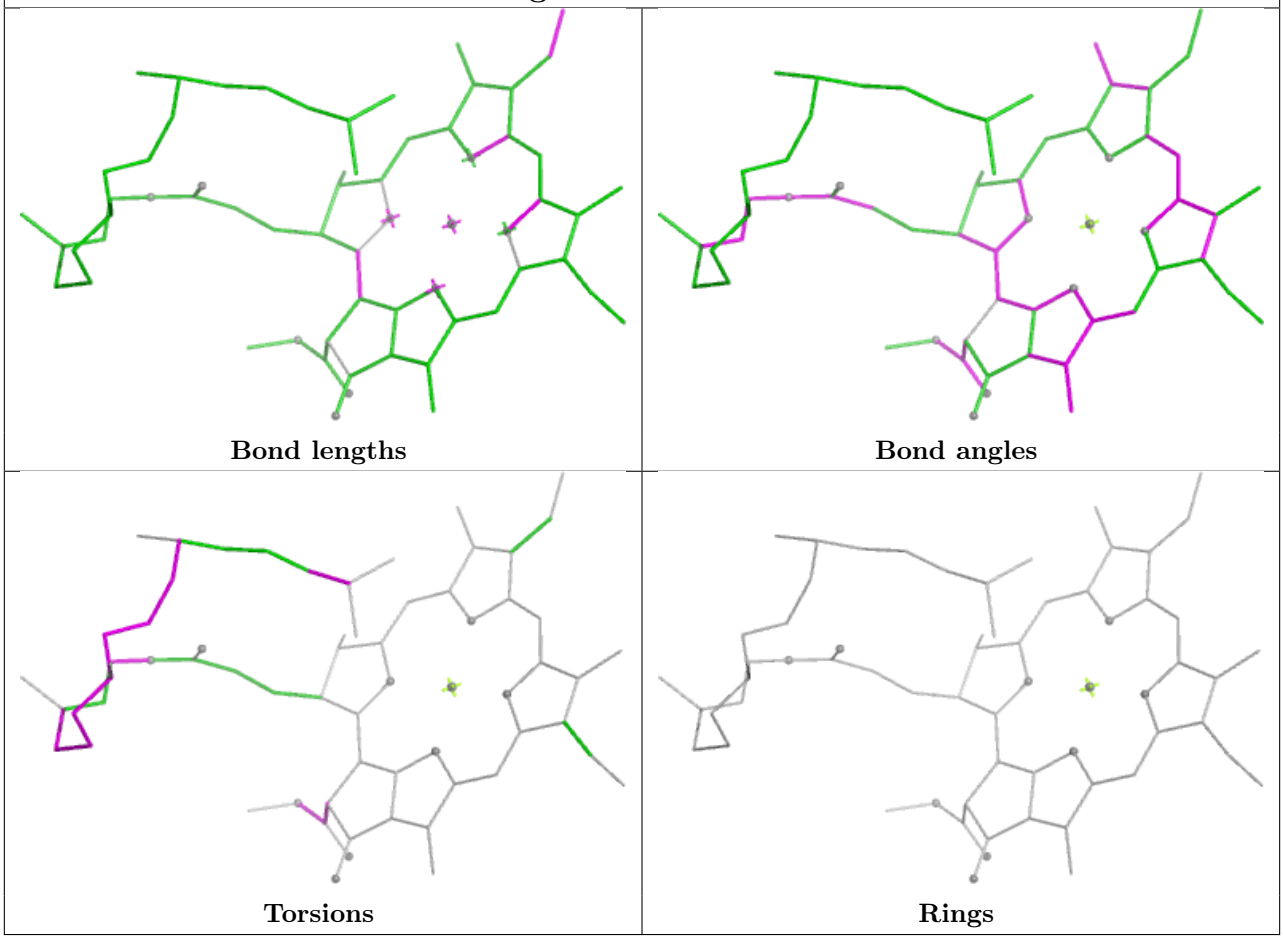
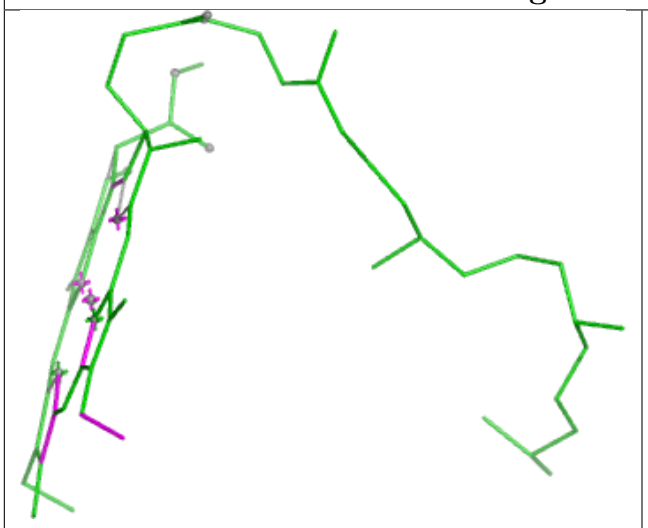


Rings

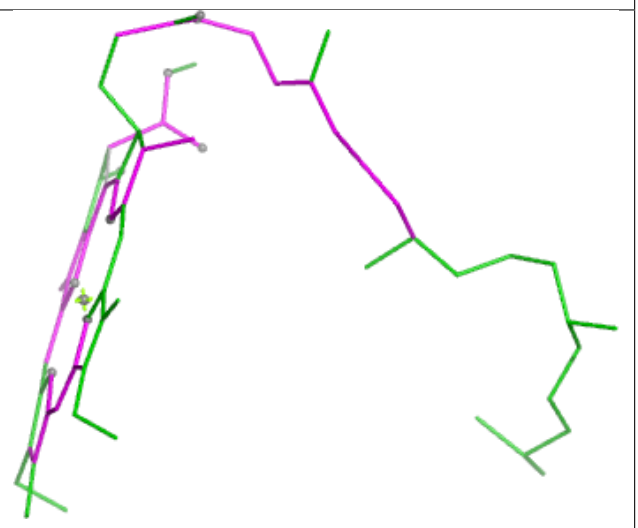
Ligand CLA 6 619



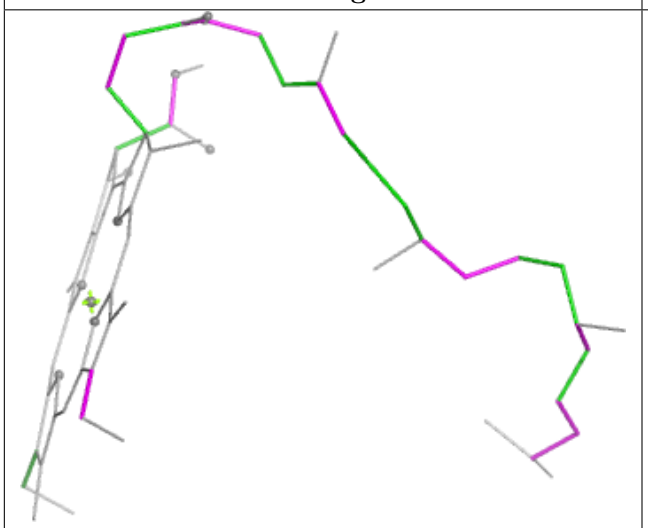
Ligand CLA 8 602



Bond lengths



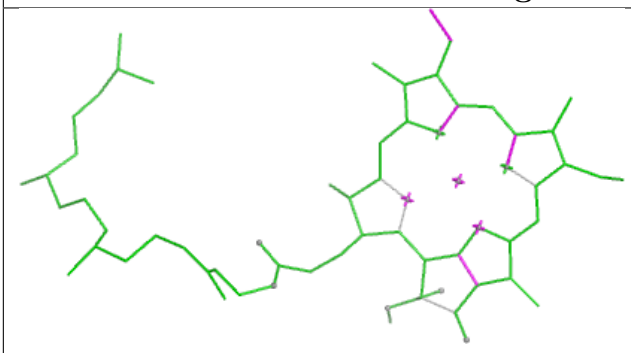
Bond angles



Torsions

Rings

Ligand CLA A 1125



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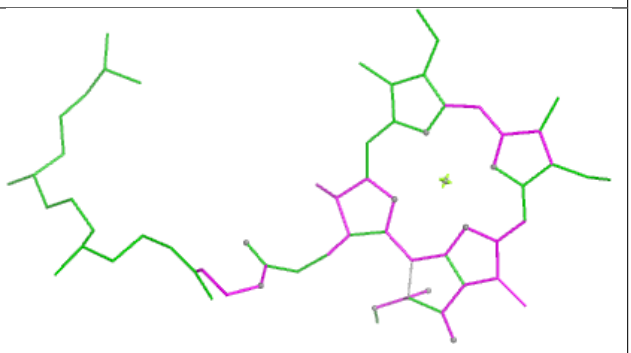
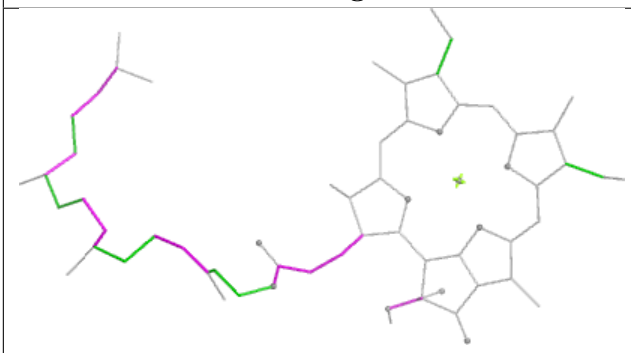
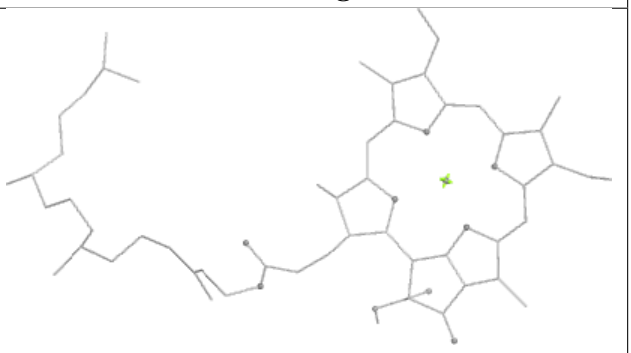


Bond angles

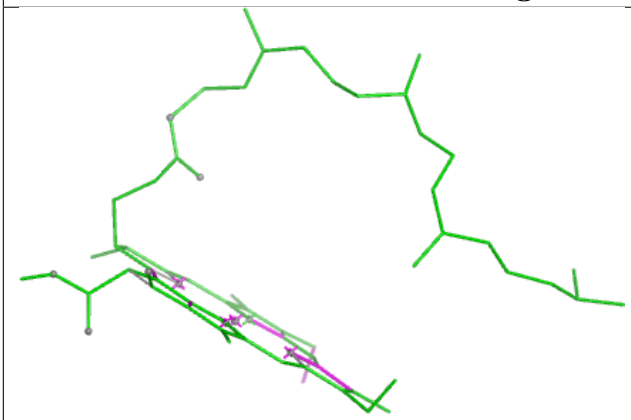


Torsions



Rings

Ligand CLA B 1241



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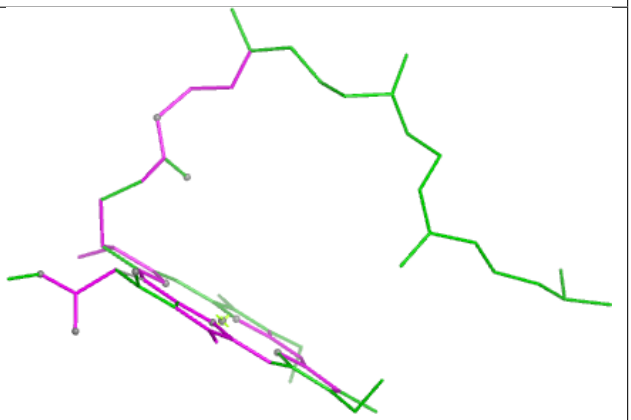
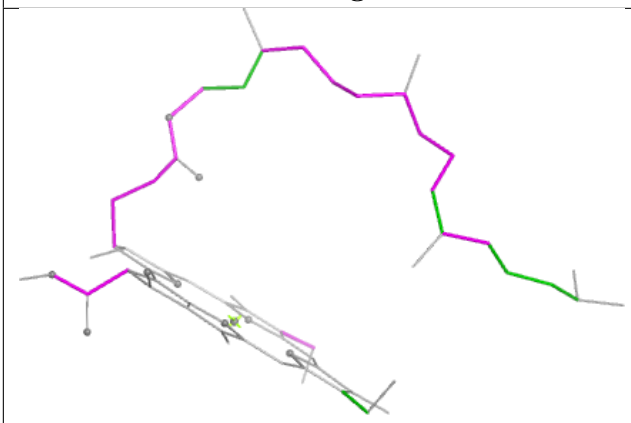
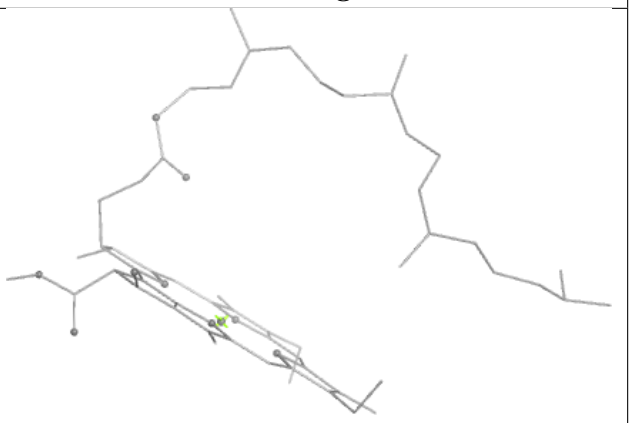


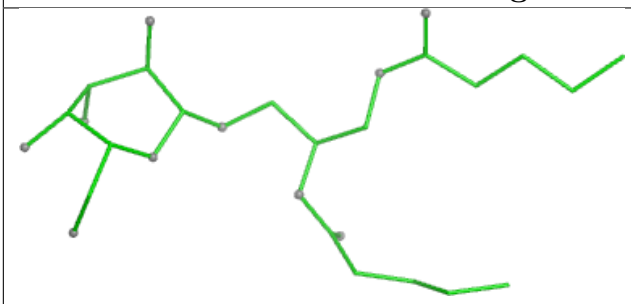
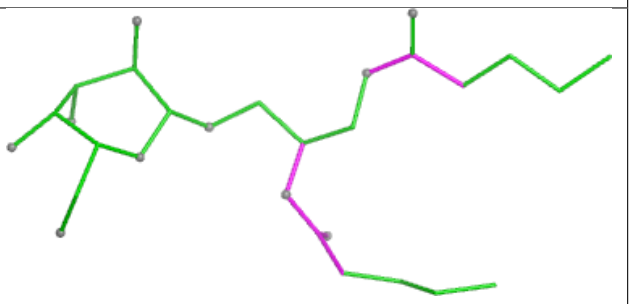
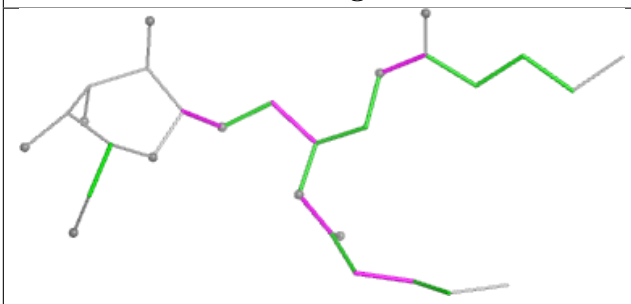
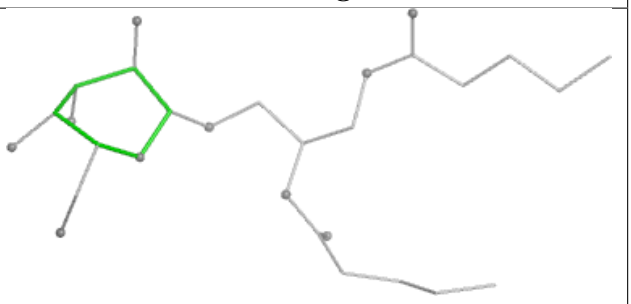
Bond angles



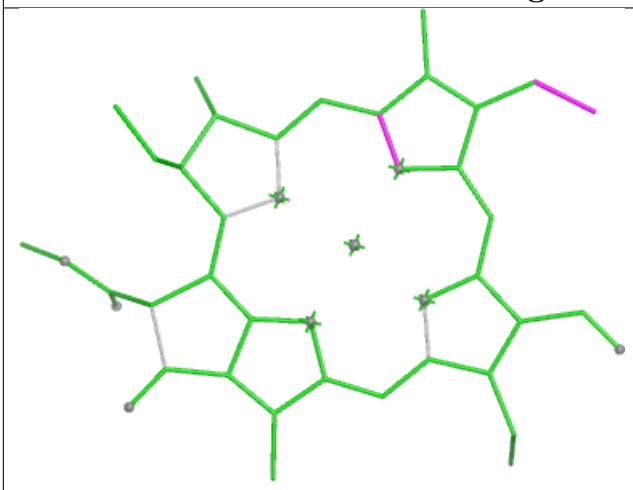
Torsions



Rings

Ligand LMG A 5003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 5 617



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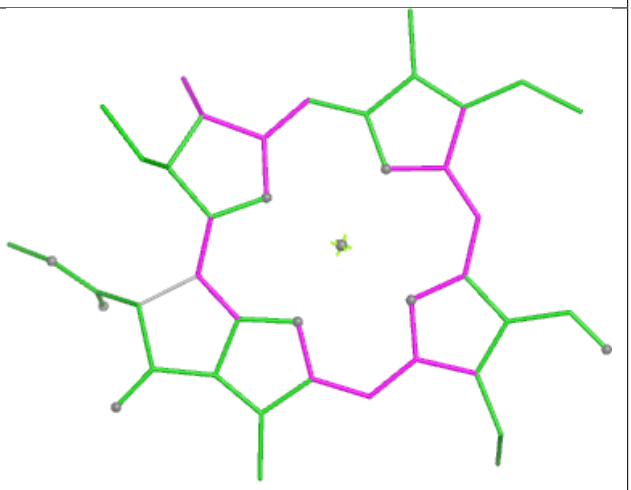
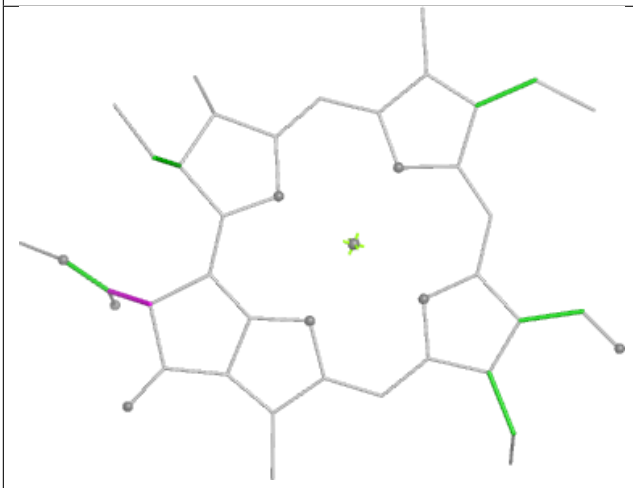


Bond angles



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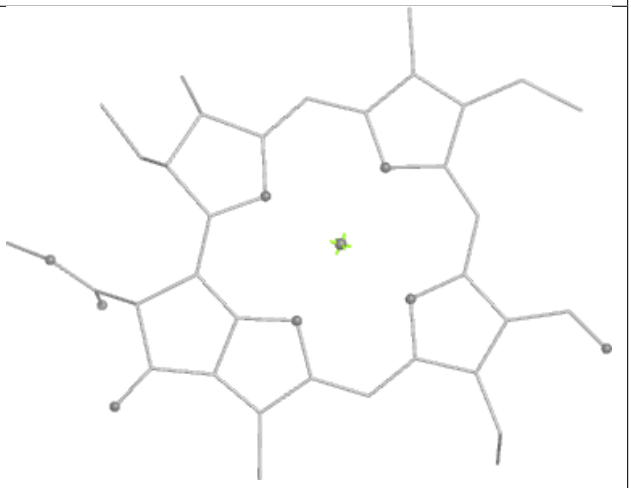
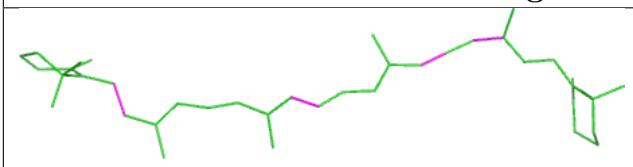
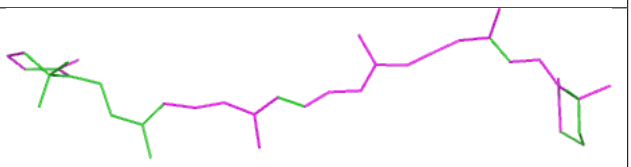


Rings

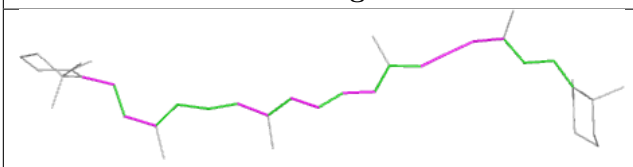
Ligand BCR 5 503



Bond lengths



Bond angles



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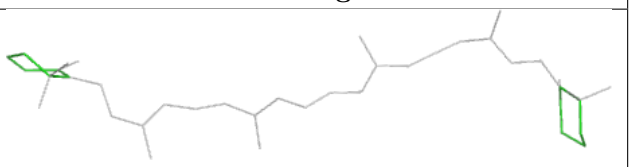
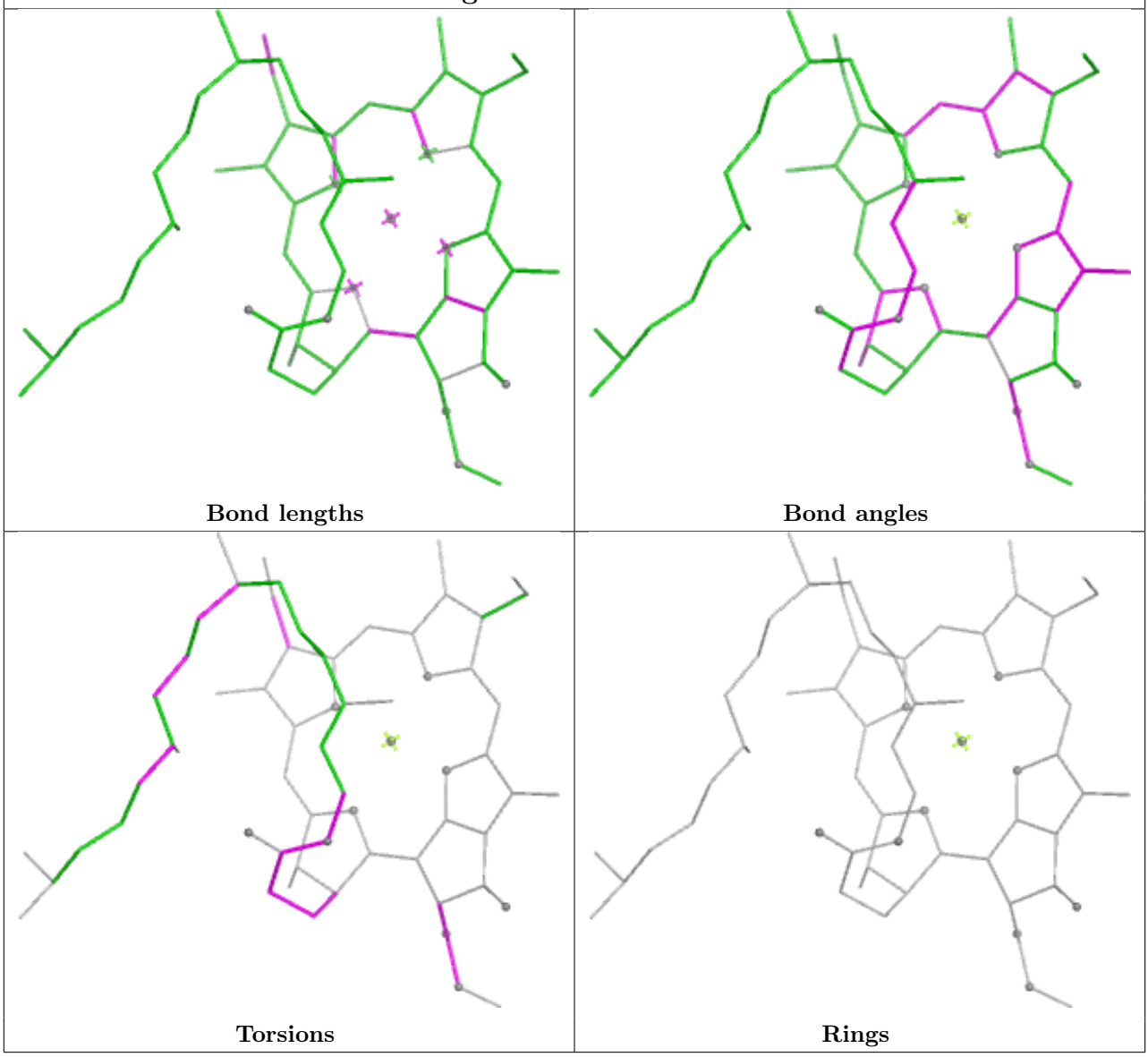
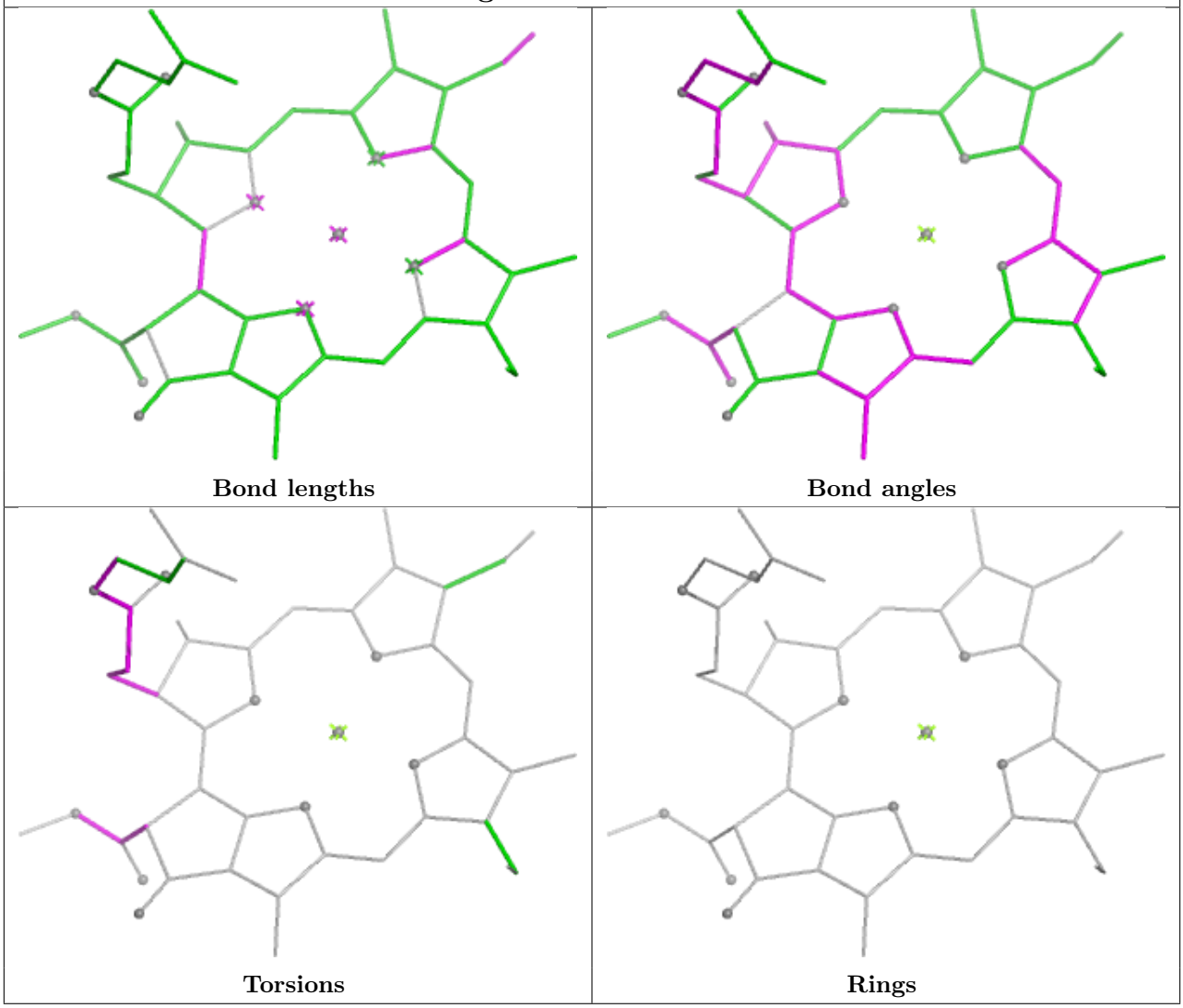


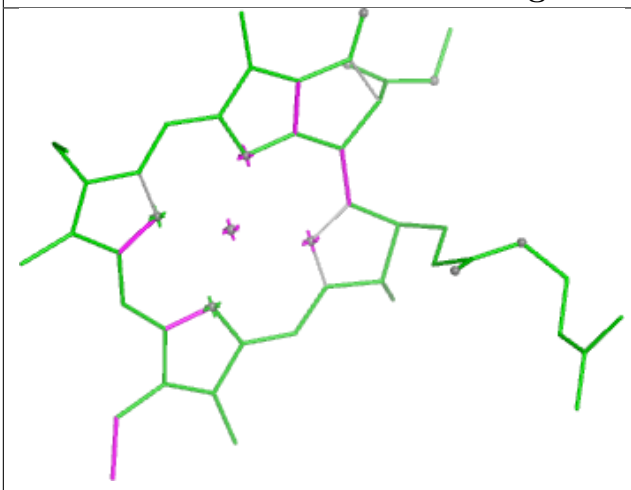
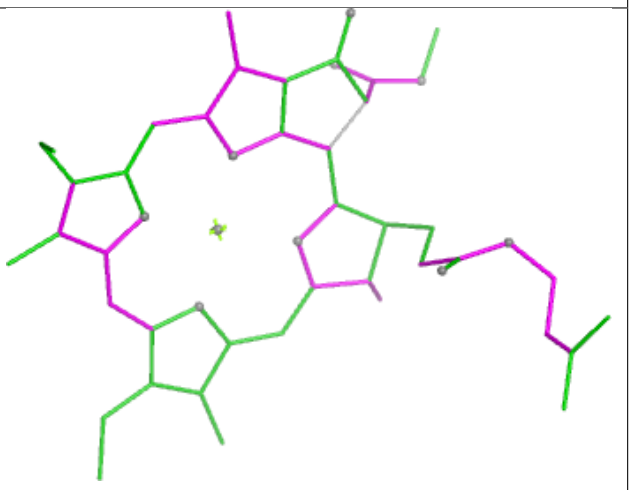
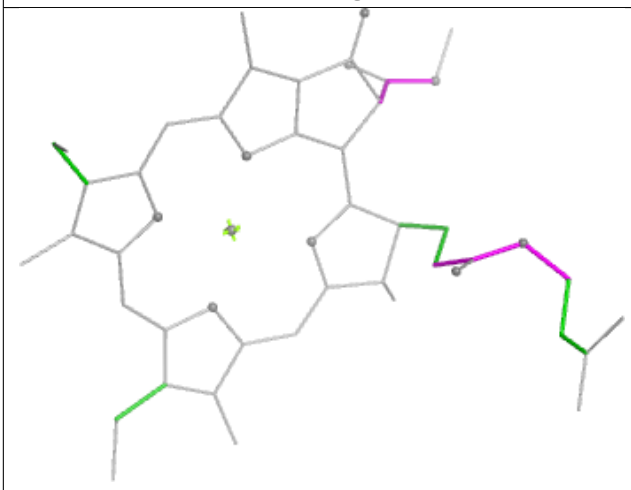
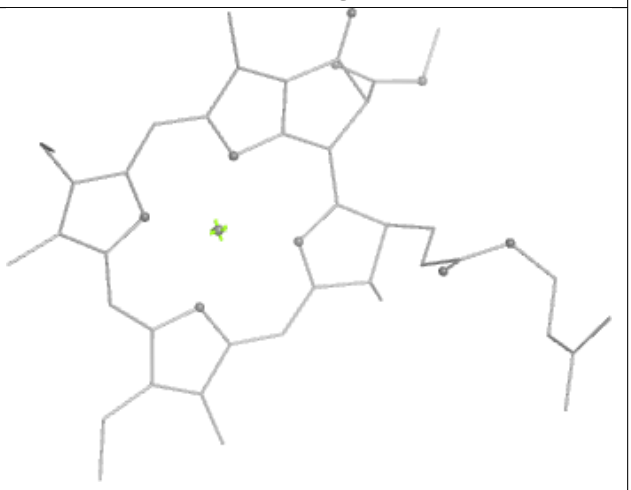
Rings

Ligand CLA B 1205



Ligand CLA L 1503



Ligand CLA 8 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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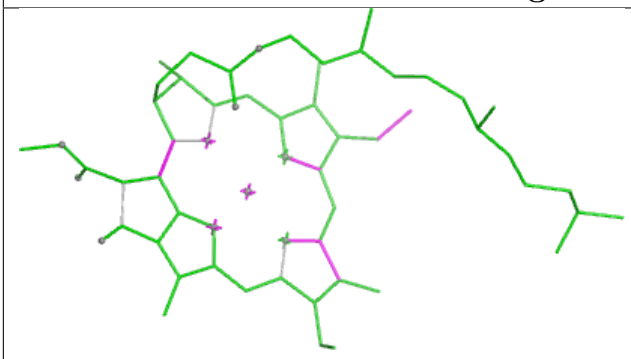
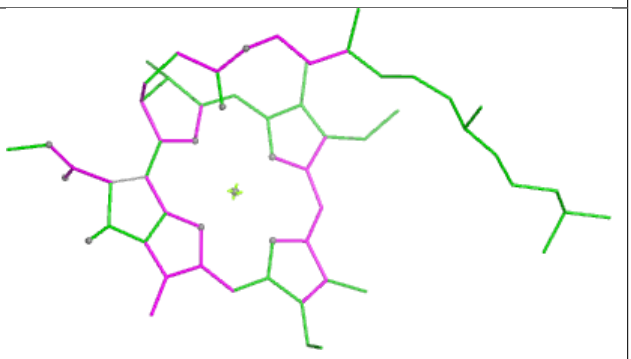
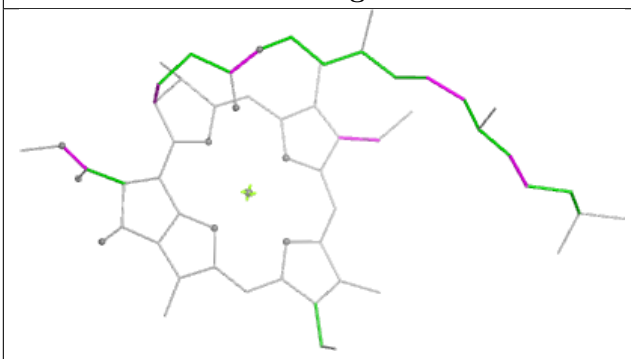
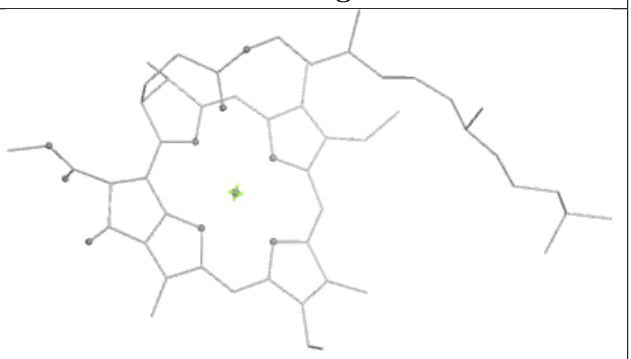
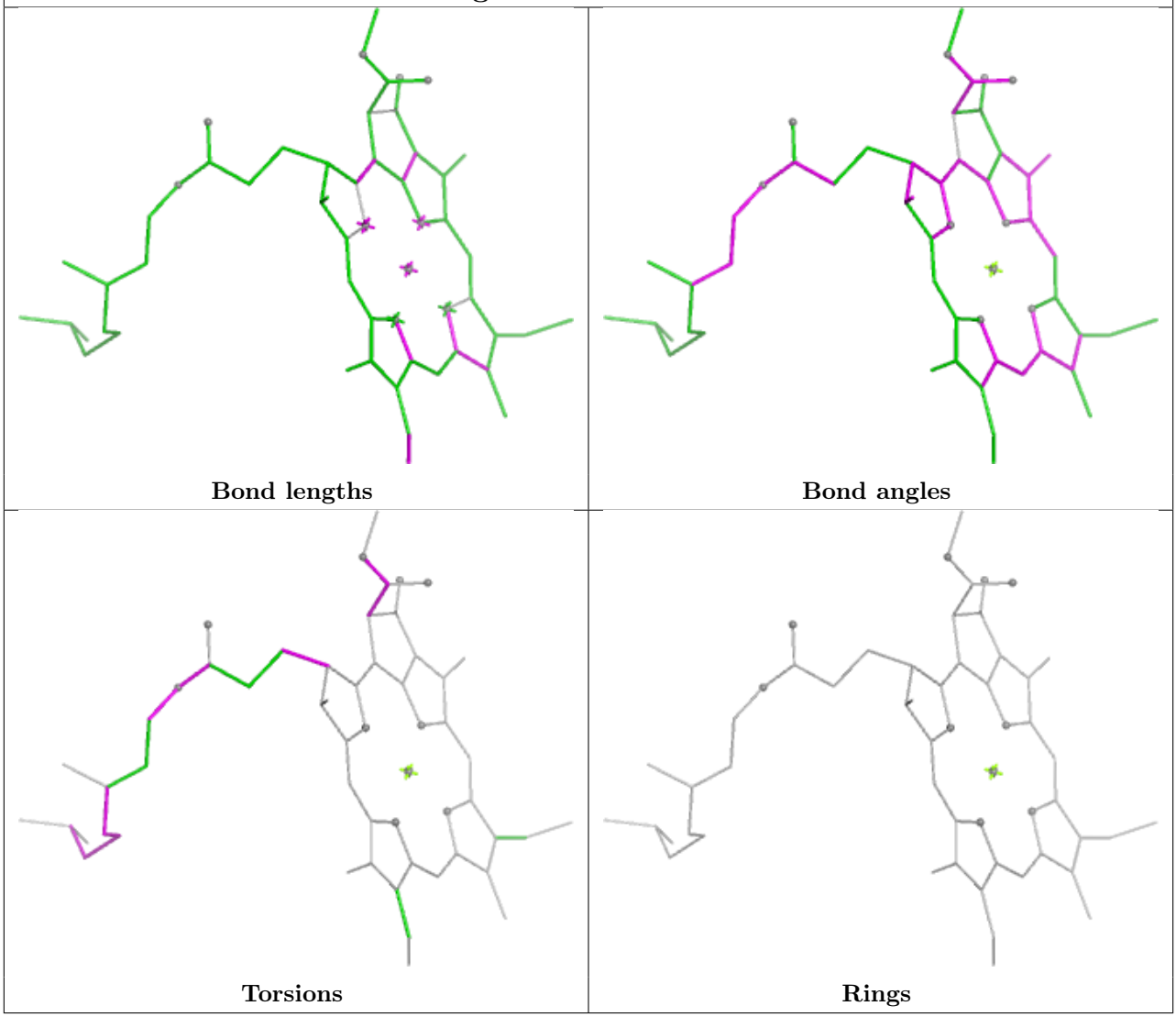
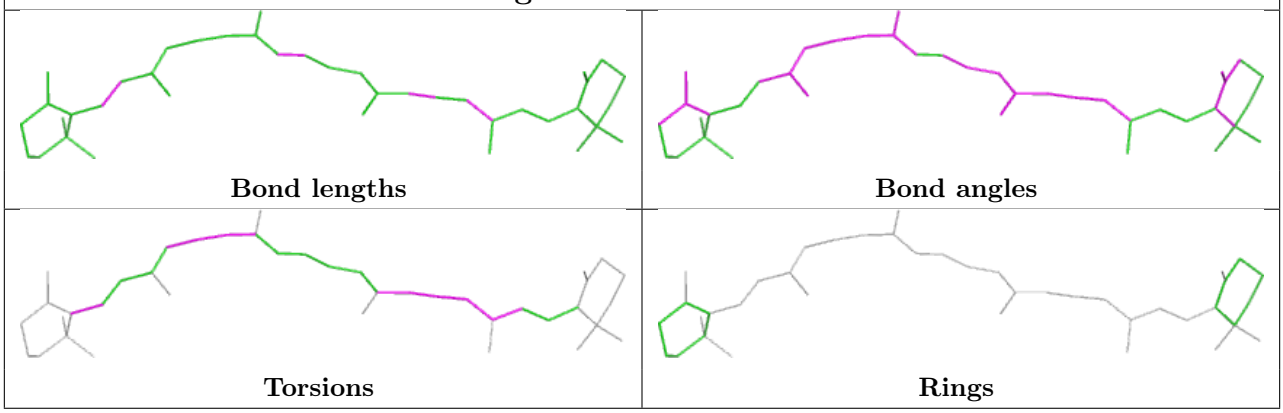
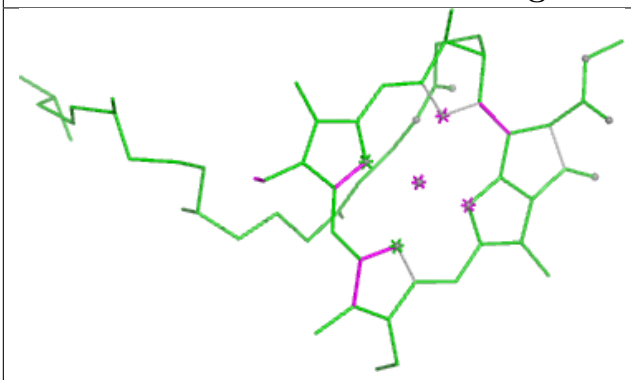
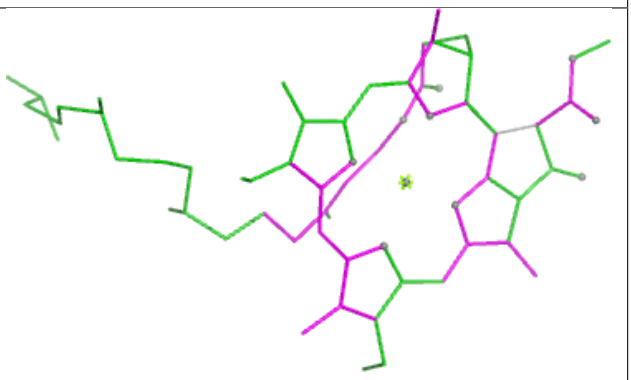
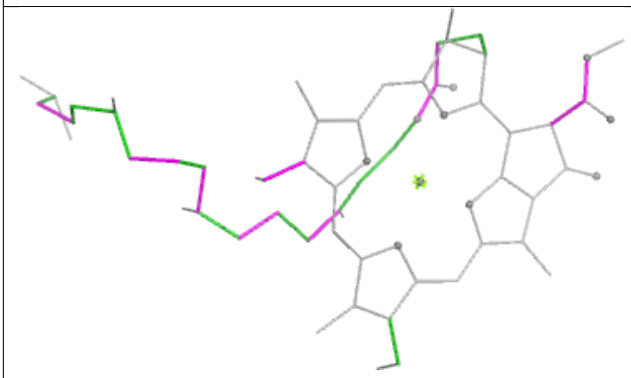
 Bond lengths	 Bond angles
 Torsions	 Rings

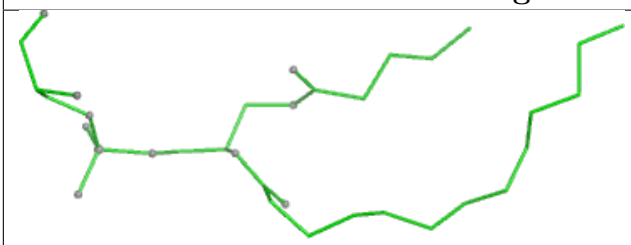
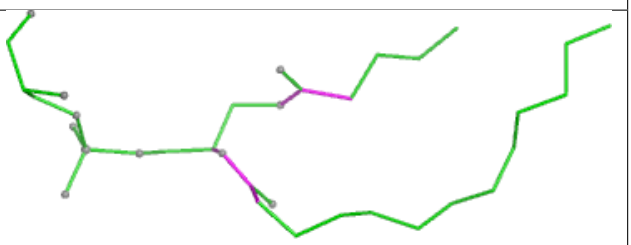
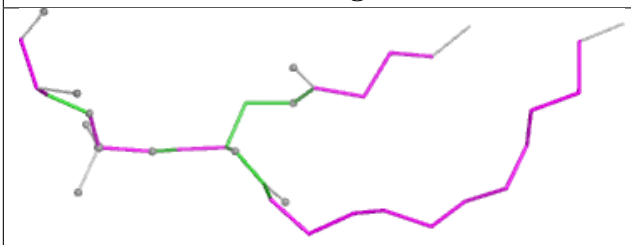
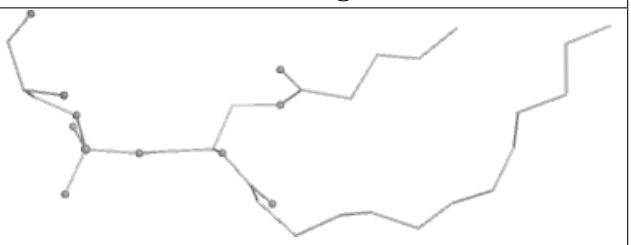
Ligand CLA A 1102

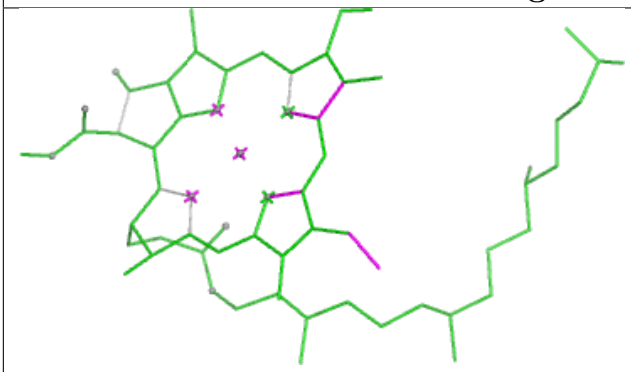
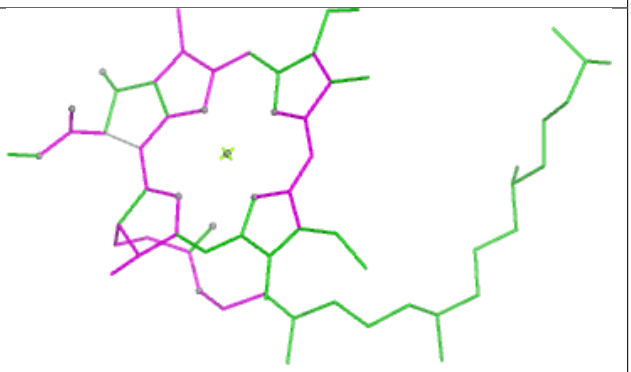
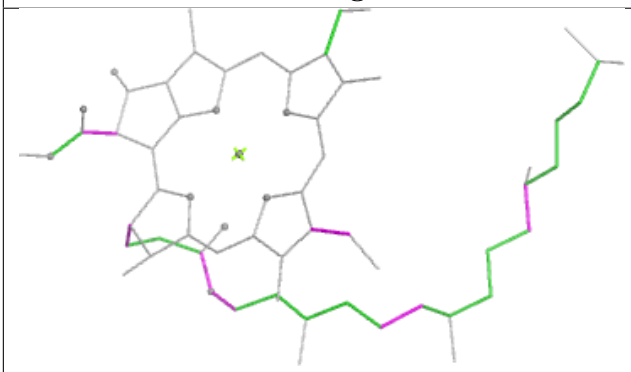
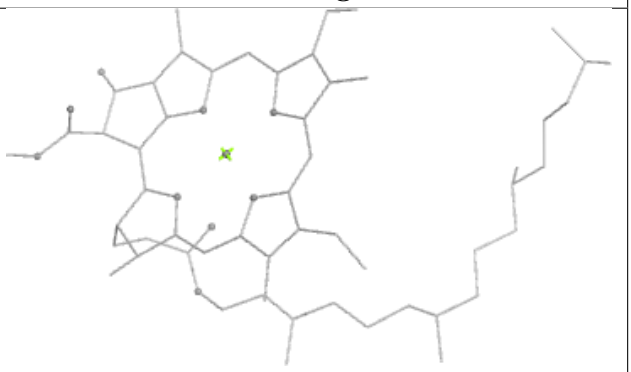


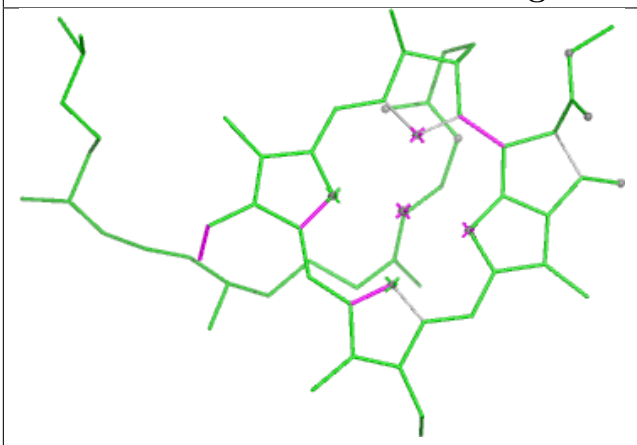
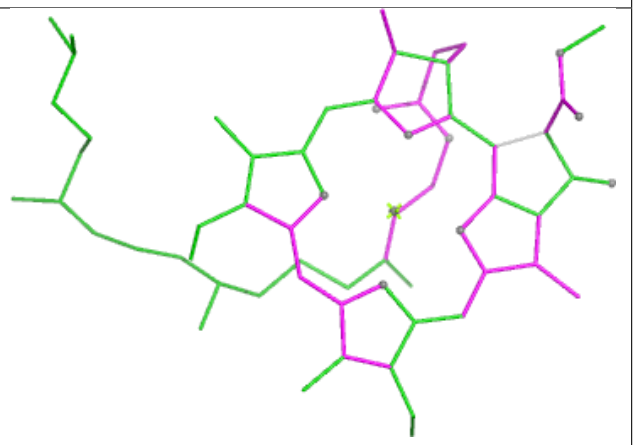
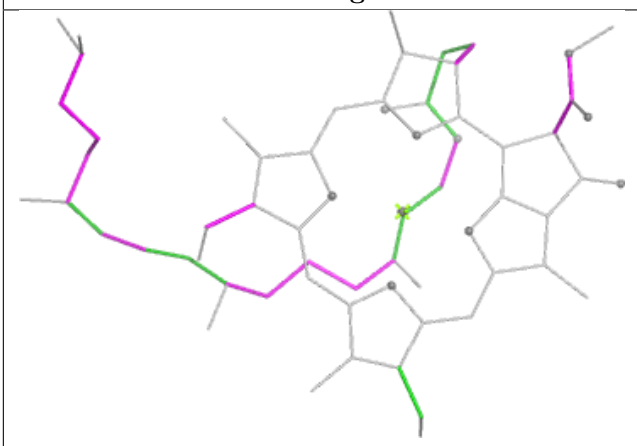
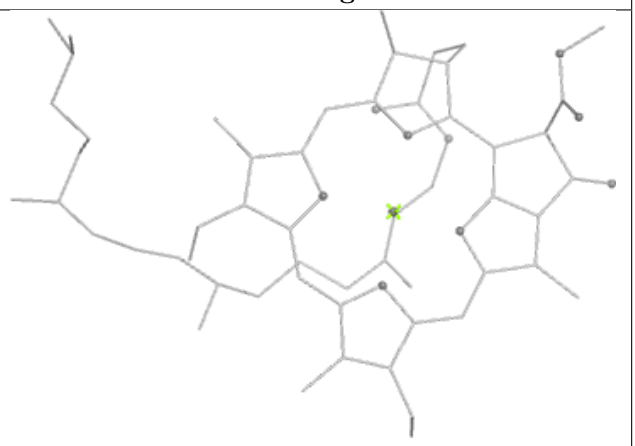
Ligand BCR B 4005



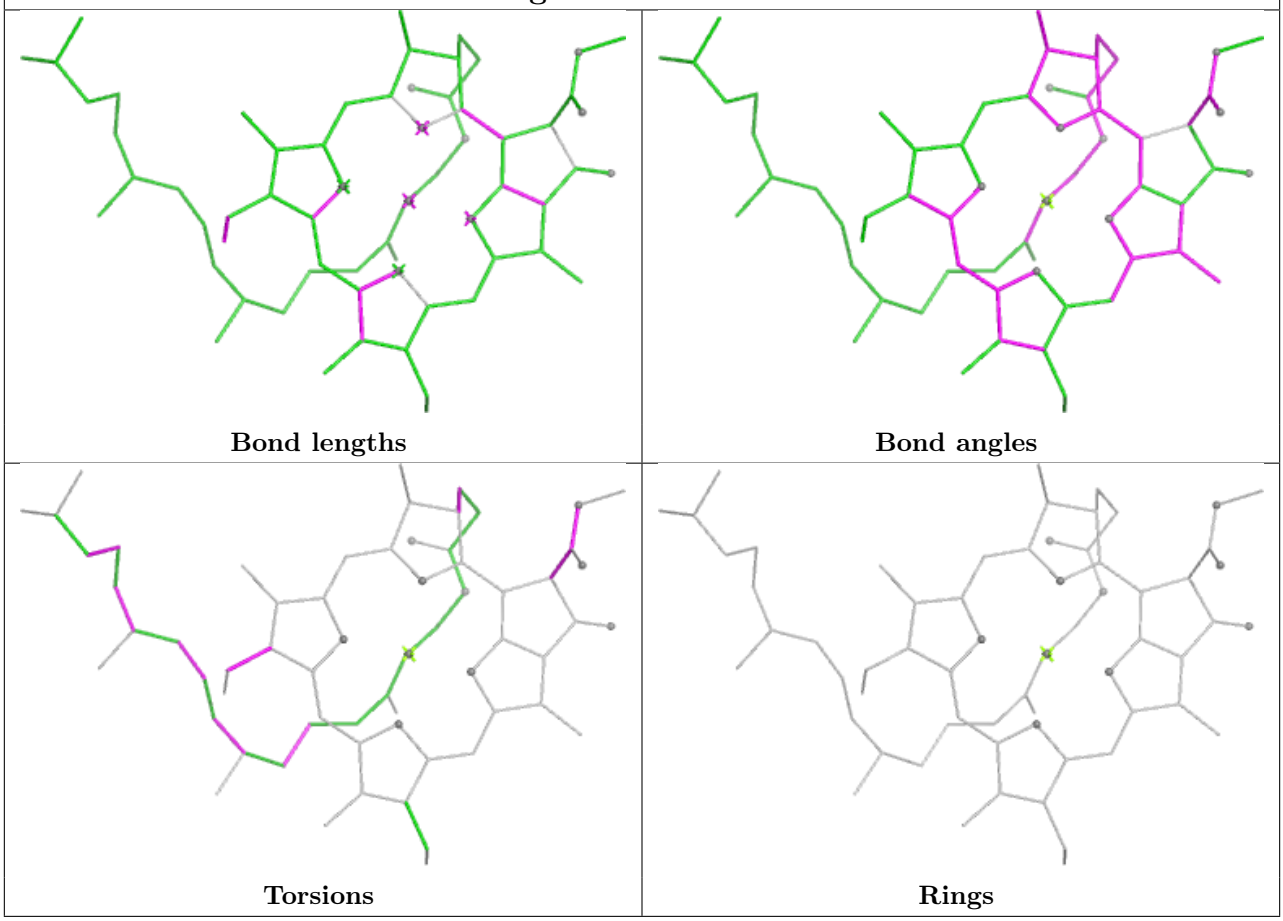
Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LHG A 5001	
 Bond lengths	 Bond angles
 Torsions	 Rings

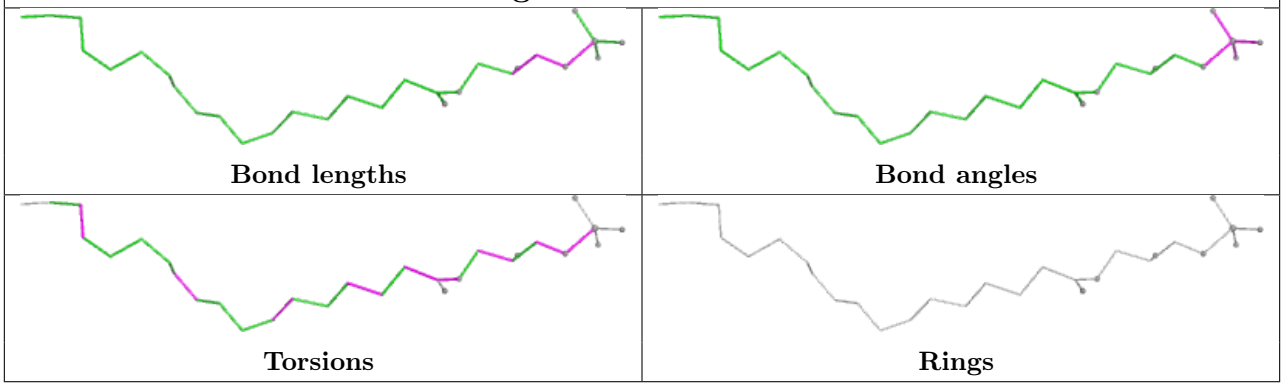
Ligand CLA 6 604	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 6 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

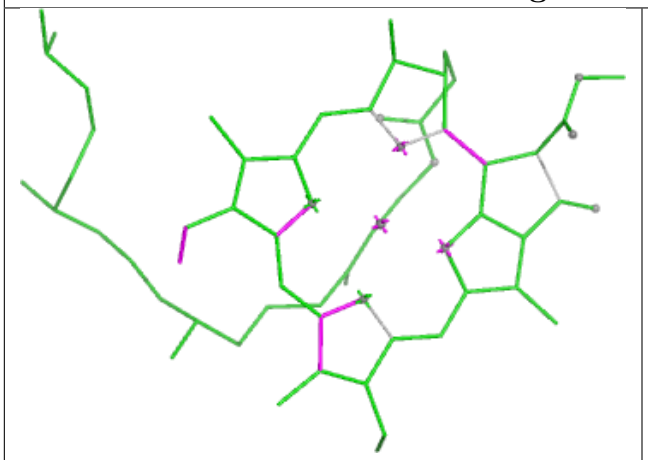
Ligand CLA 7 603



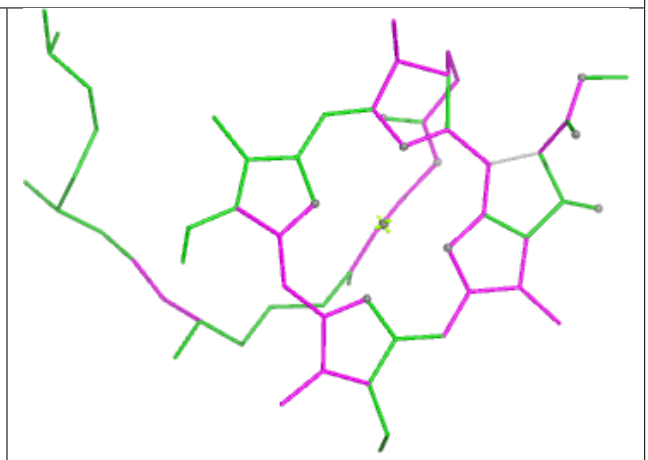
Ligand NKP A 5004



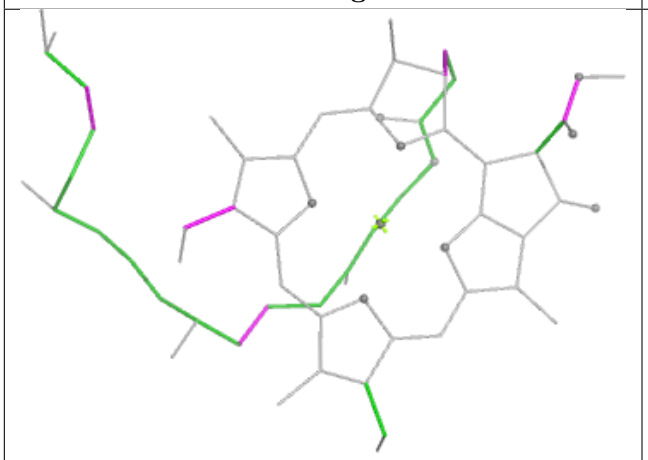
Ligand CLA 8 603



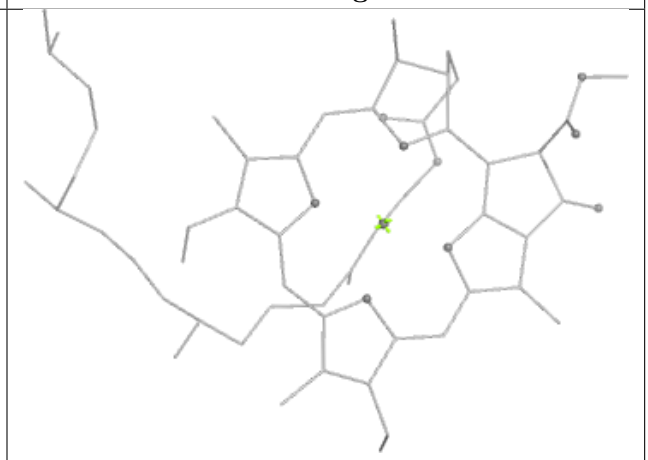
Bond lengths



Bond angles

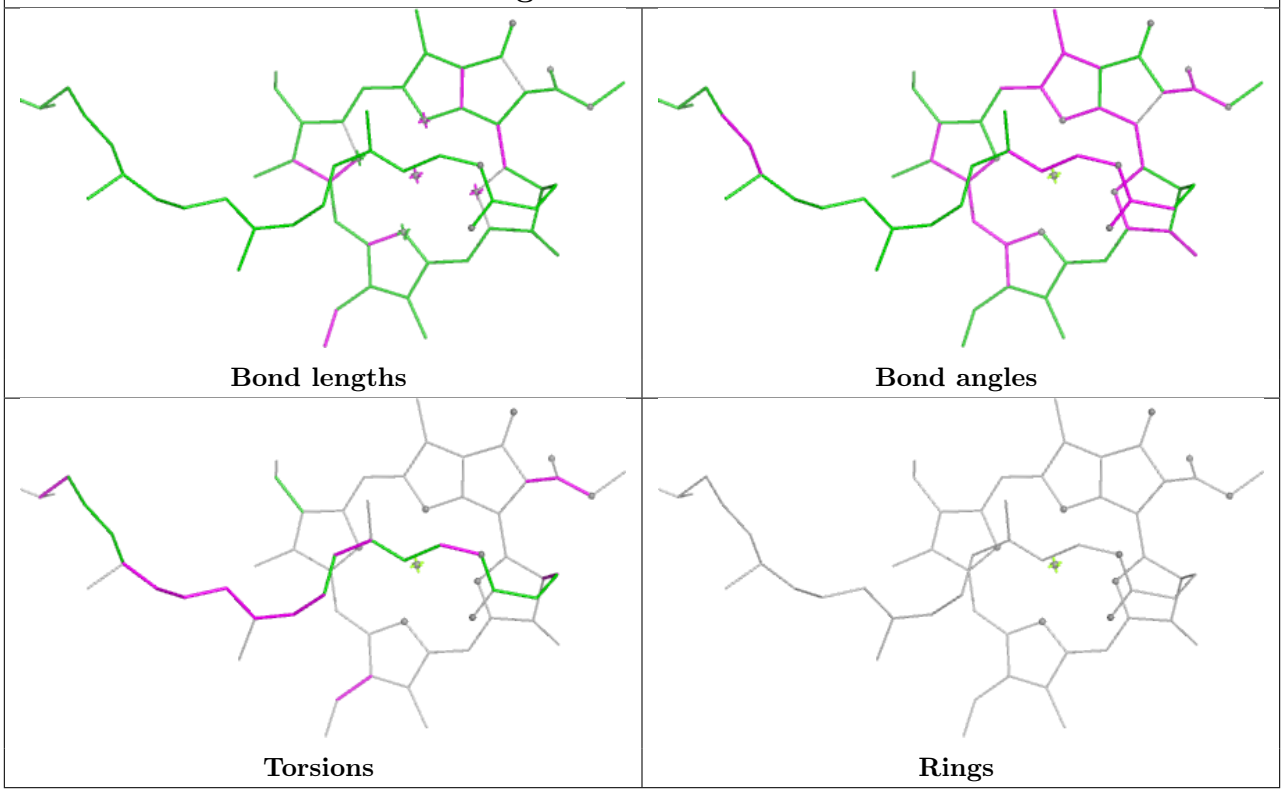


Torsions

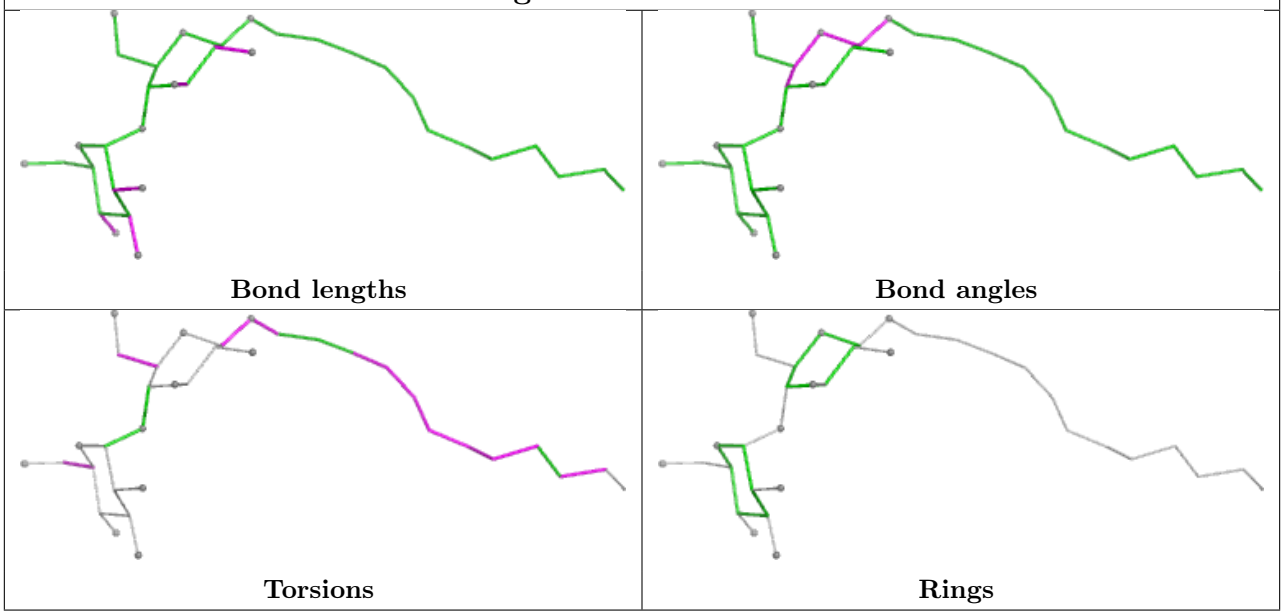


Rings

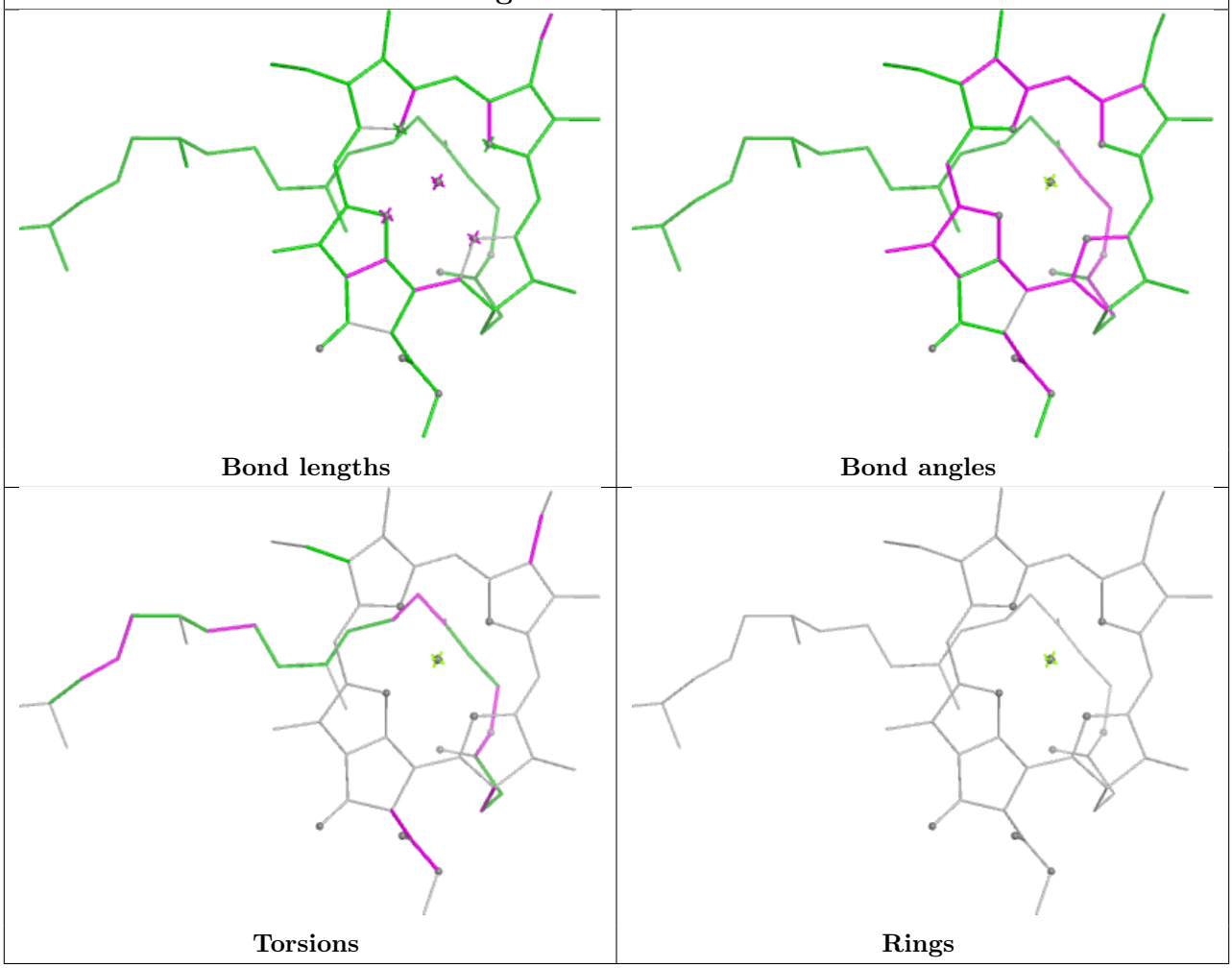
Ligand CLA B 1213

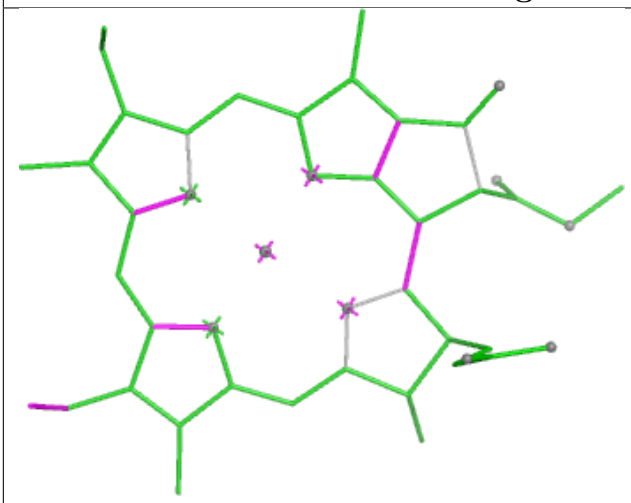
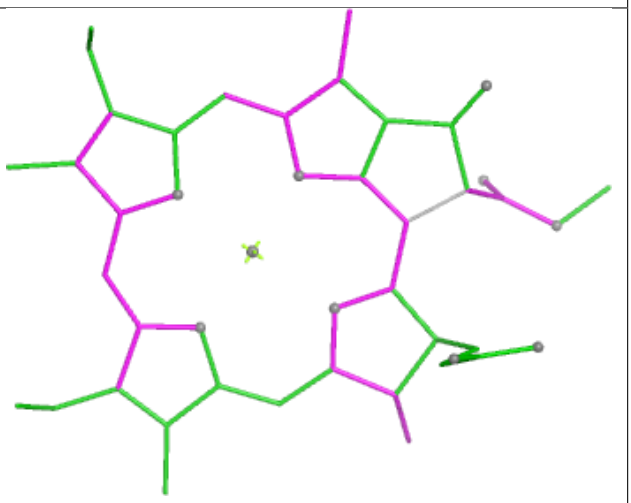
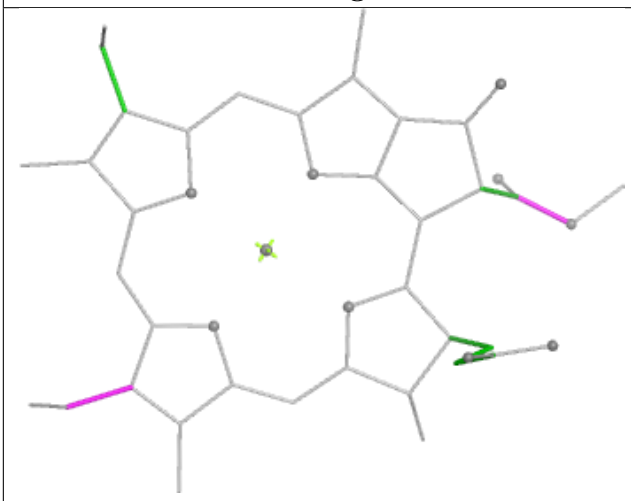
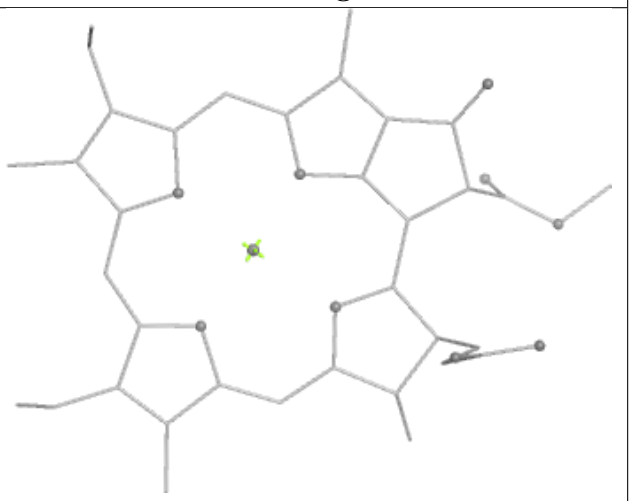


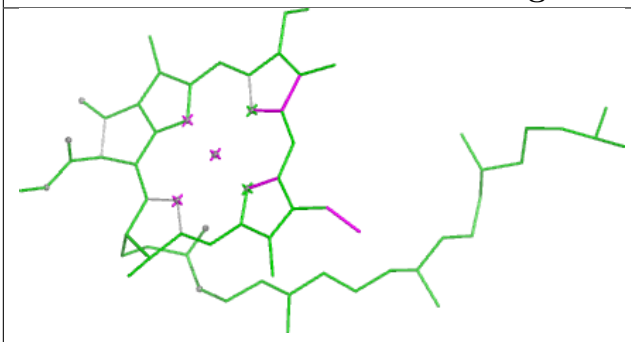
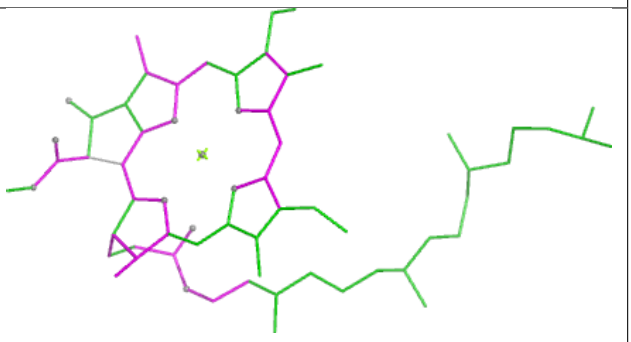
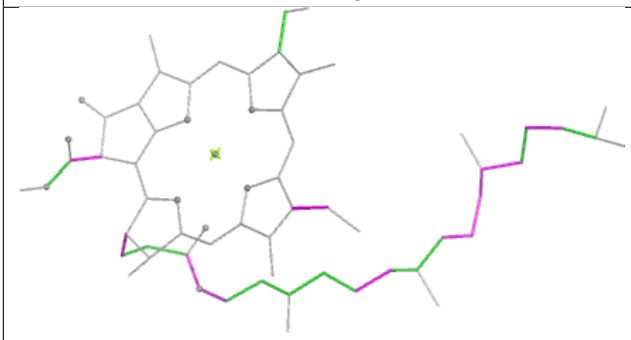
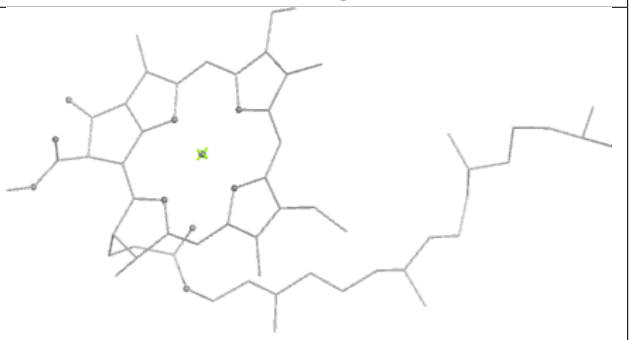
Ligand LMT B 5005



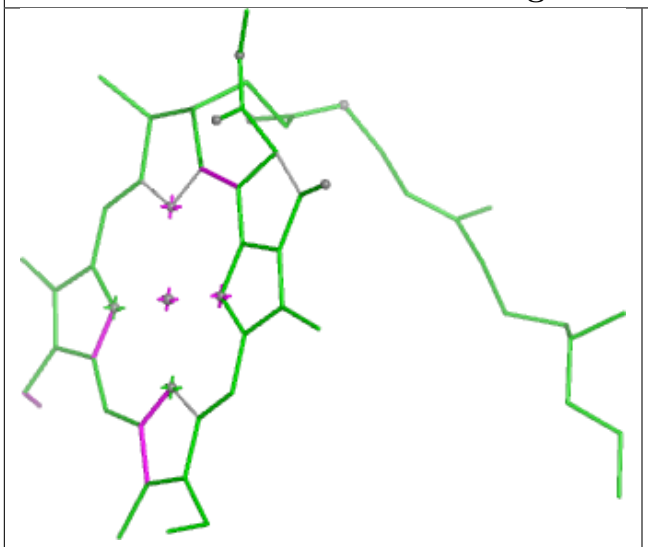
Ligand CLA B 1224



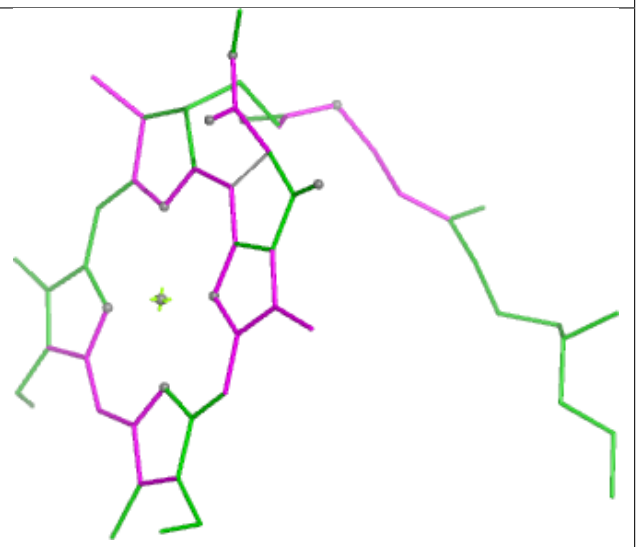
Ligand CLA B 1232	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 604	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

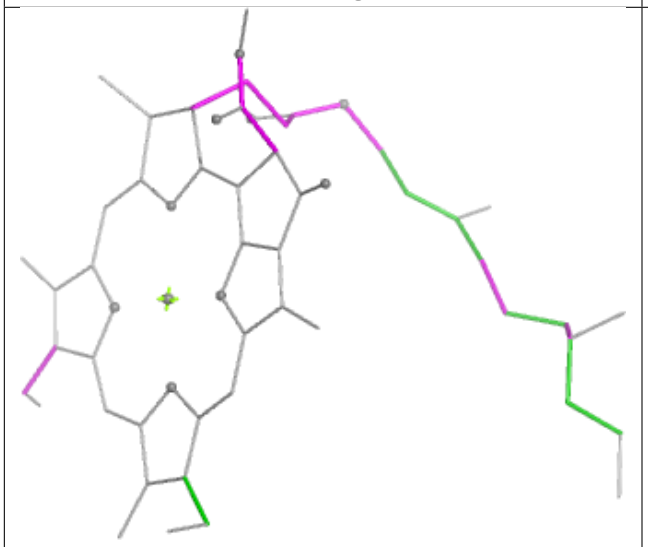
Ligand CLA Z 607



Bond lengths



Bond angles



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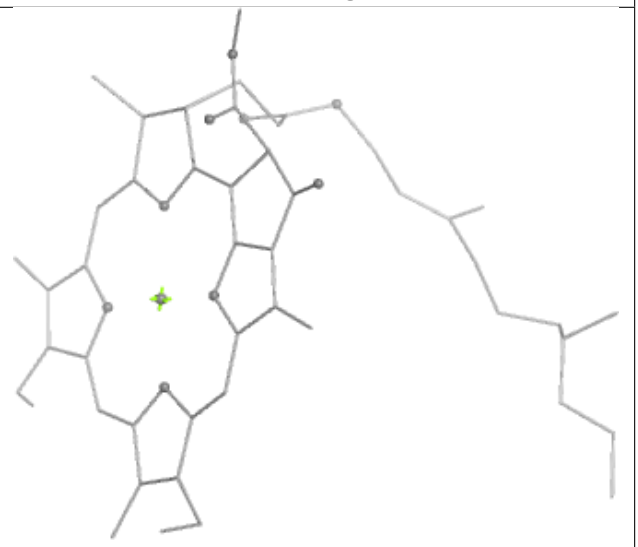
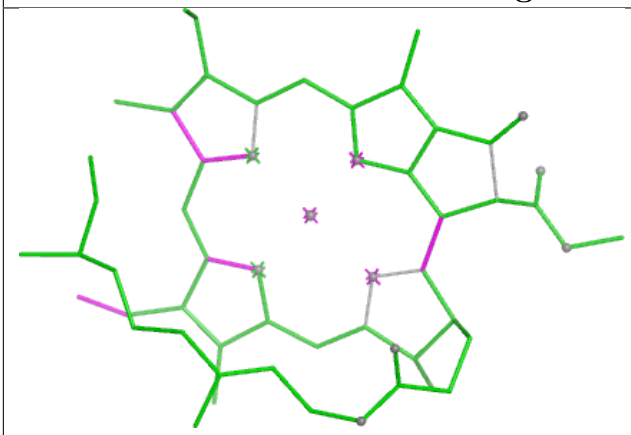


Rings

Ligand CLA B 1217



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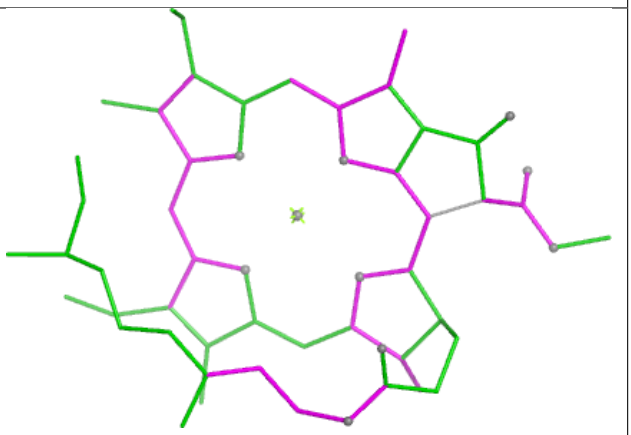
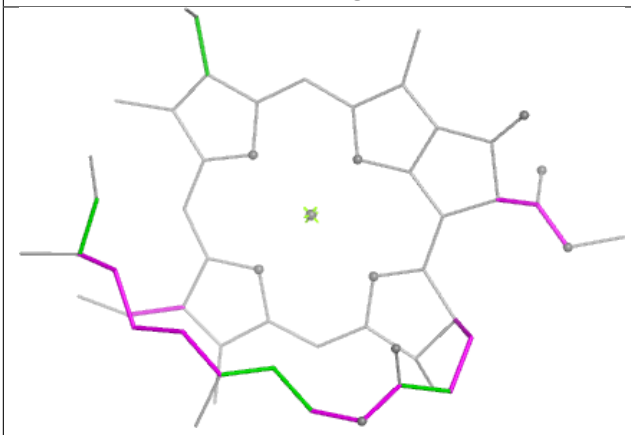


Bond angles



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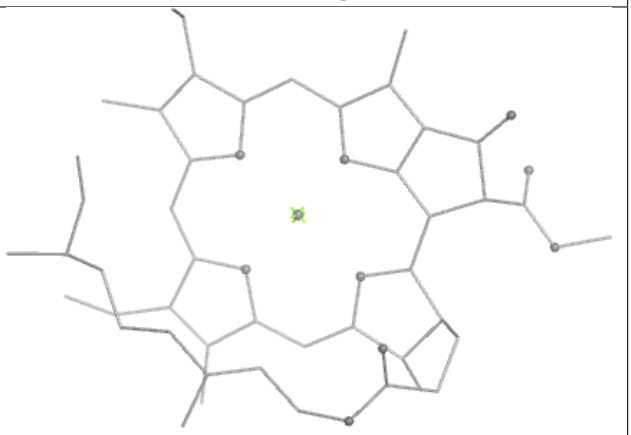
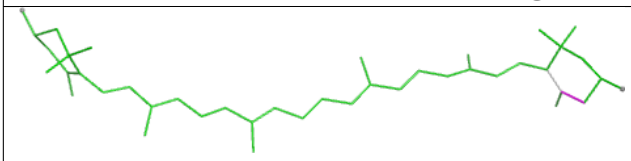


Rings

Ligand LUT 6 501



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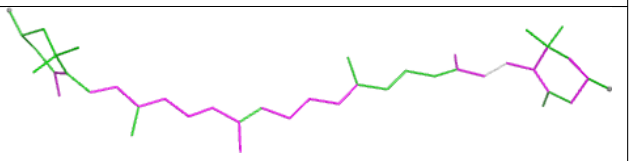

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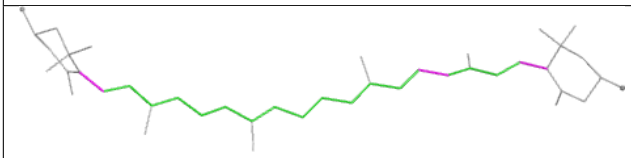

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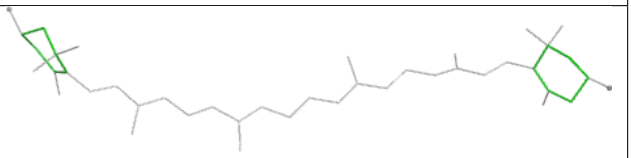
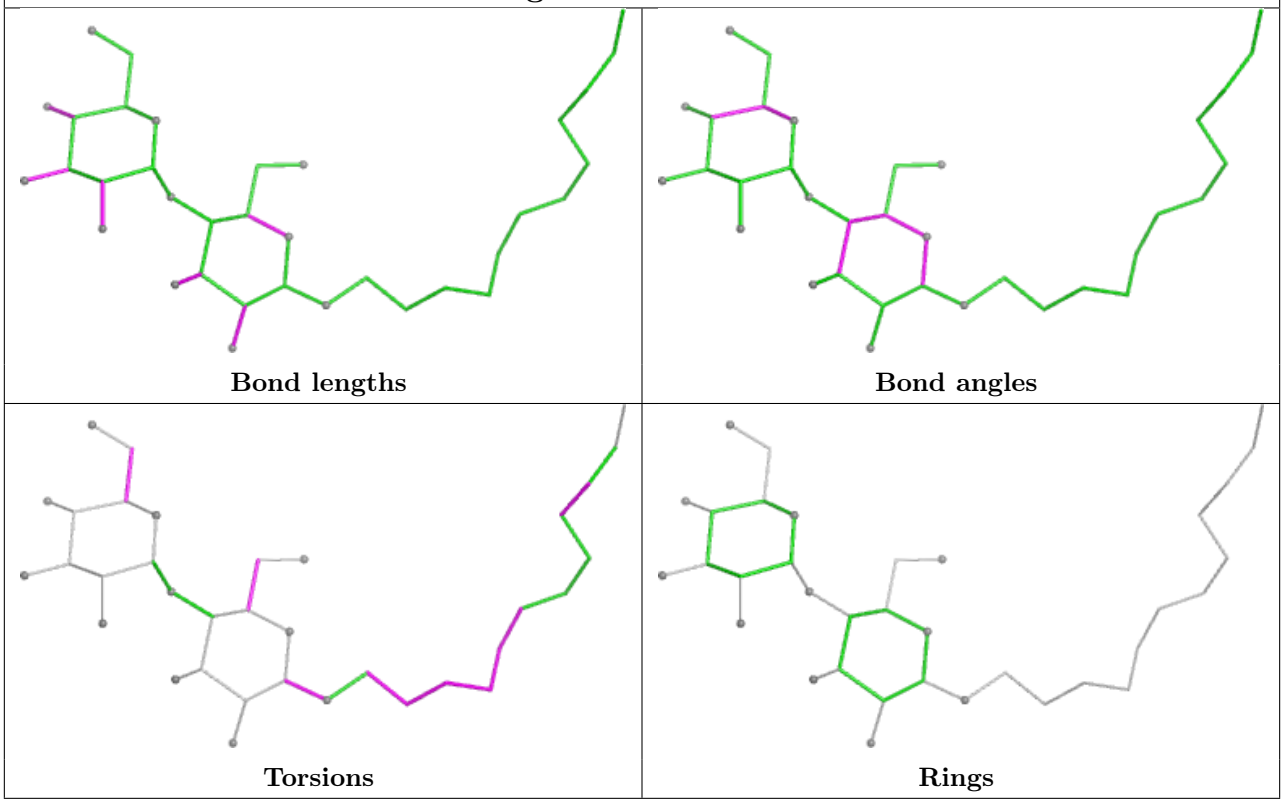
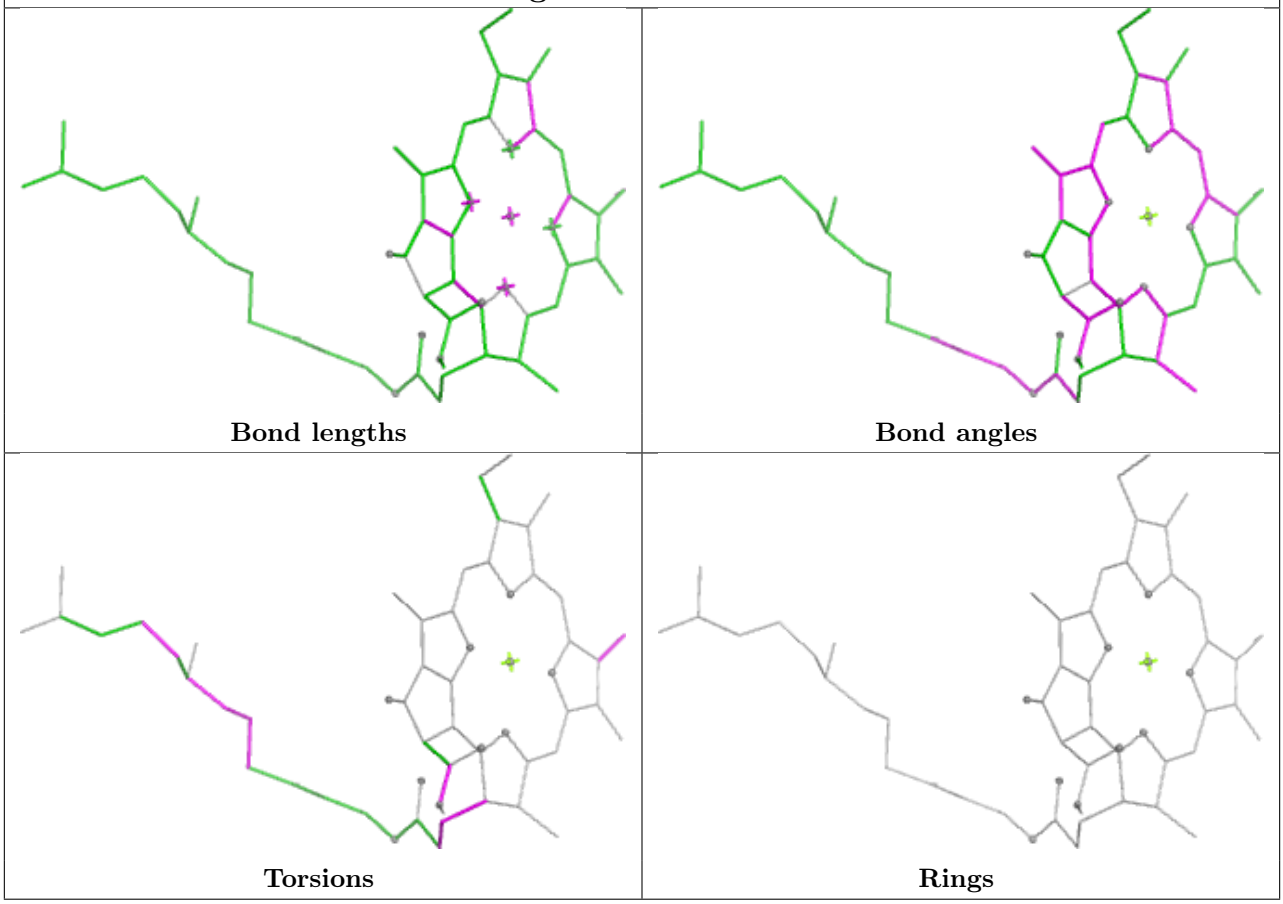


Rings

Ligand LMT 4 803



Ligand CLA 3 612



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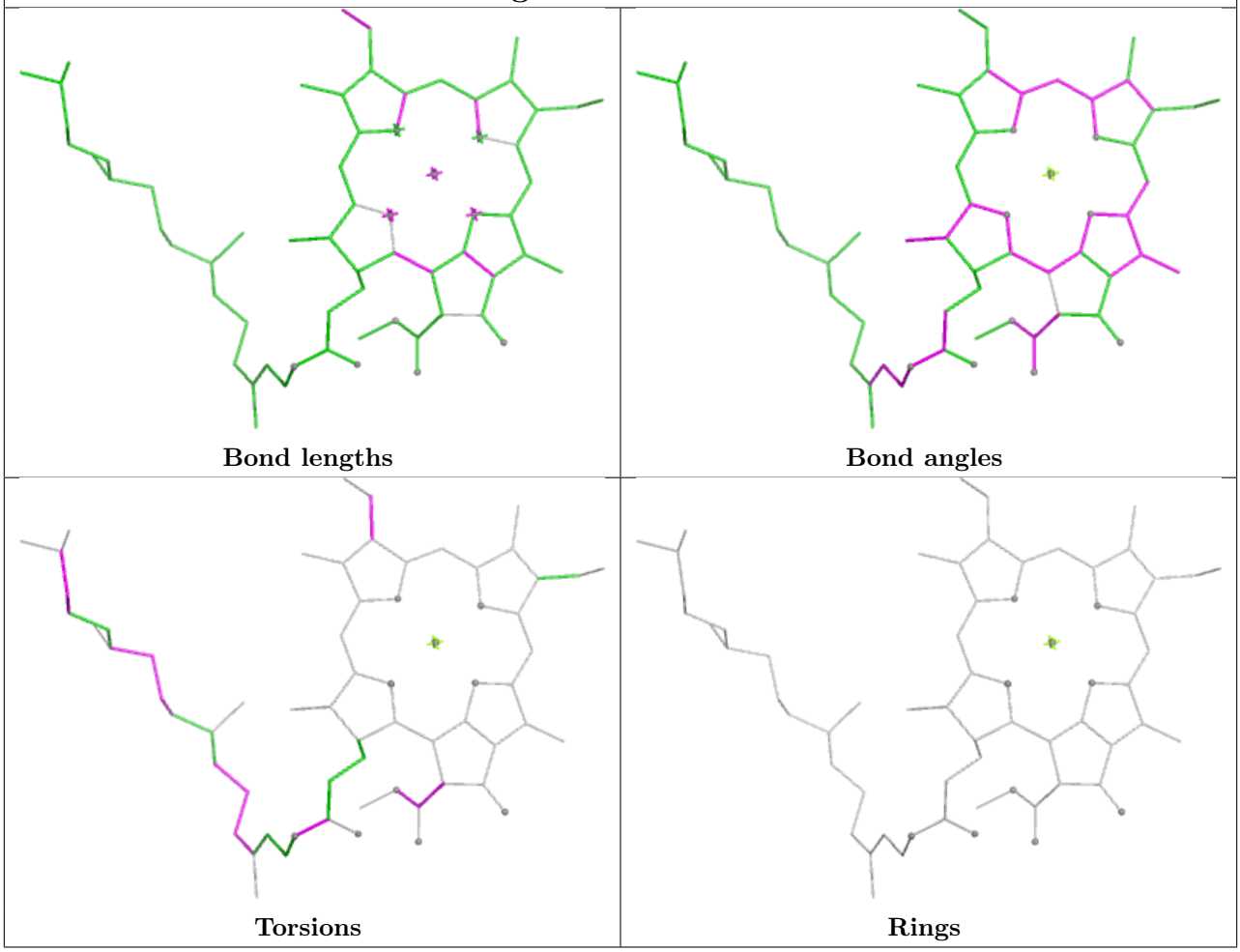
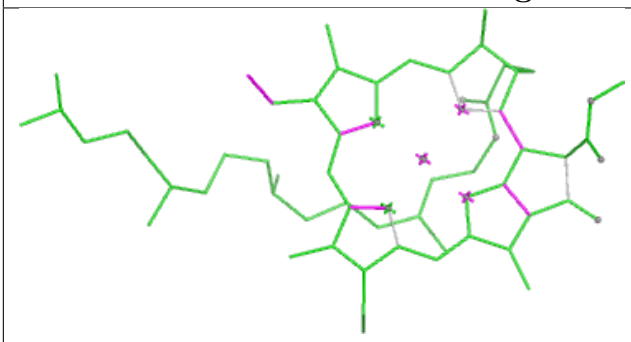
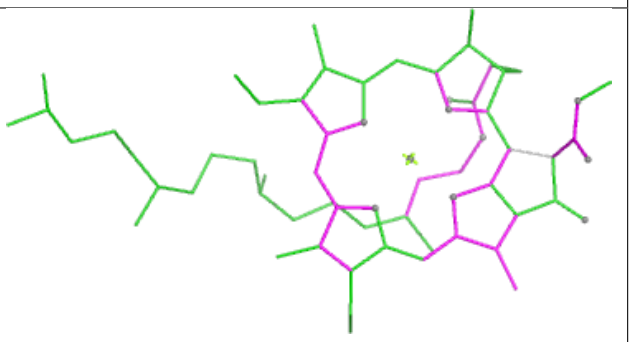
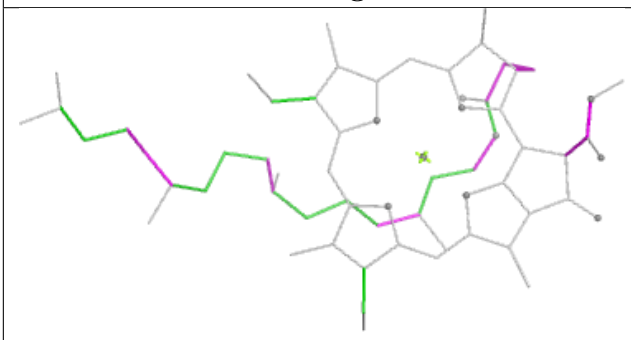
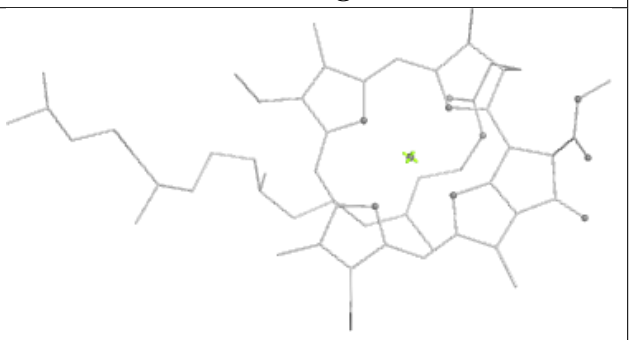
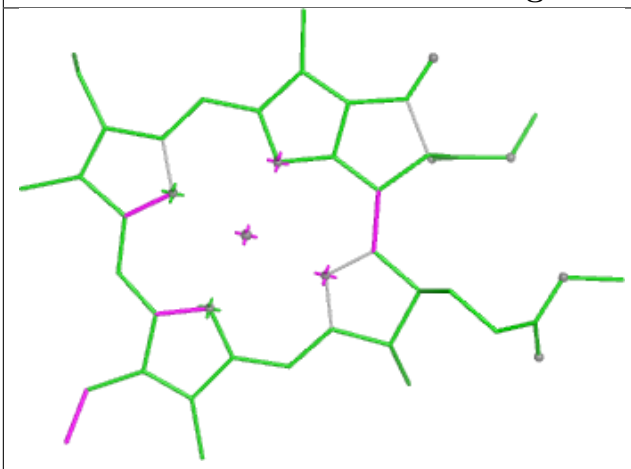
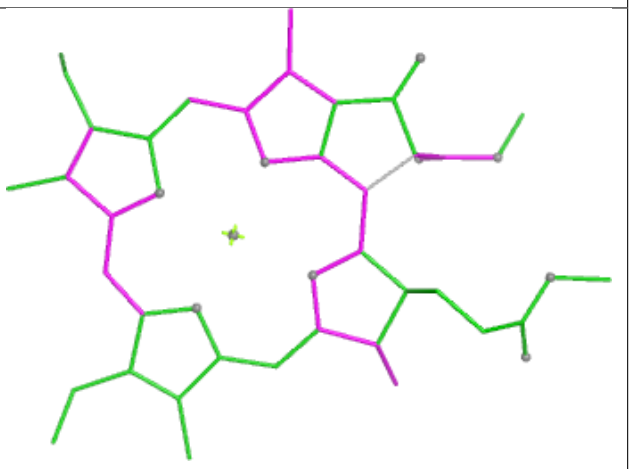


Ligand CLA A 1138	
 Bond lengths	 Bond angles
 Torsions	 Rings

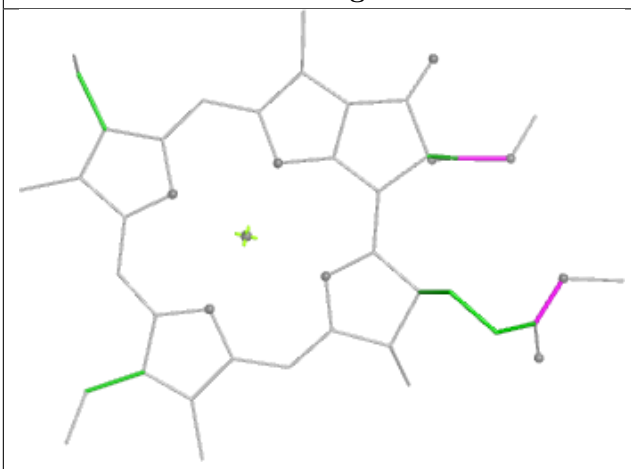
Ligand CLA Z 602



Bond lengths



Bond angles



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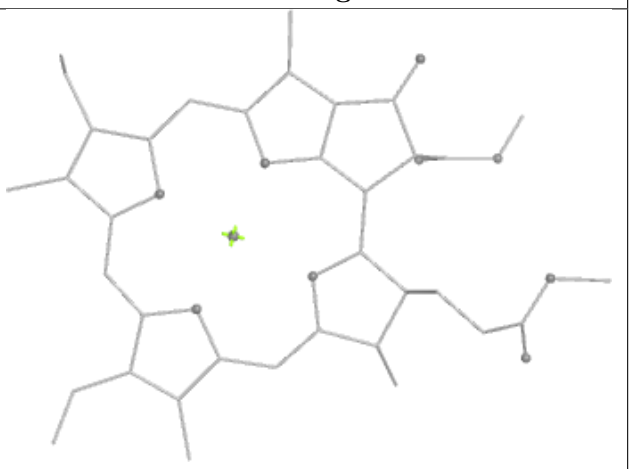
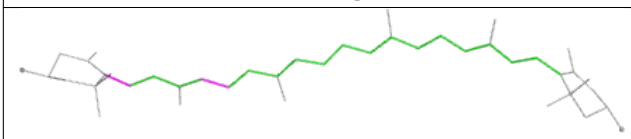


Rings

Ligand LUT Z 501

Bond lengths

Bond angles



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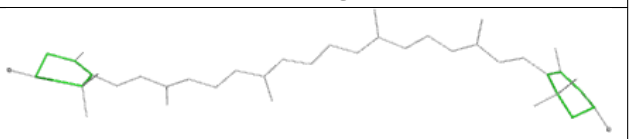
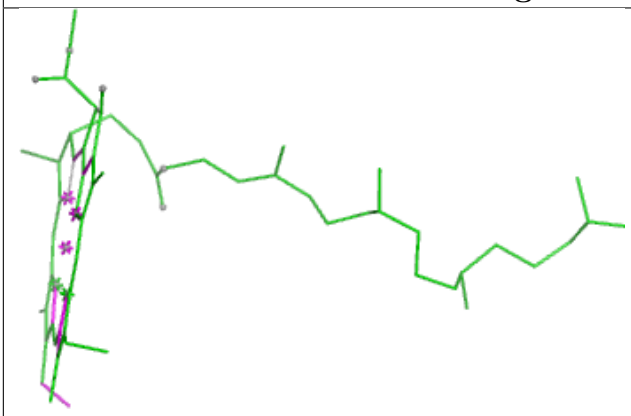
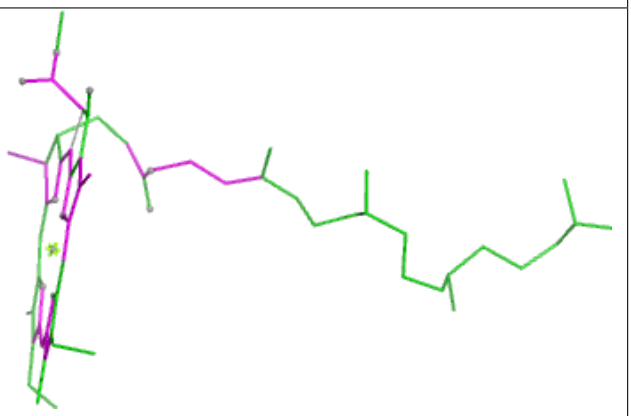
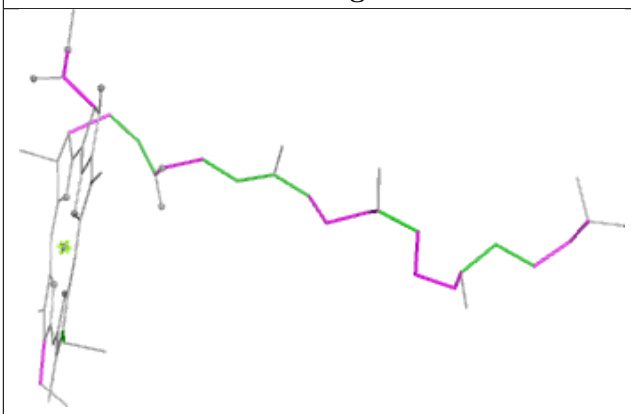
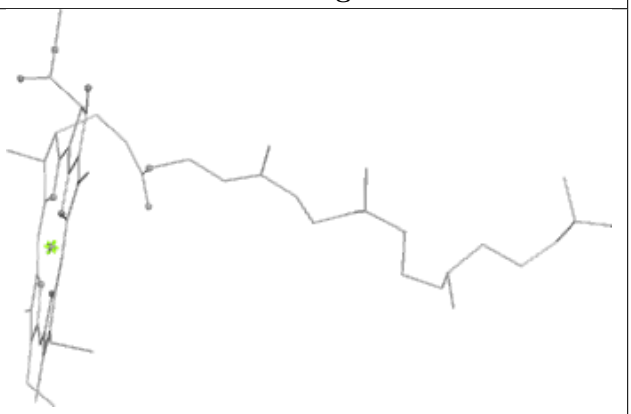
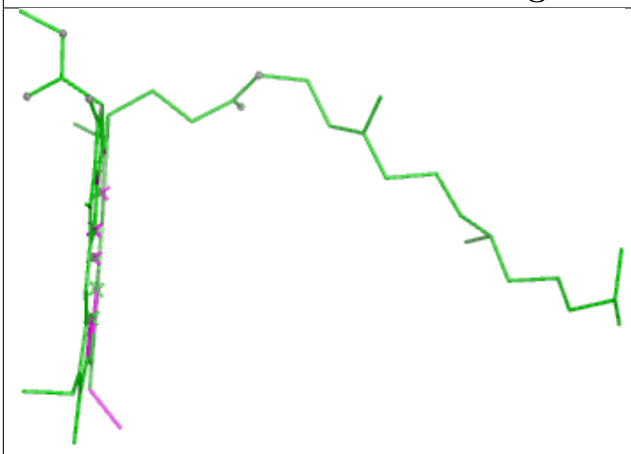


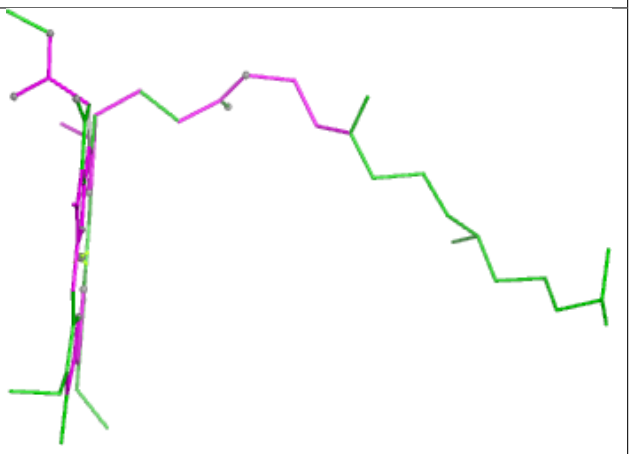
Rings

Ligand CLA A 1126	
 Bond lengths	 Bond angles
 Torsions	 Rings

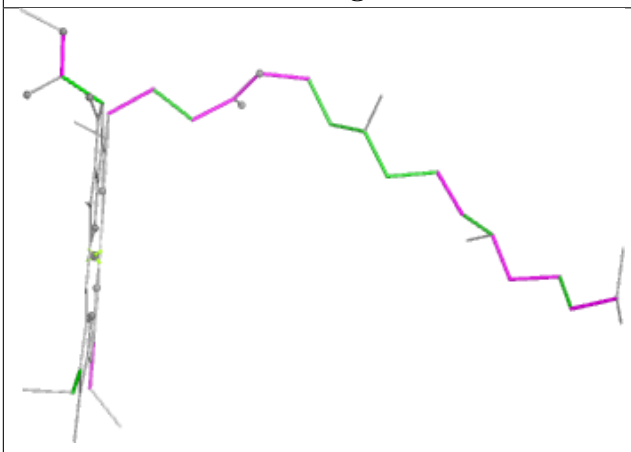
Ligand CLA 4 609



Bond lengths



Bond angles



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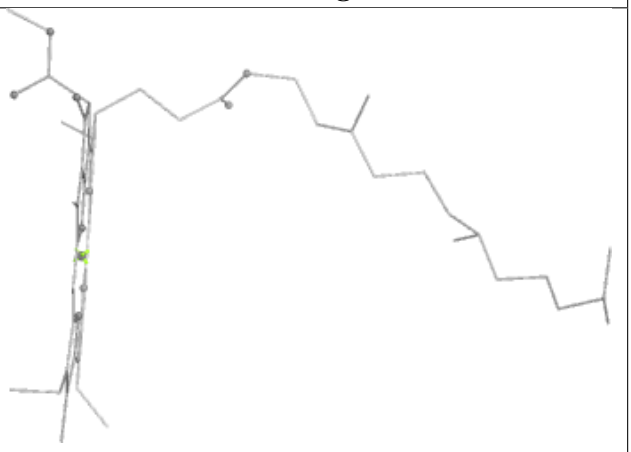
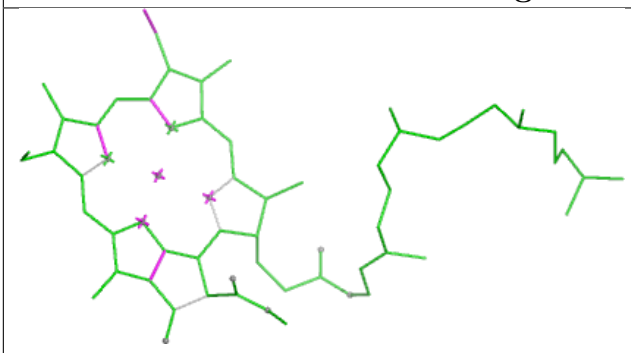
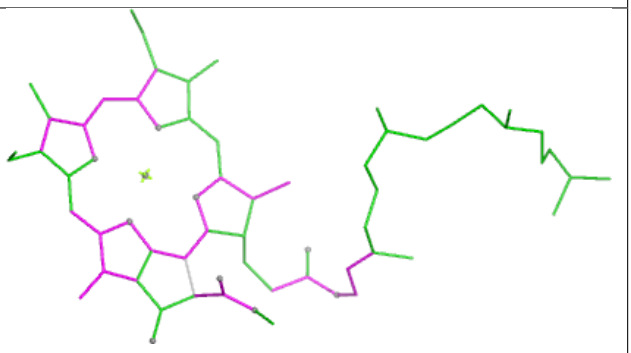
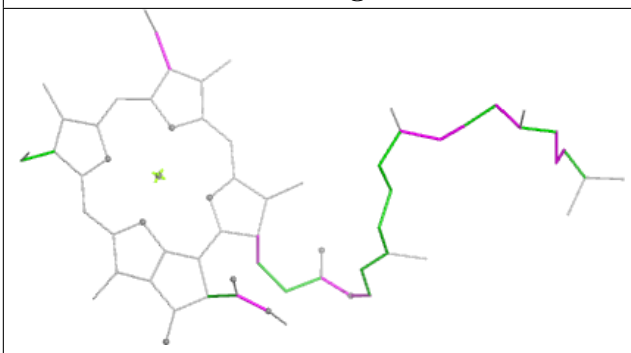
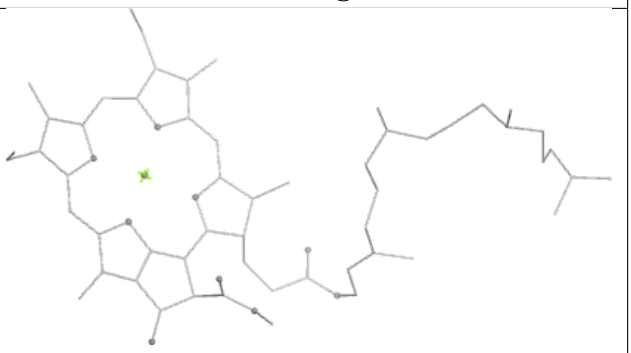
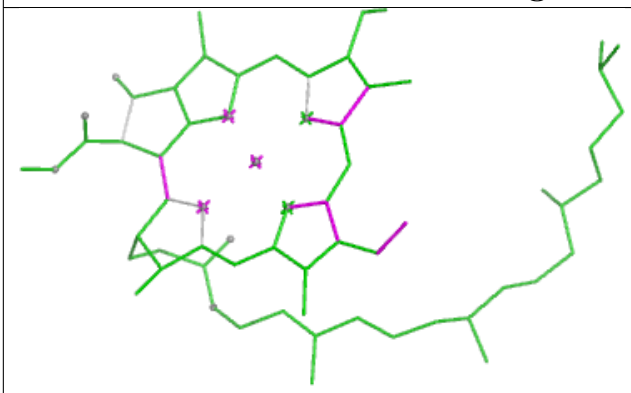
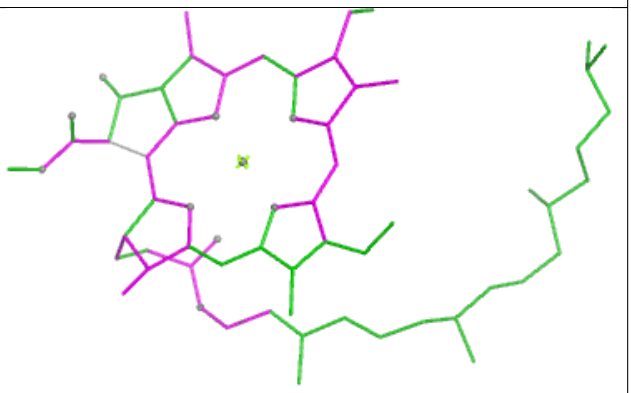
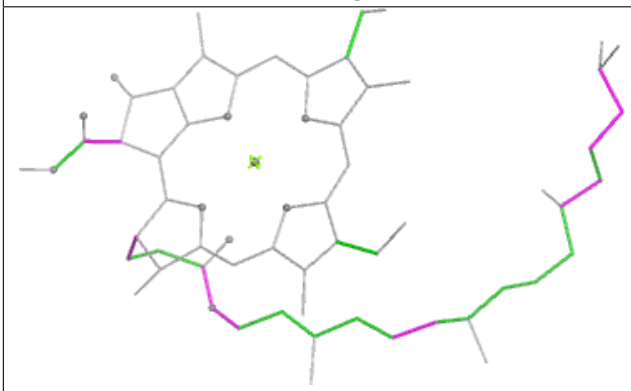
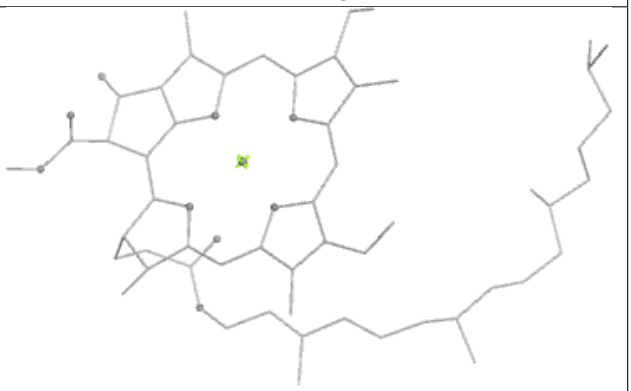
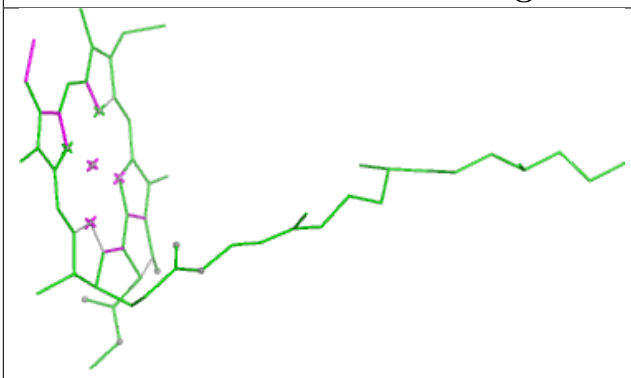
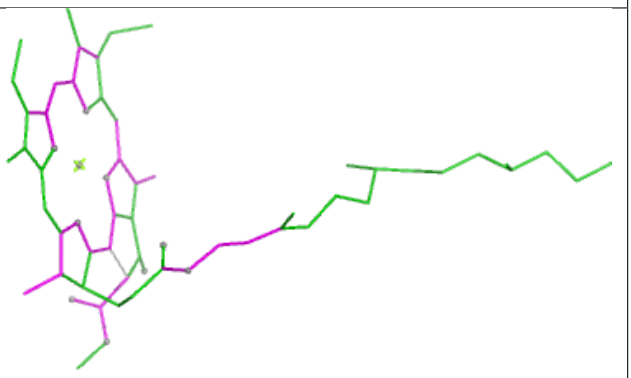
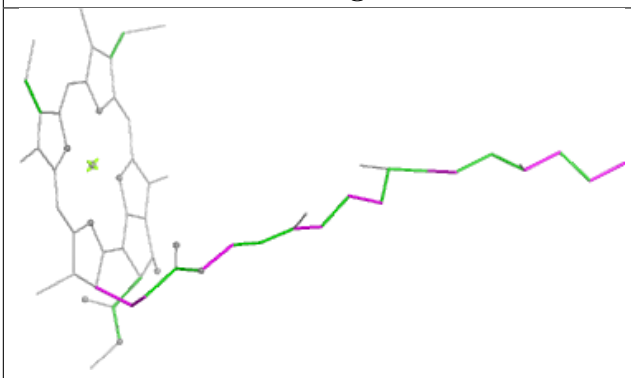


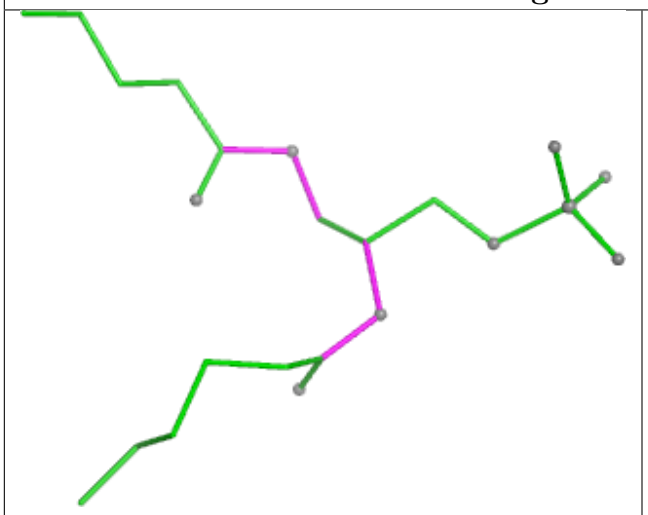
Rings

Ligand CLA A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

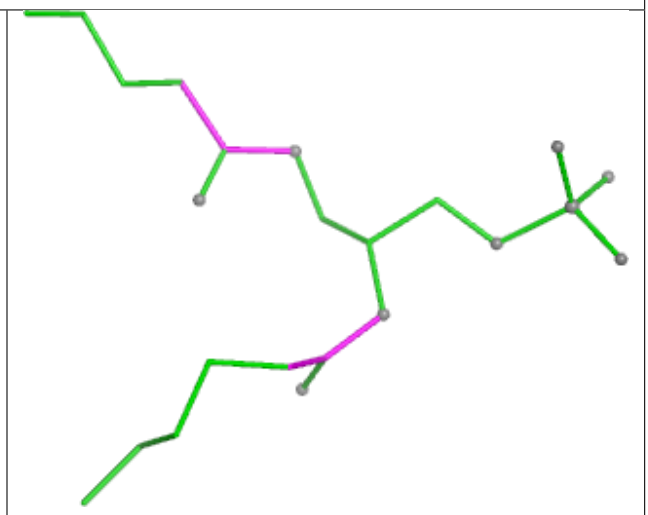
Ligand CLA 5 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1225	
 Bond lengths	 Bond angles
 Torsions	Rings

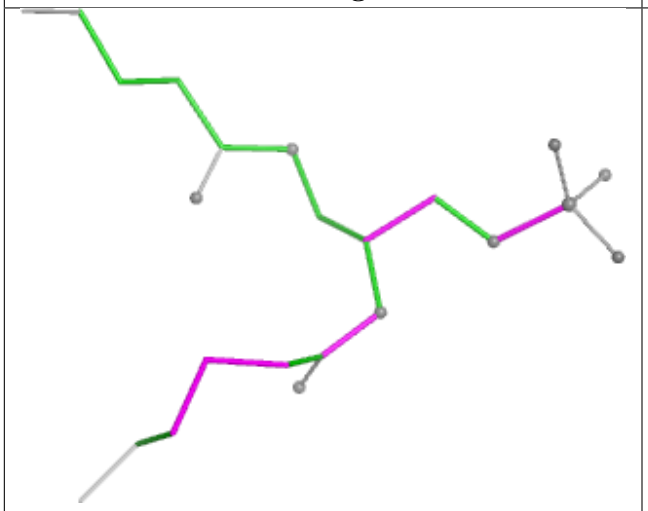
Ligand 3PH 5 802



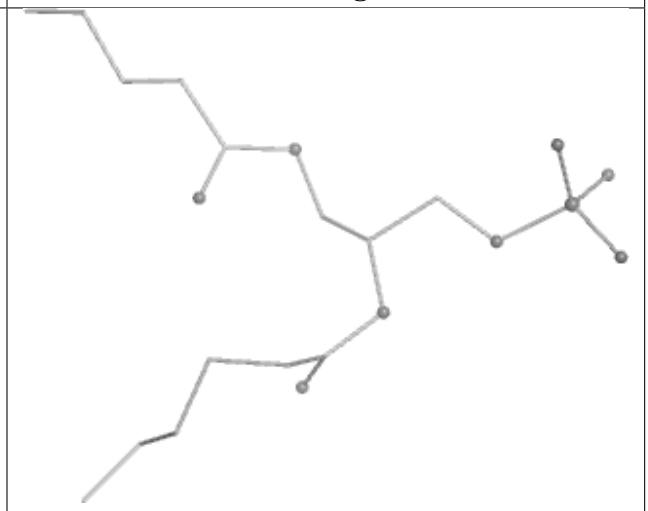
Bond lengths



Bond angles

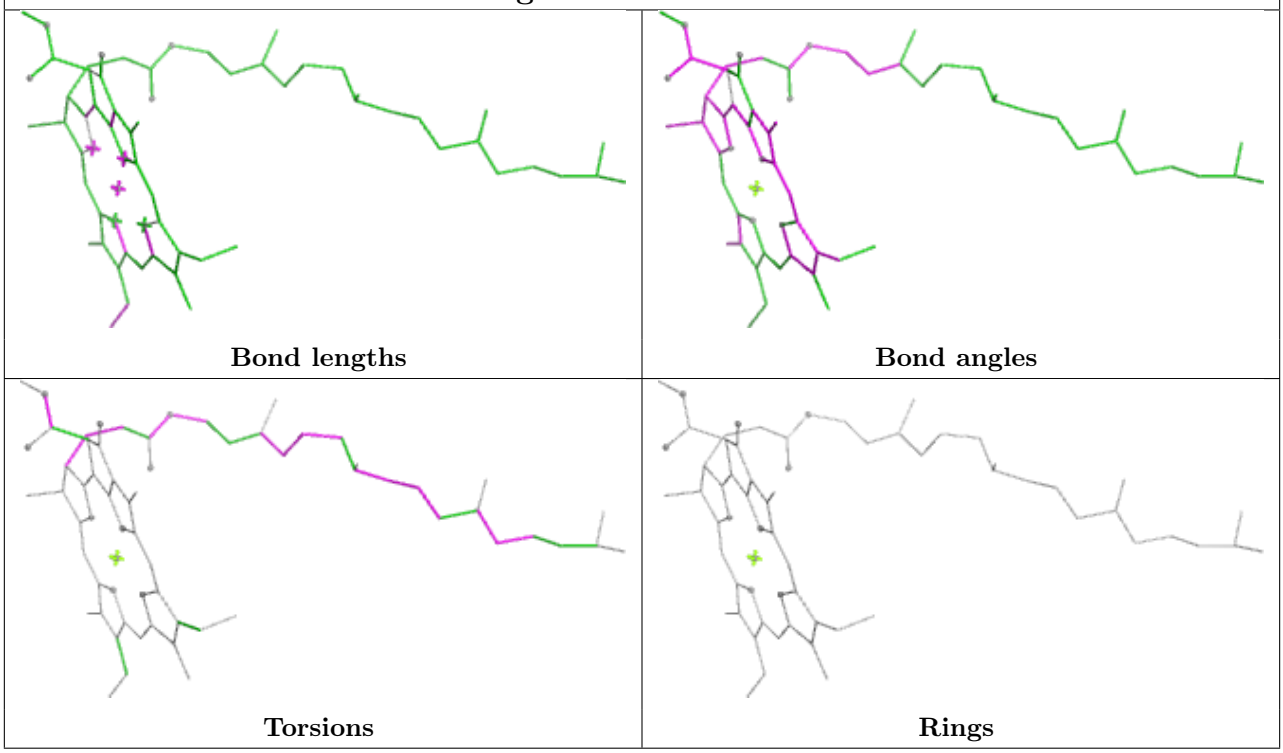


Torsions

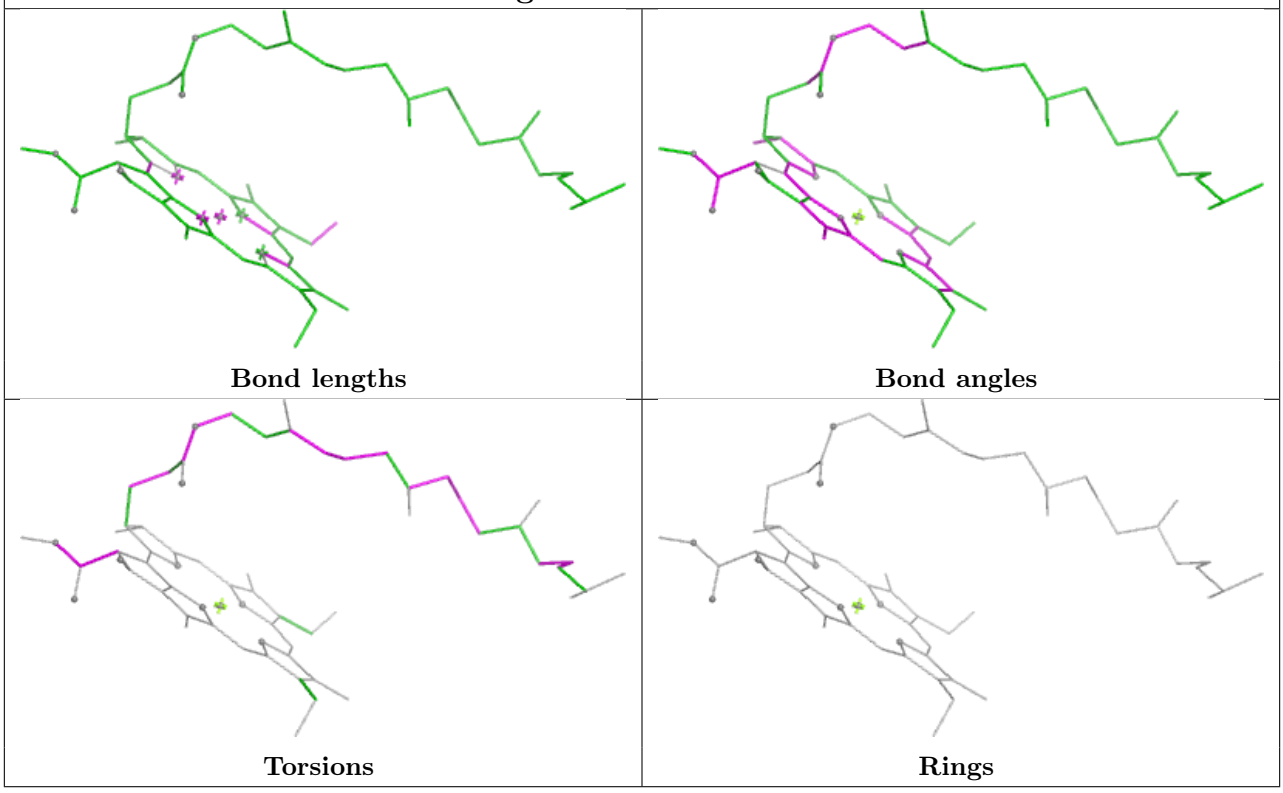


Rings

Ligand CLA B 1226



Ligand CLA B 1228



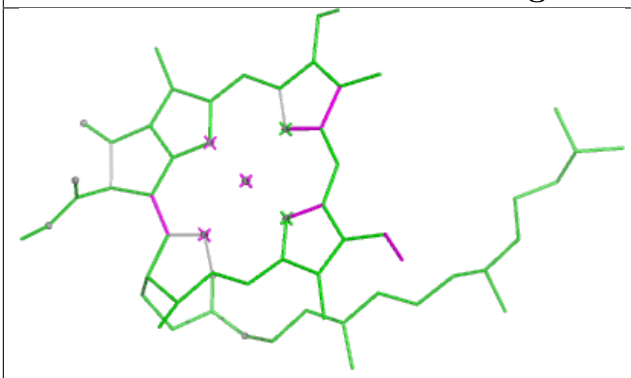
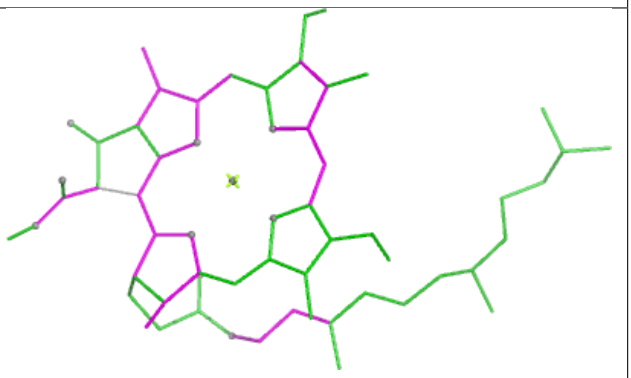
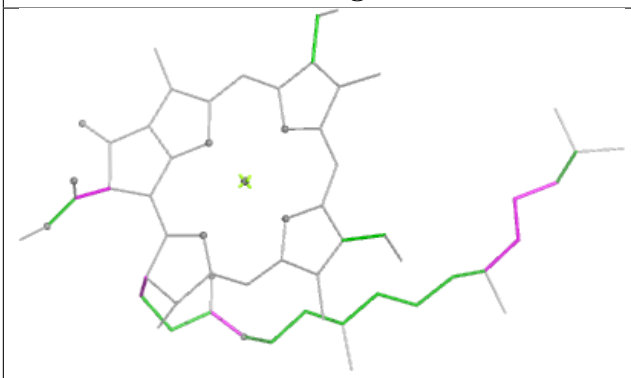
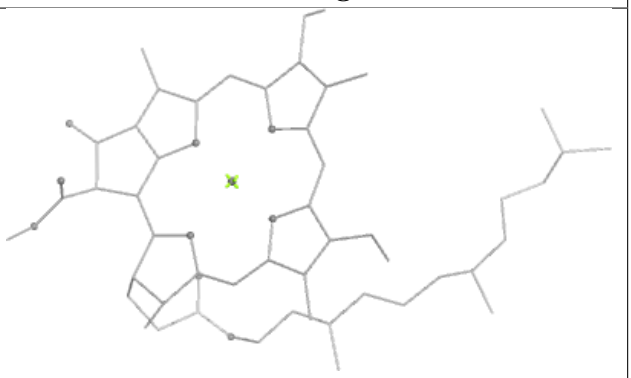
Ligand CLA A 1120

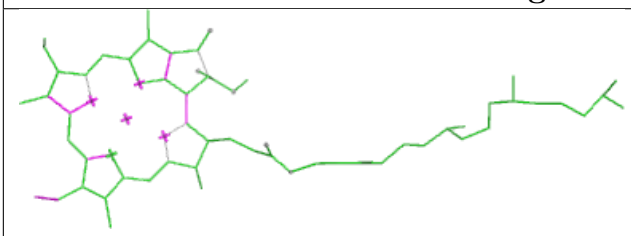
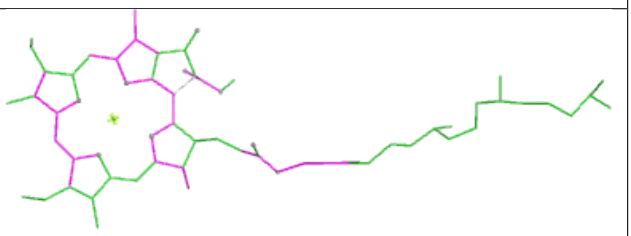
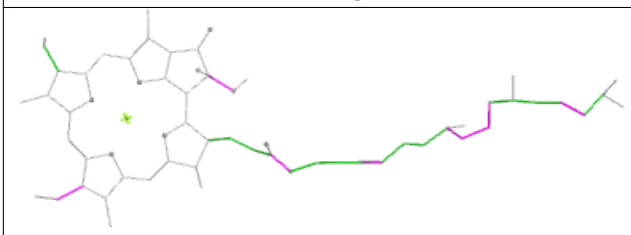
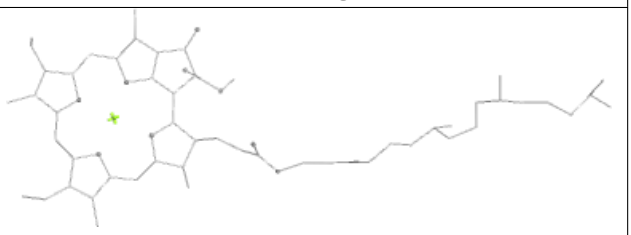
Bond lengths

Bond angles

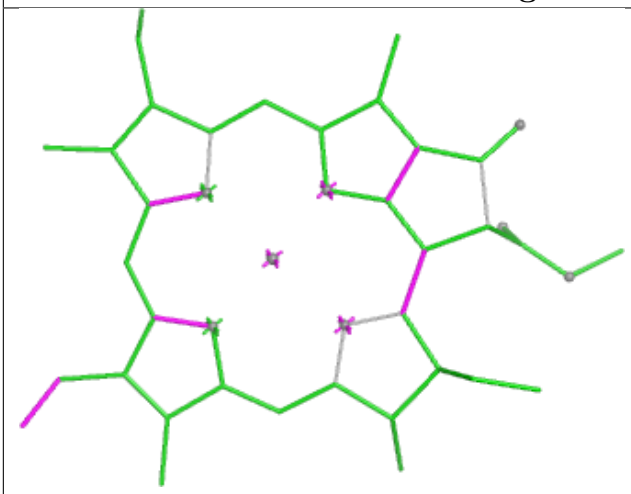
Torsions

Rings

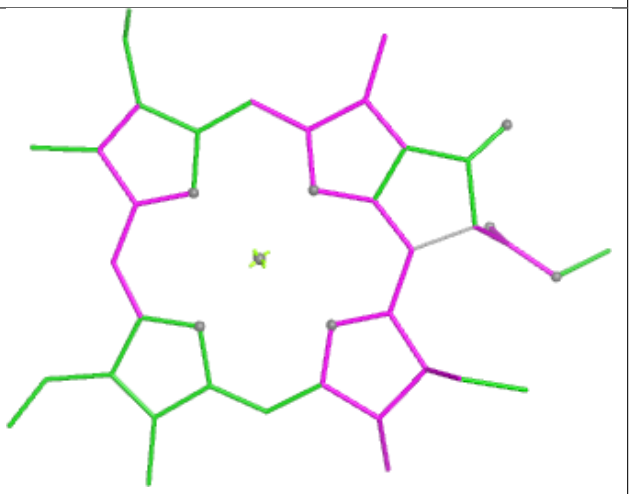
Ligand CLA 4 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 1901



Bond lengths



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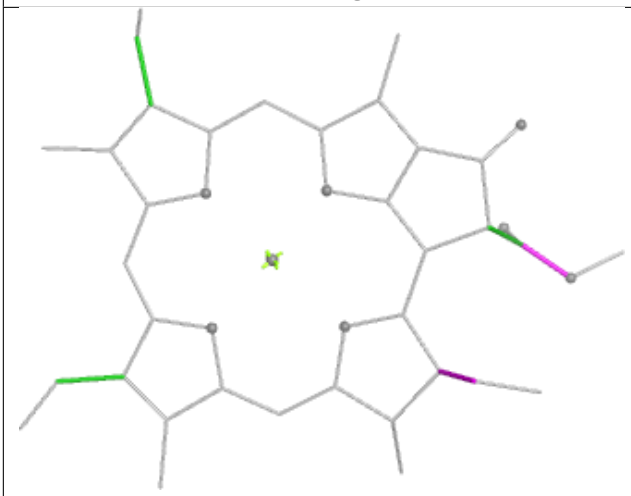
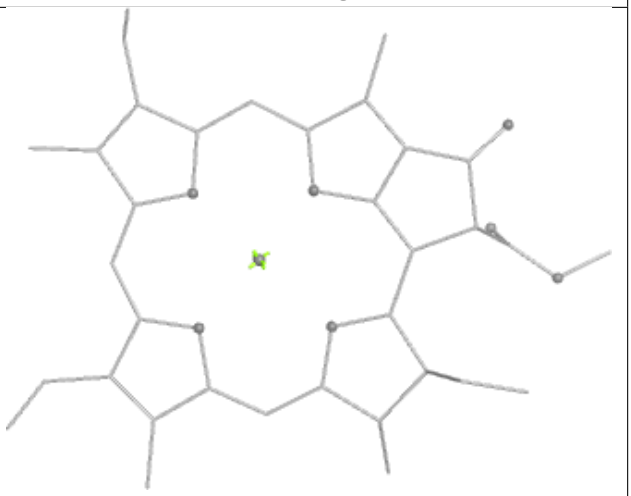
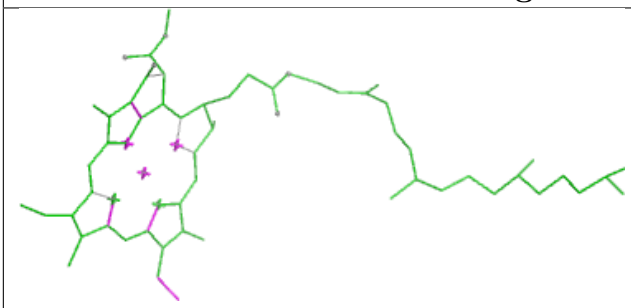
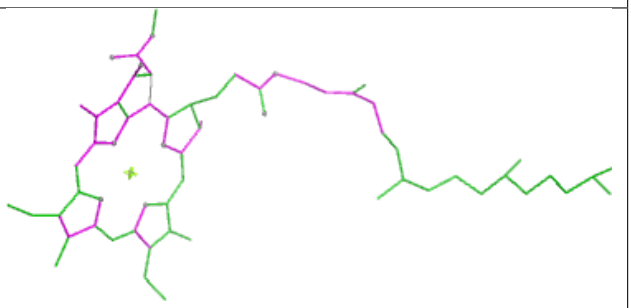
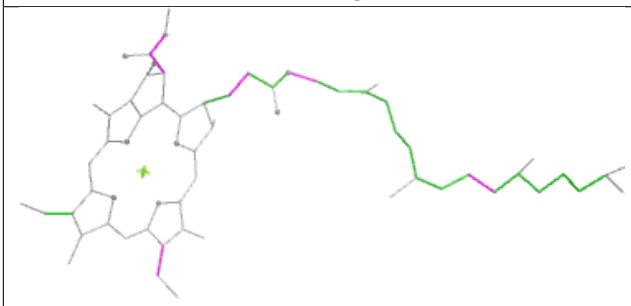
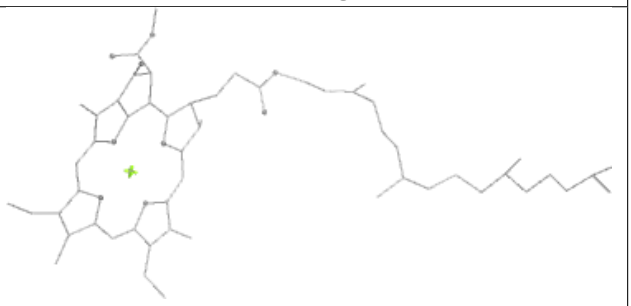
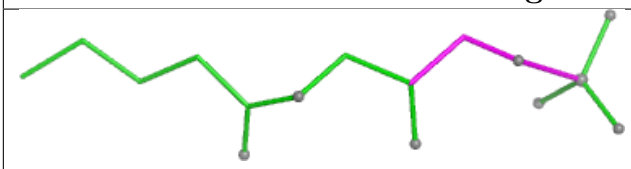
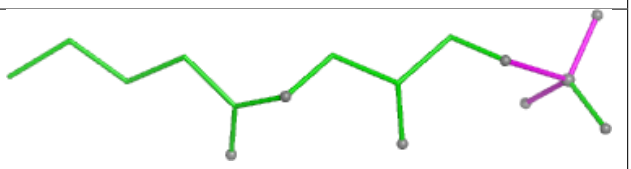
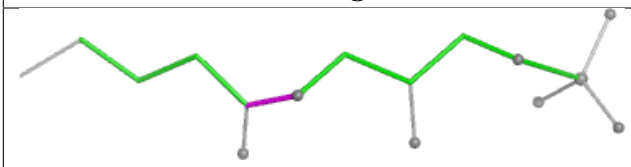
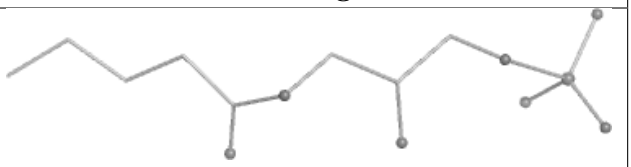


Torsions

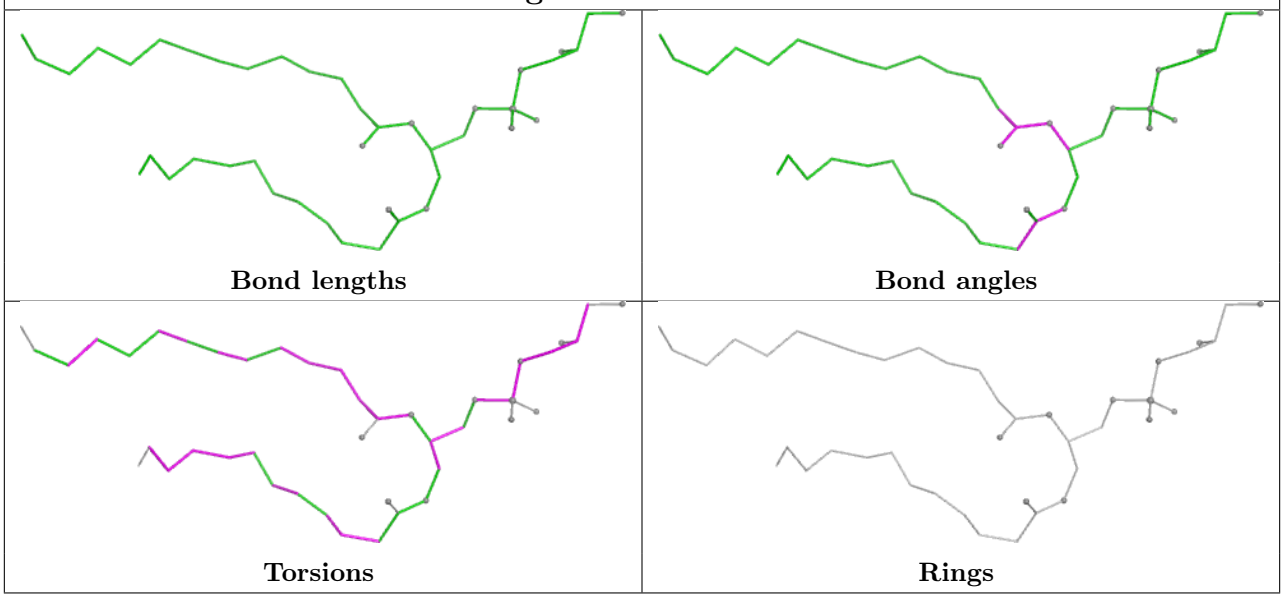


Rings

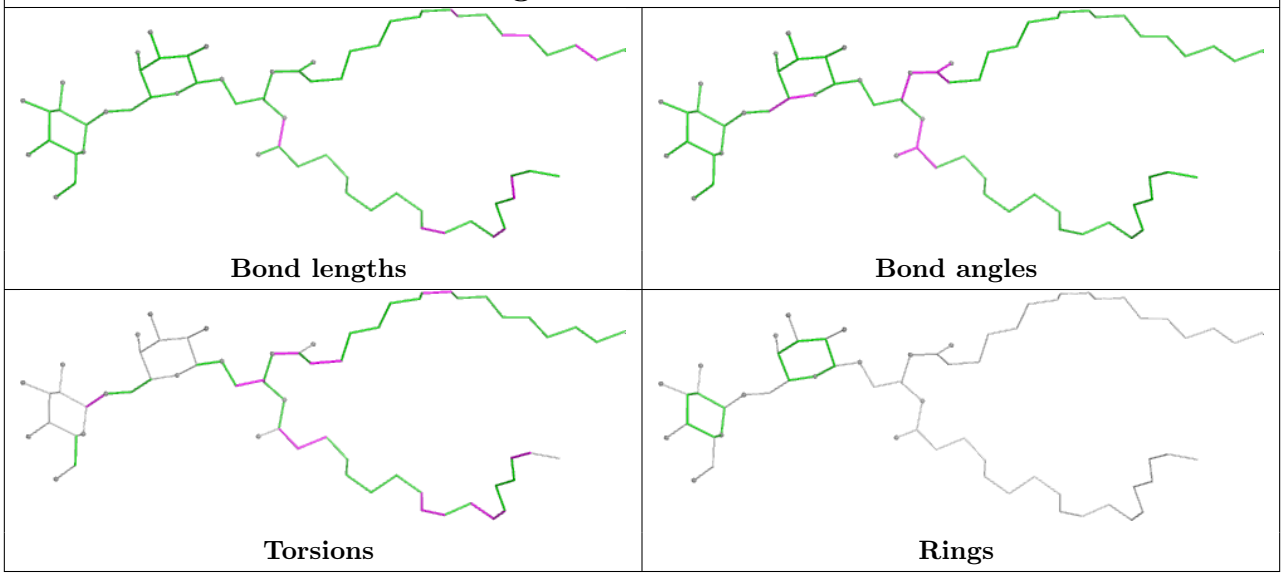
Ligand CLA B 1022	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NKP 3 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

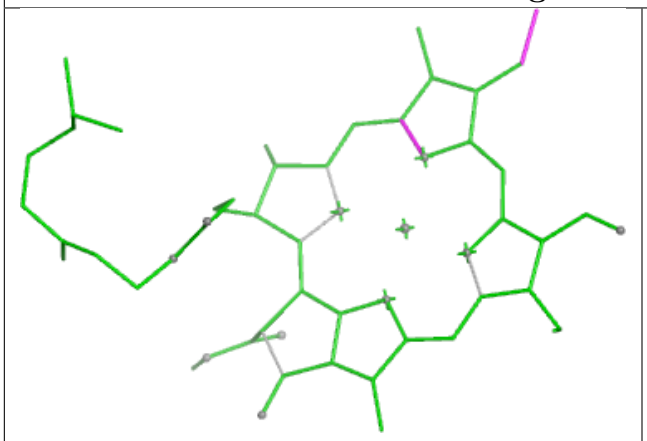
Ligand LHG Z 801



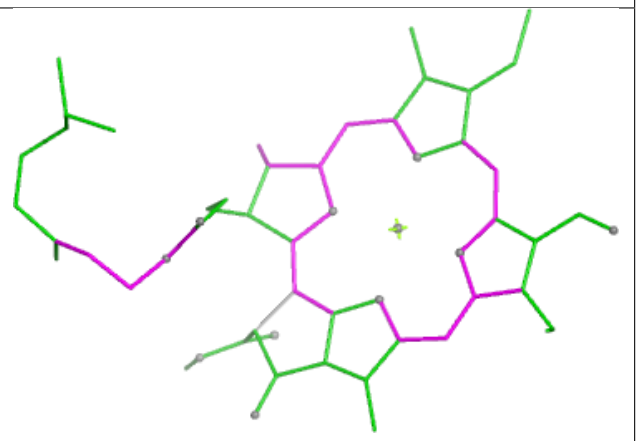
Ligand DGD B 5003



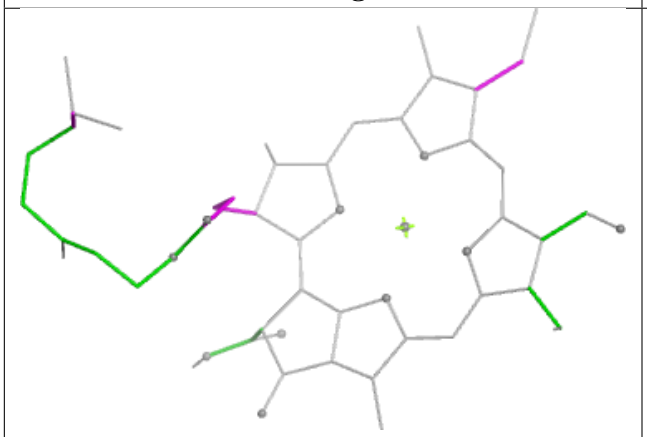
Ligand CHL 8 610



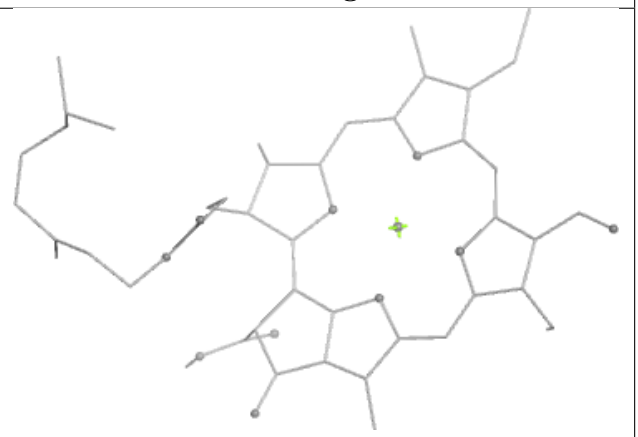
Bond lengths



Bond angles

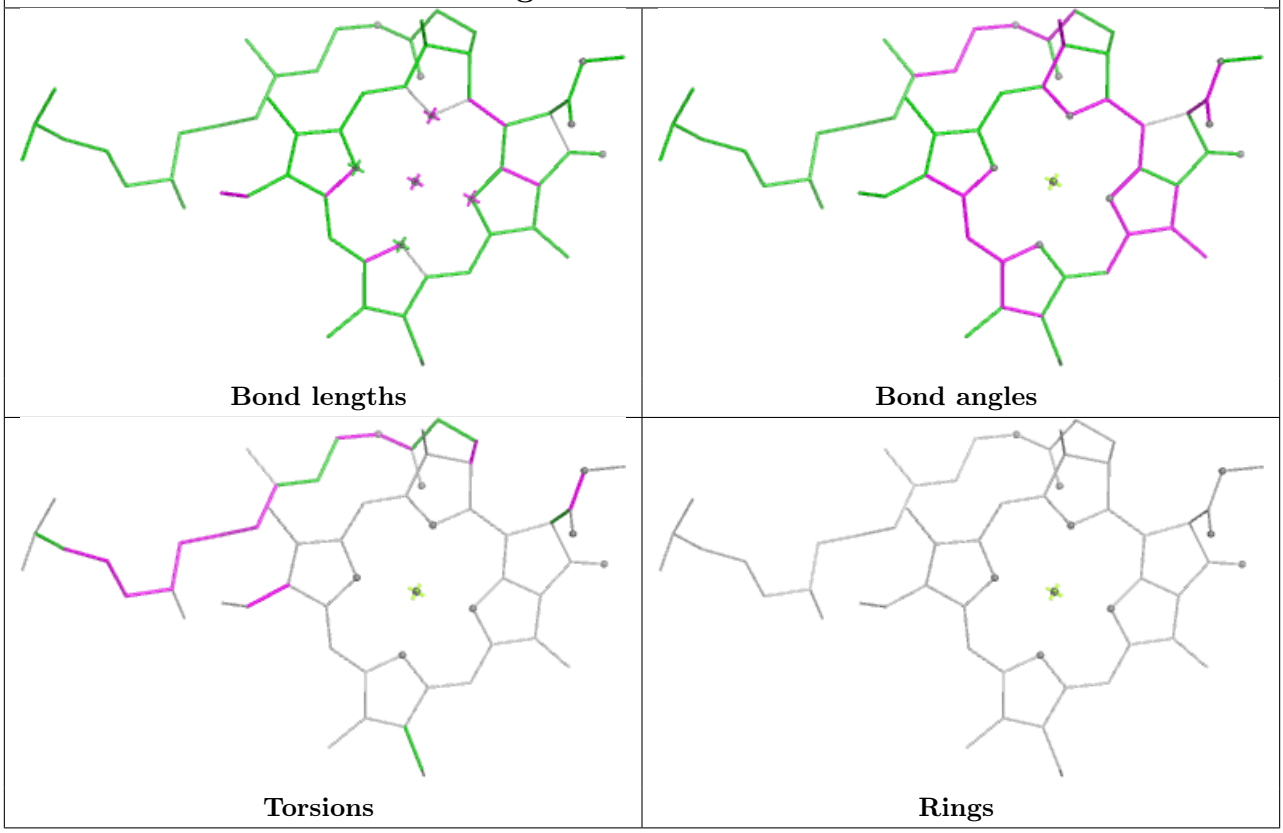


Torsions

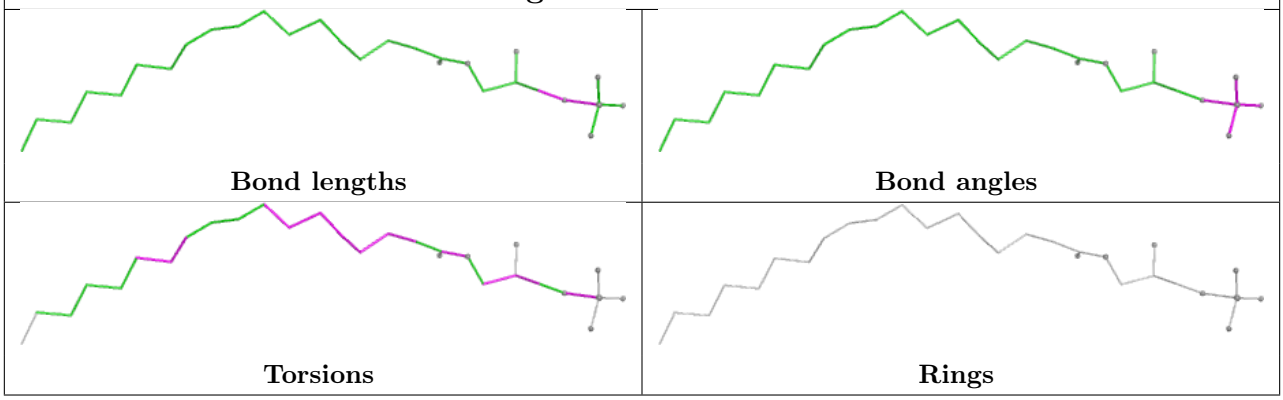


Rings

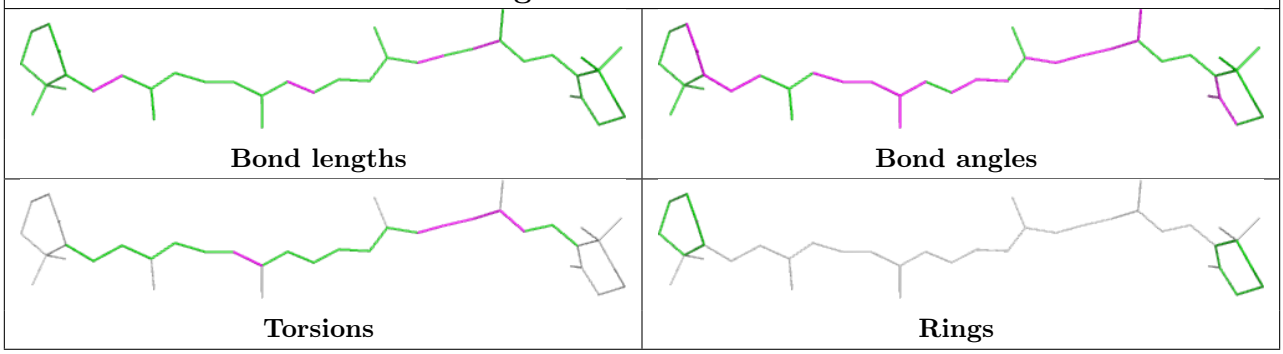
Ligand CLA B 1215

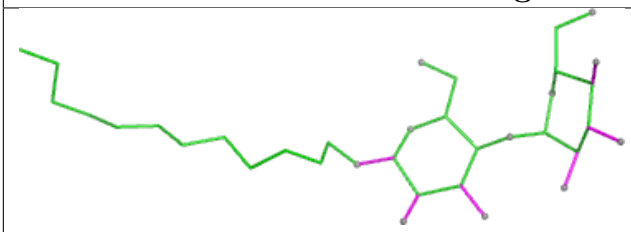
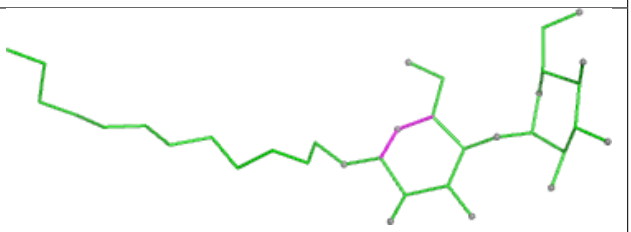
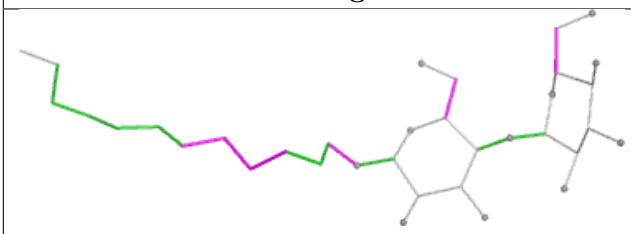
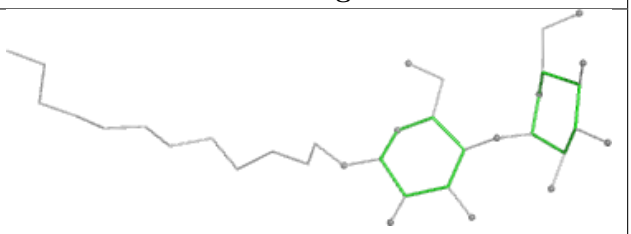


Ligand NKP 8 802



Ligand BCR A 4002



Ligand LMT F 5001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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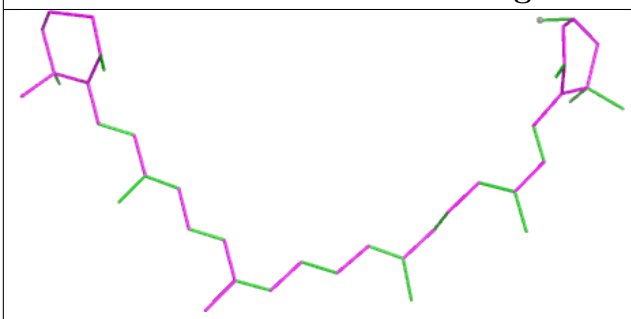
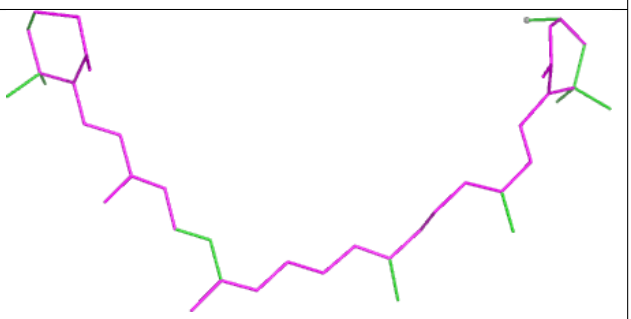
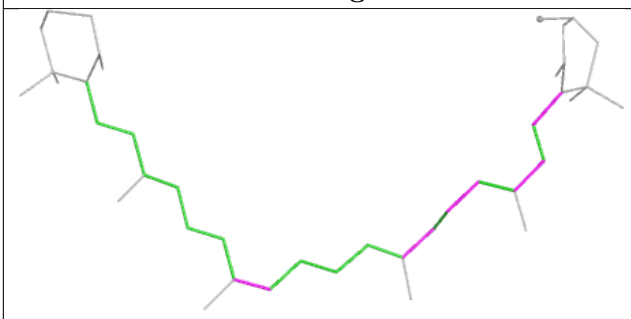
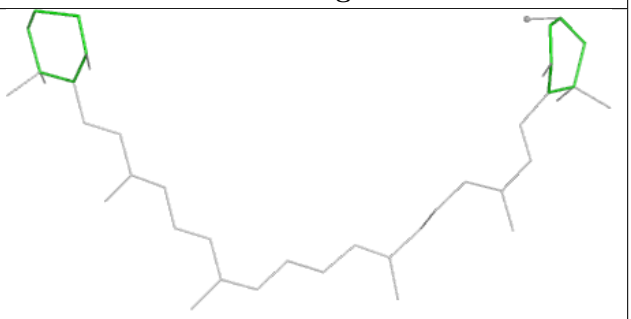
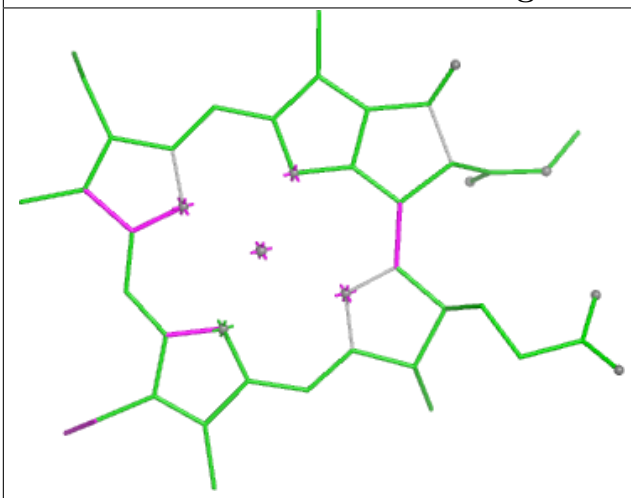
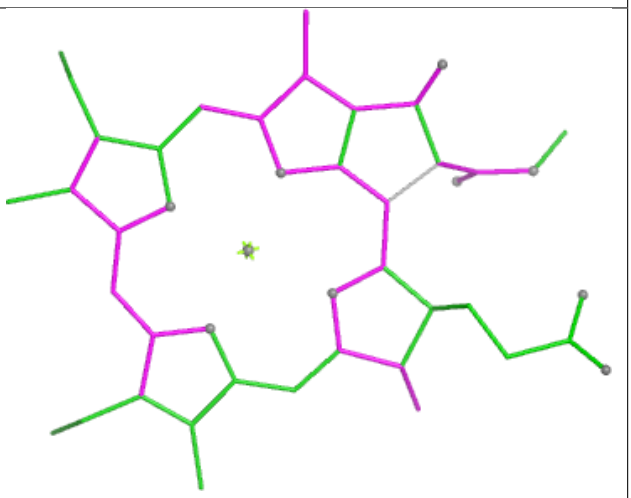
 Bond lengths	 Bond angles
 Torsions	 Rings

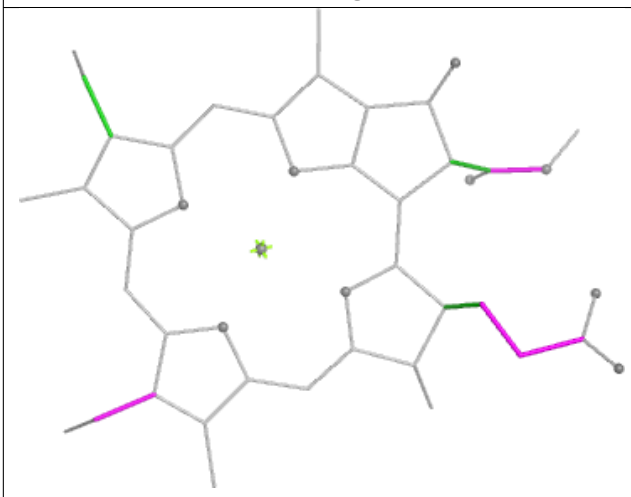
Ligand CLA F 1302



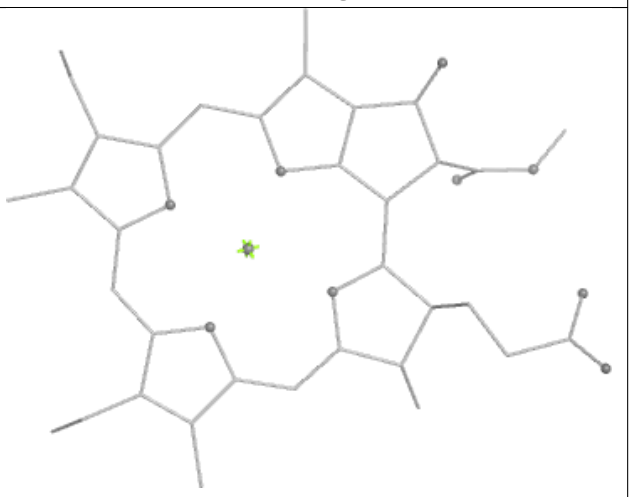
Bond lengths



Bond angles

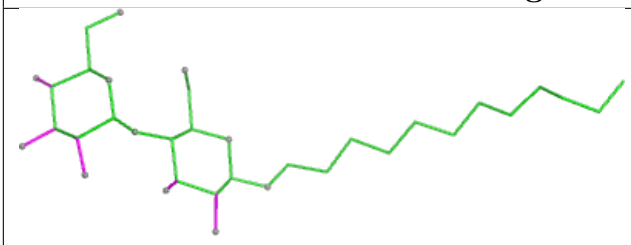


Torsions



Rings

Ligand LMT 1 803



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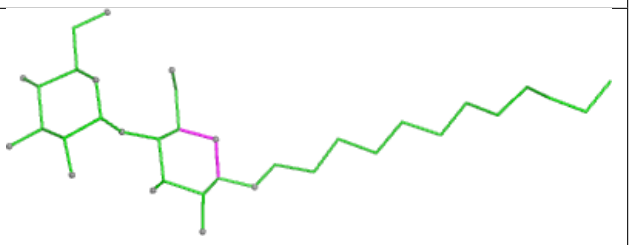
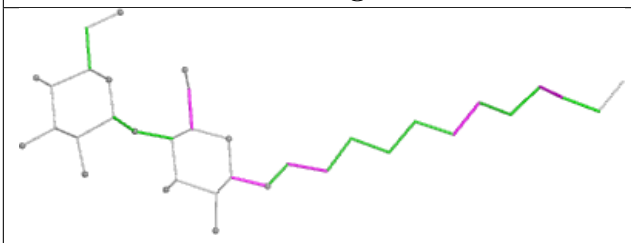
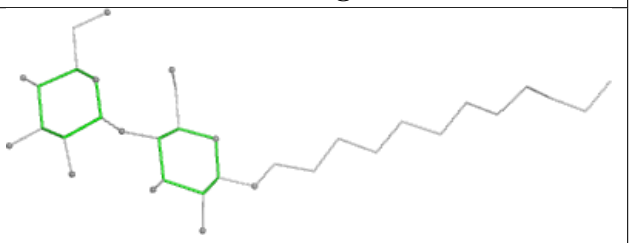


Bond angles

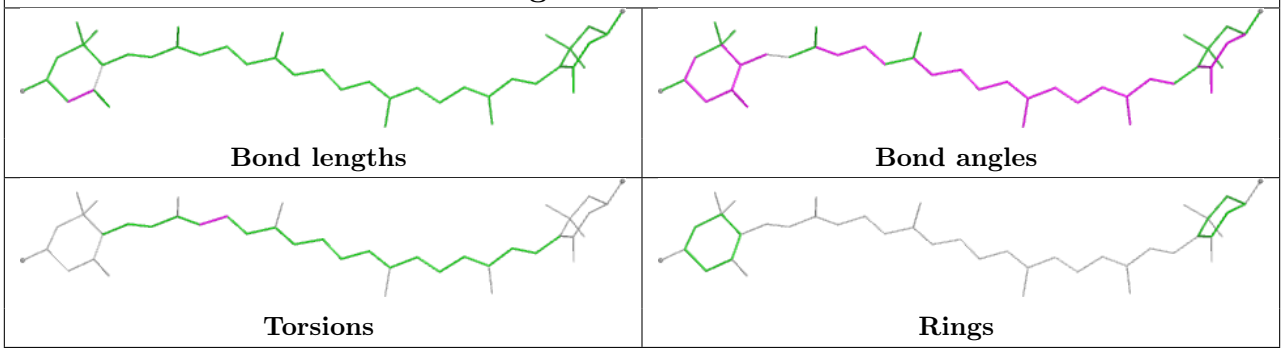


Torsions

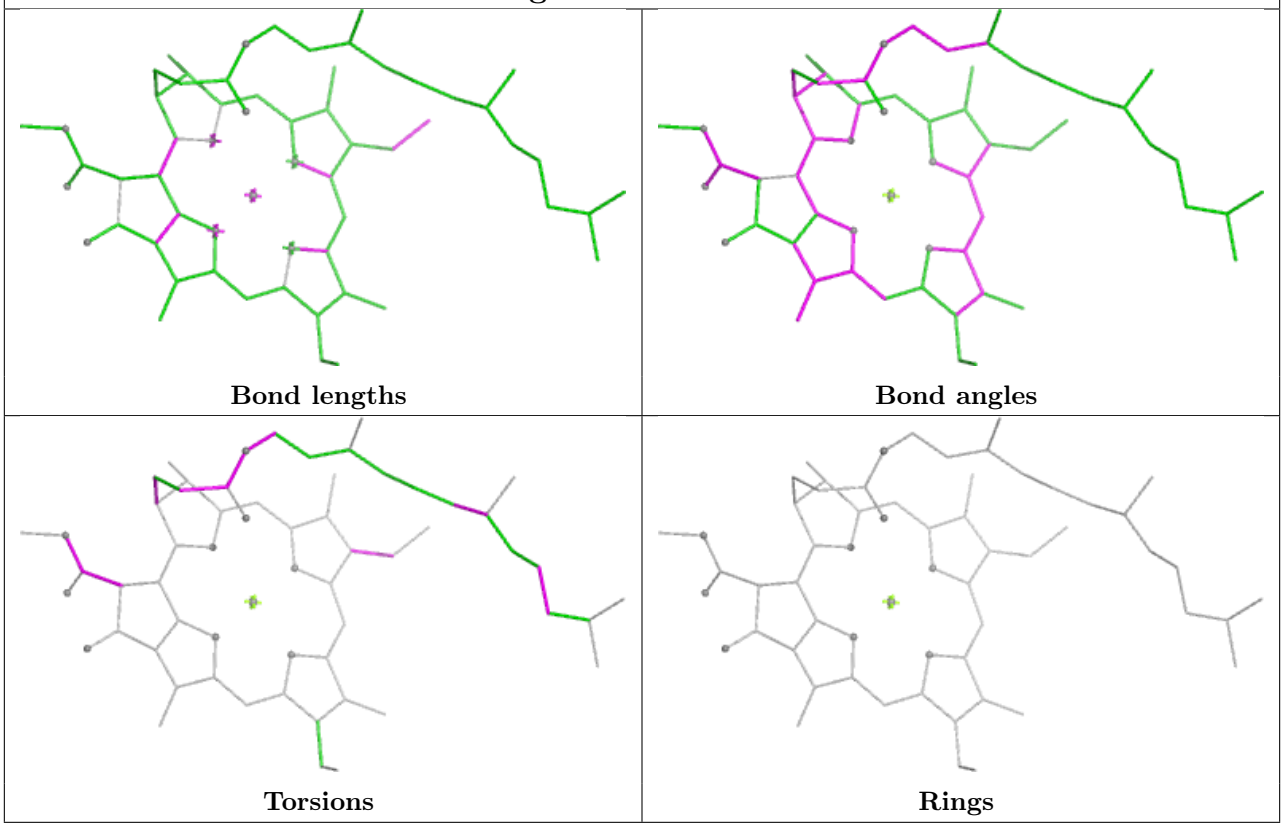


Rings

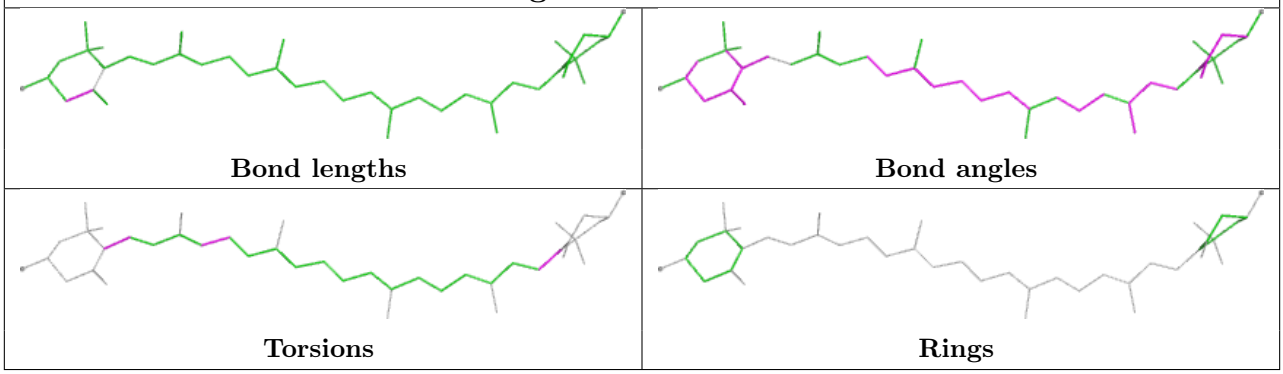
Ligand LUT 1 502



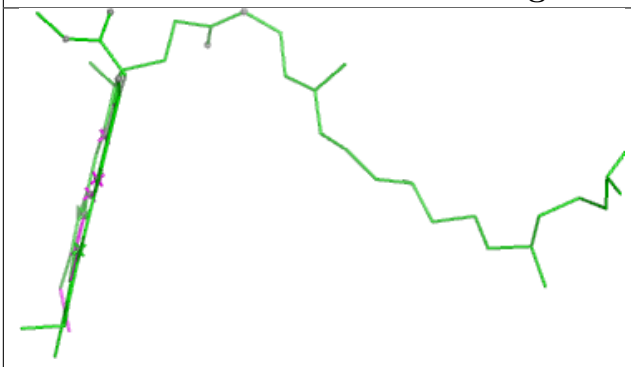
Ligand CLA 6 601



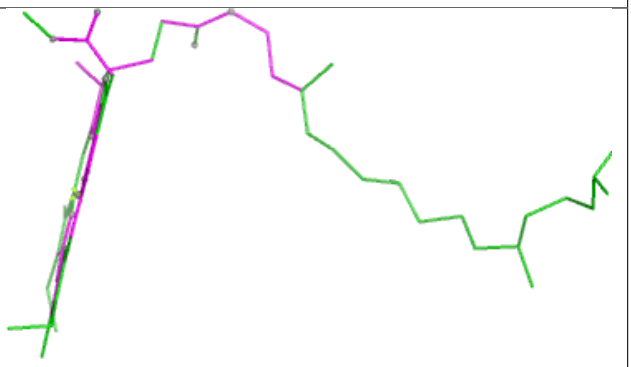
Ligand LUT 4 502



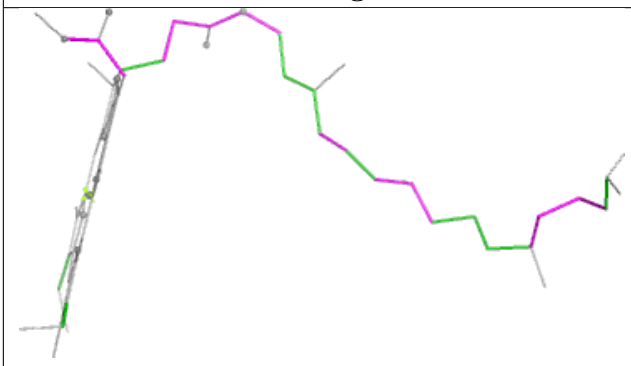
Ligand CLA 8 609



Bond lengths



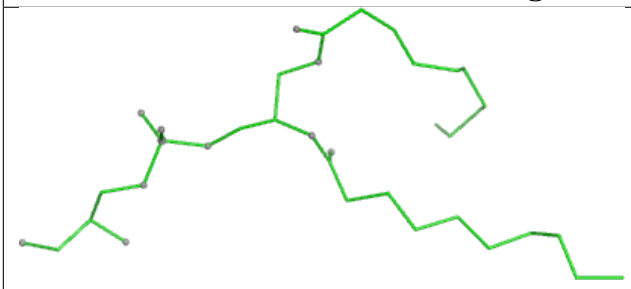
Bond angles



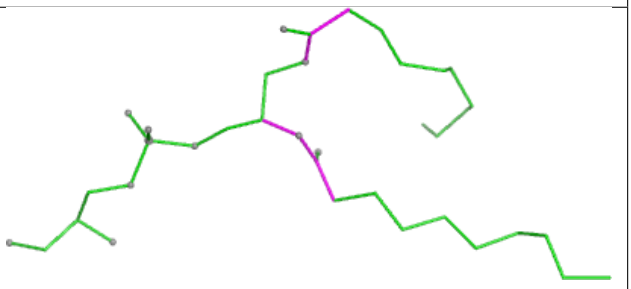
Torsions

Rings

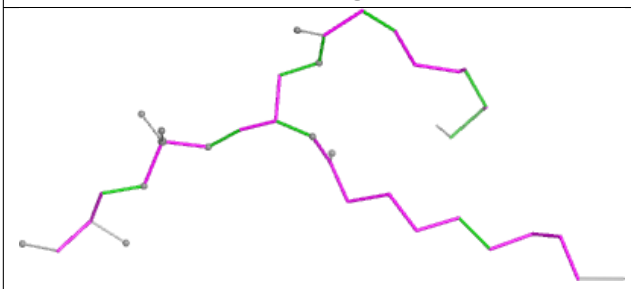
Ligand LHG 5 801



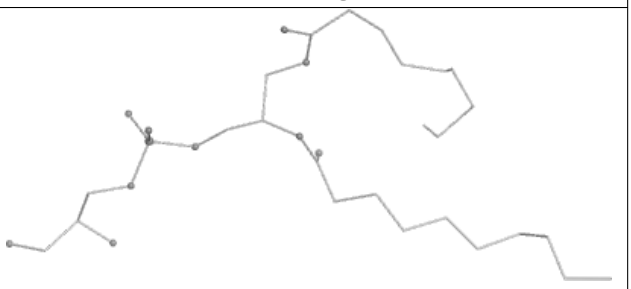
Bond lengths



Bond angles

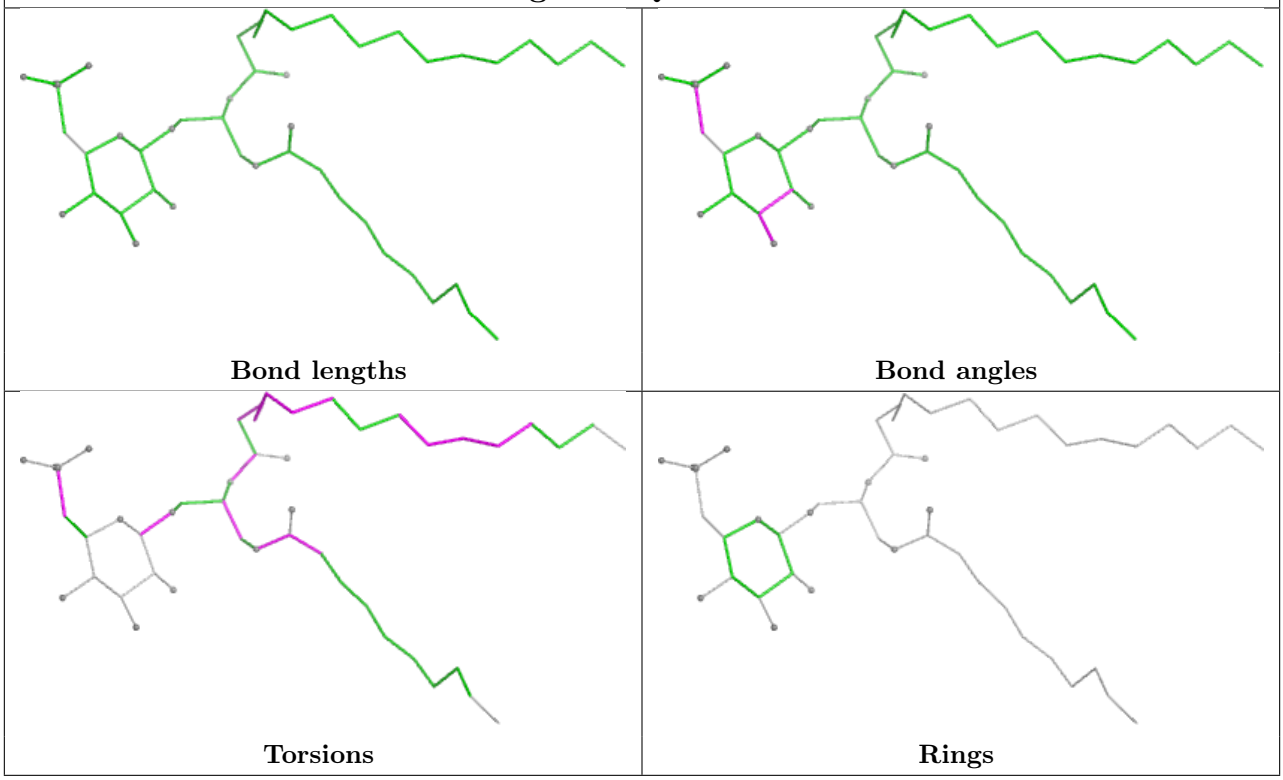


Torsions

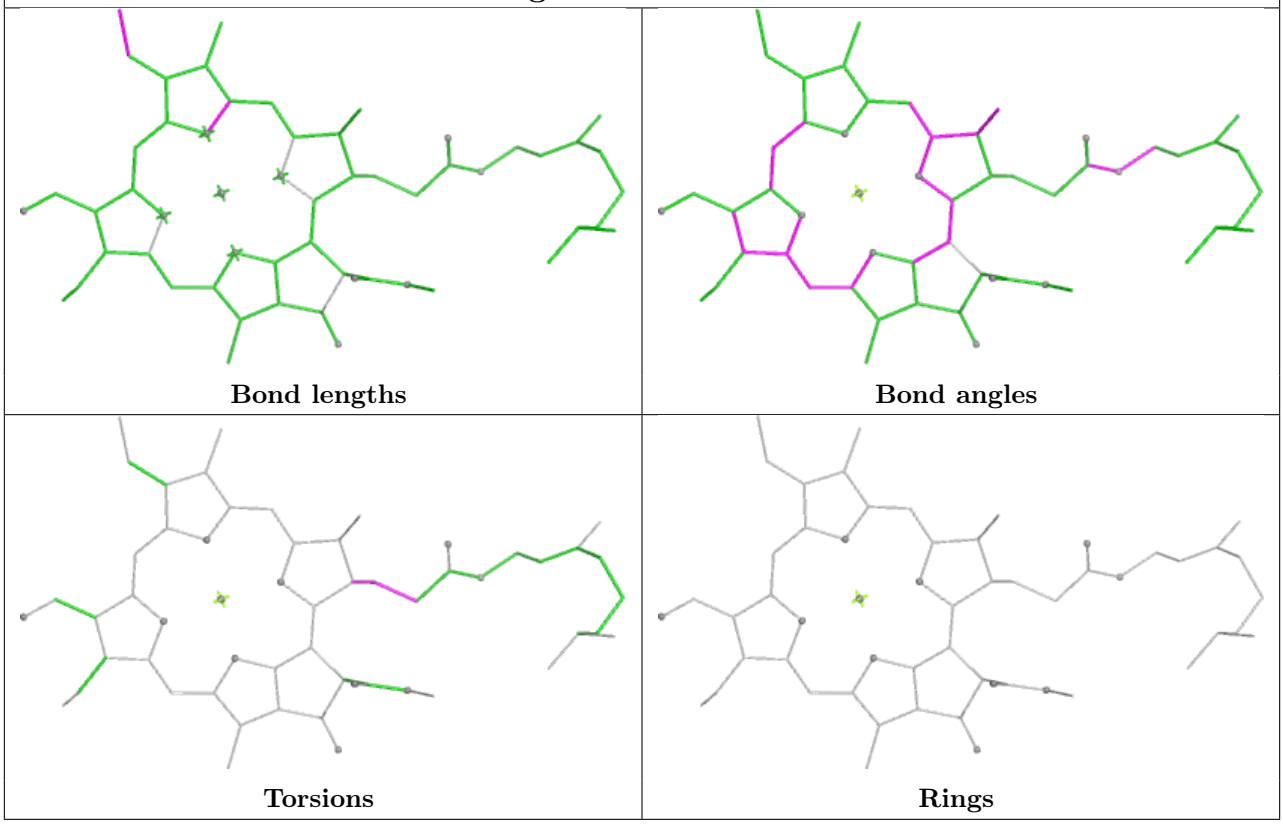


Rings

Ligand SQD 1 802



Ligand CHL 4 613



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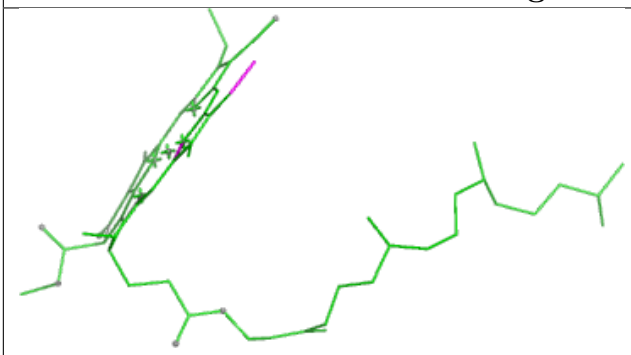
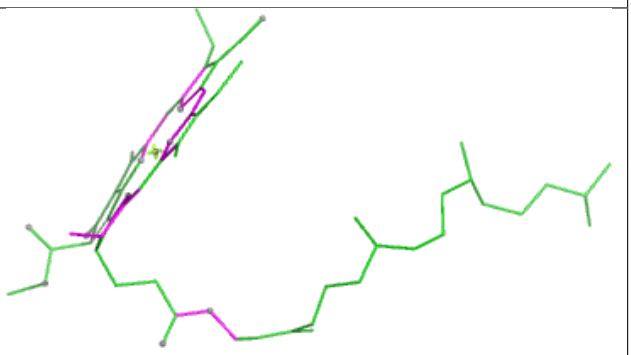
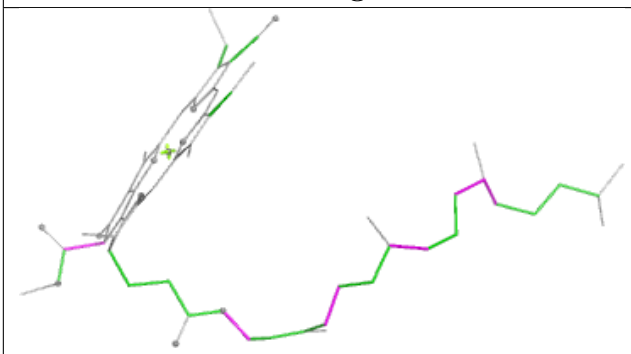
 Bond lengths	 Bond angles
 Torsions	Rings

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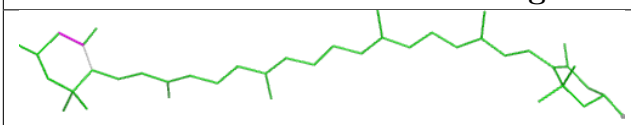
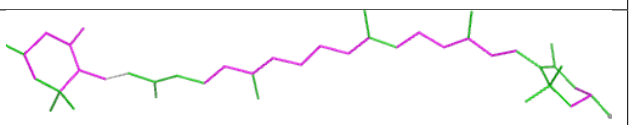
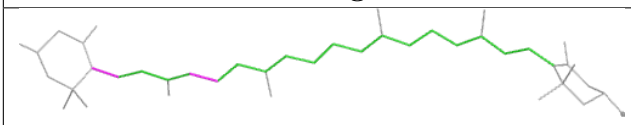
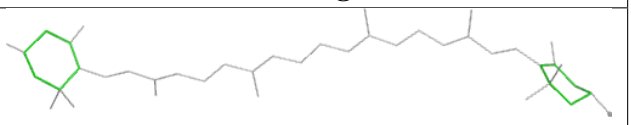
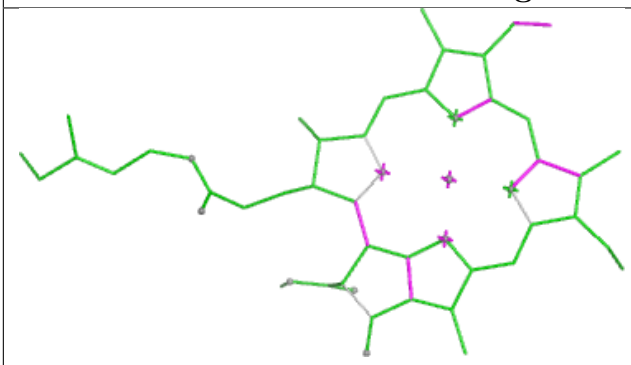
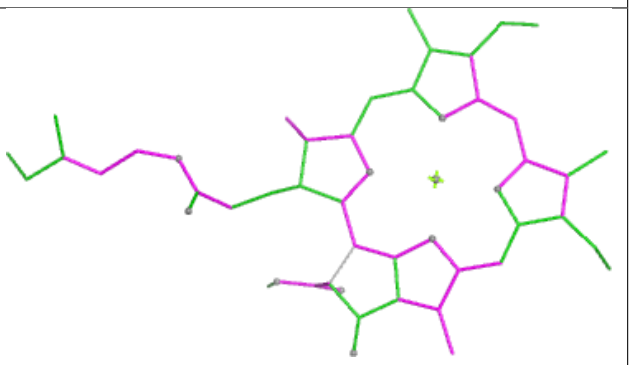
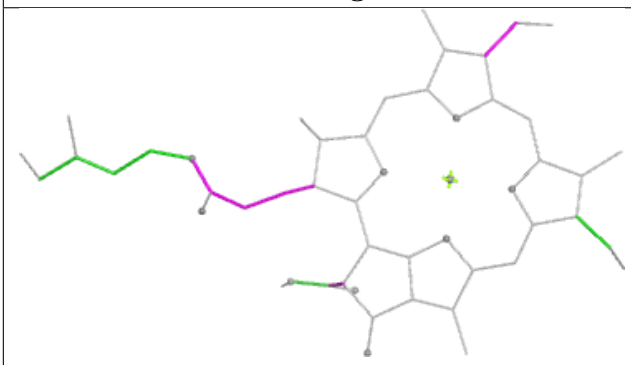
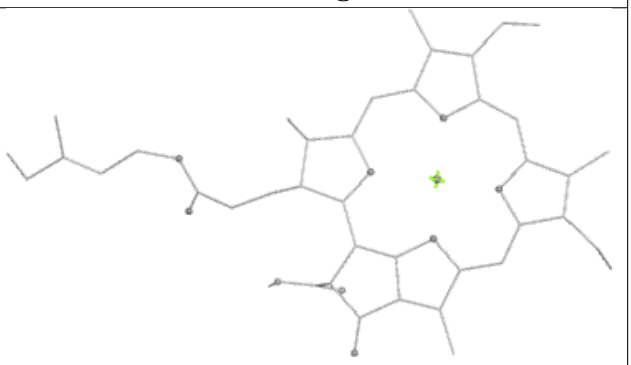
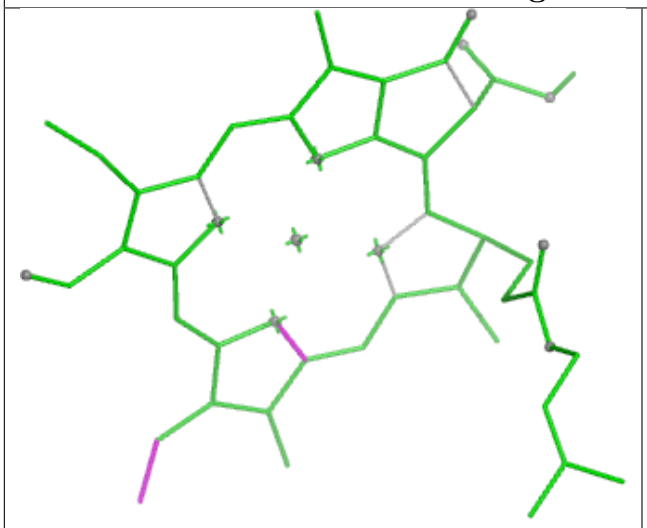
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1135	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 4 610



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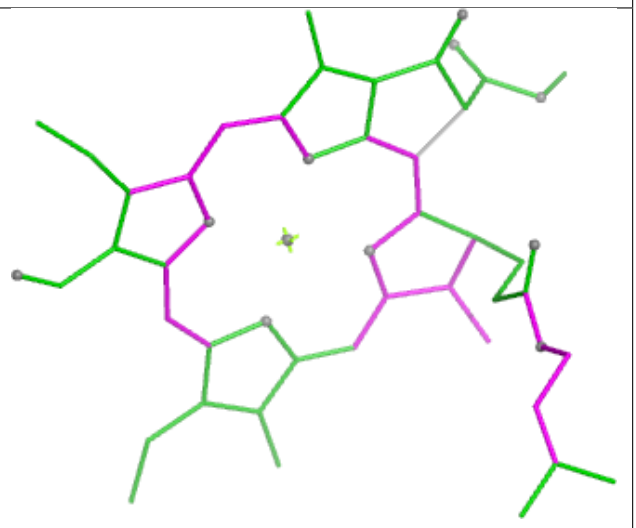

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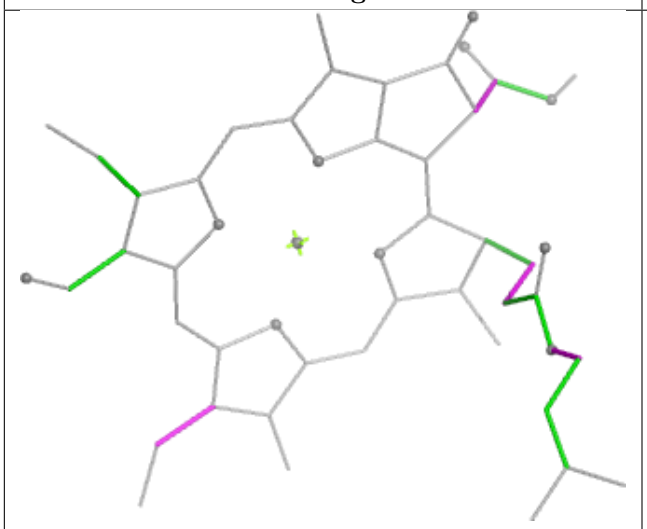
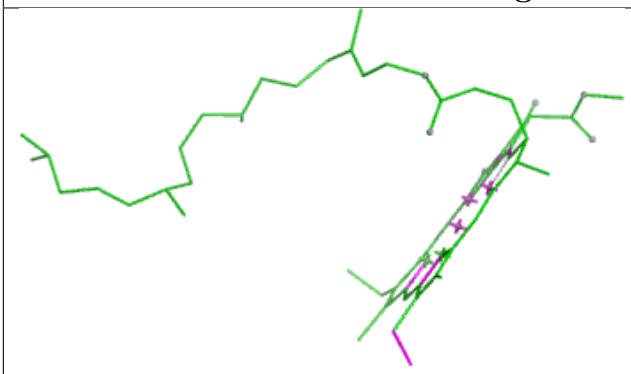
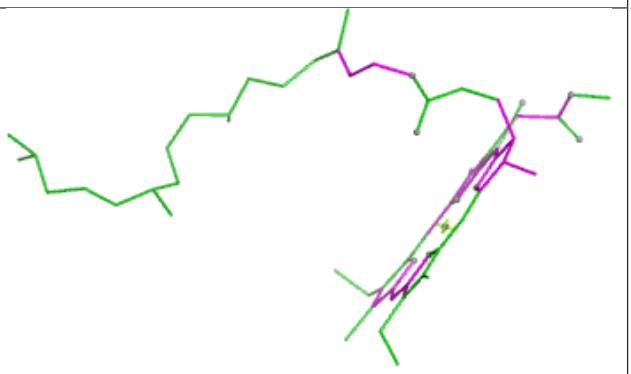
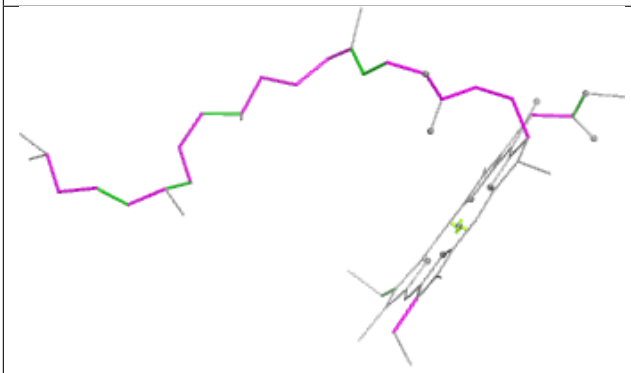
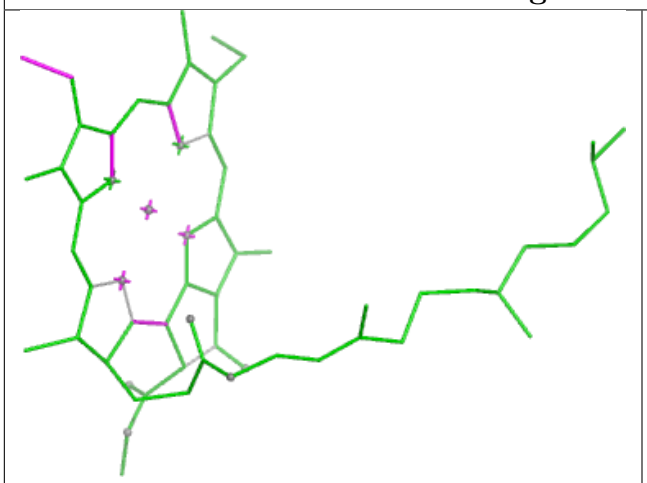


Torsions

Rings

Ligand CLA A 1108	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 1 607



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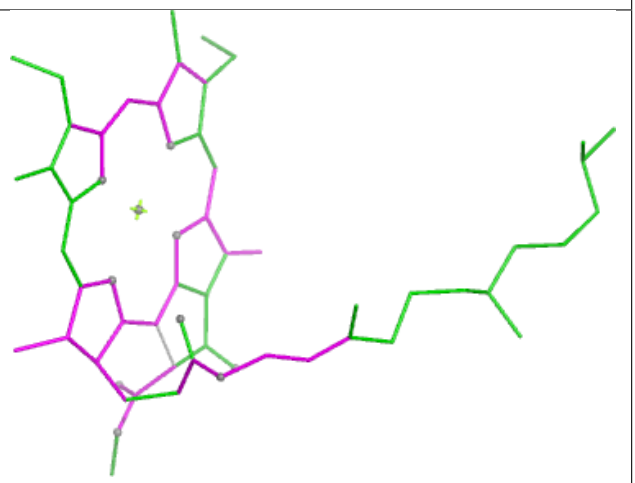

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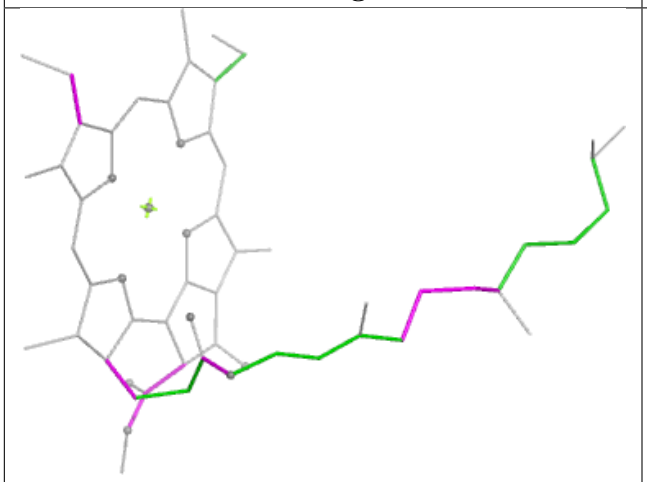

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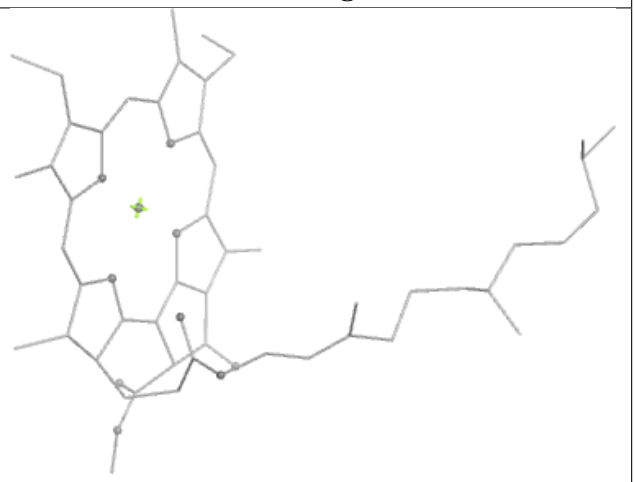
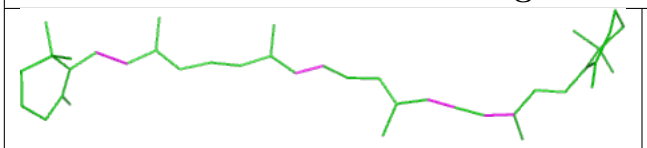


Rings

Ligand BCR B 4007



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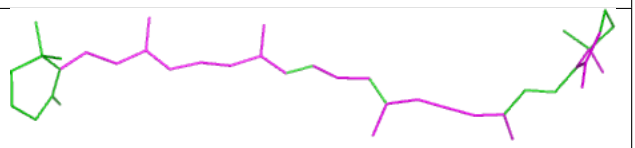

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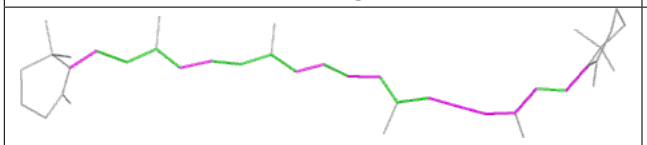

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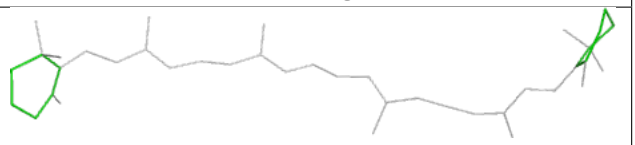
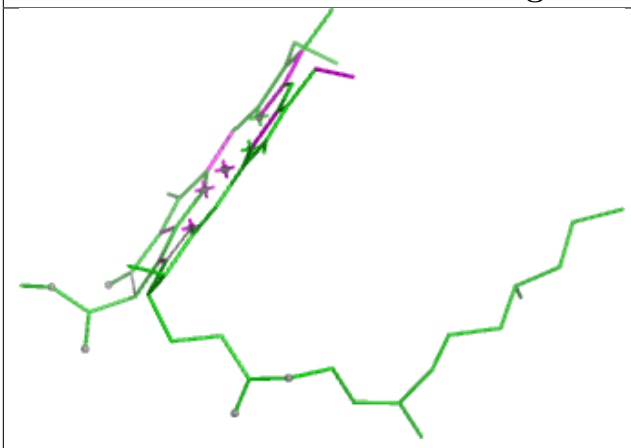
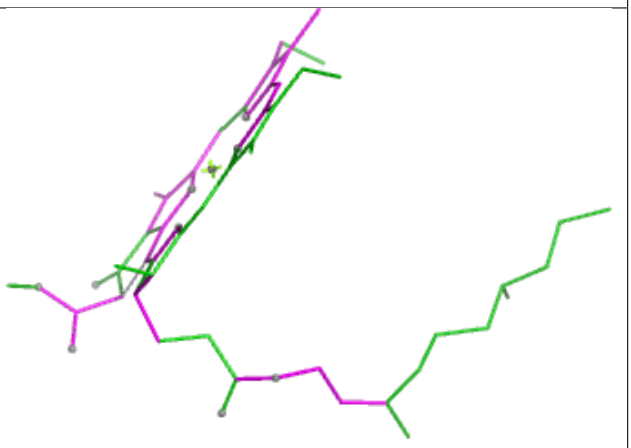
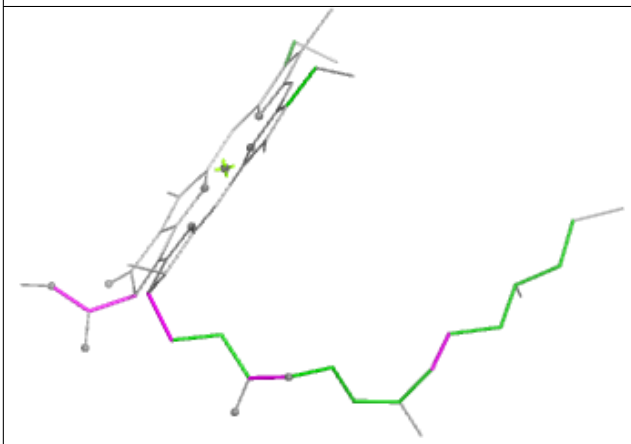
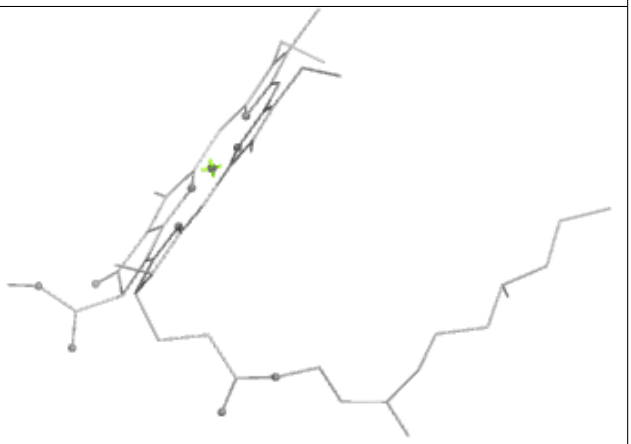


Rings

Ligand CLA Z 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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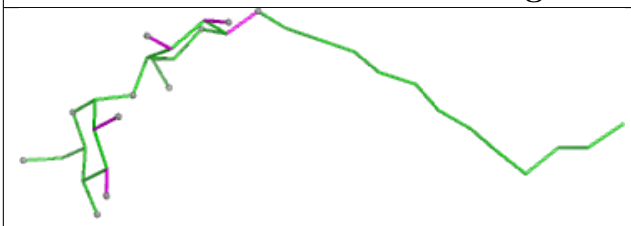
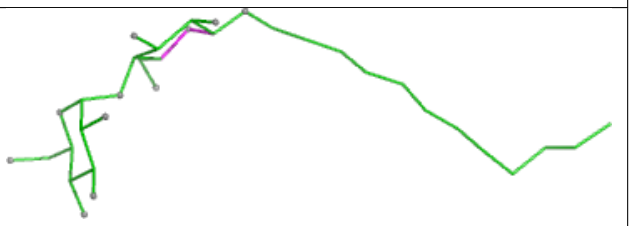
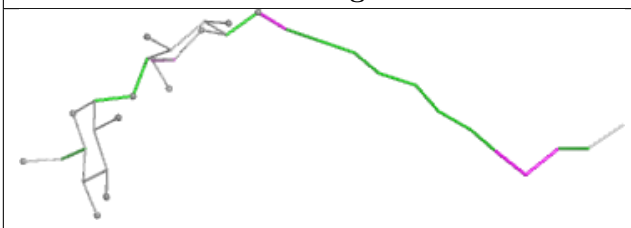
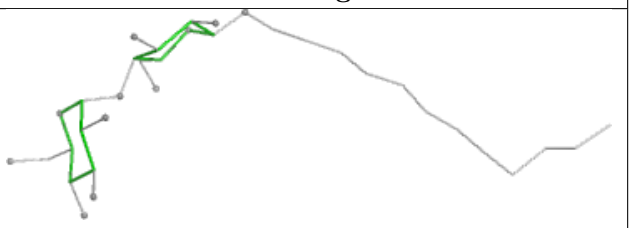
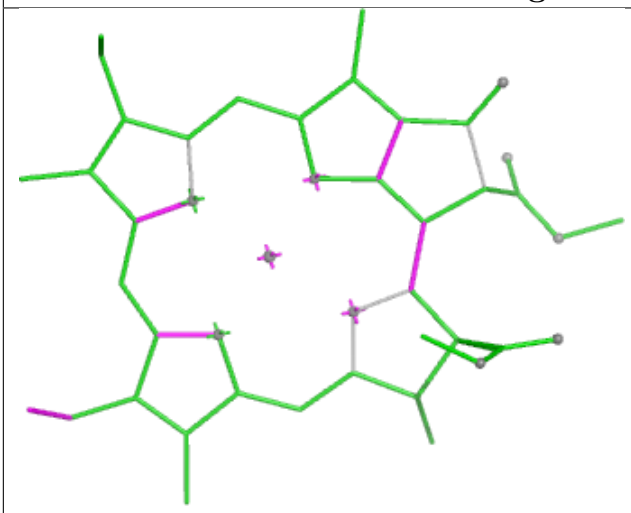
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 615



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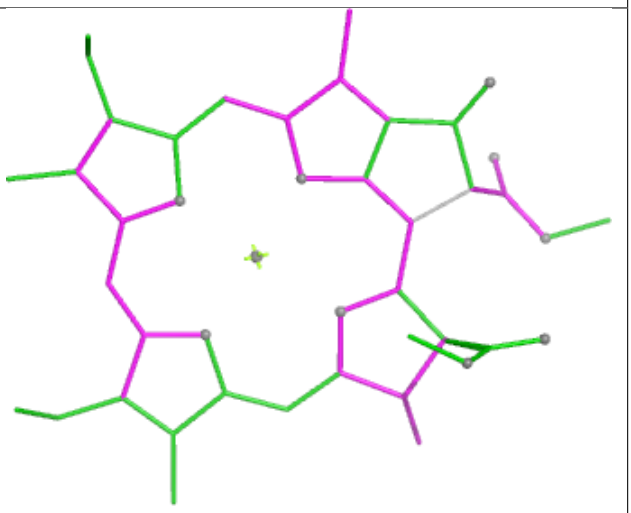

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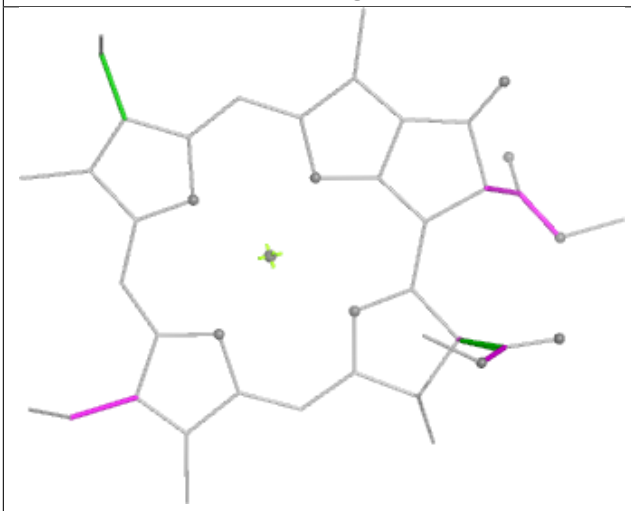

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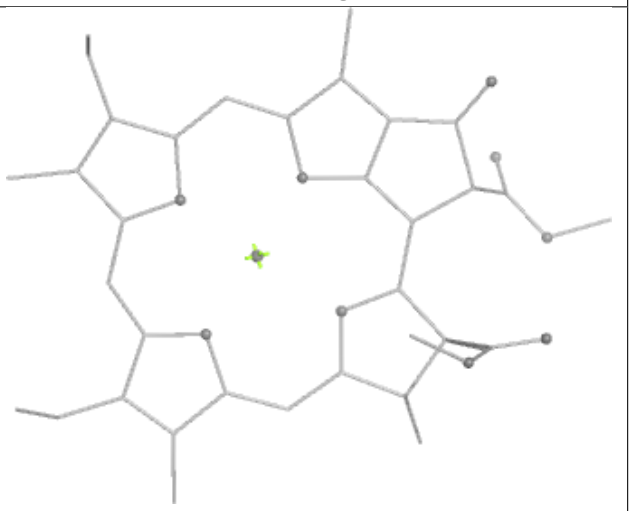
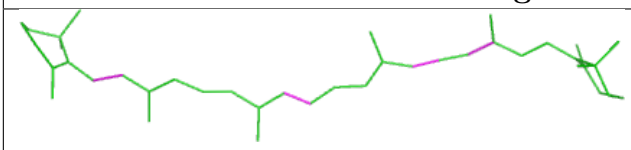


Rings

Ligand BCR B 4004



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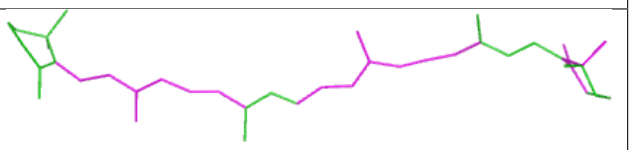

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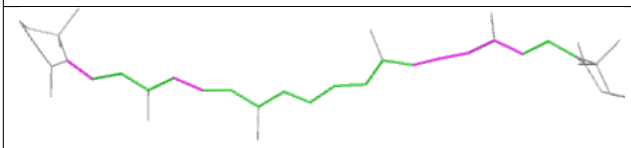

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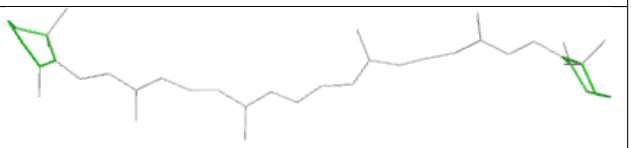
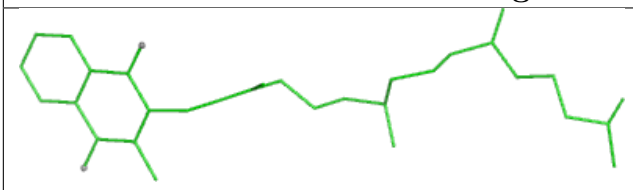


Rings

Ligand PQN A 2001



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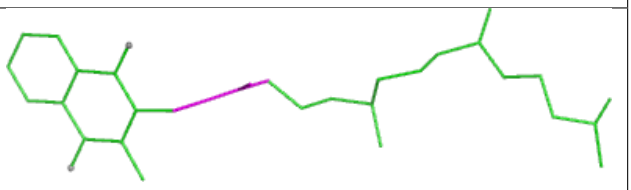

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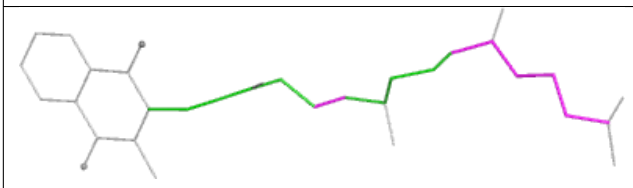

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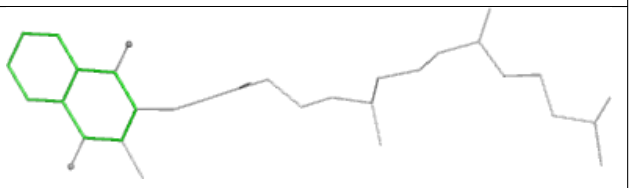
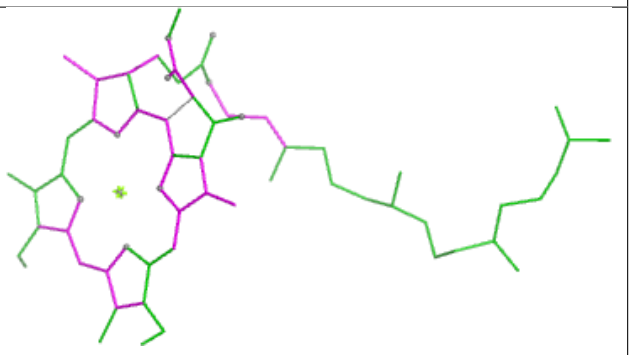


Rings

Ligand CLA 7 607

Bond lengths



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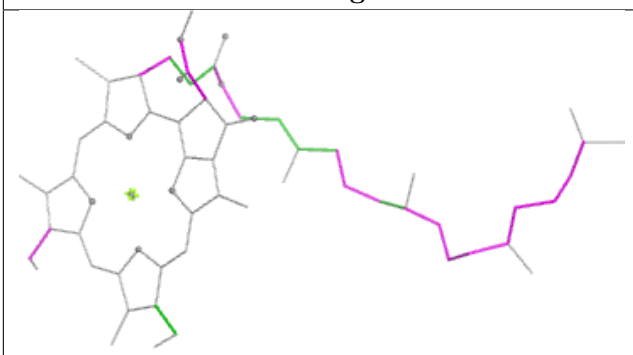

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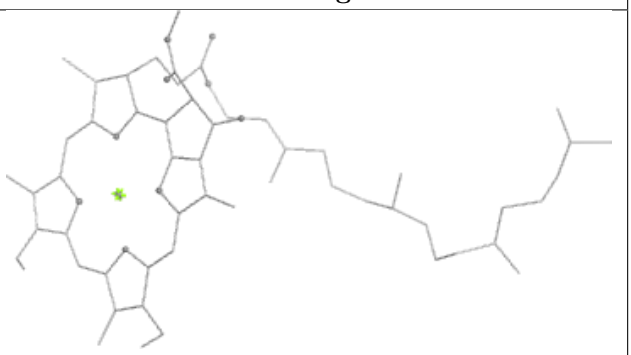
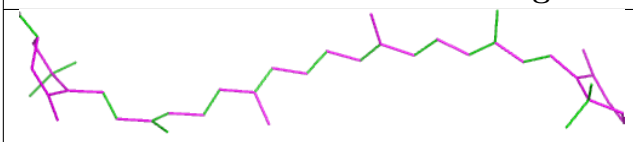


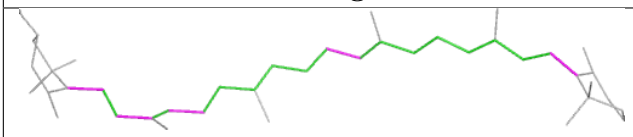
Rings

Ligand C7Z 1 503



Bond lengths

Bond angles



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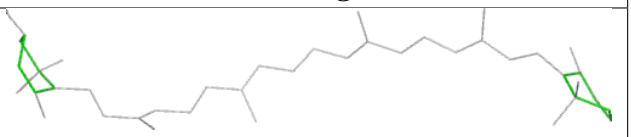
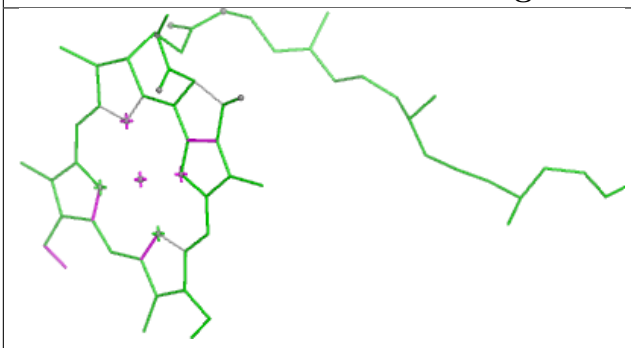


Rings

Ligand CLA A 1121



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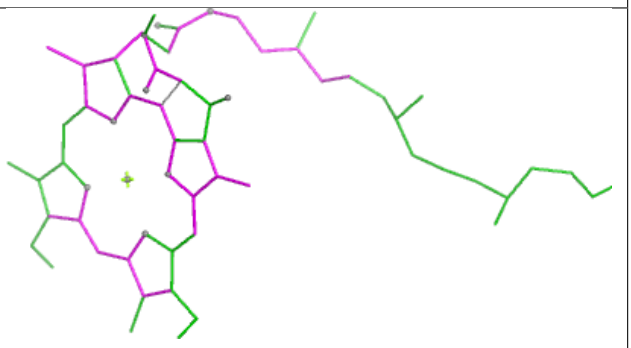
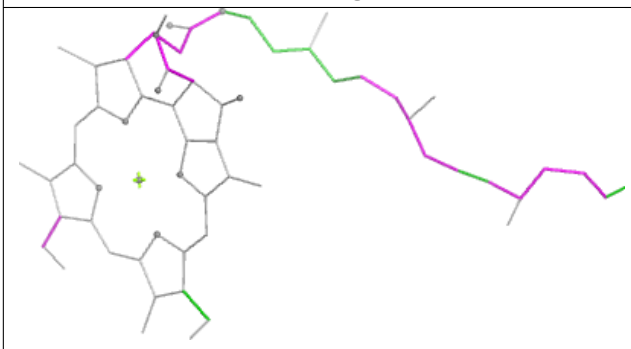


Bond angles



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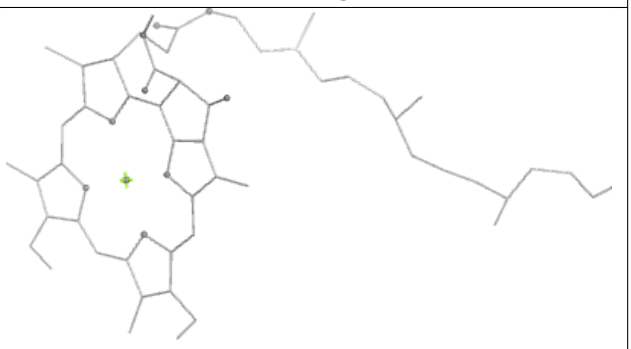
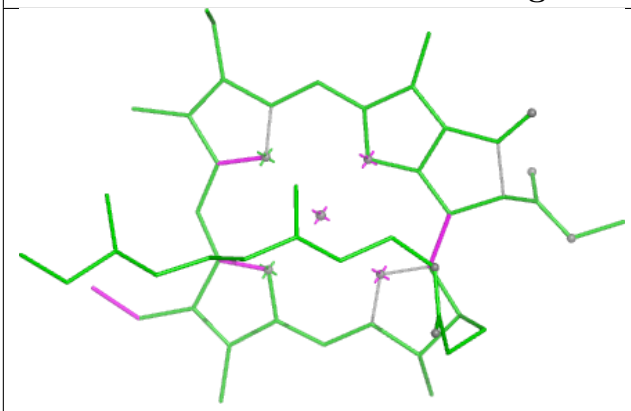
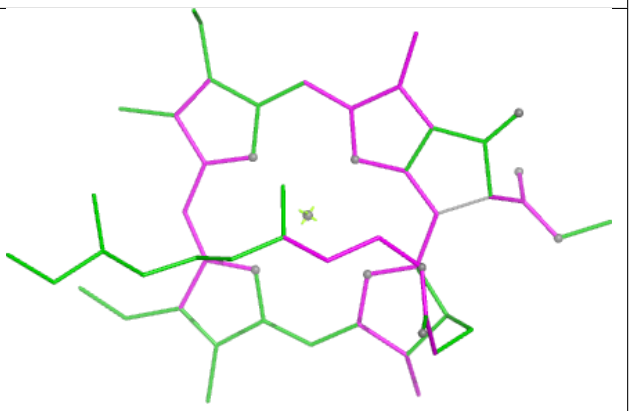


Rings

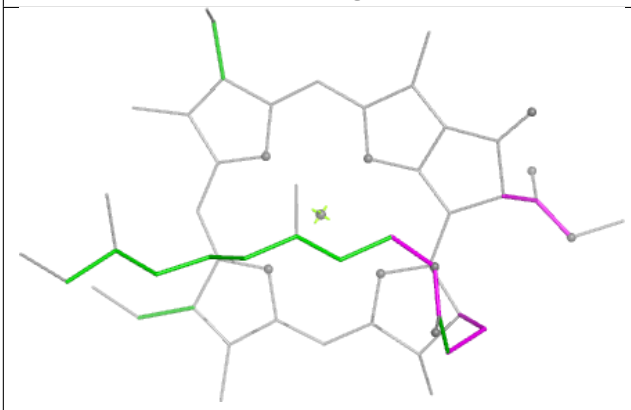
Ligand CLA 3 616



Bond lengths



Bond angles



Torsions

Rings

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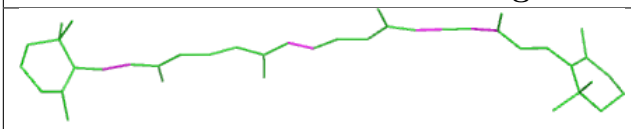
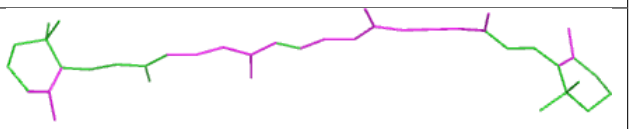
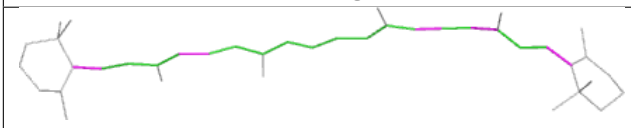
 Bond lengths	 Bond angles
 Torsions	Rings

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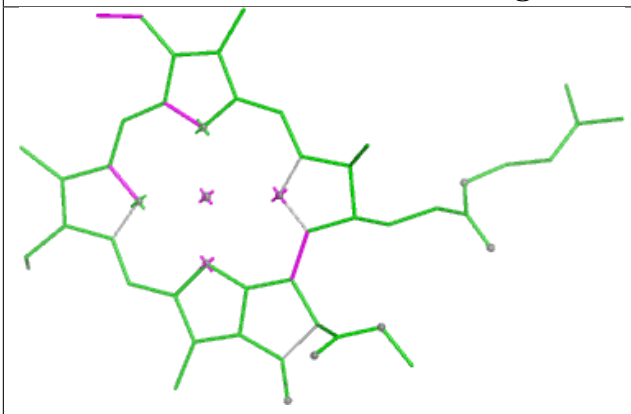
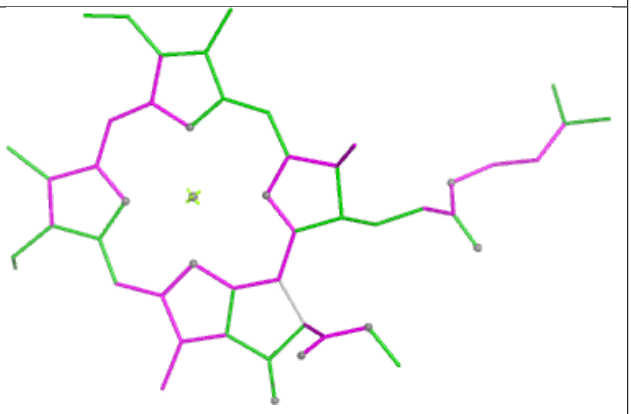
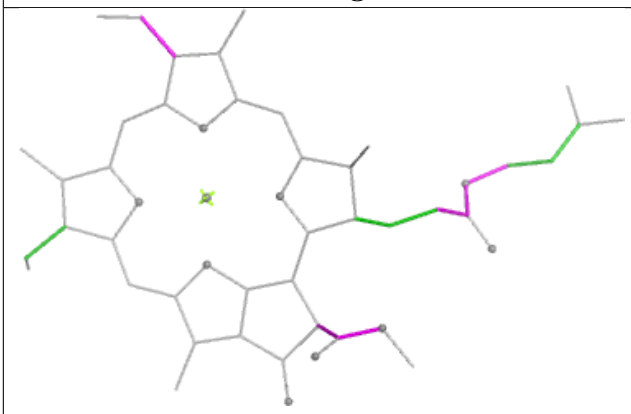
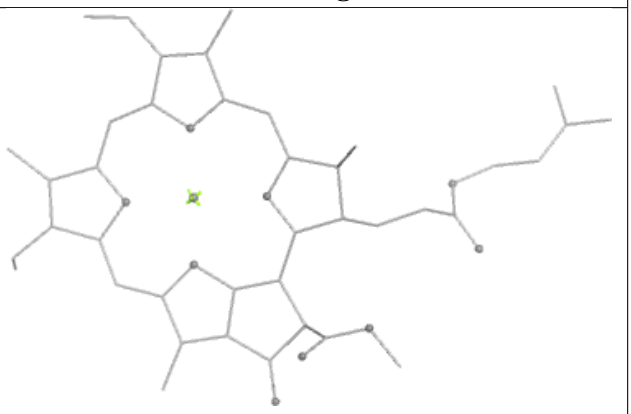
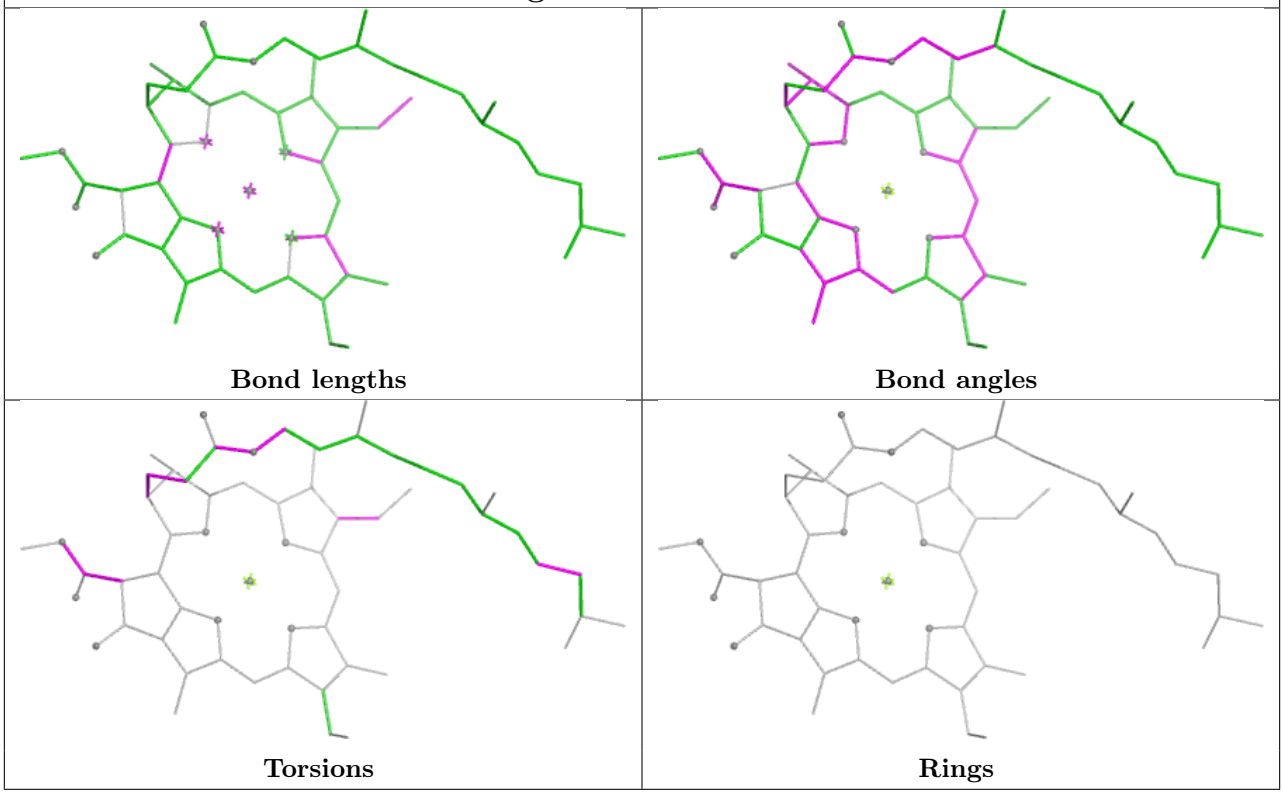
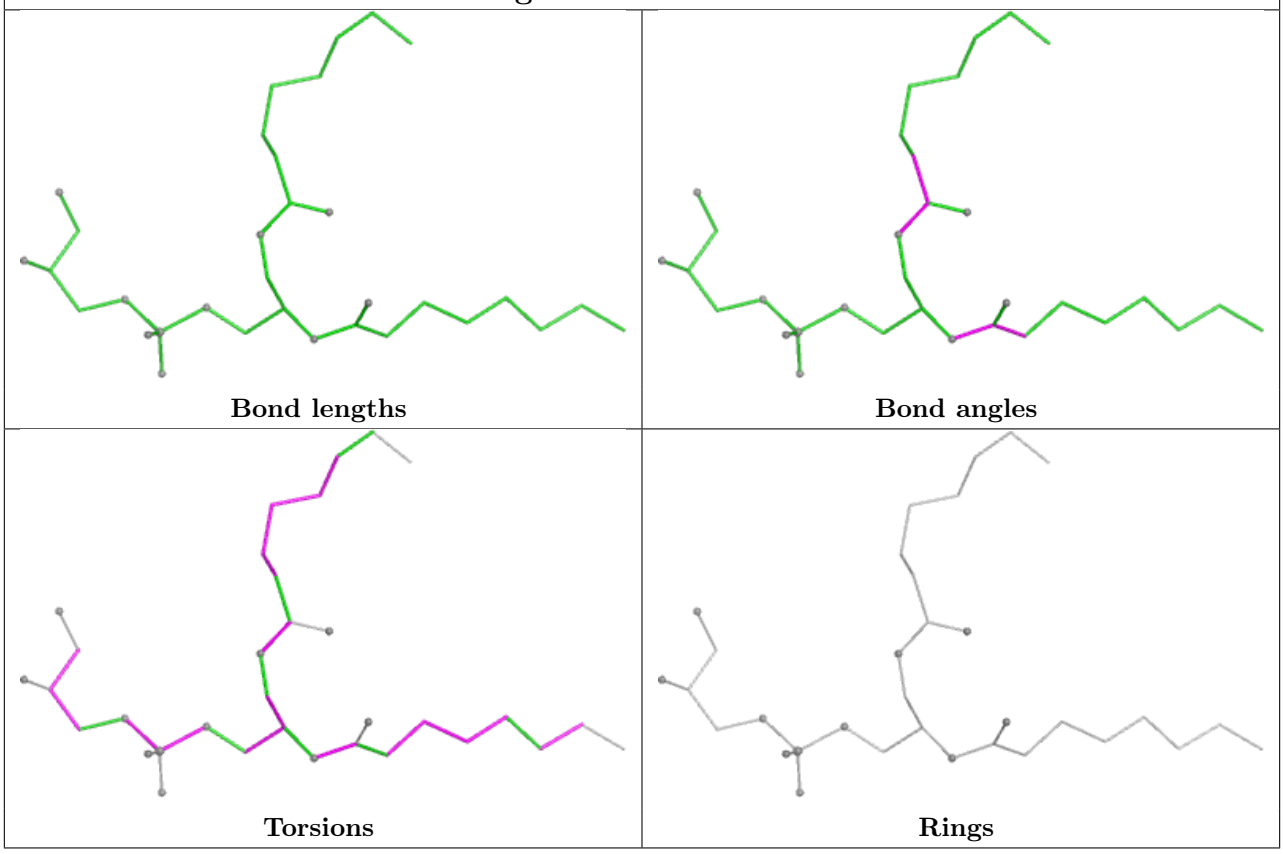
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 601



Ligand LHG B 5006



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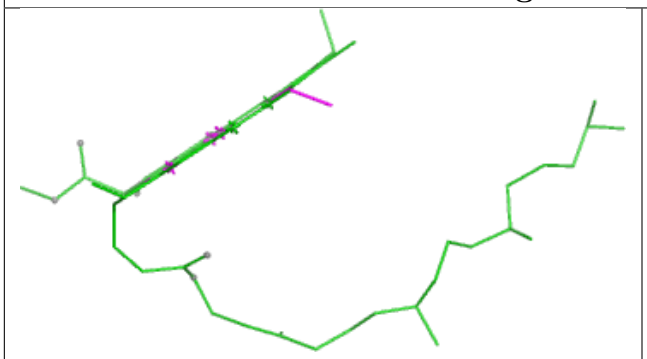

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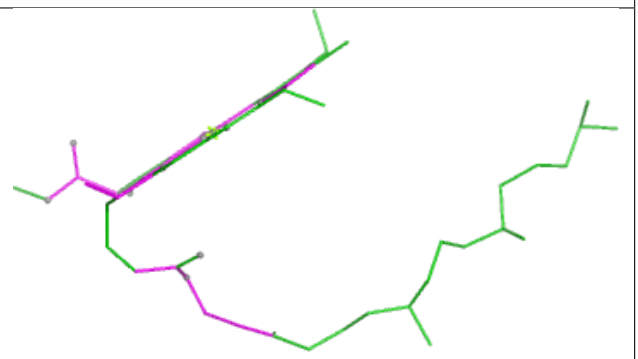
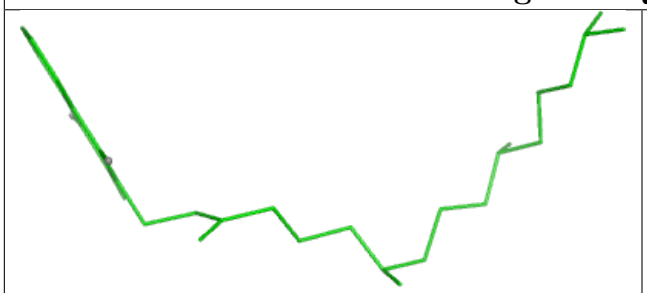


Bond angles

Torsions

Rings

Ligand PQN B 2002



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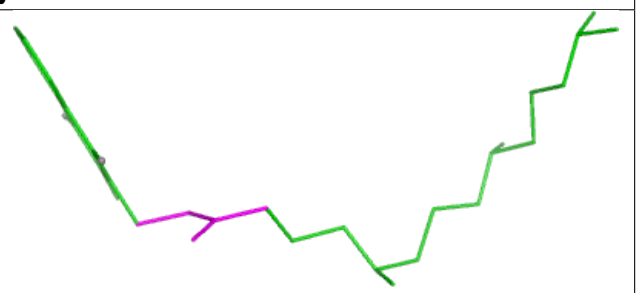
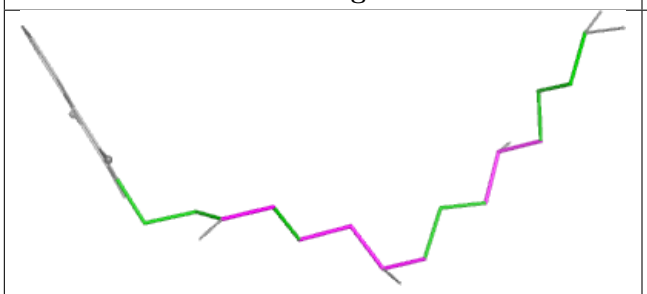
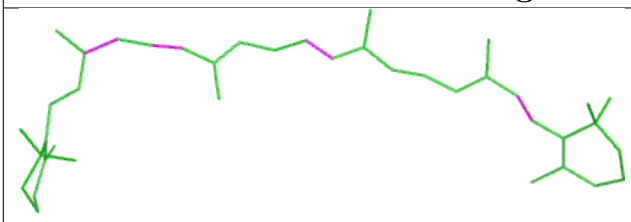
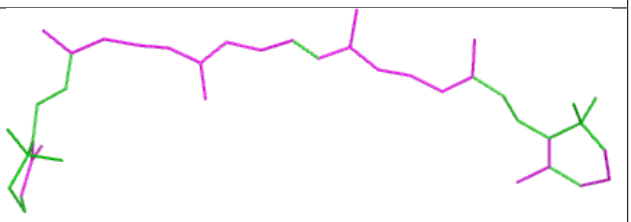
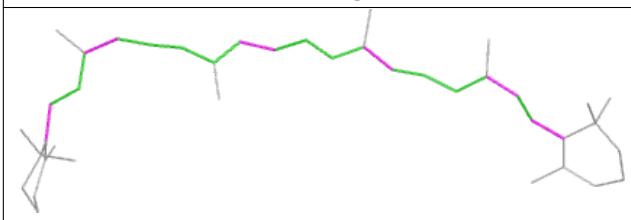
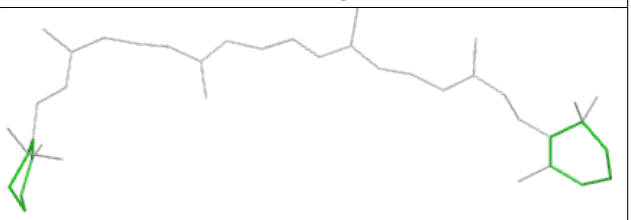


Bond angles



Torsions

Rings

Ligand BCR L 4002	
 Bond lengths	 Bond angles
 Torsions	 Rings

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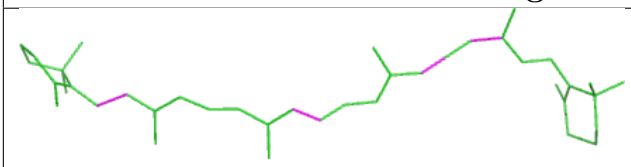
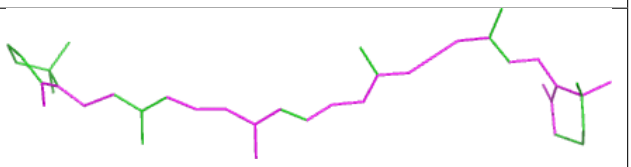
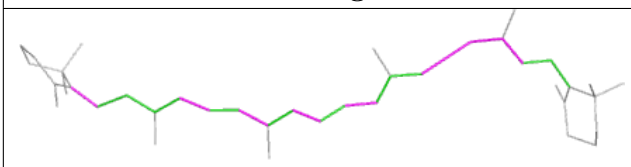
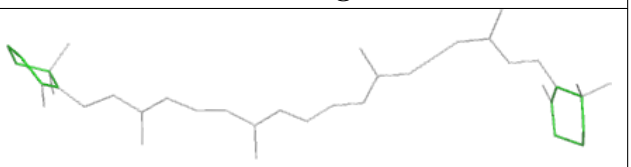
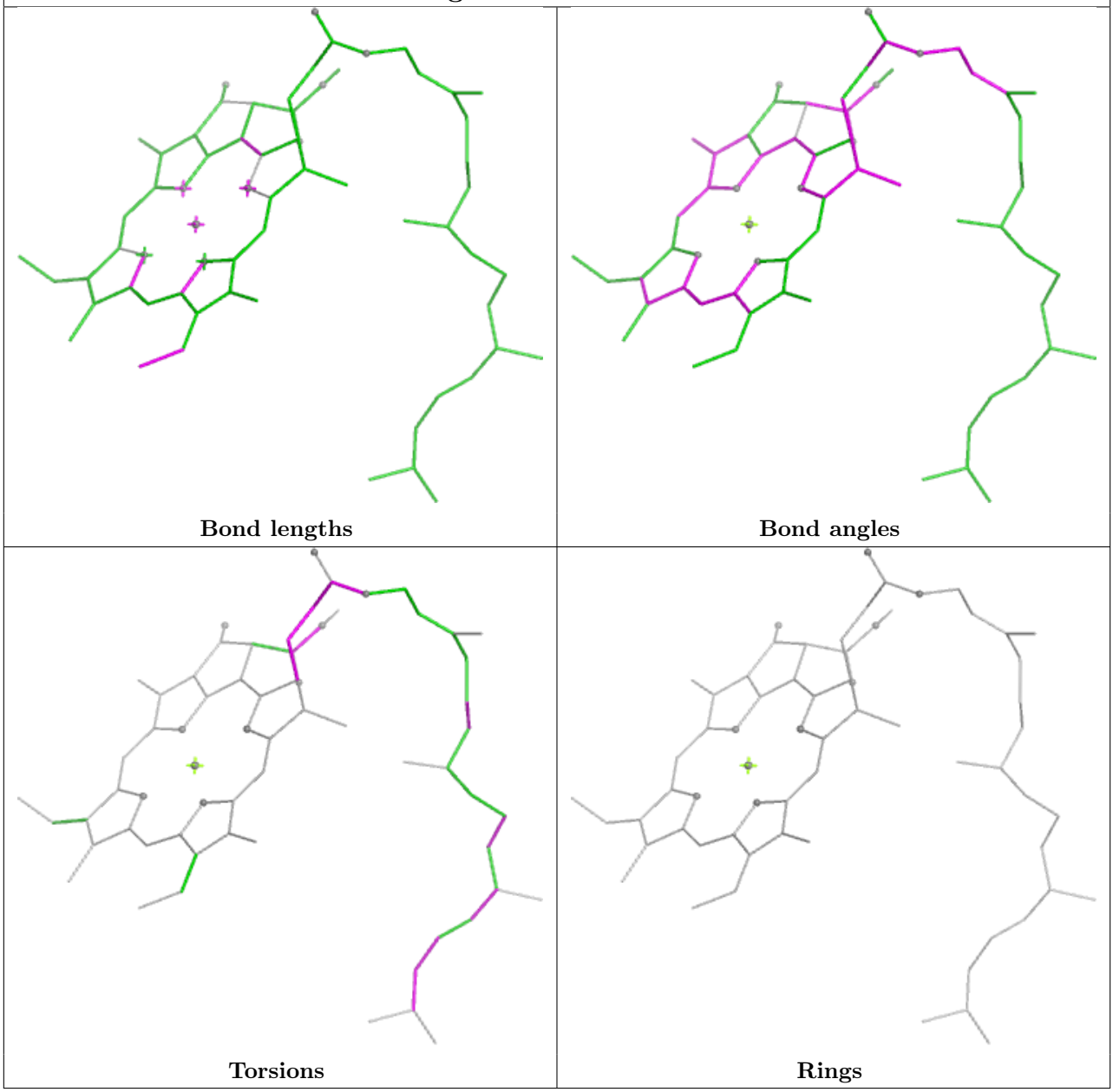
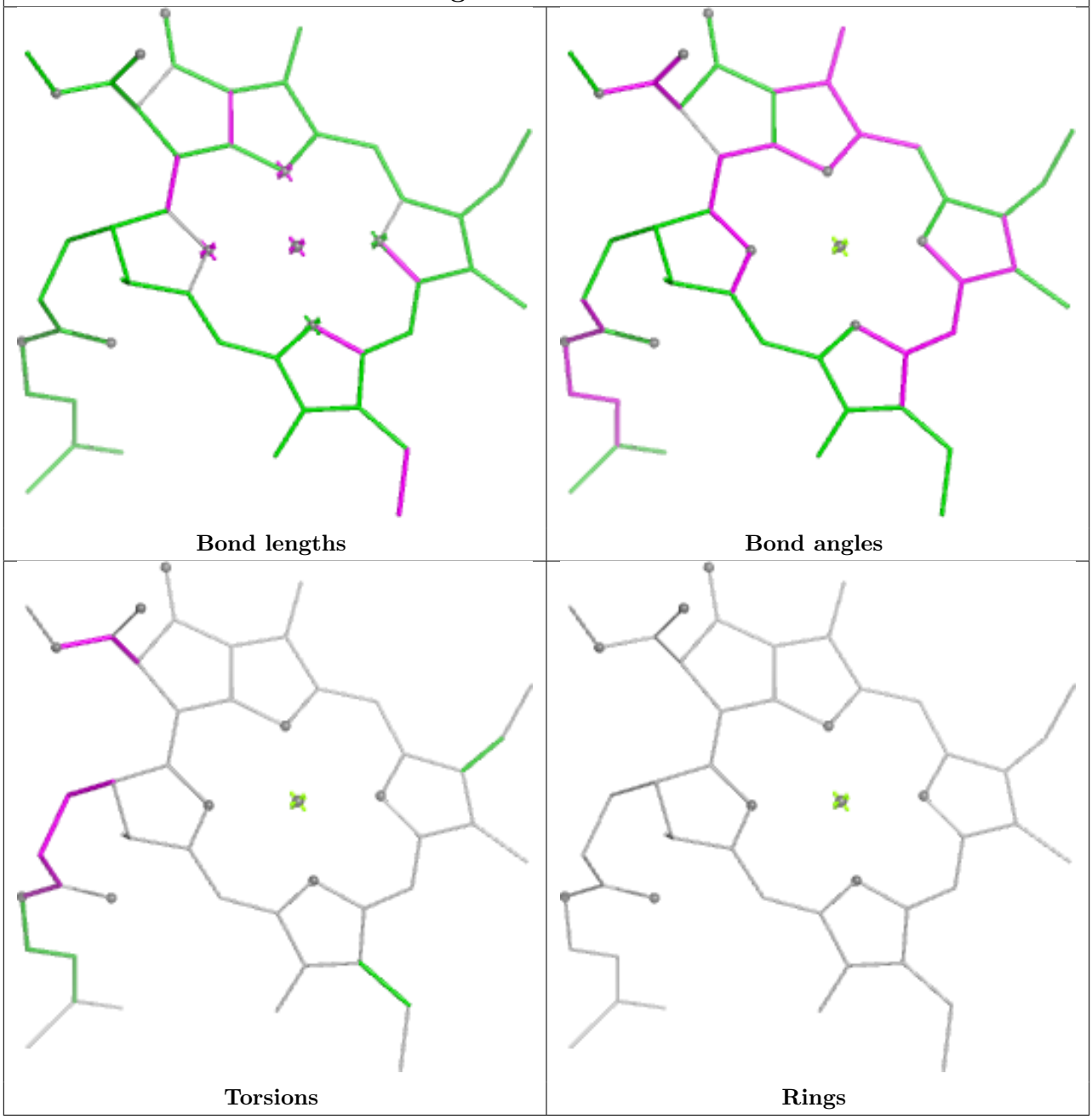
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1207



Ligand CLA 7 612



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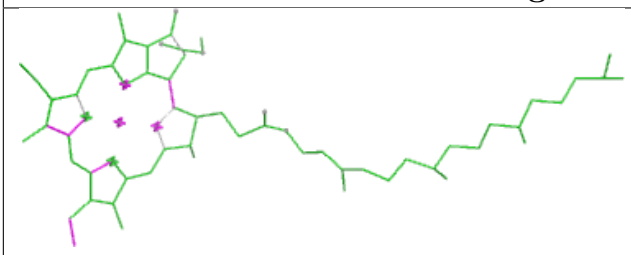
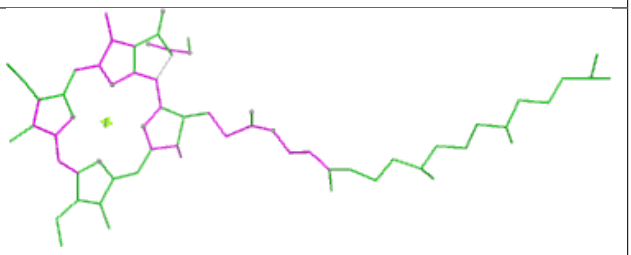
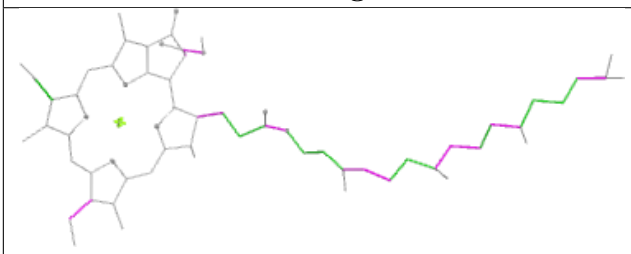
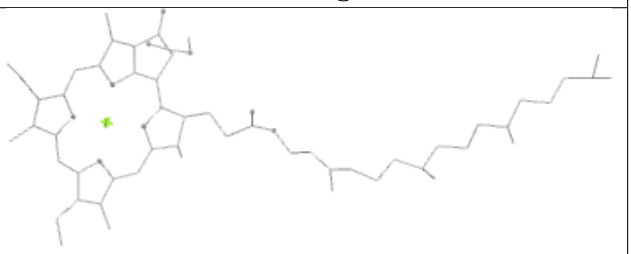
 Bond lengths	 Bond angles
 Torsions	 Rings

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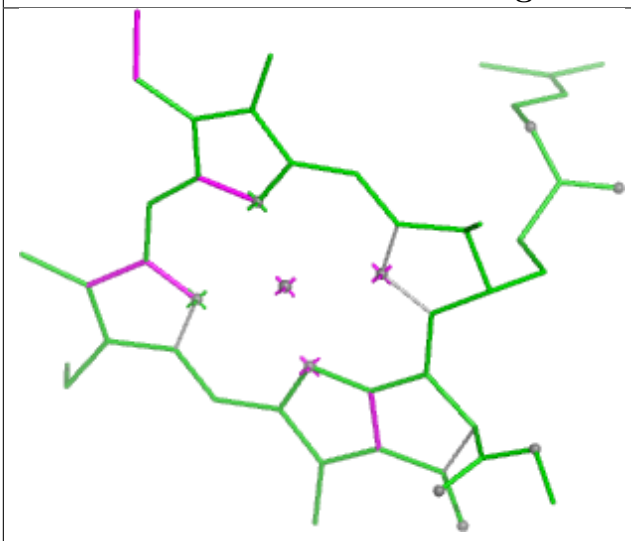
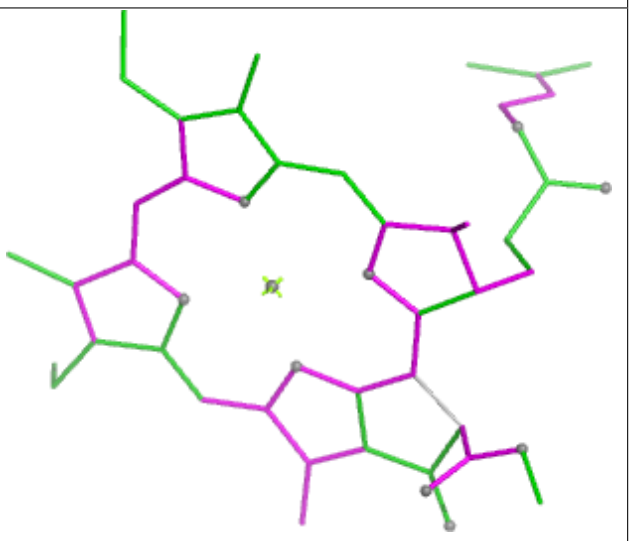
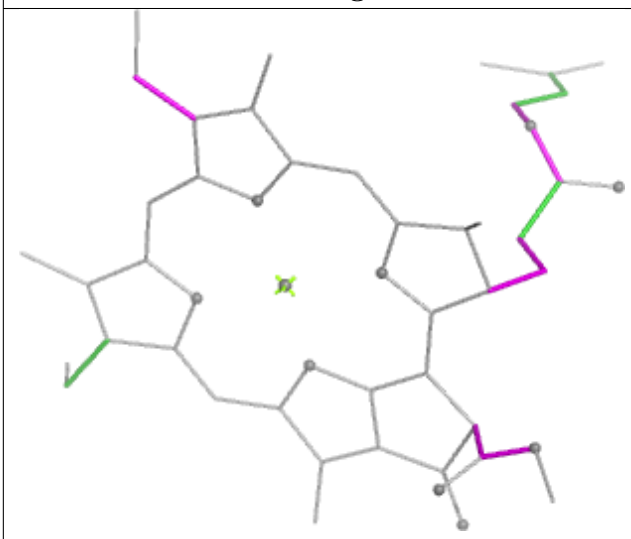
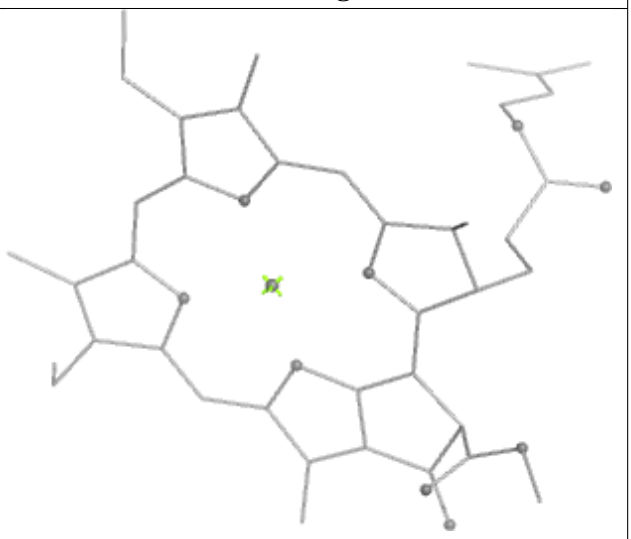
 Bond lengths	 Bond angles
 Torsions	 Rings

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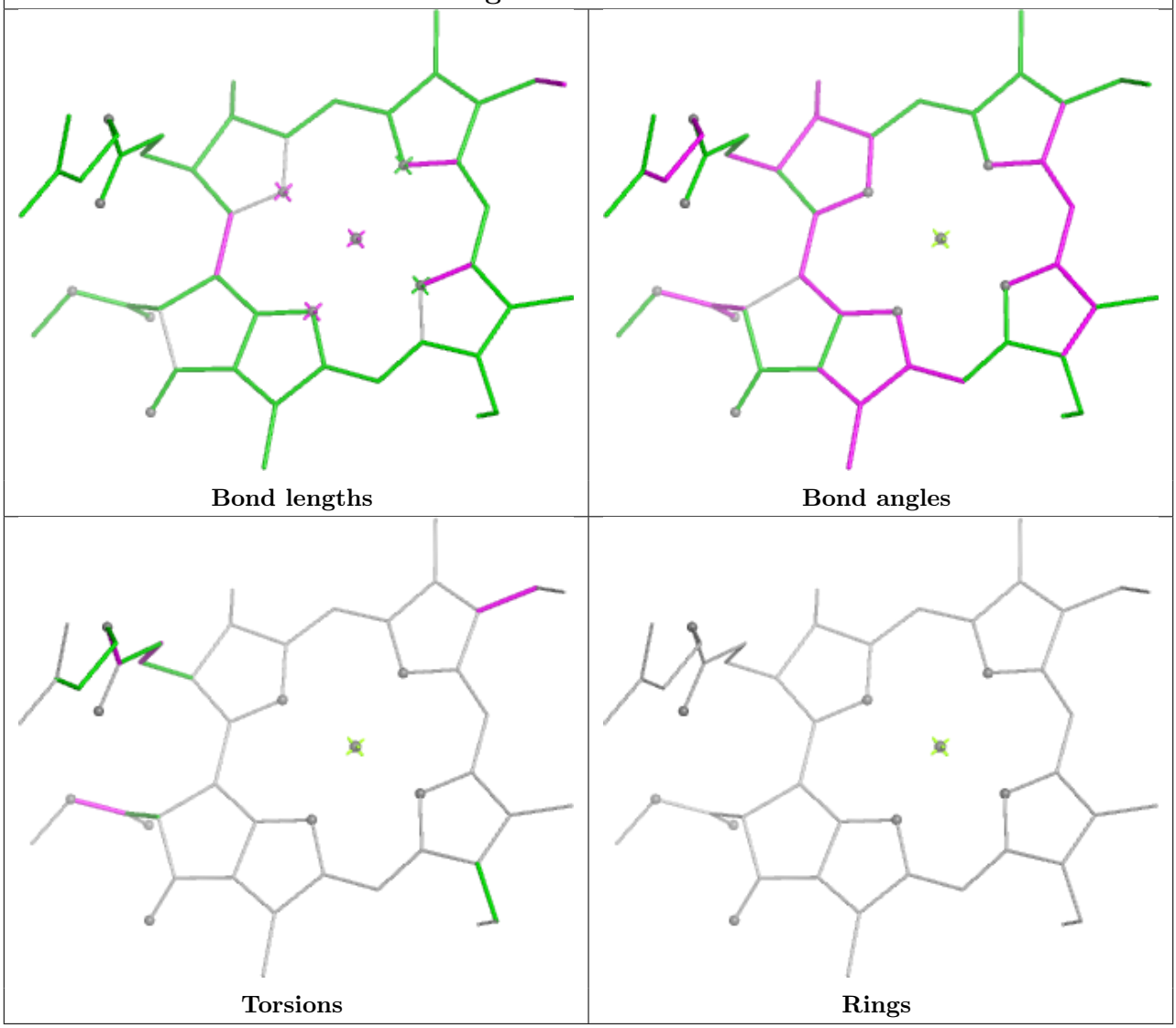

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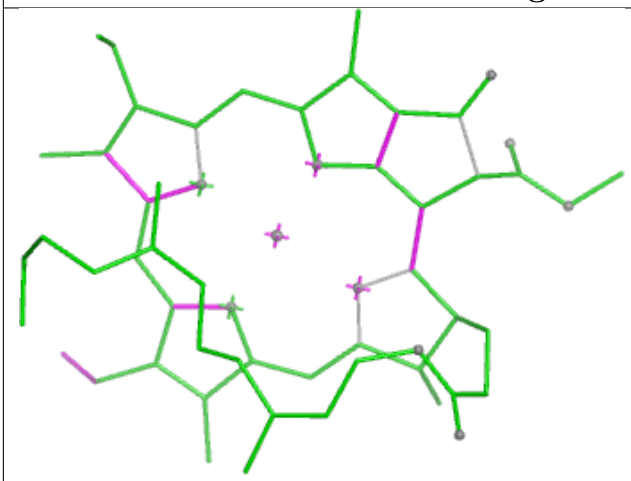

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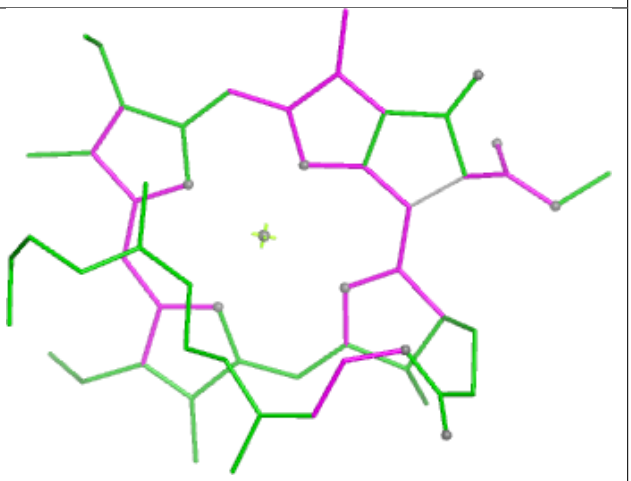
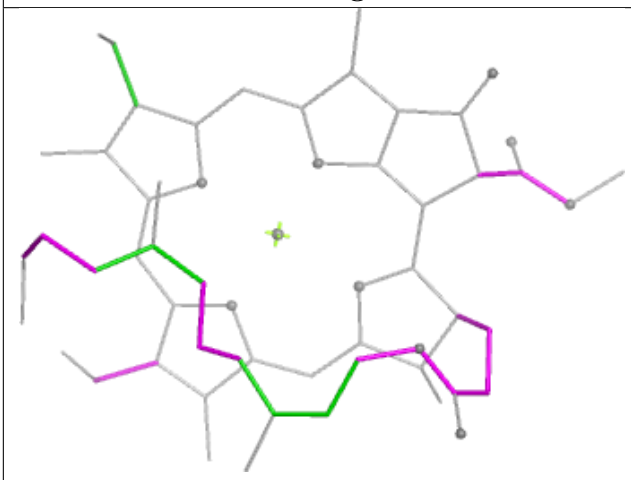
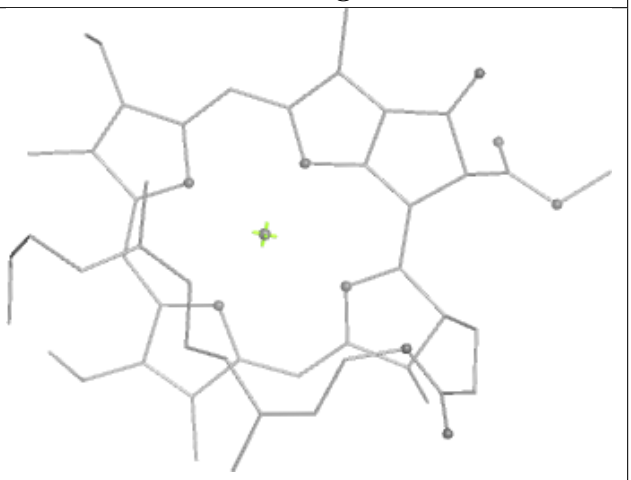


Bond angles



Torsions



Rings

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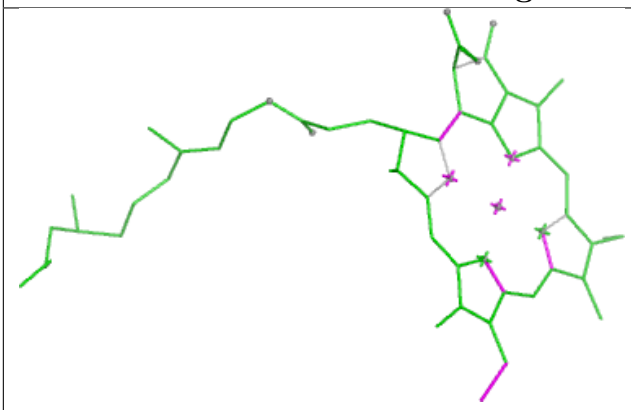
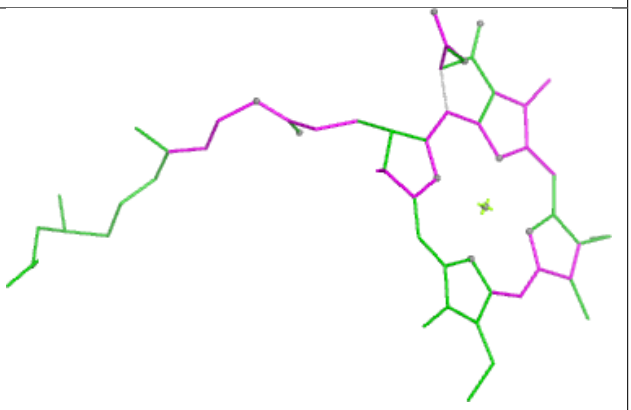
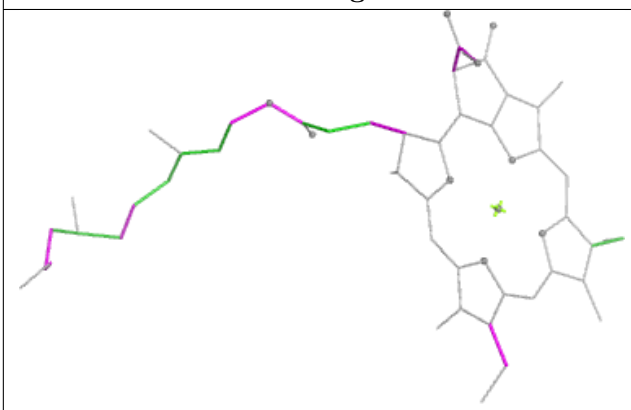
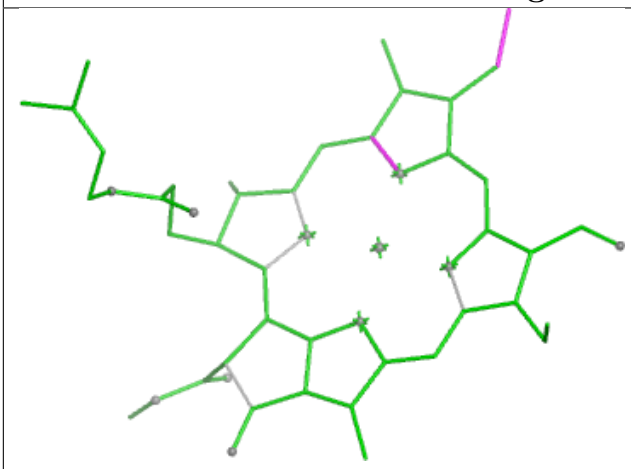
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL 4 611



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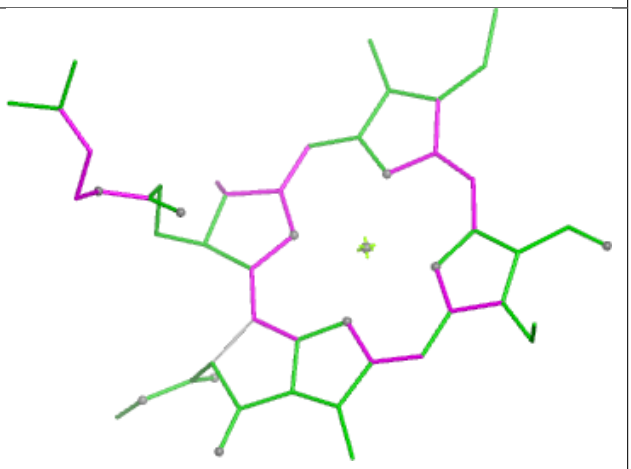
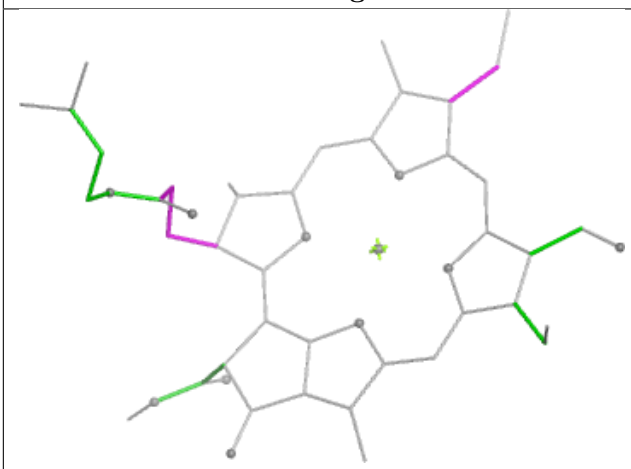
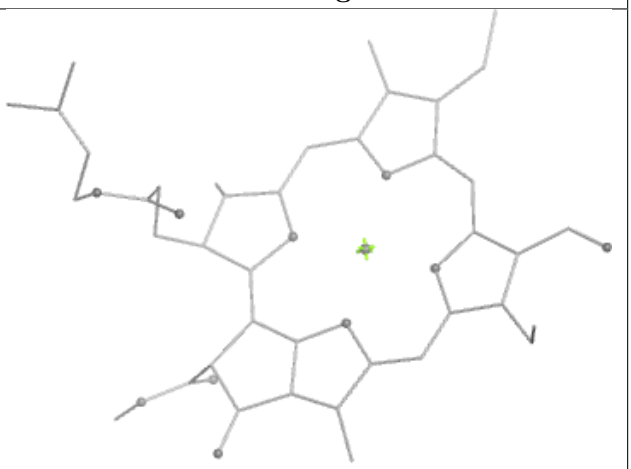


Bond angles

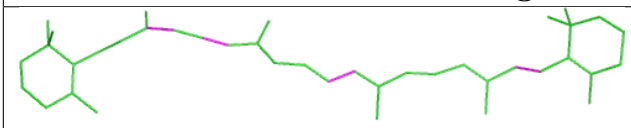


Torsions

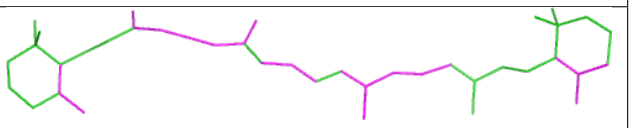


Rings

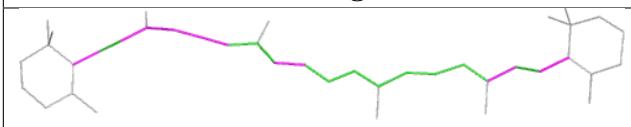
Ligand BCR L 4001



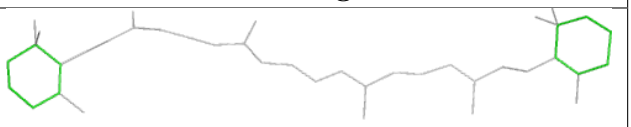
Bond lengths



Bond angles

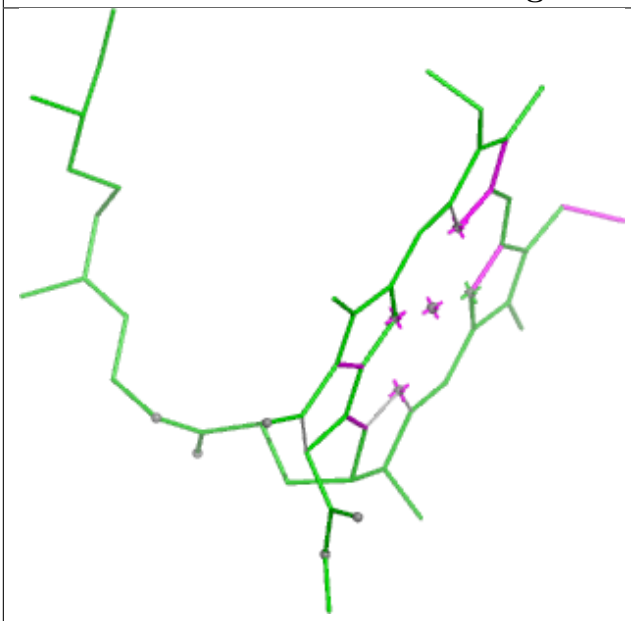


Torsions



Rings

Ligand CLA Z 608



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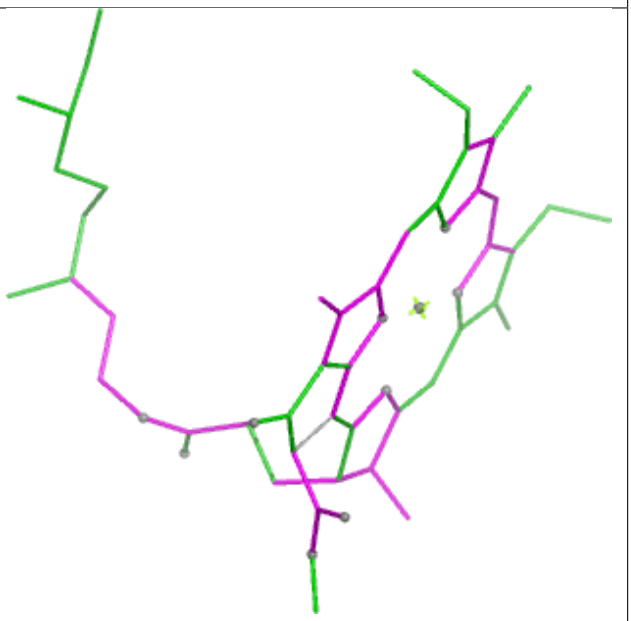
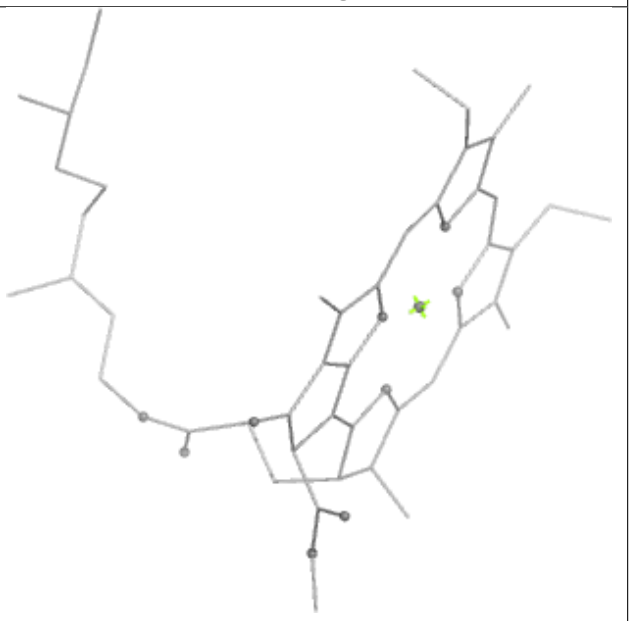


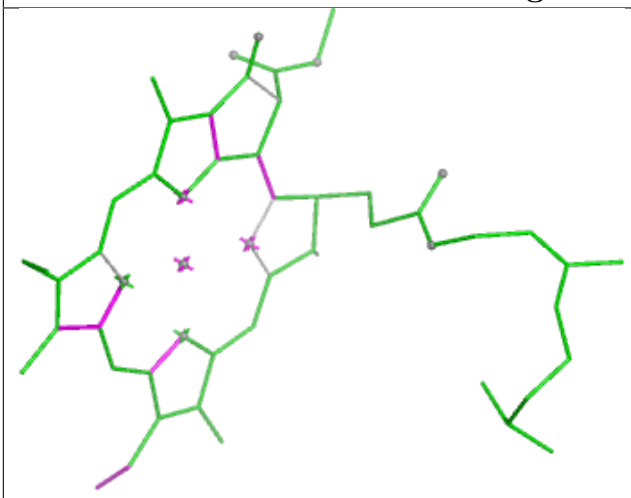
Bond angles

Torsions



Rings

Ligand CLA Z 611



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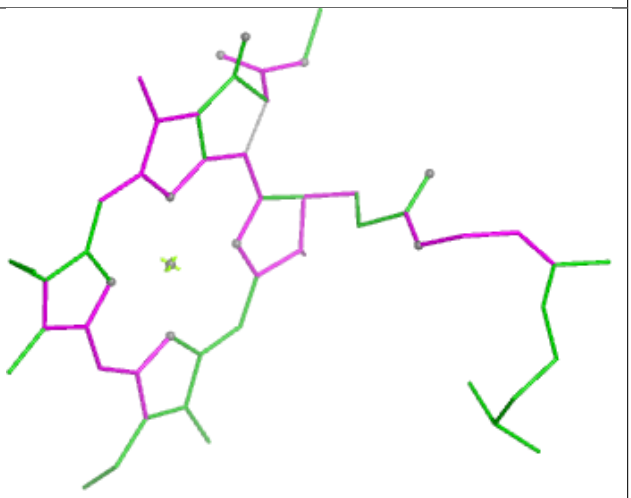
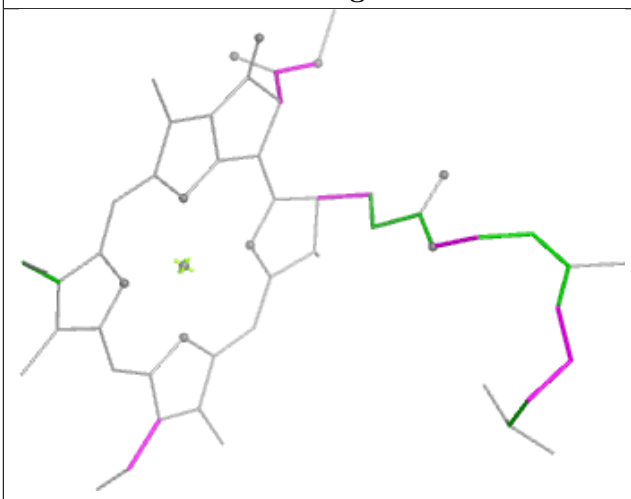
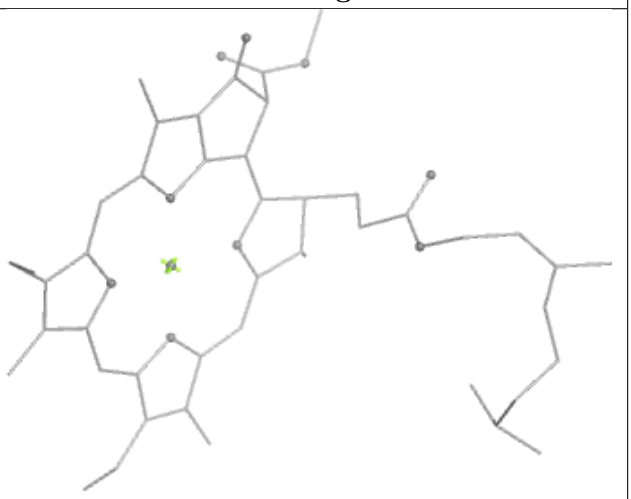


Bond angles

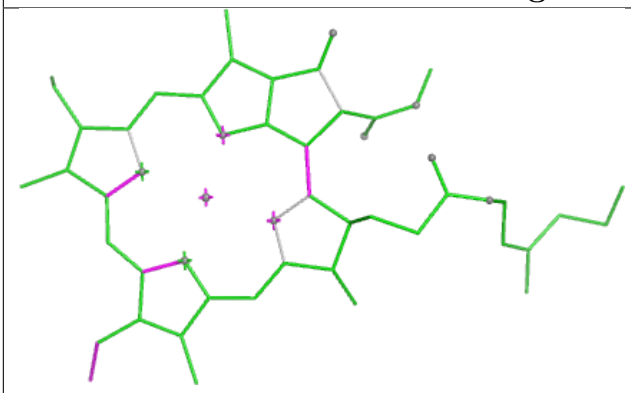


Torsions

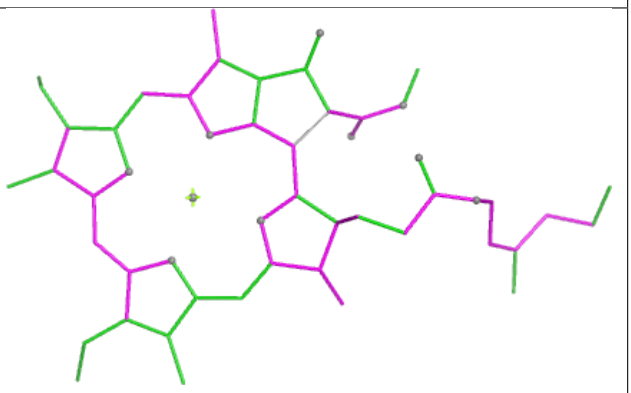


Rings

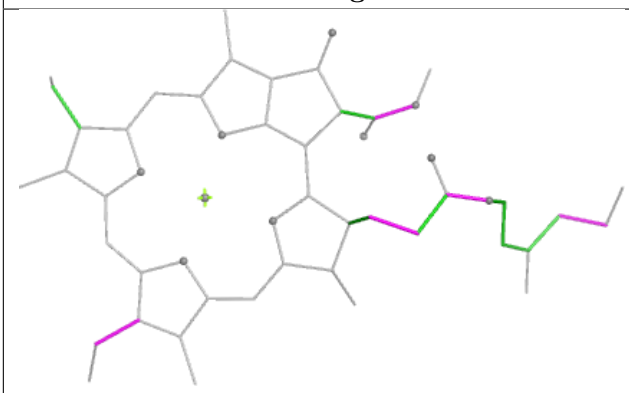
Ligand CLA 6 602



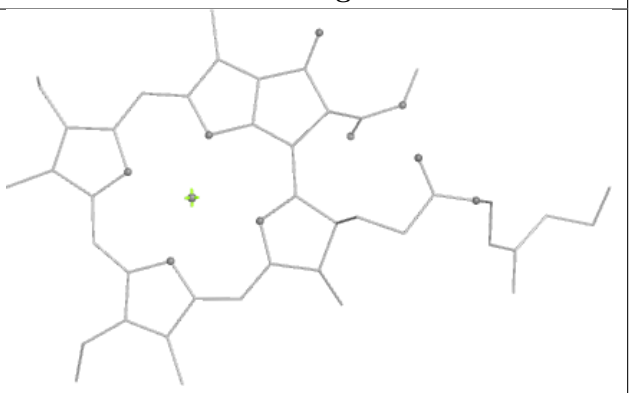
Bond lengths



Bond angles

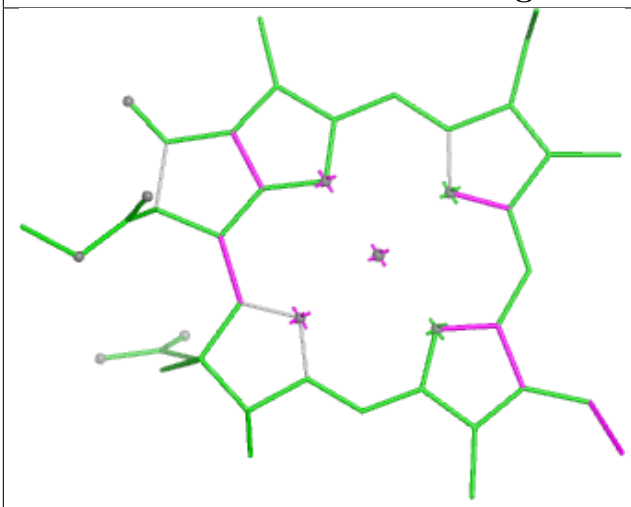


Torsions

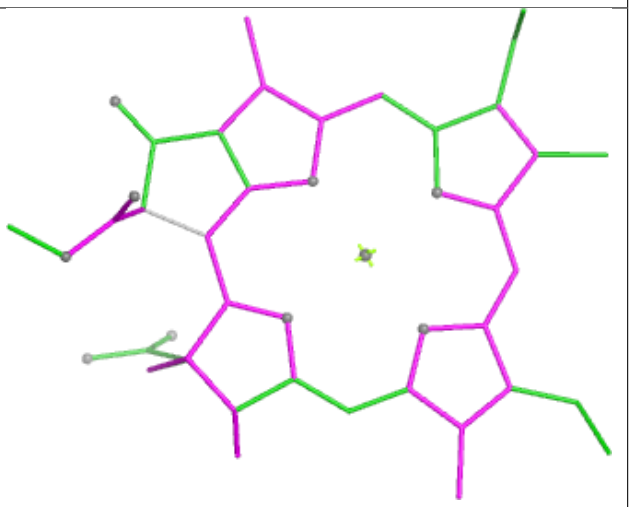


Rings

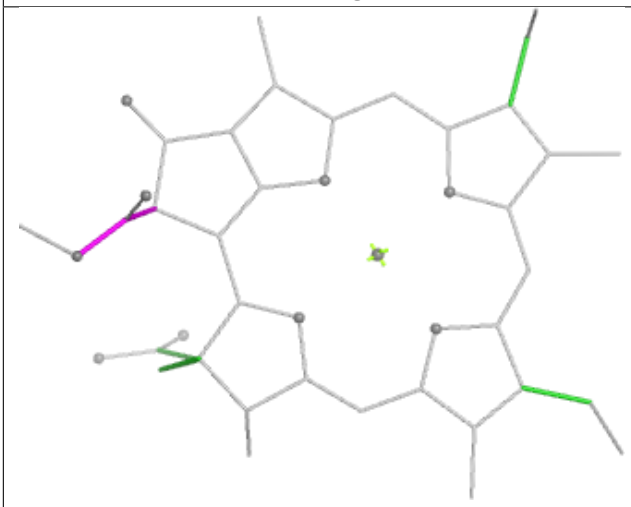
Ligand CLA B 1201



Bond lengths



Bond angles



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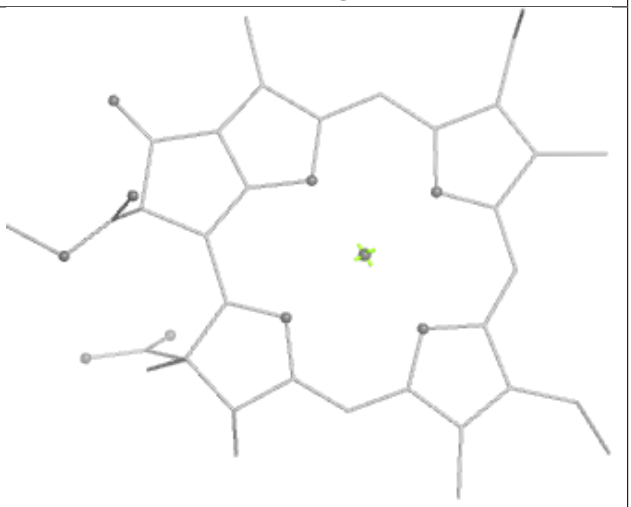
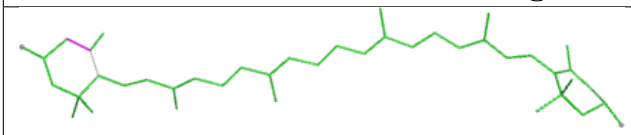


Rings

Ligand LUT 8 502



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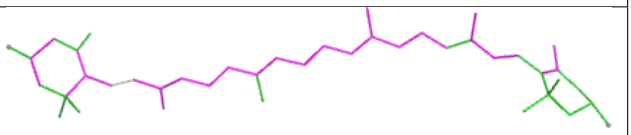
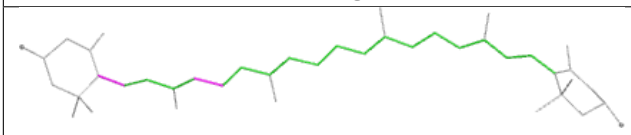


Bond angles



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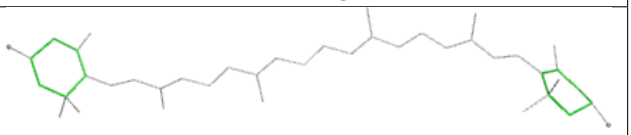
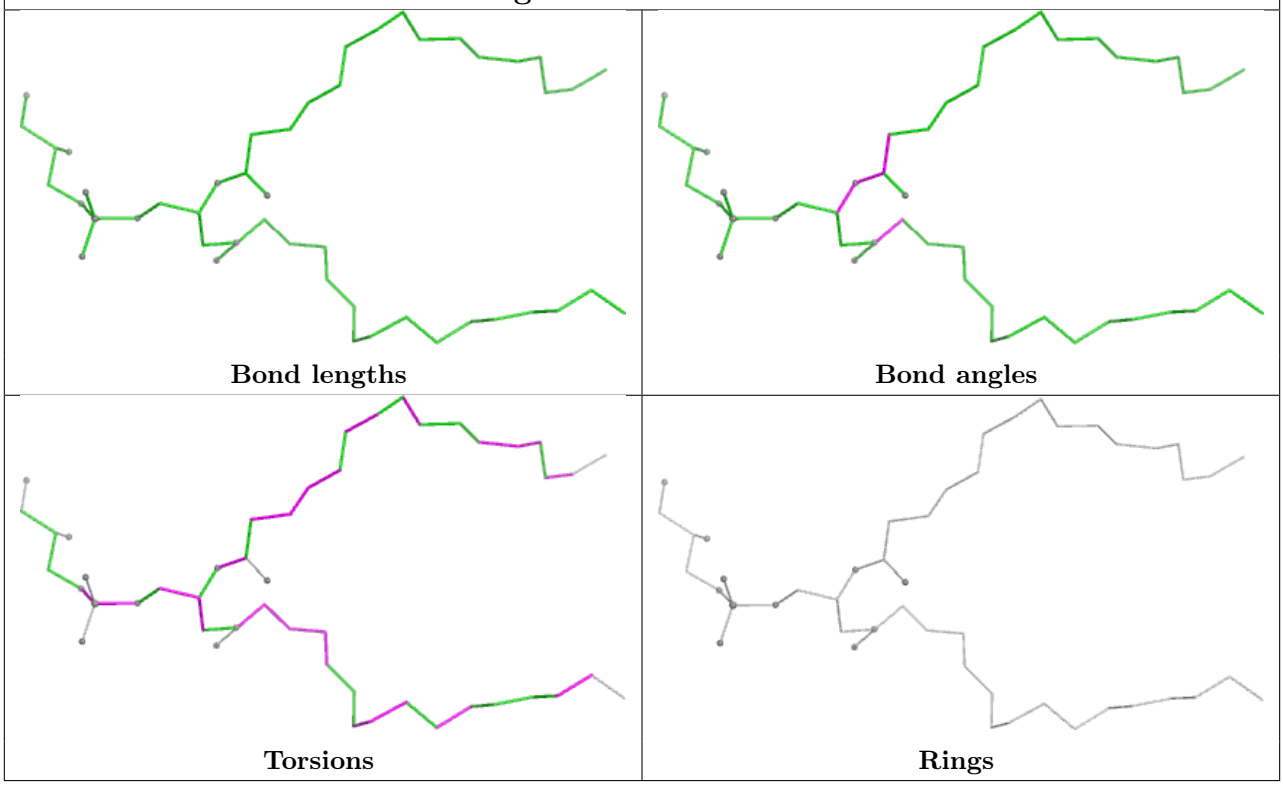


Rings

Ligand LHG A 5002



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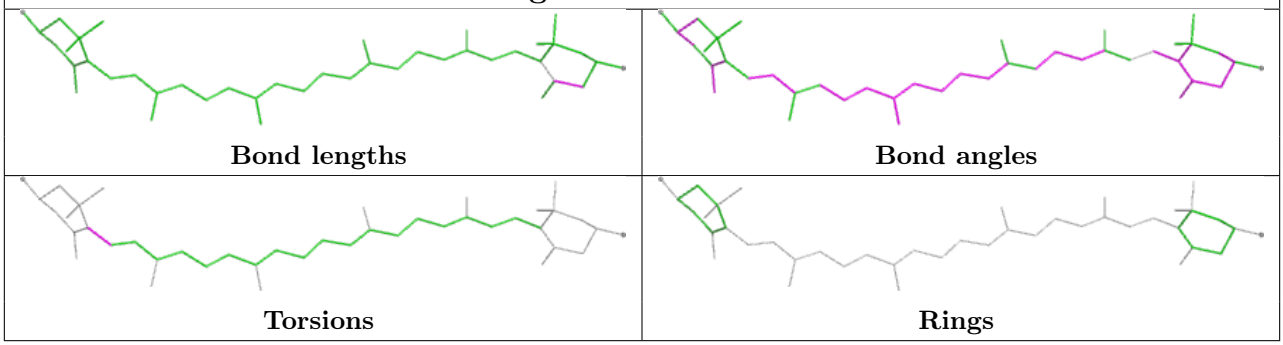
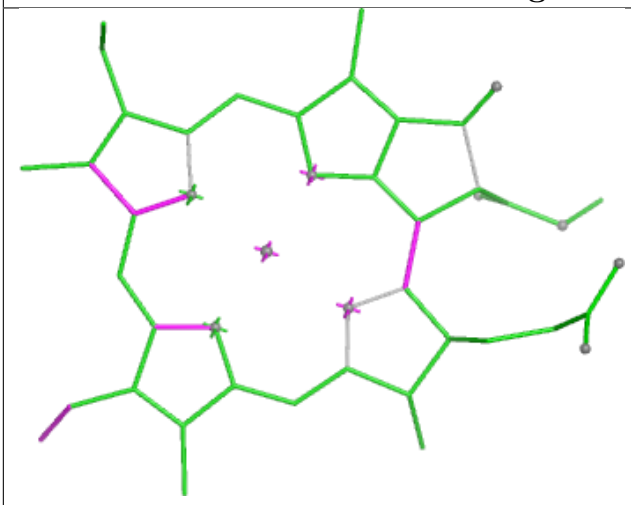


Ligand CLA 3 608



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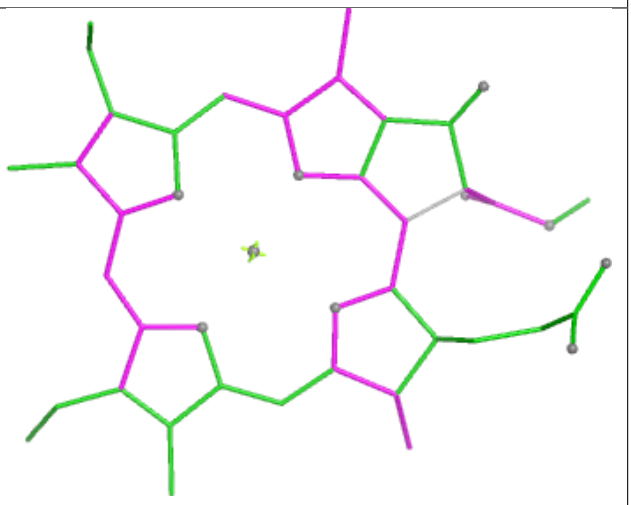

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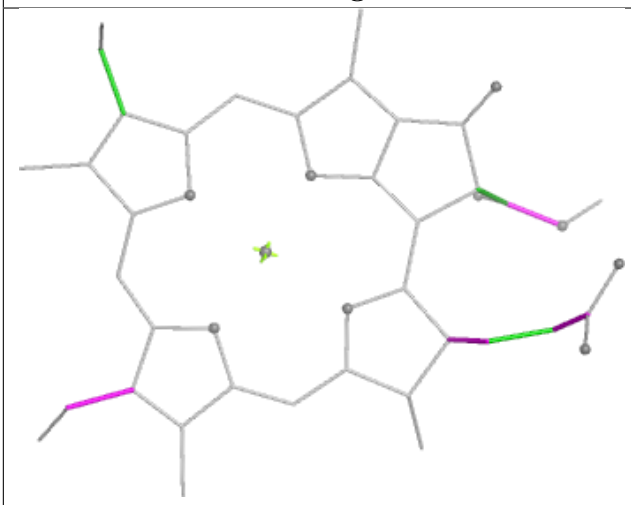

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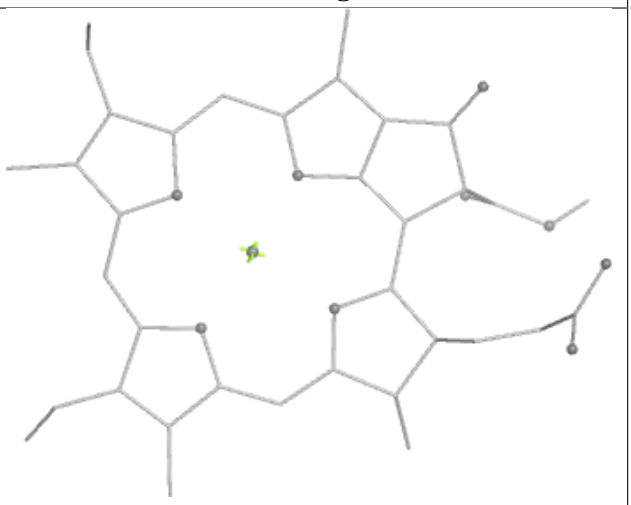
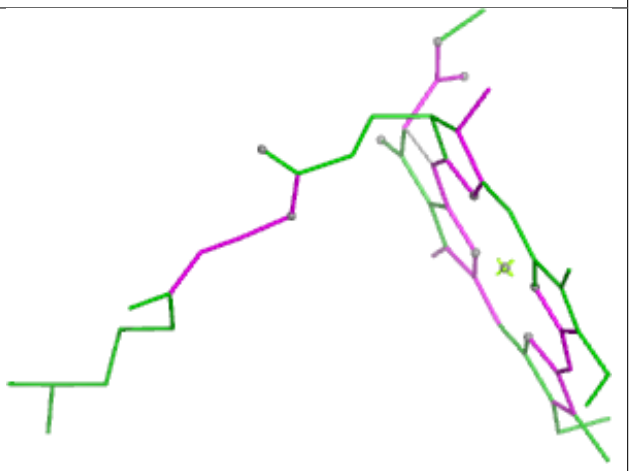


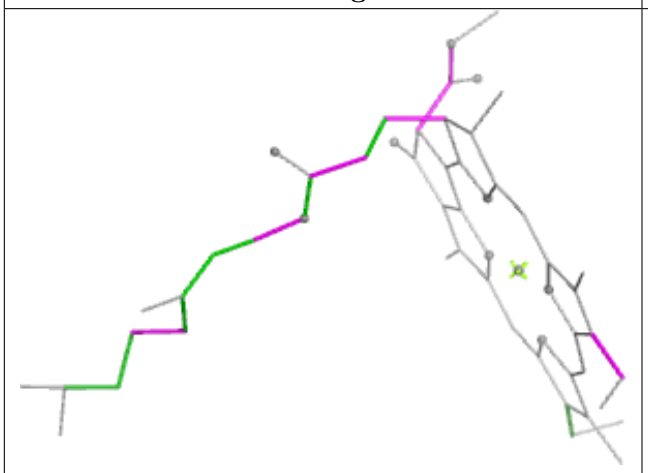
Rings

Ligand CLA A 1134

Bond lengths



Bond angles



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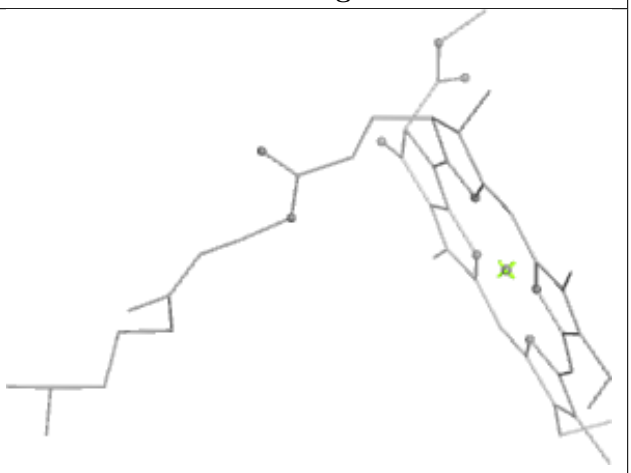
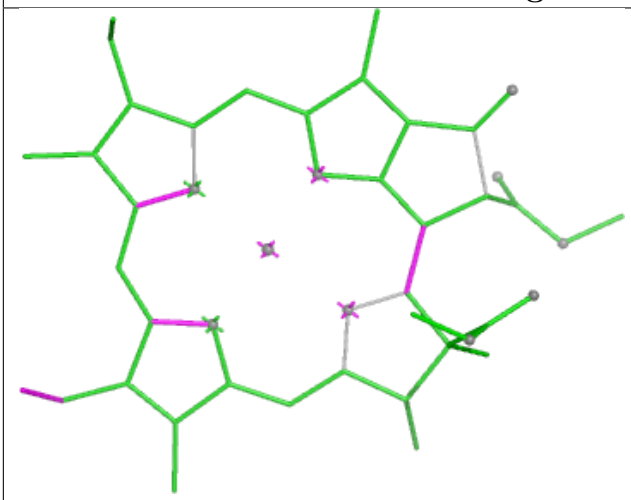


Rings

Ligand CLA Z 615



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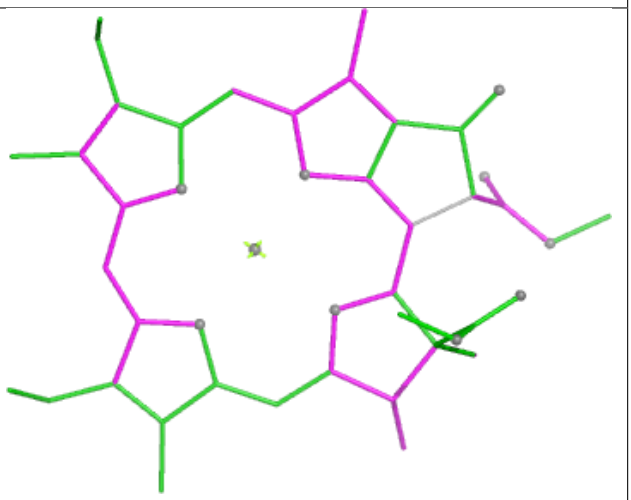
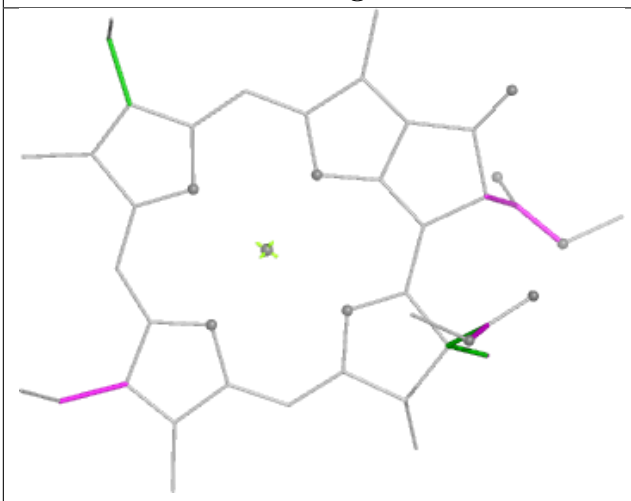


Bond angles



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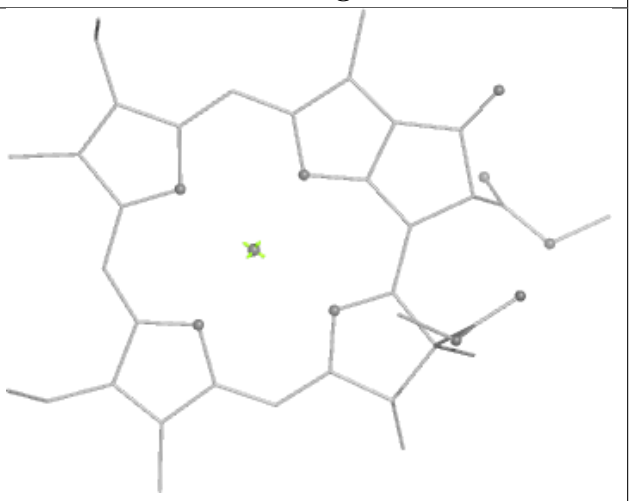
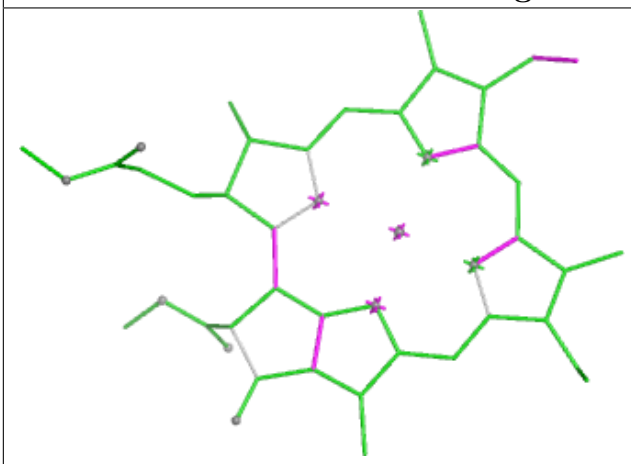


Rings

Ligand CLA K 1401



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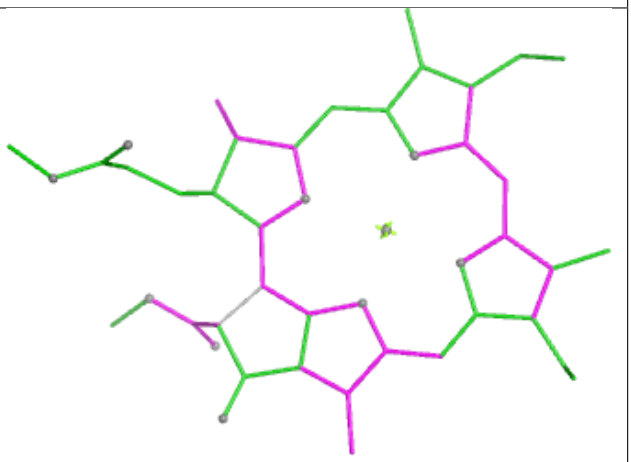
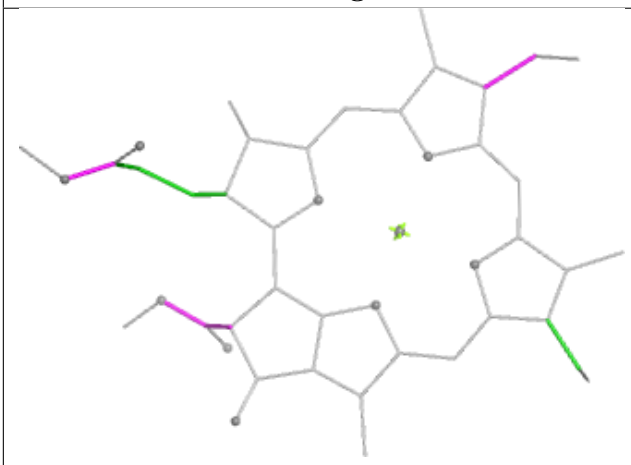
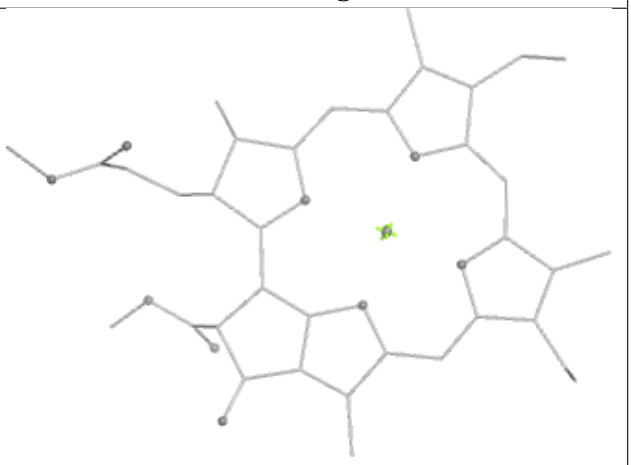


Bond angles

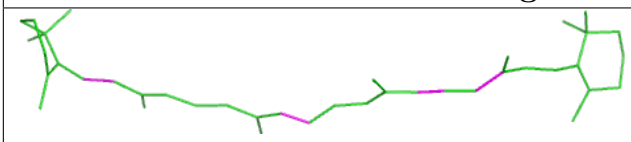


Torsions

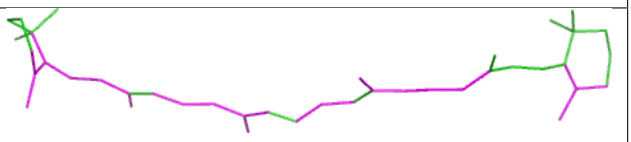


Rings

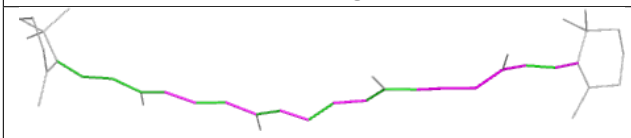
Ligand BCR I 4001



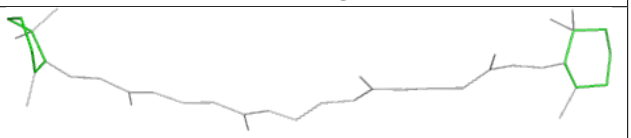
Bond lengths



Bond angles

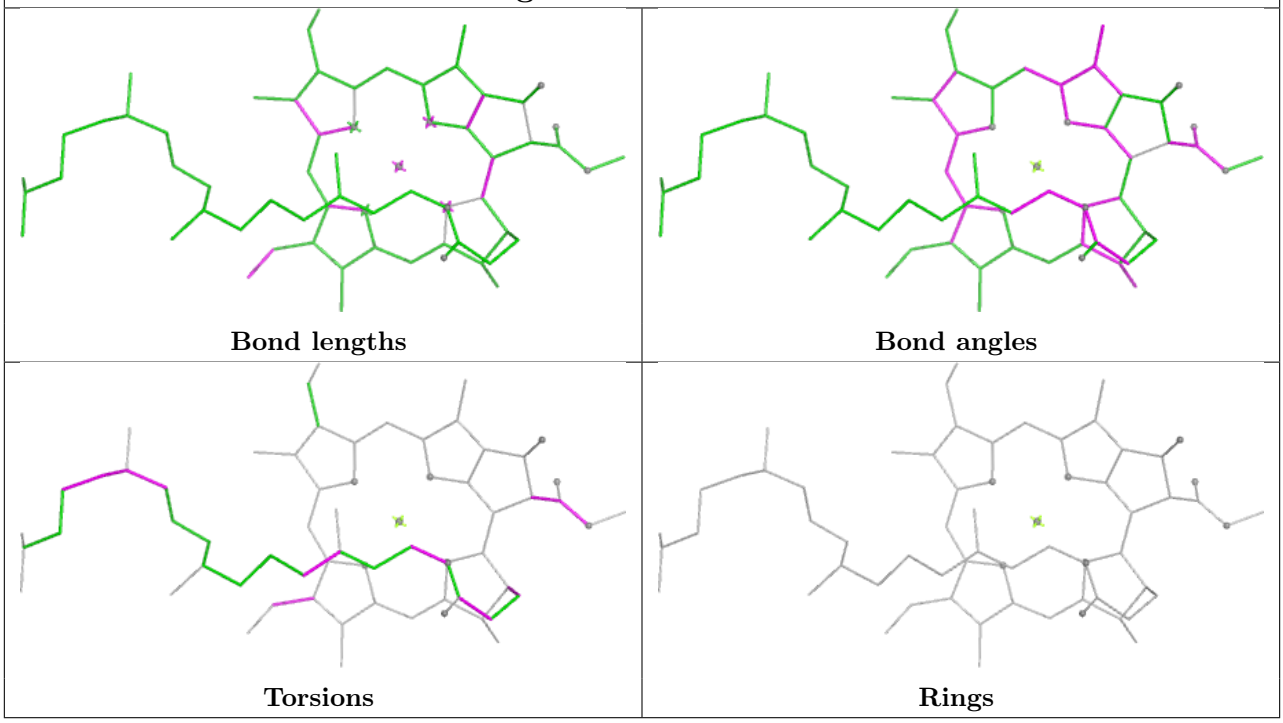


Torsions

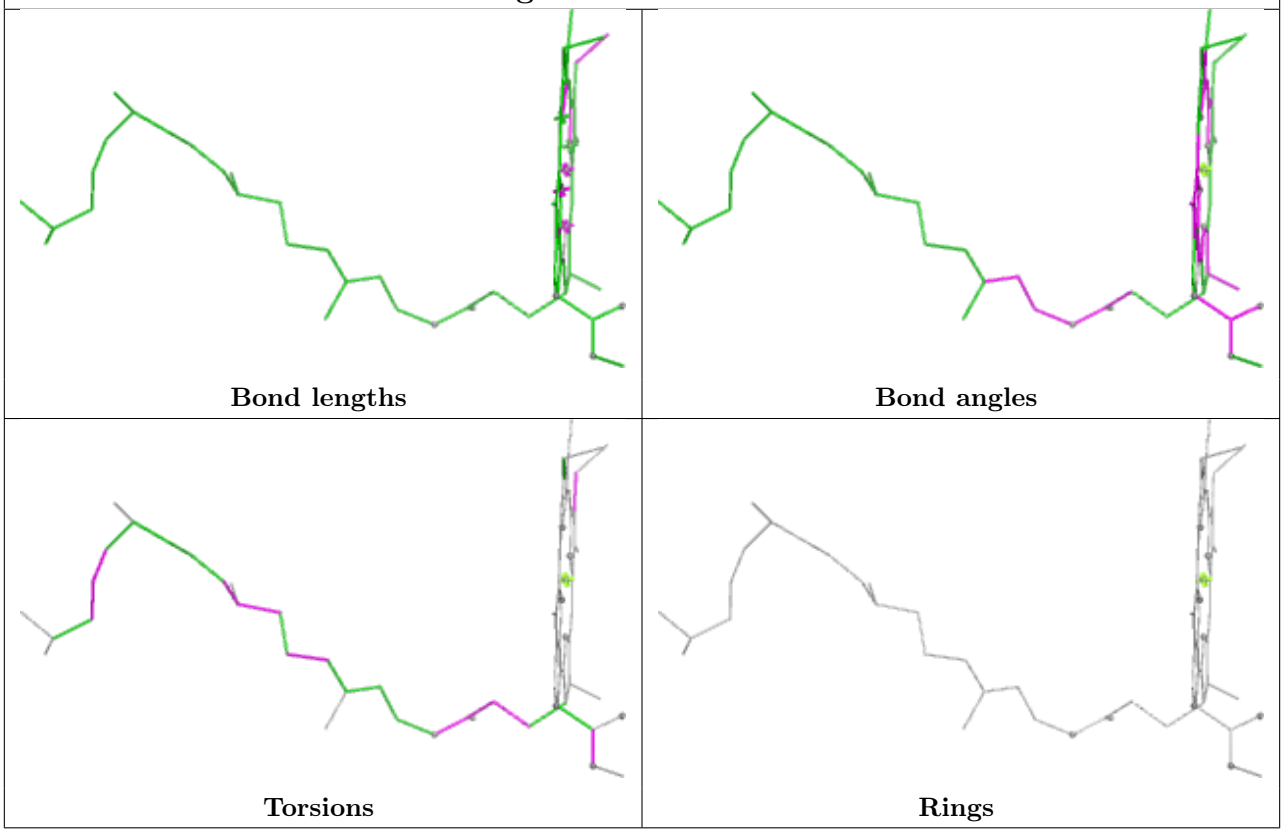


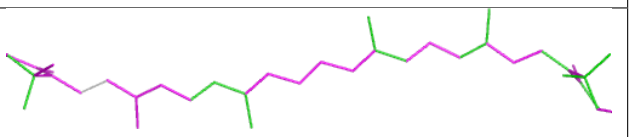
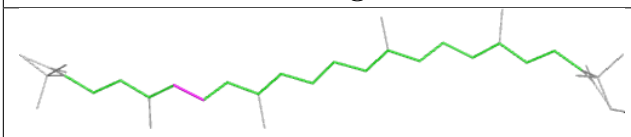
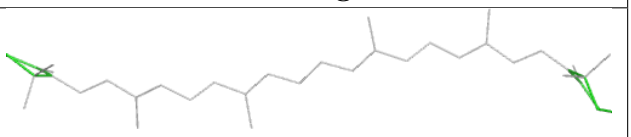
Rings

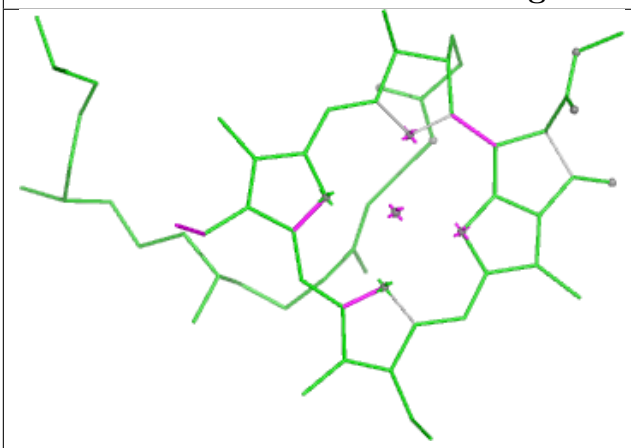
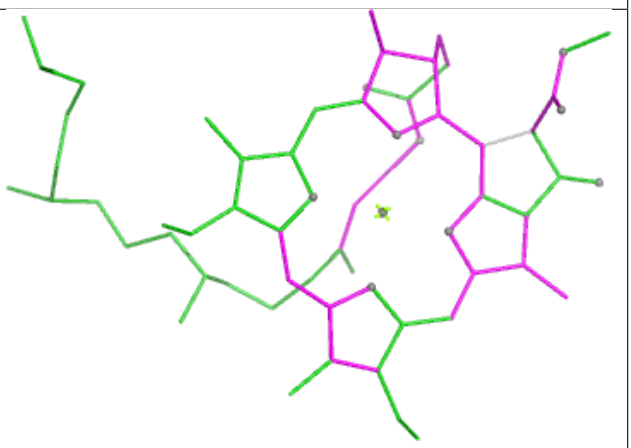
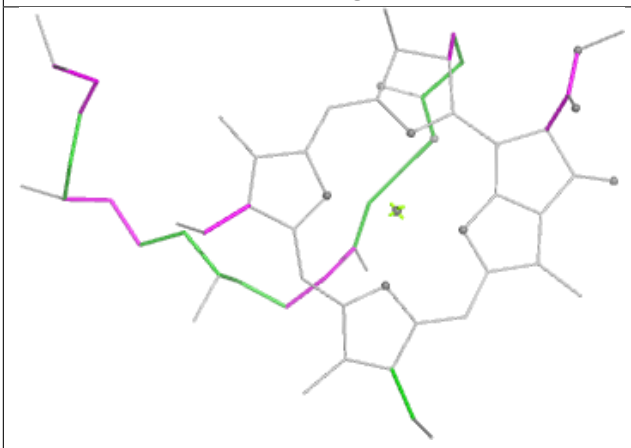
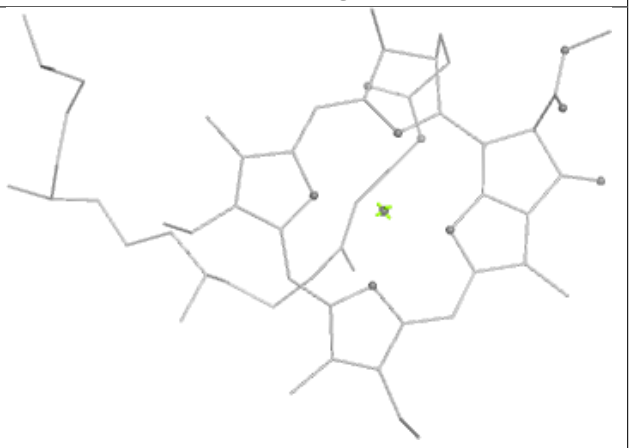
Ligand CLA B 1235



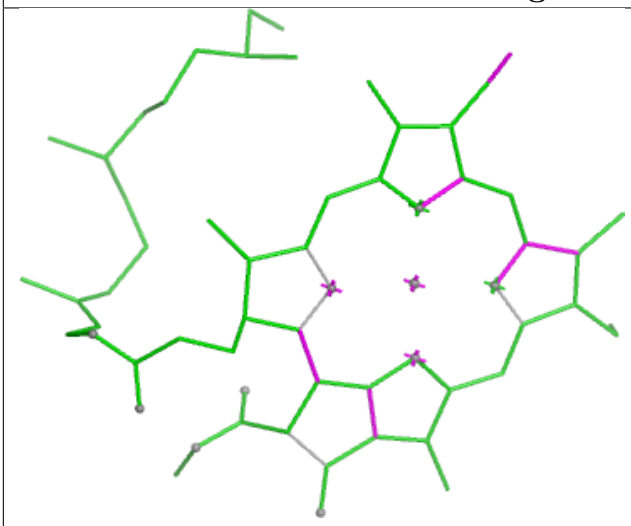
Ligand CLA B 1239



Ligand LUT 3 502	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 602



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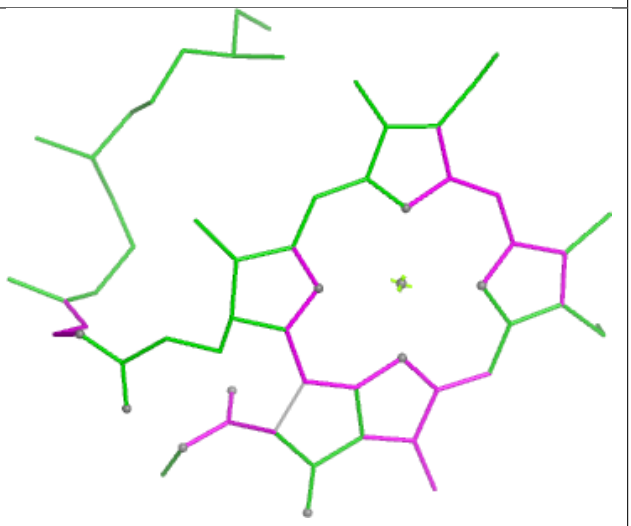
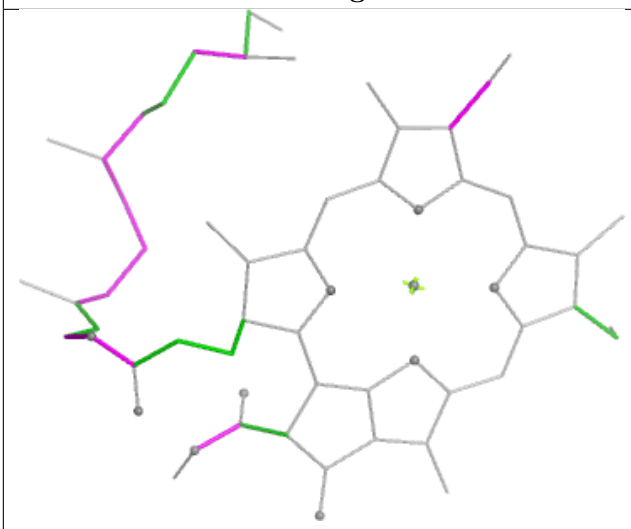


Bond angles



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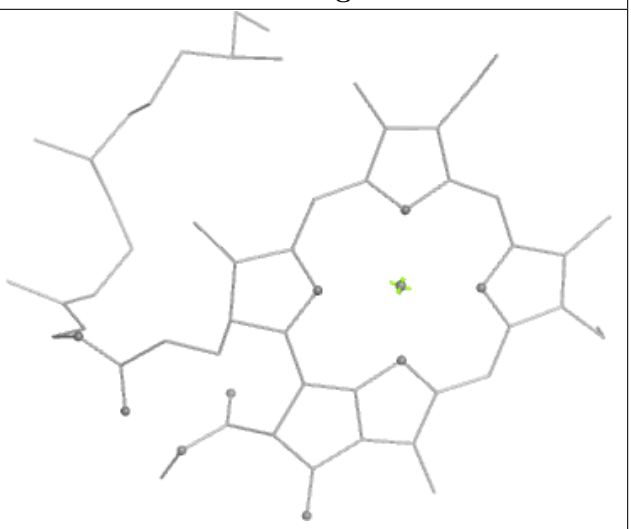
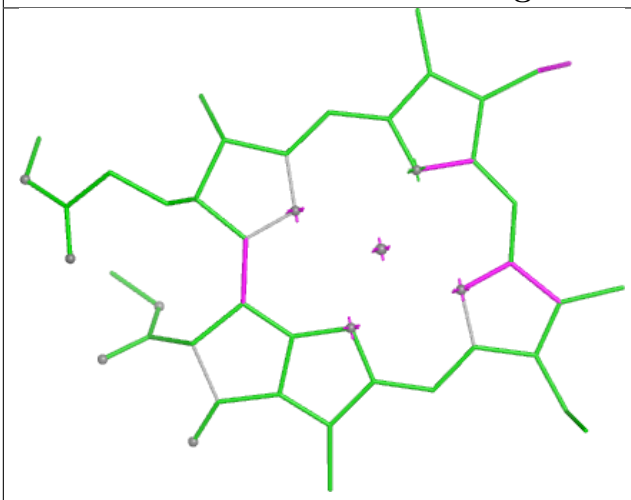
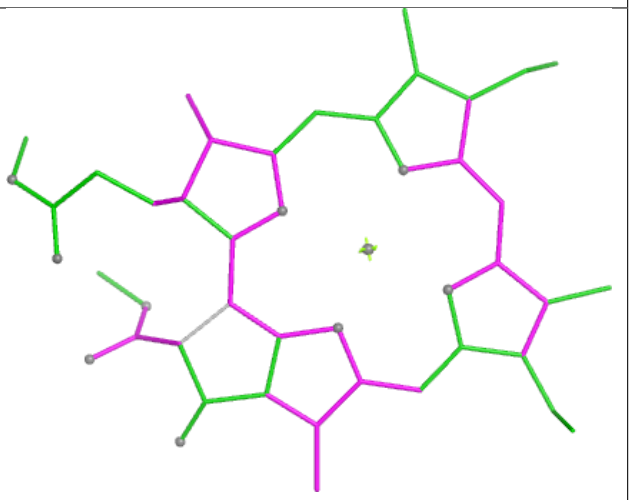


Rings

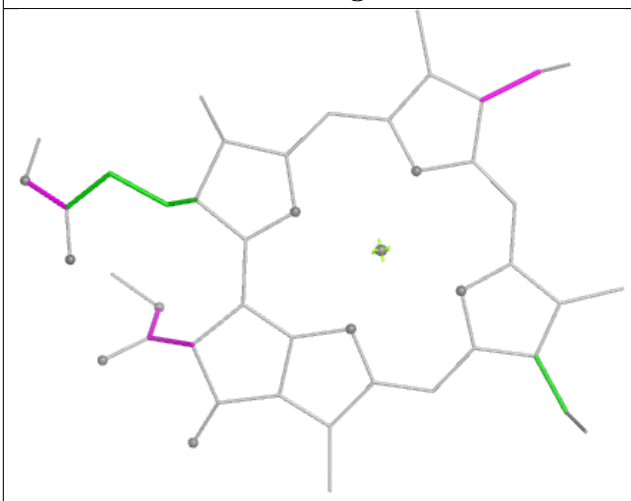
Ligand CLA G 1602



Bond lengths



Bond angles



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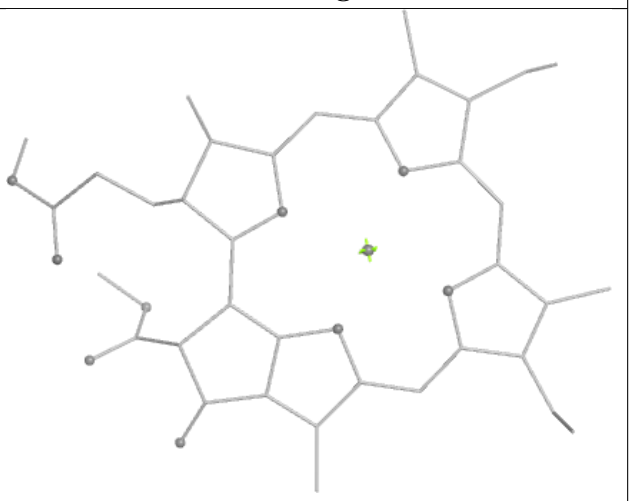
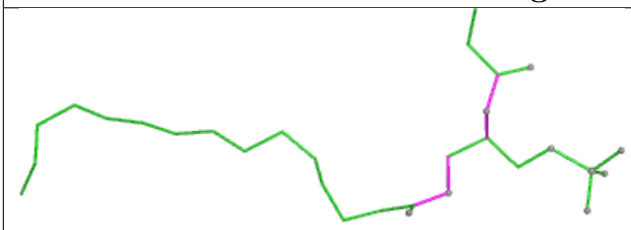


Rings

Ligand 3PH 8 806



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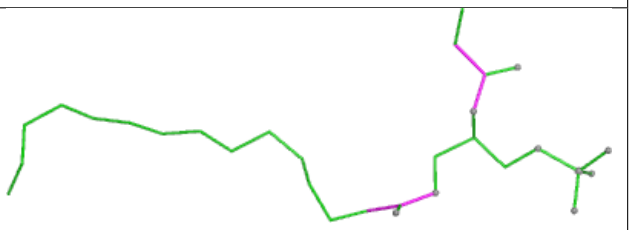
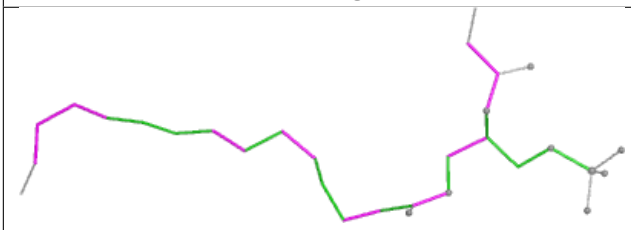


Bond angles



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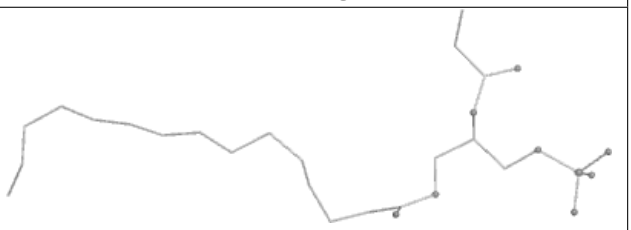
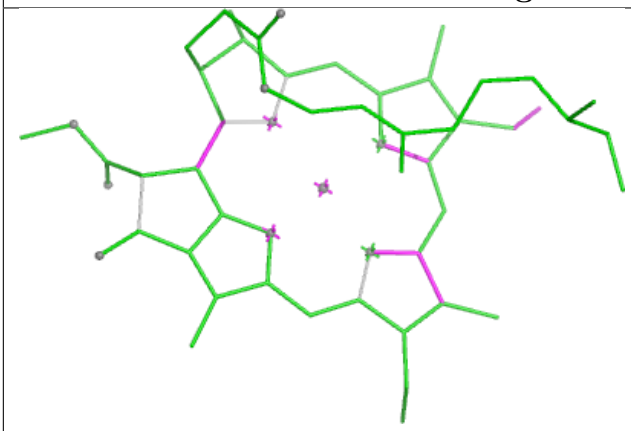
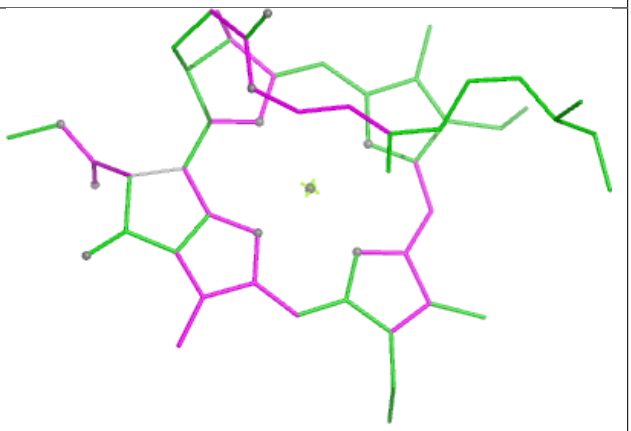


Rings

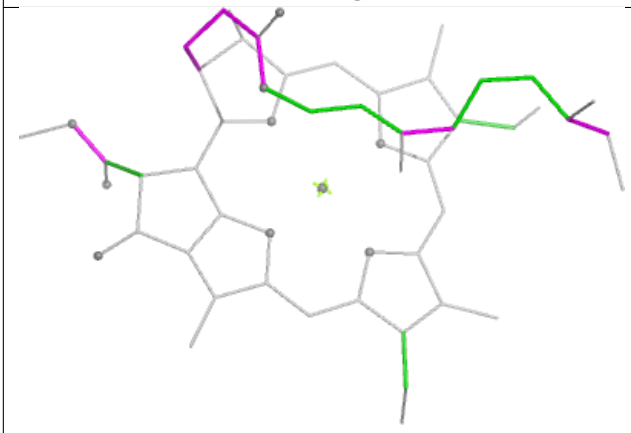
Ligand CLA B 1208



Bond lengths



Bond angles



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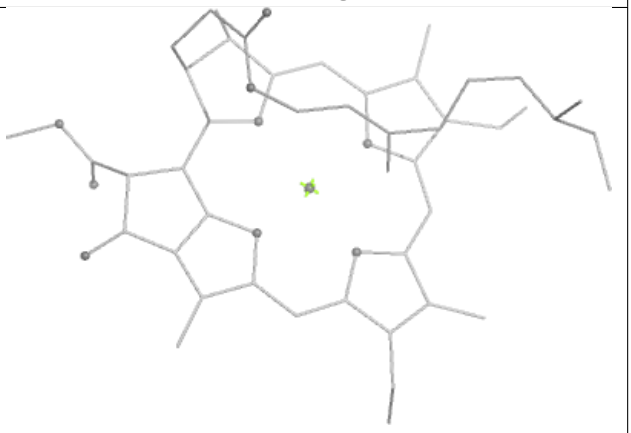
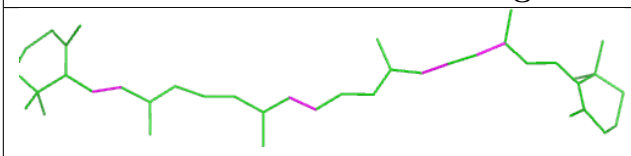
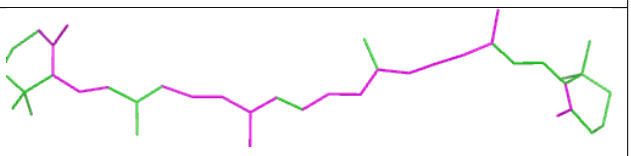


Rings

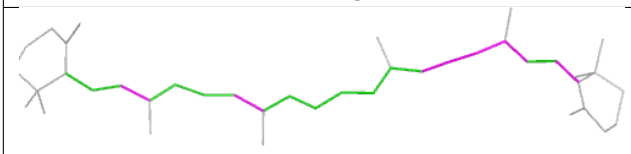
Ligand BCR B 4002



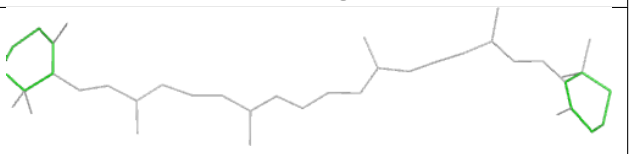
Bond lengths



Bond angles

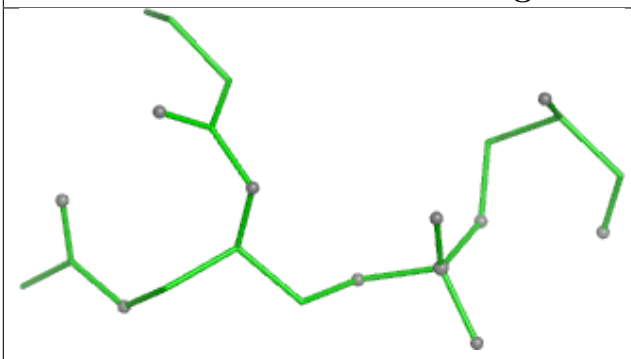


Torsions



Rings

Ligand LHG B 5001



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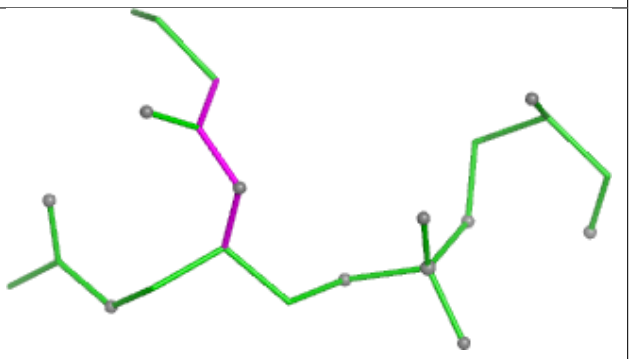

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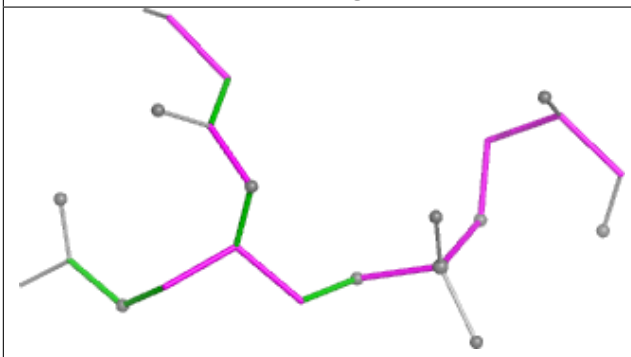

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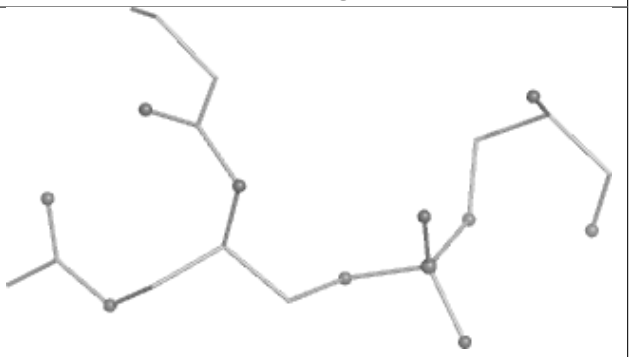
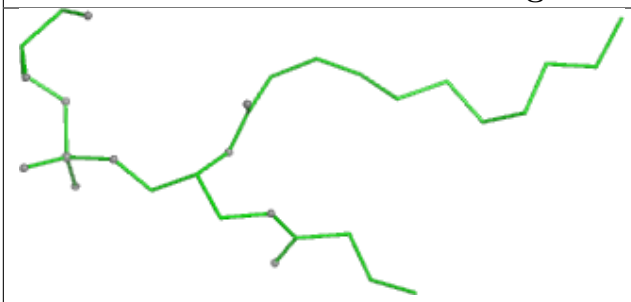


Rings

Ligand LHG 4 802



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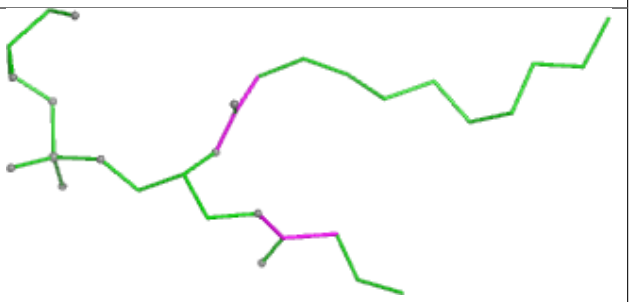
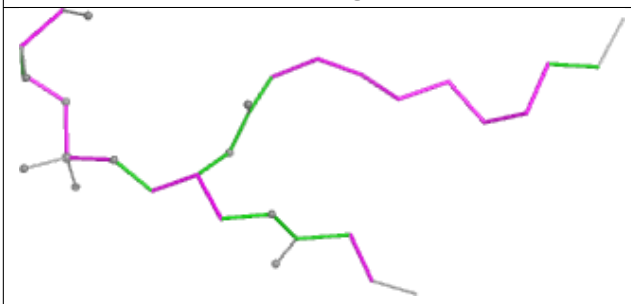


Bond angles



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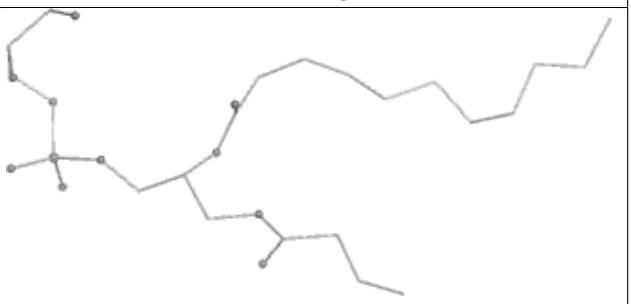
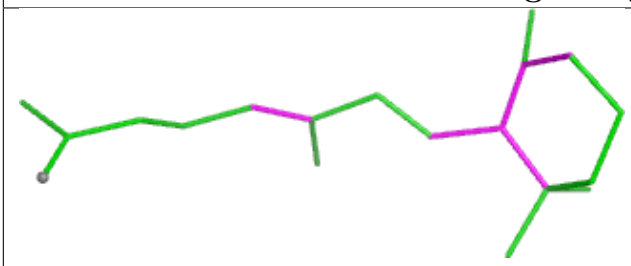
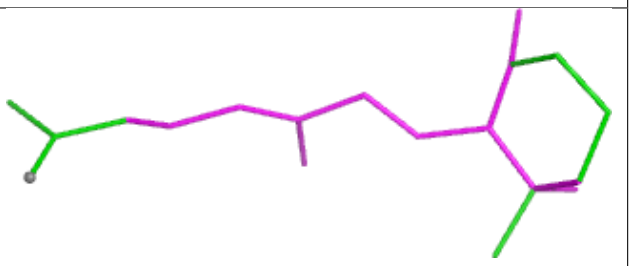
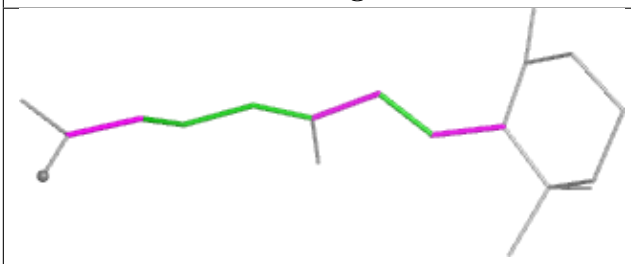
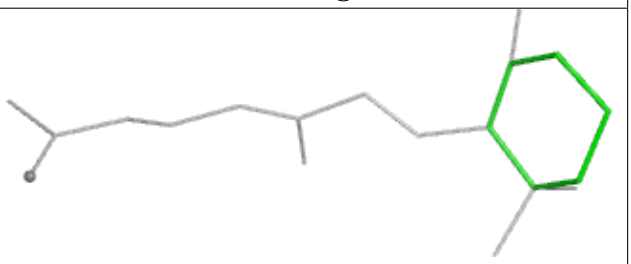
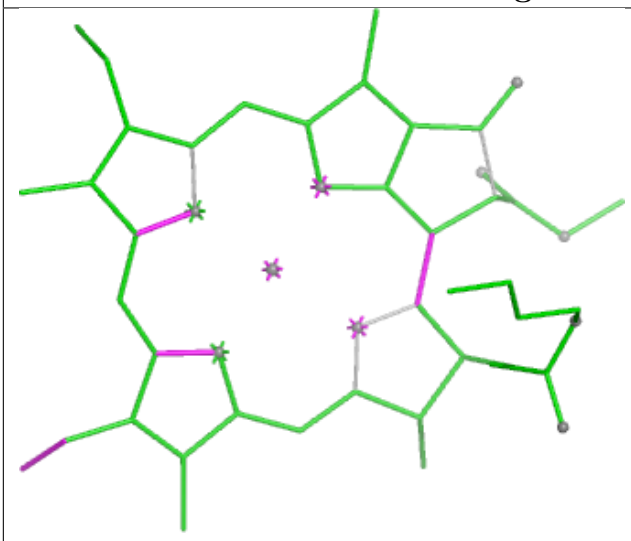


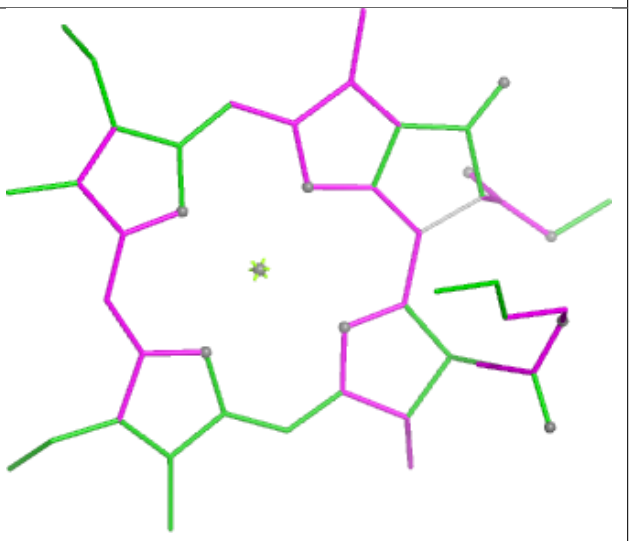
Rings

Ligand QTB Z 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

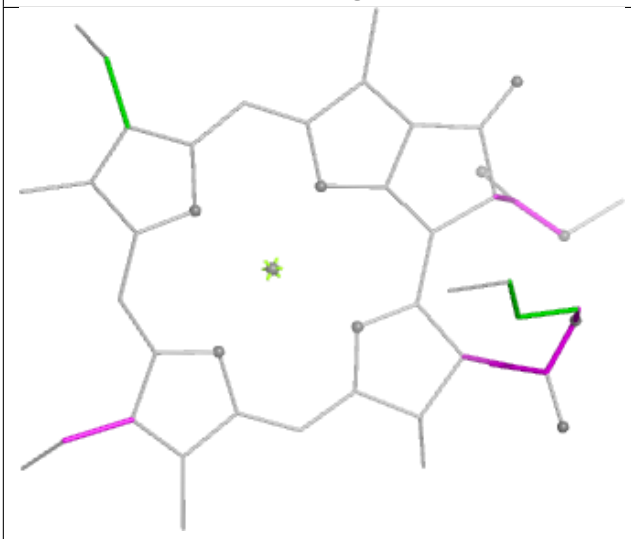
Ligand CLA K 1403



Bond lengths



Bond angles



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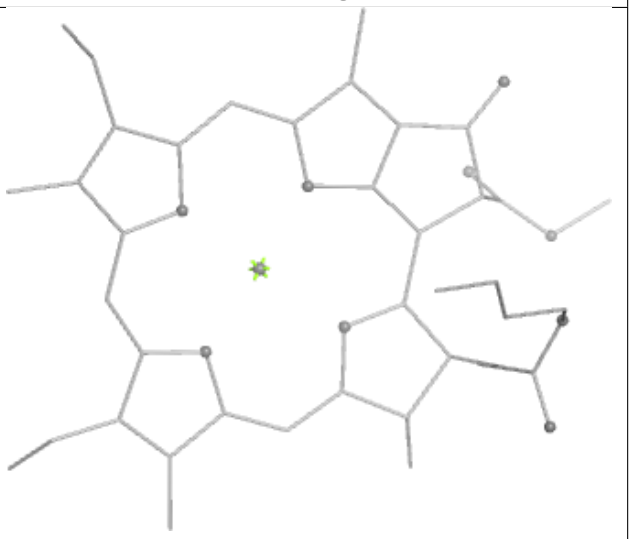
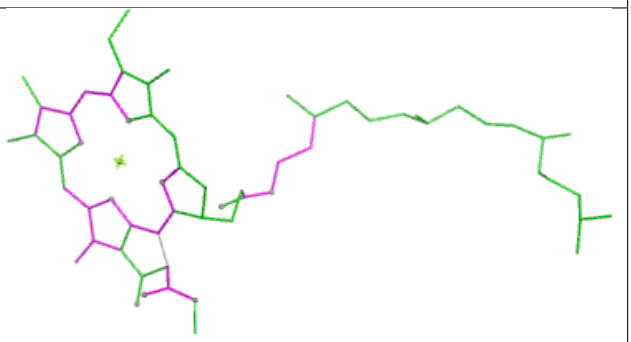
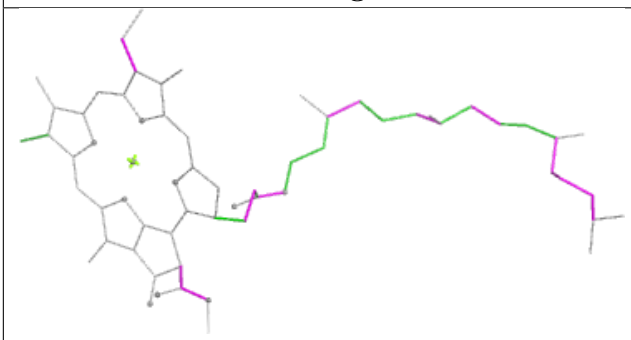
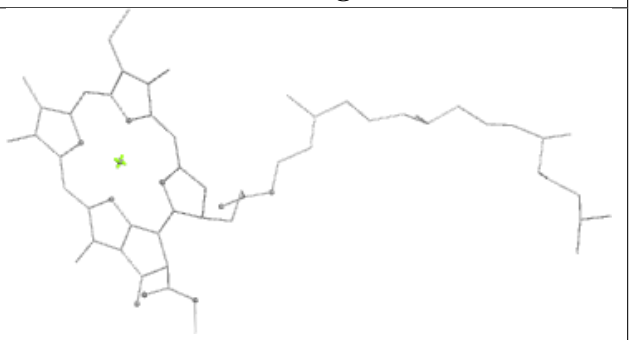
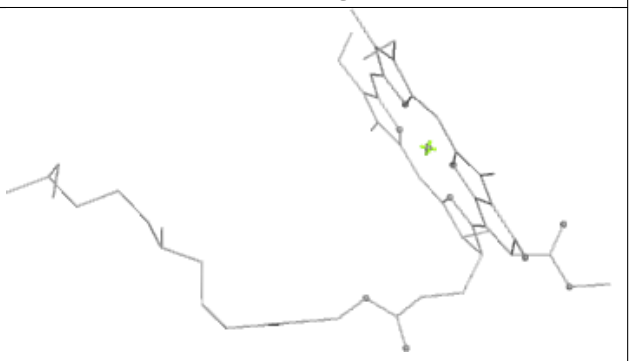
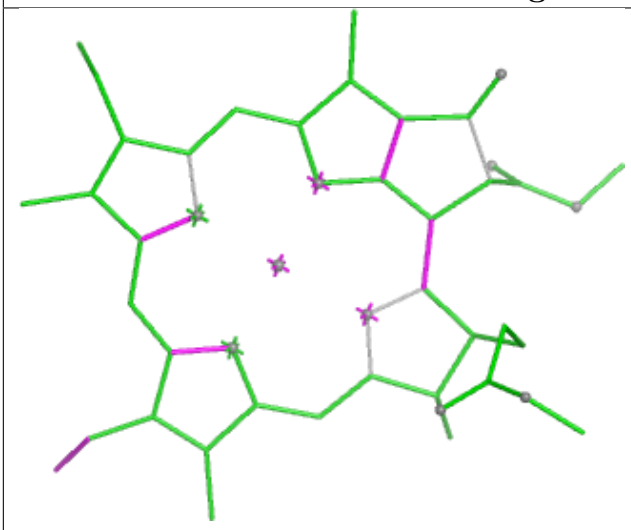


Rings

Ligand CLA A 1119	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 606	
Bond lengths	Bond angles
Torsions	 Rings

Ligand CLA 3 618



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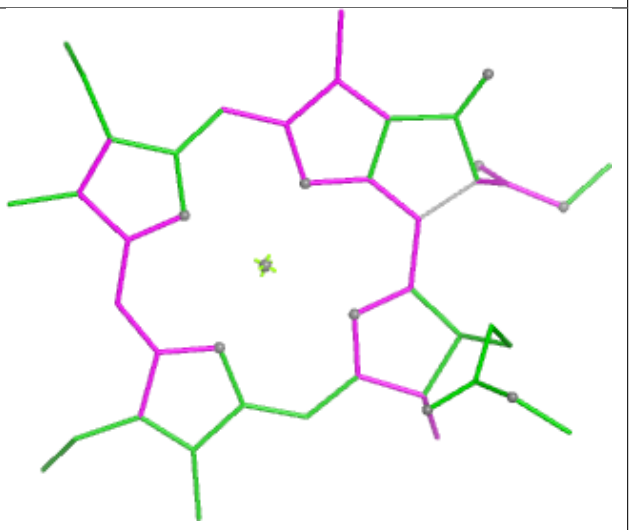

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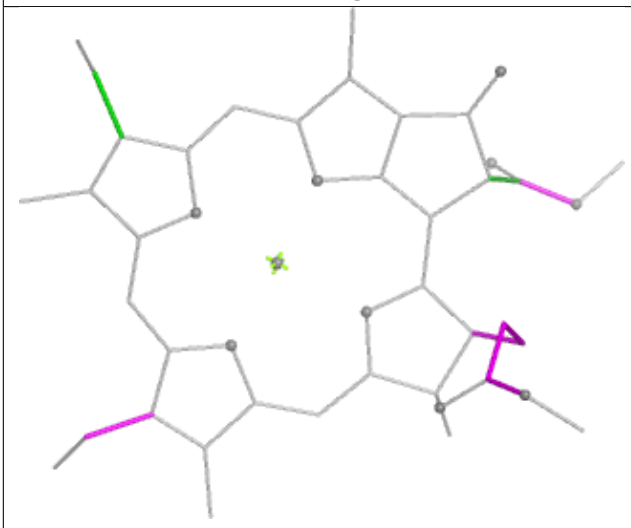

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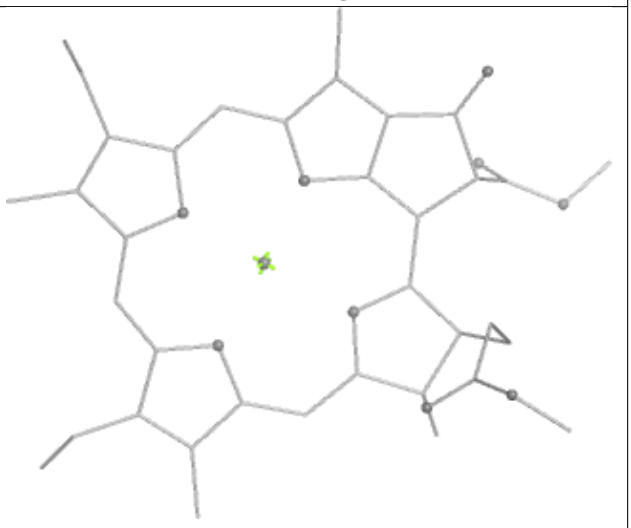

Rings

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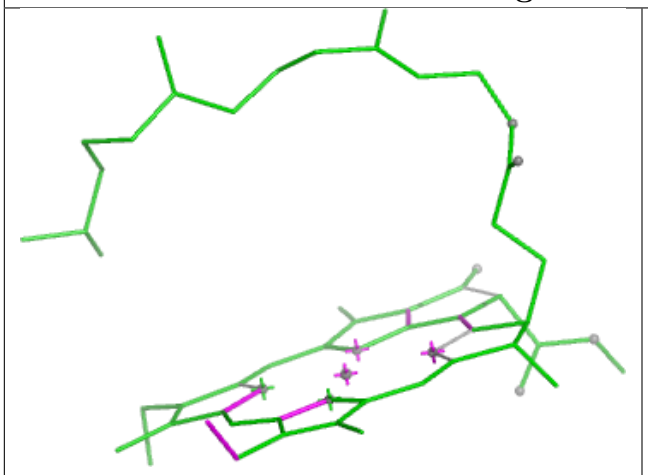

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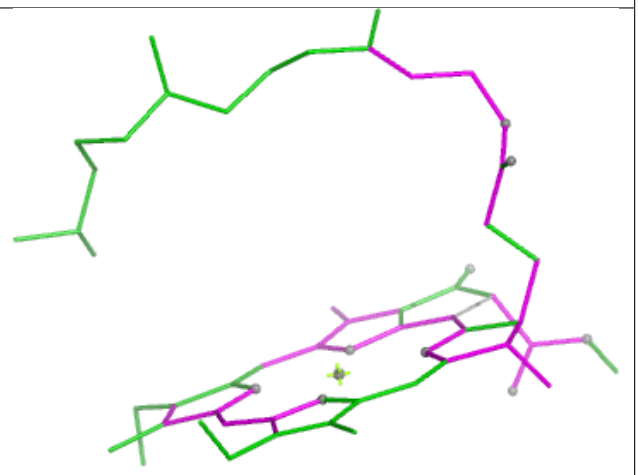
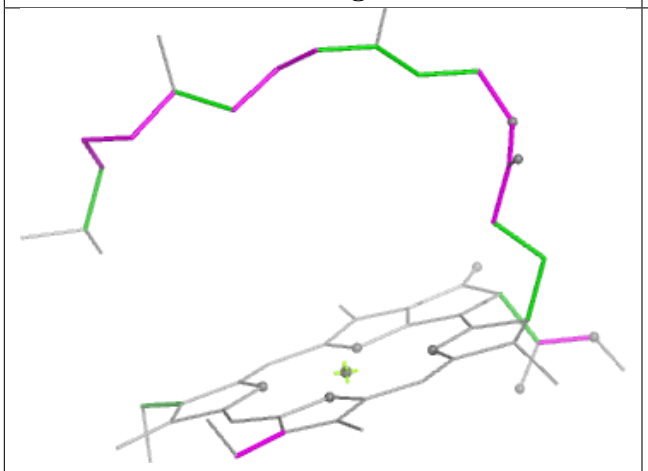
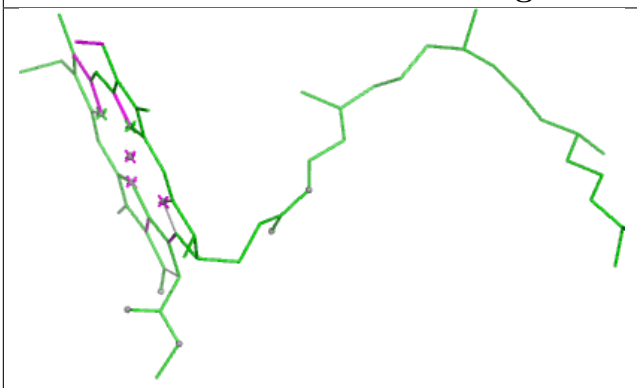
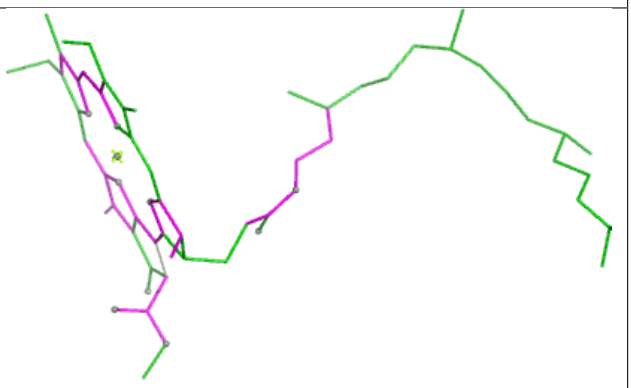
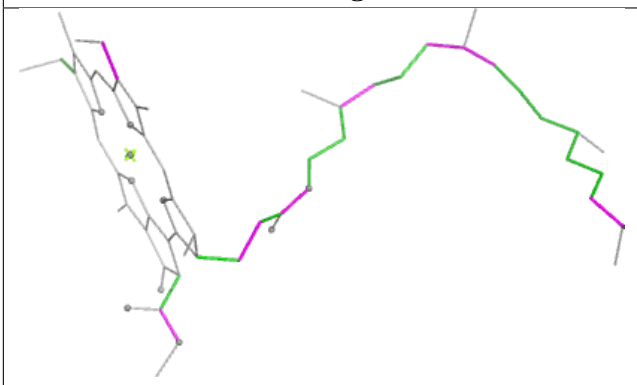


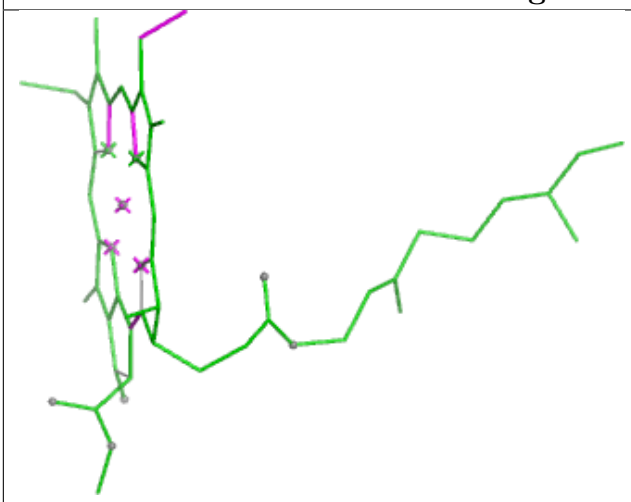
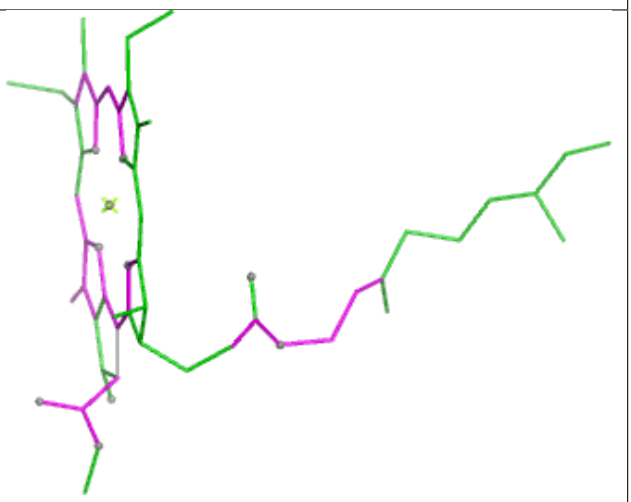
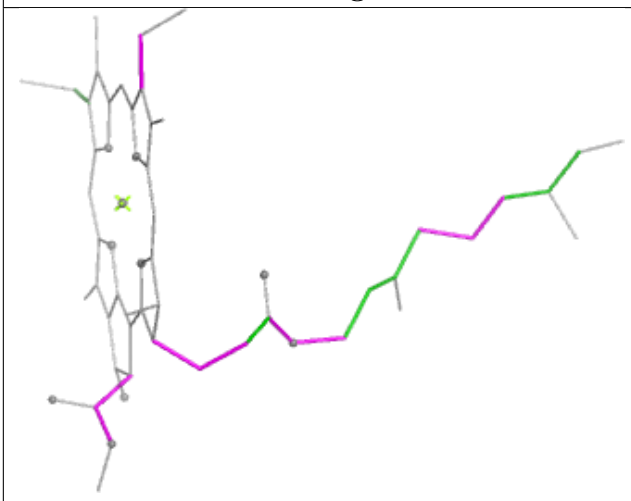
Bond angles



Torsions

Rings

Ligand CLA B 1238	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 7 606	
 Bond lengths	 Bond angles
 Torsions	Rings

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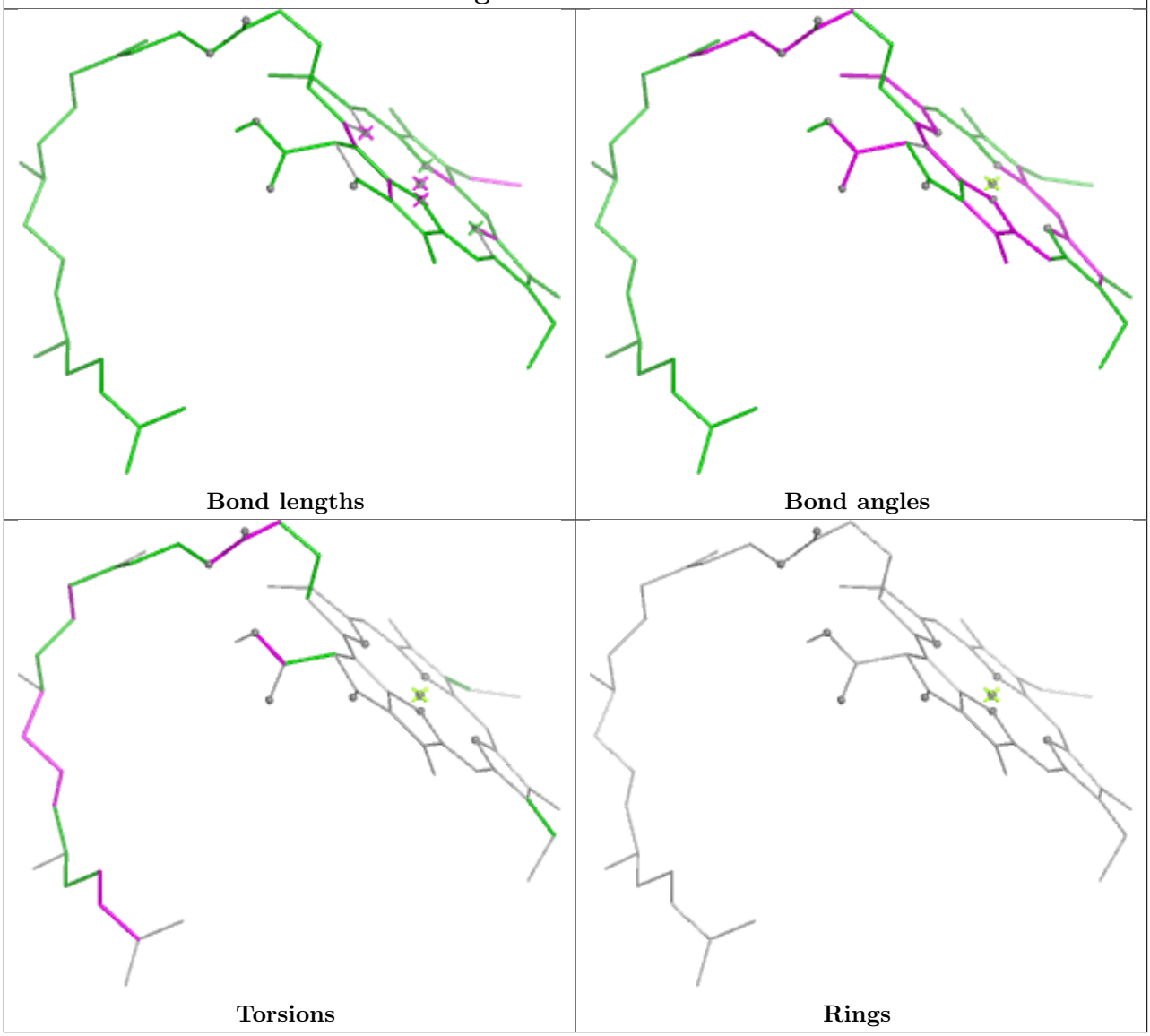

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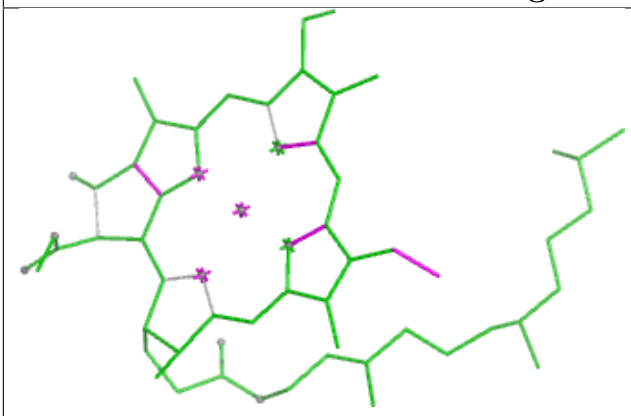
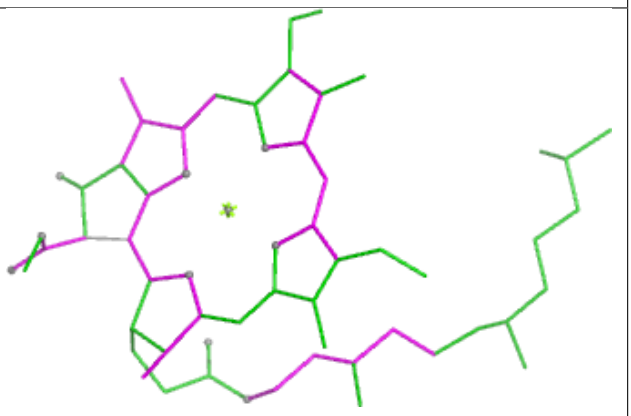
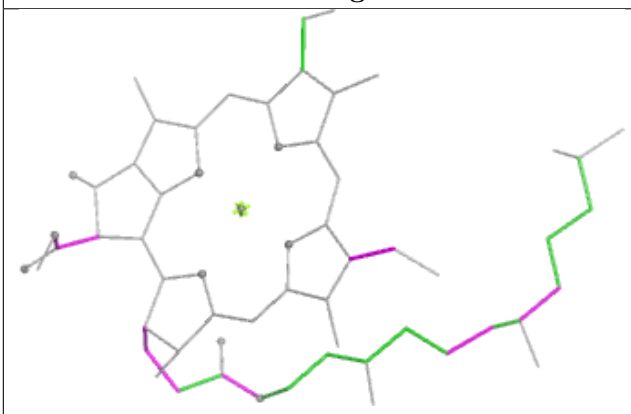
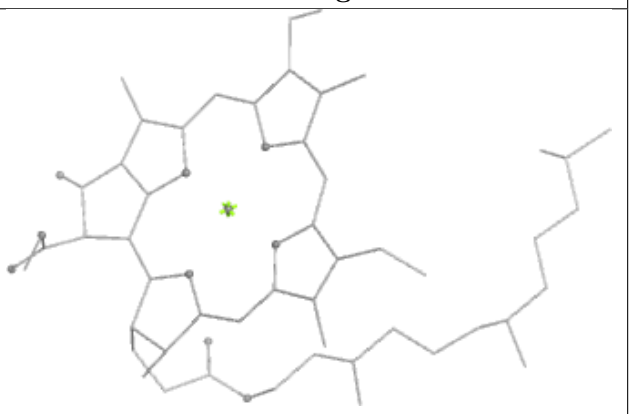
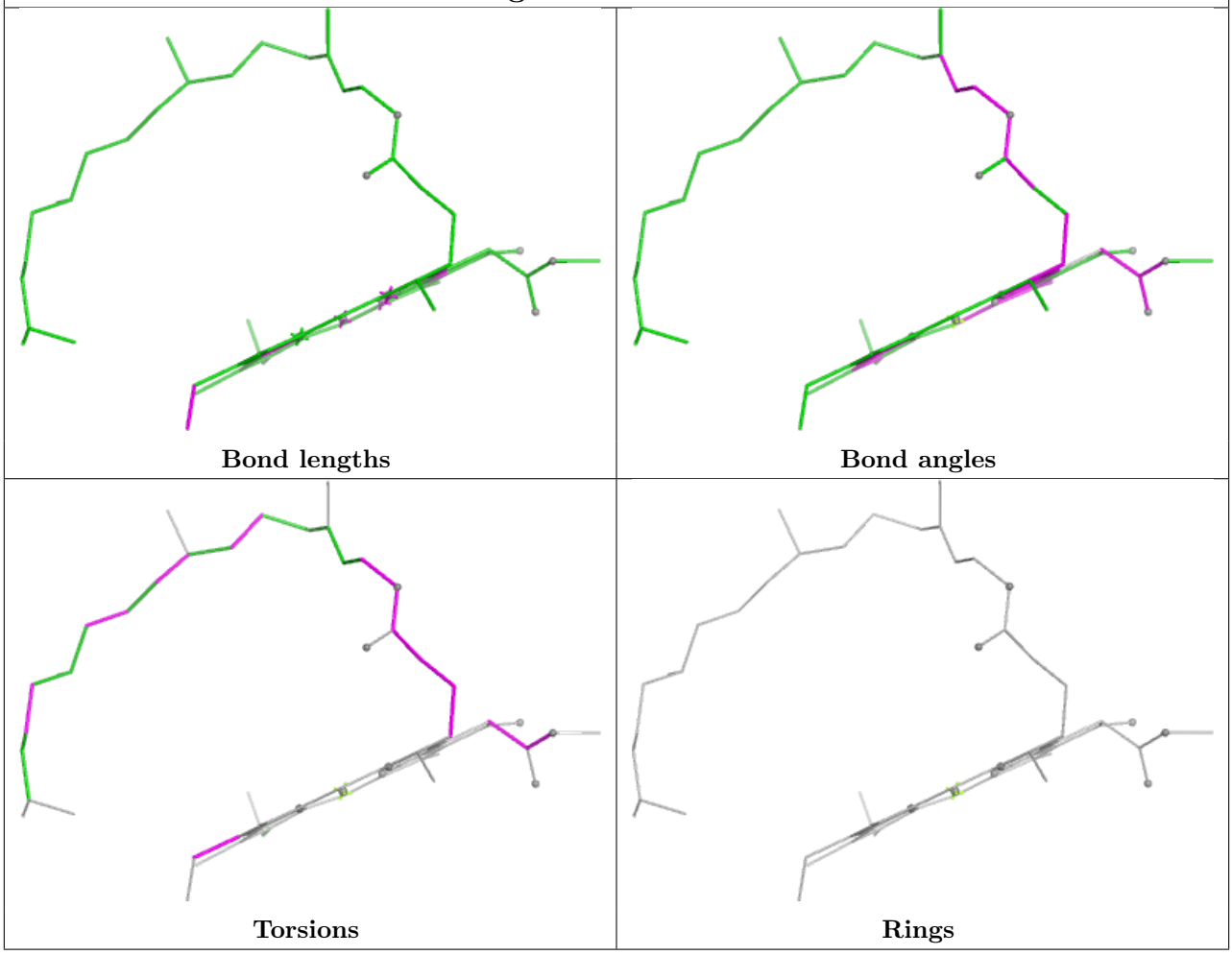
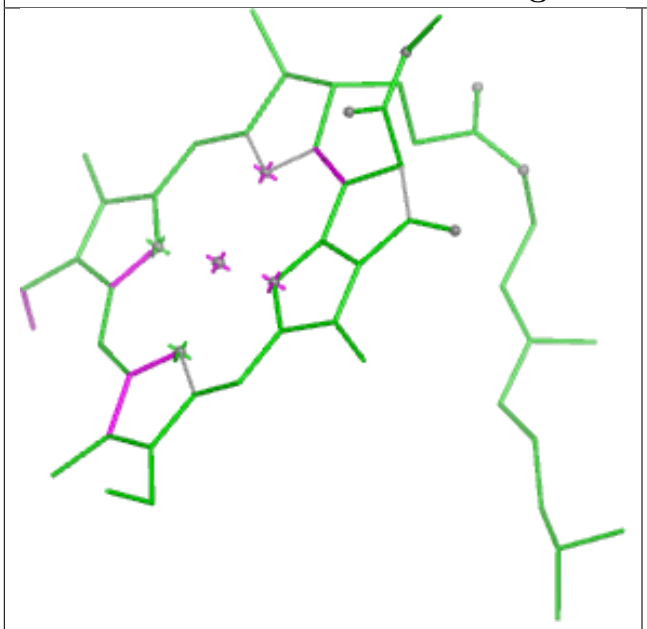
 Bond lengths	 Bond angles
 Torsions	 Rings

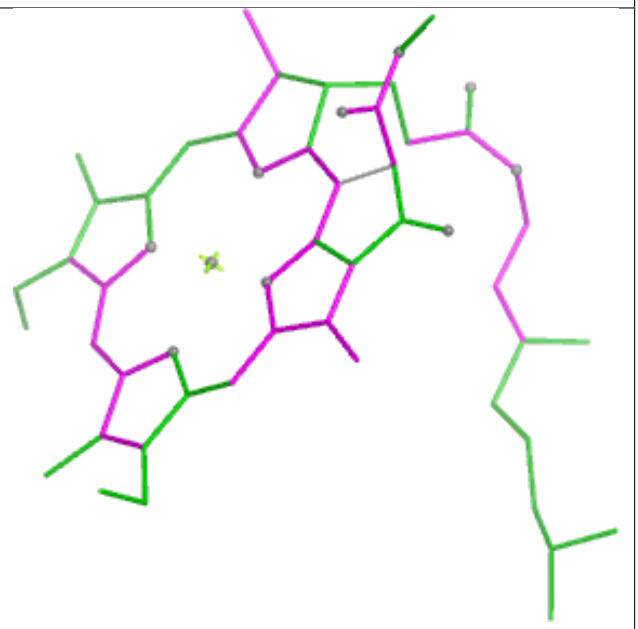
Ligand CLA 6 606



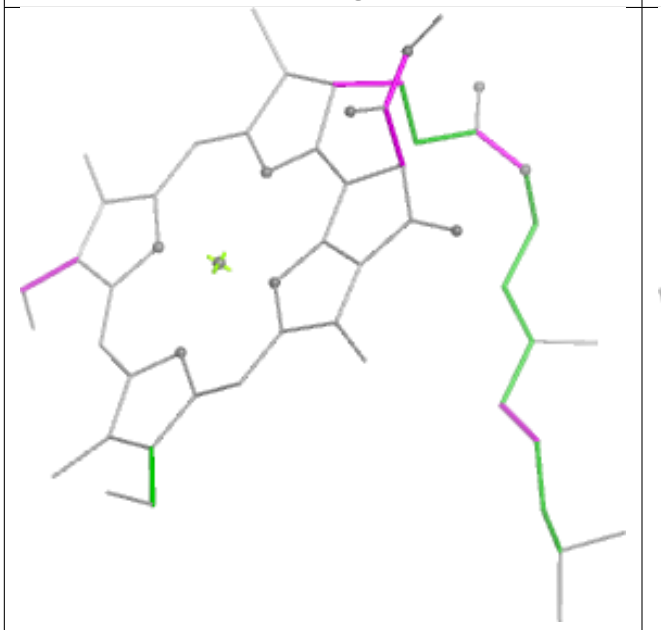
Ligand CLA 4 607



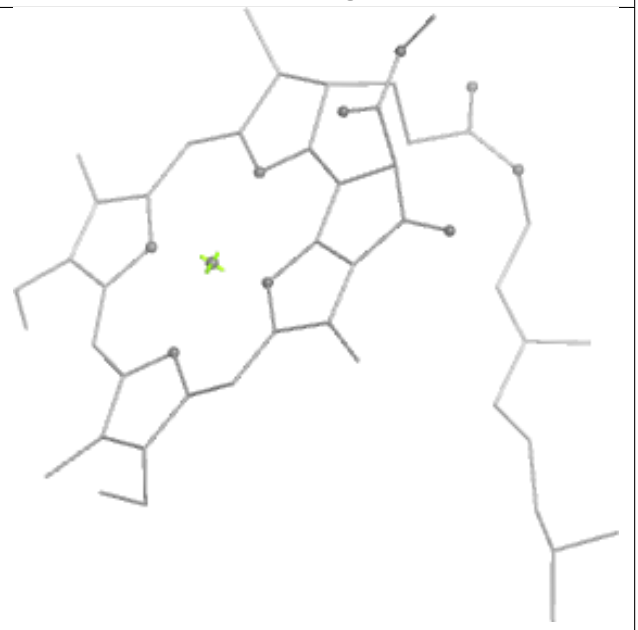
Bond lengths



Bond angles



Torsions



Rings

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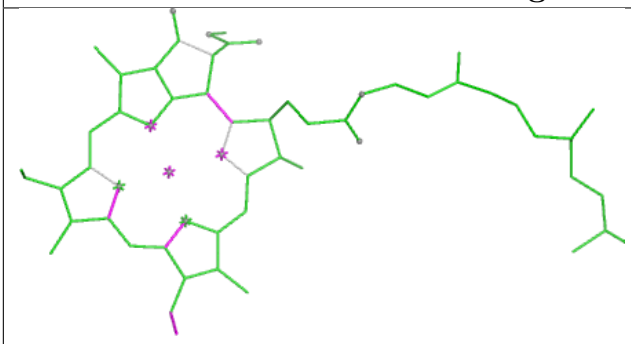

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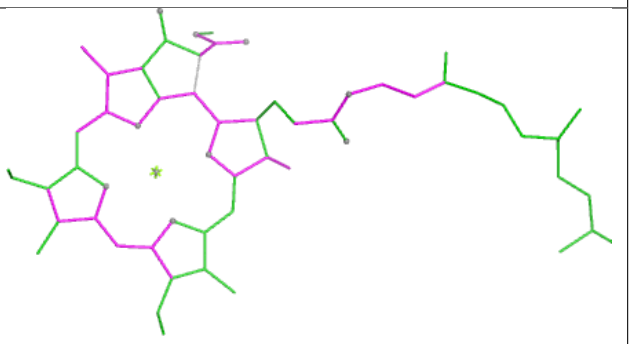

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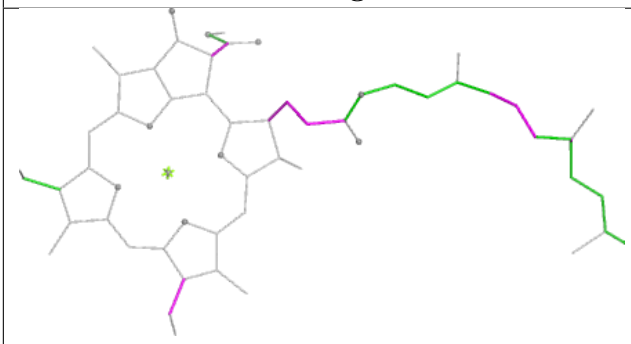

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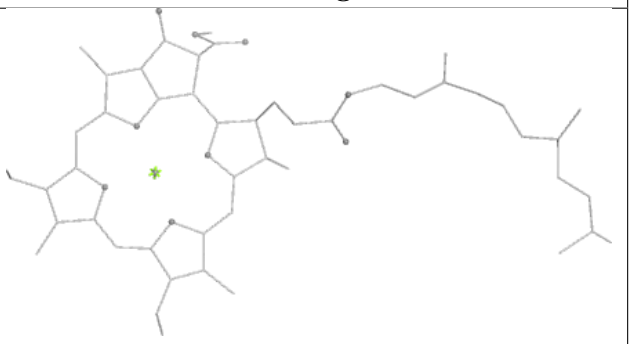
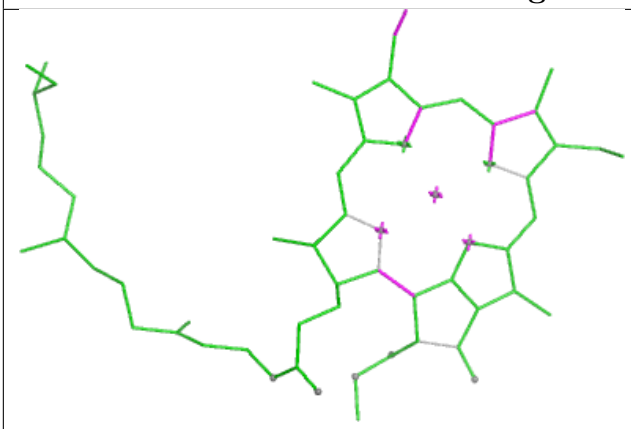


Rings

Ligand CLA 7 605



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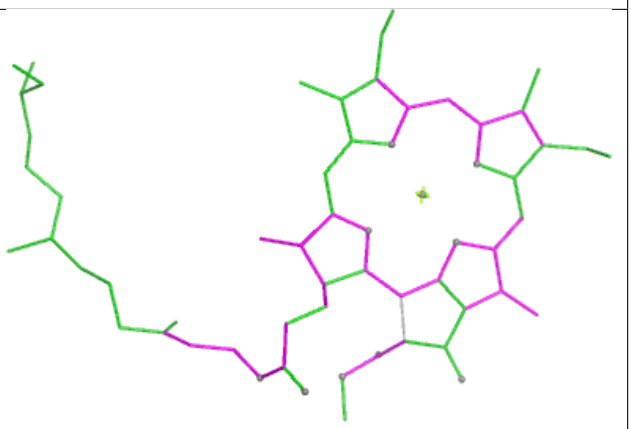
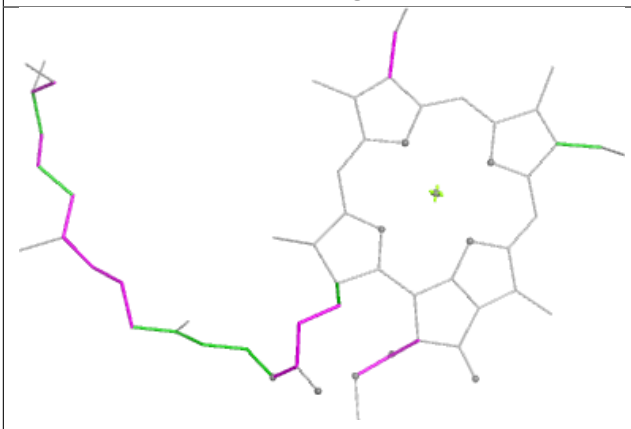


Bond angles



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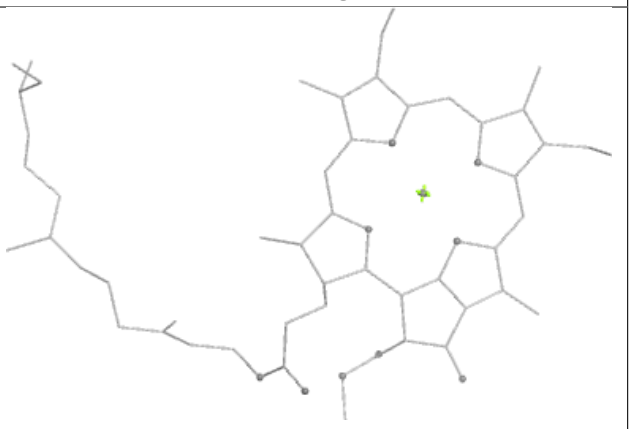
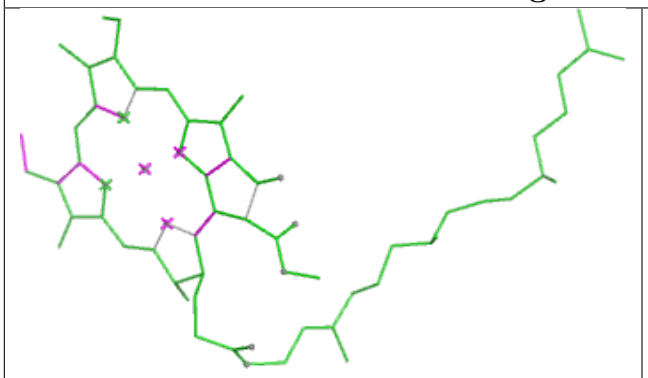
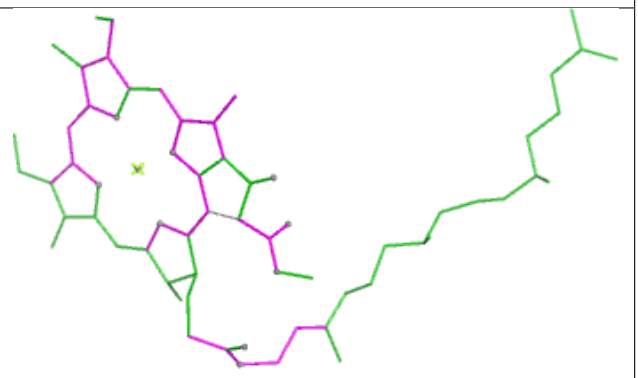


Rings

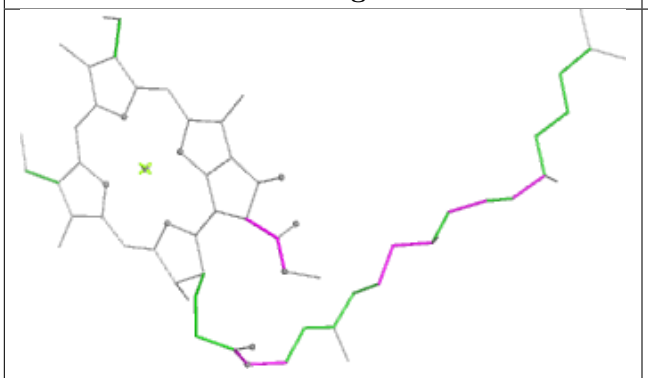
Ligand CLA 3 605



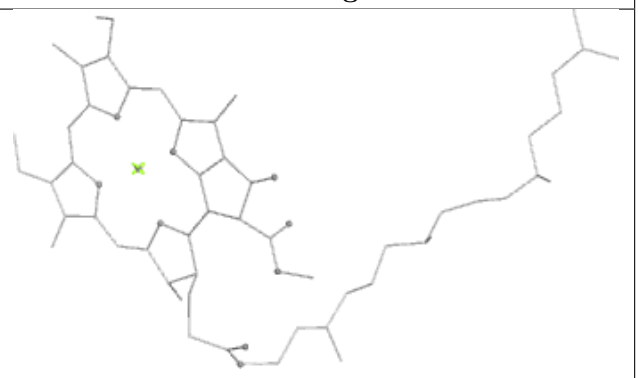
Bond lengths



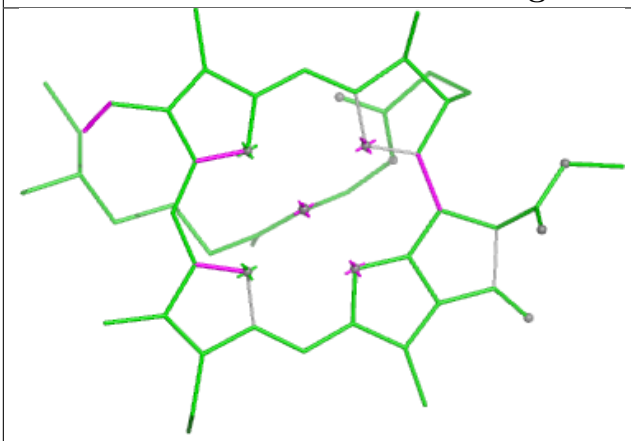
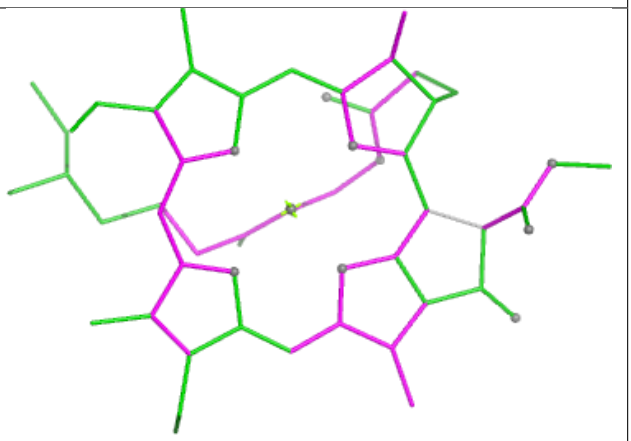
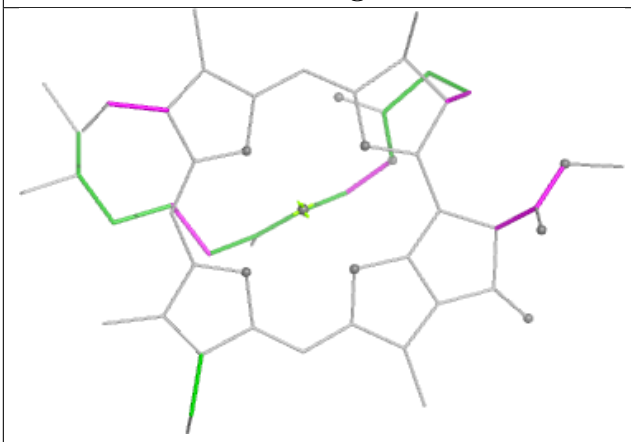
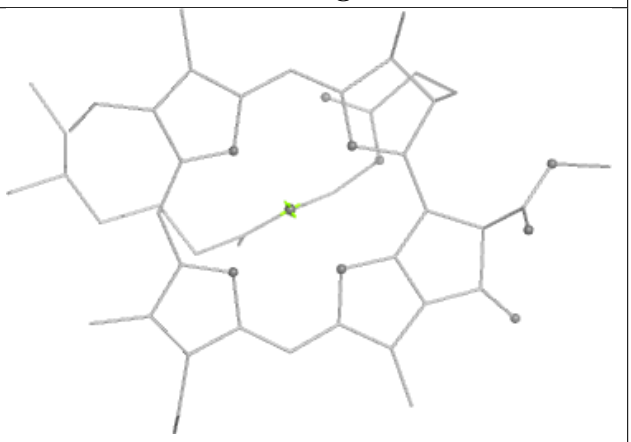
Bond angles



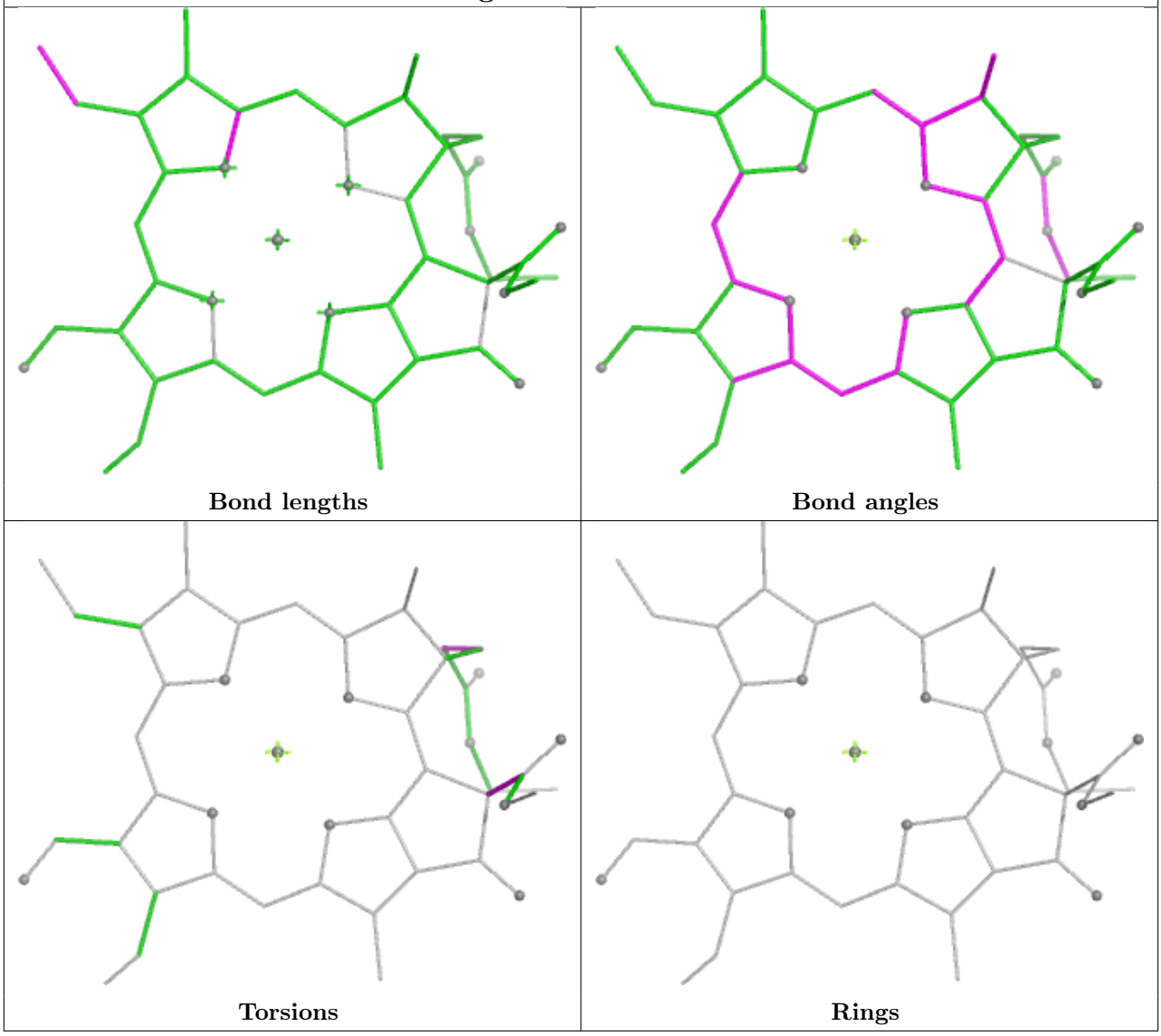
Torsions



Rings

Ligand CLA 5 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CHL 1 610



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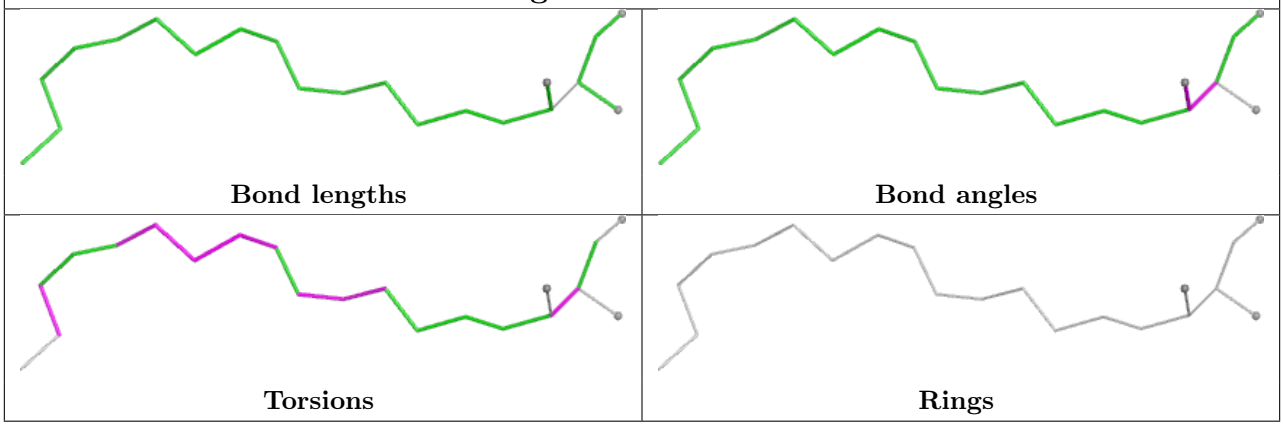
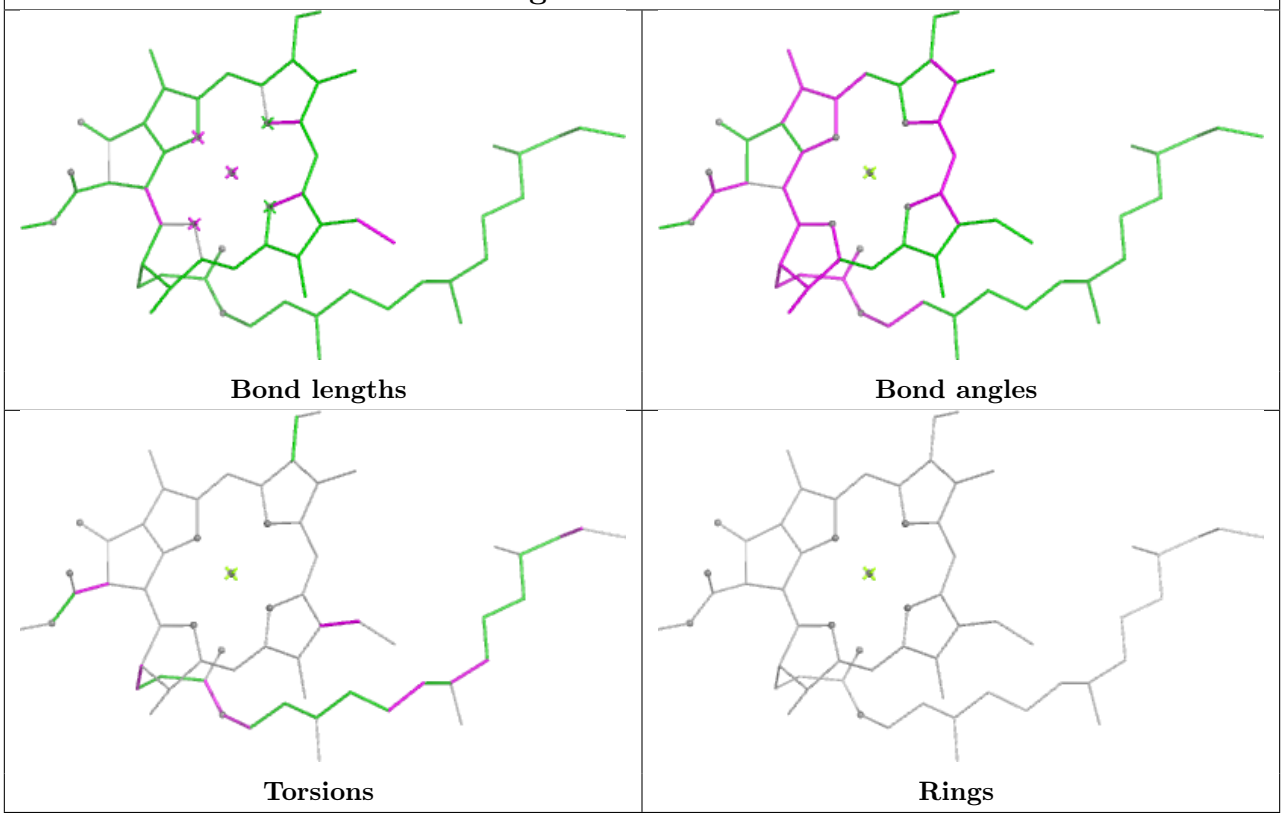


Ligand CLA 8 604



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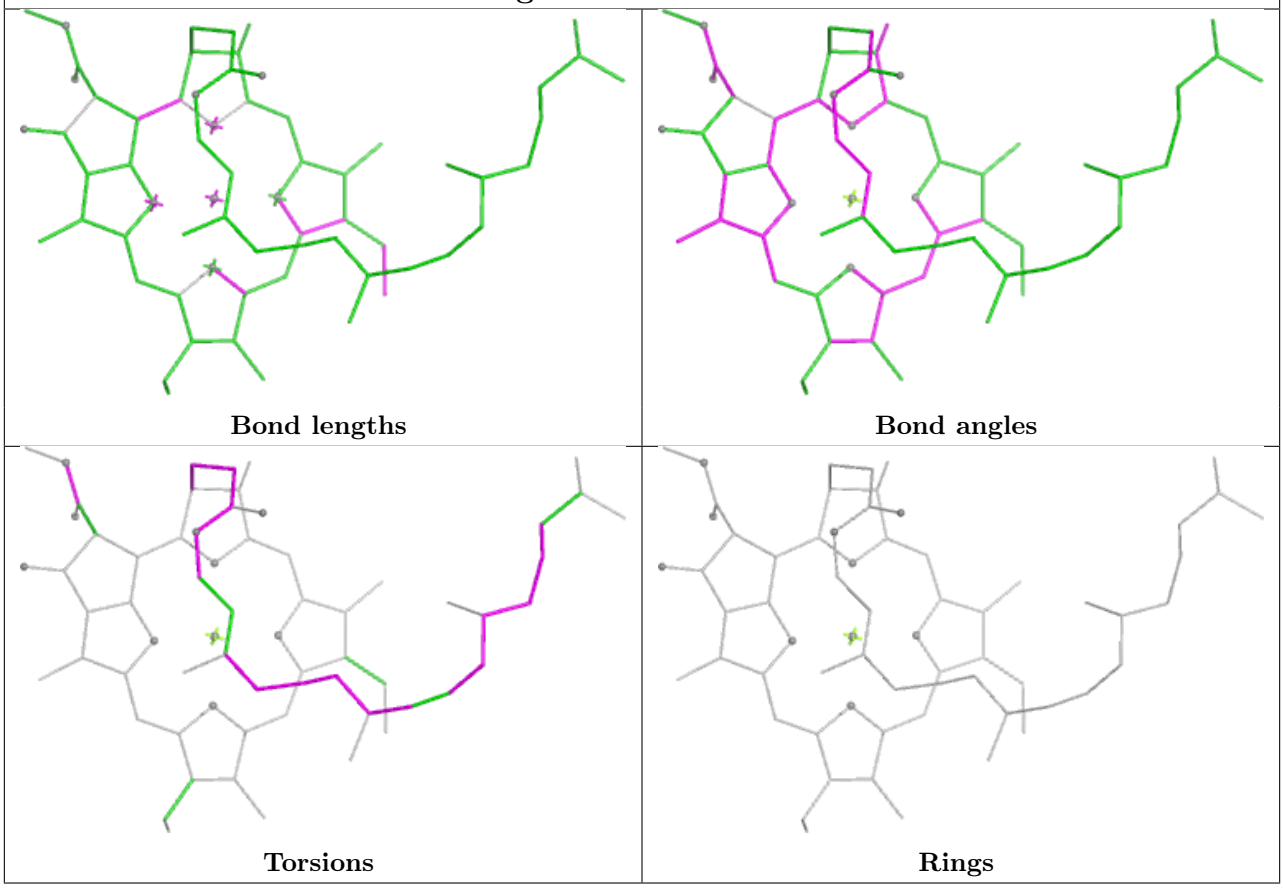

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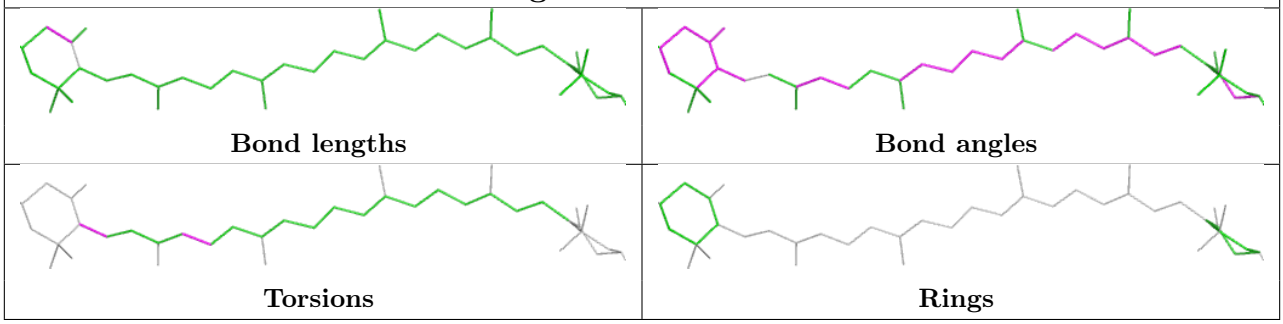

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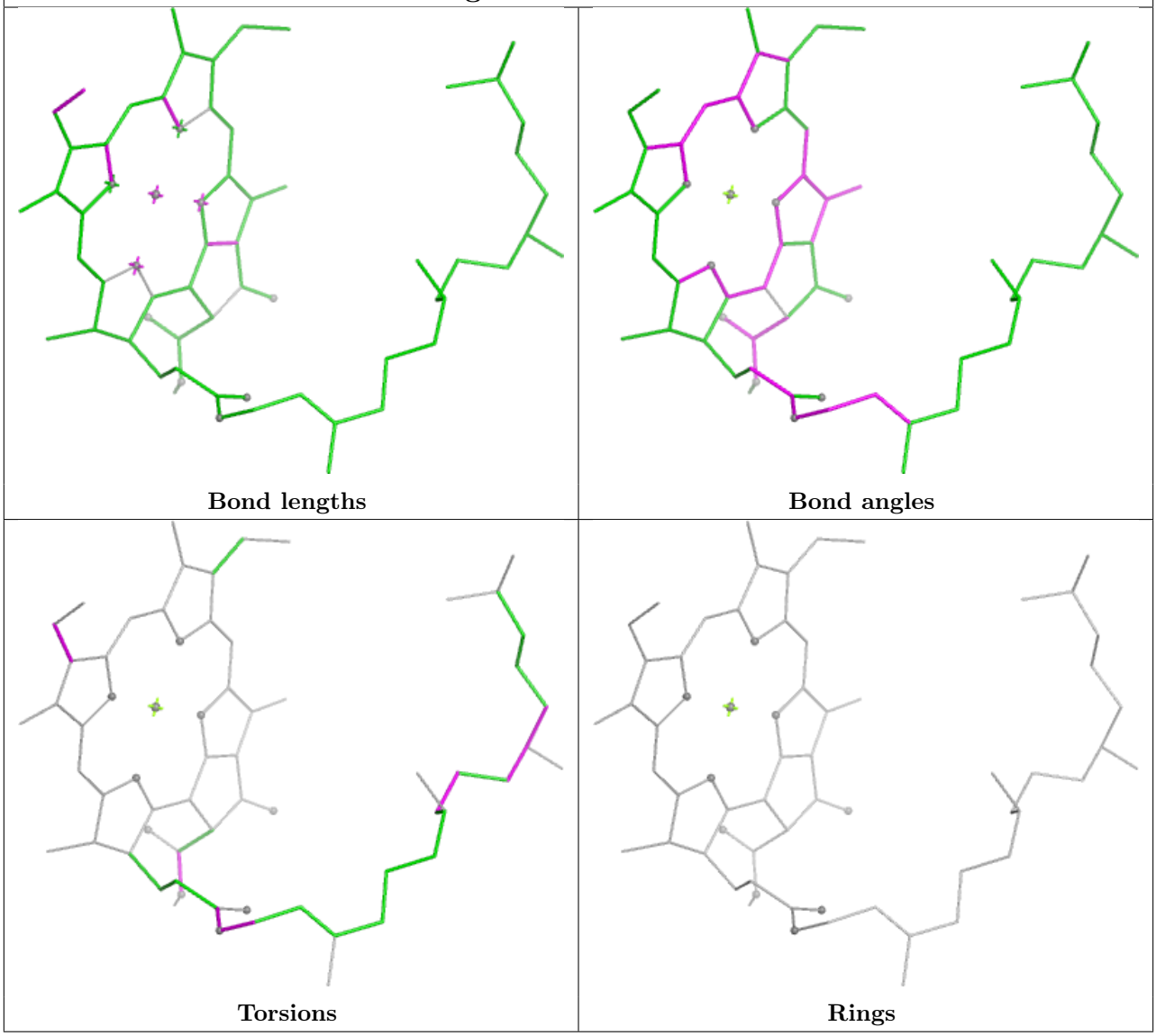

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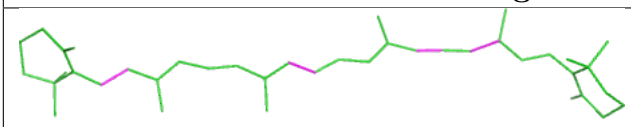
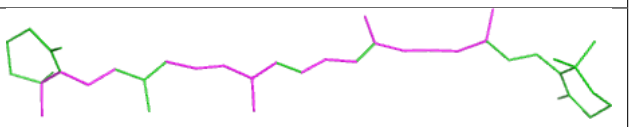
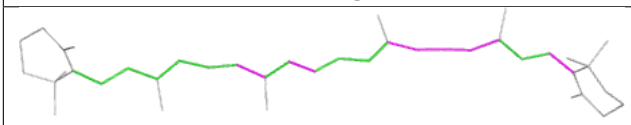
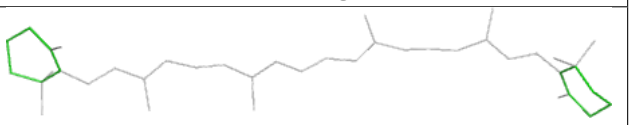
 Bond lengths	 Bond angles
 Torsions	 Rings

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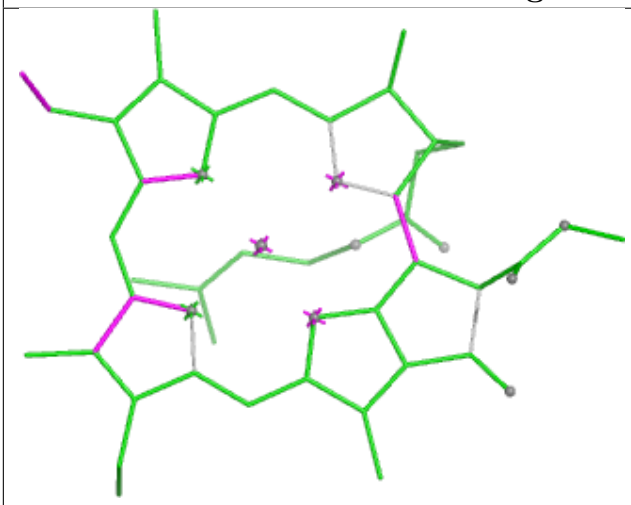
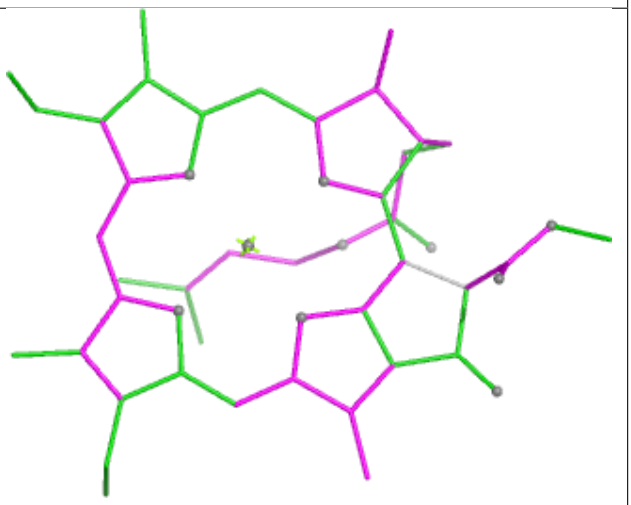
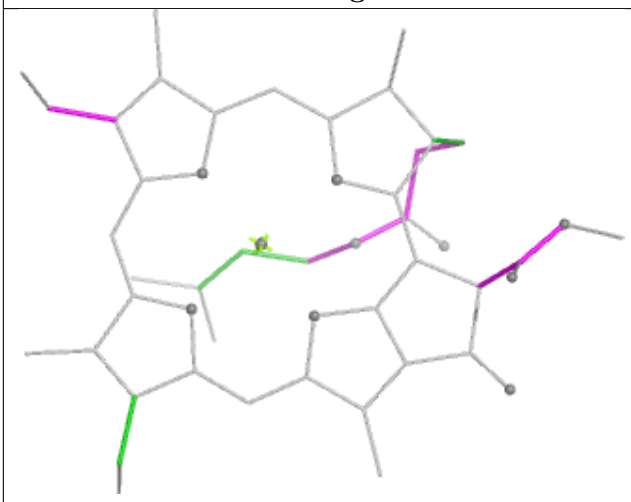
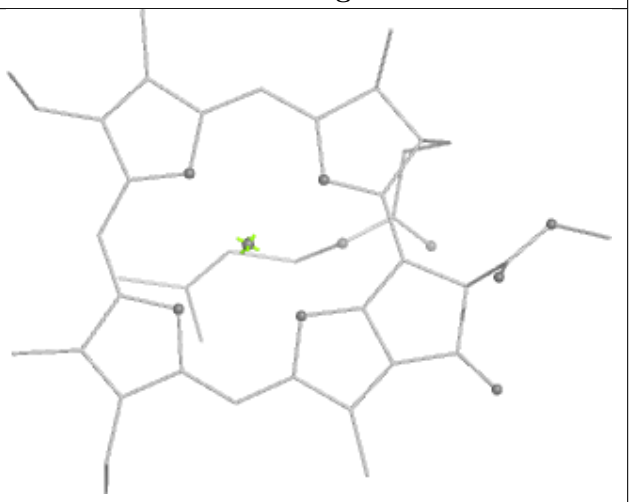
 Bond lengths	 Bond angles
 Torsions	 Rings

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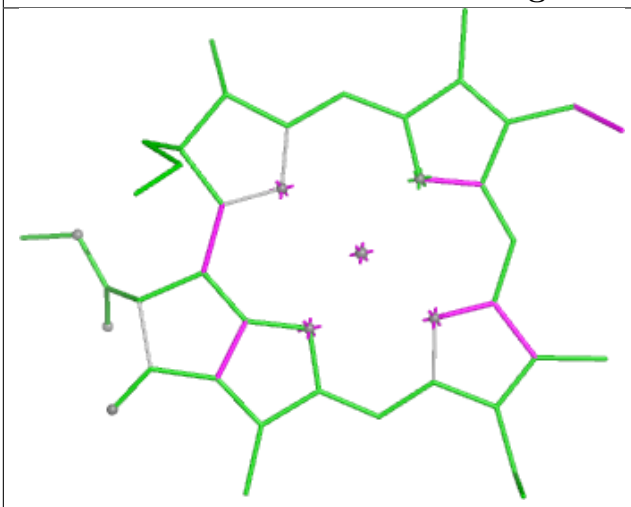	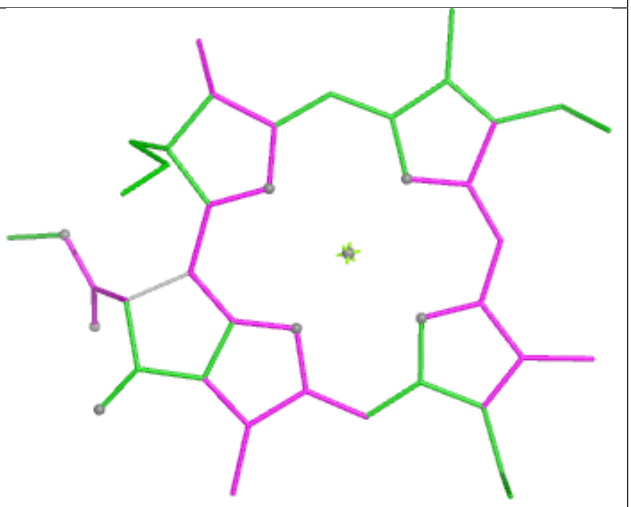
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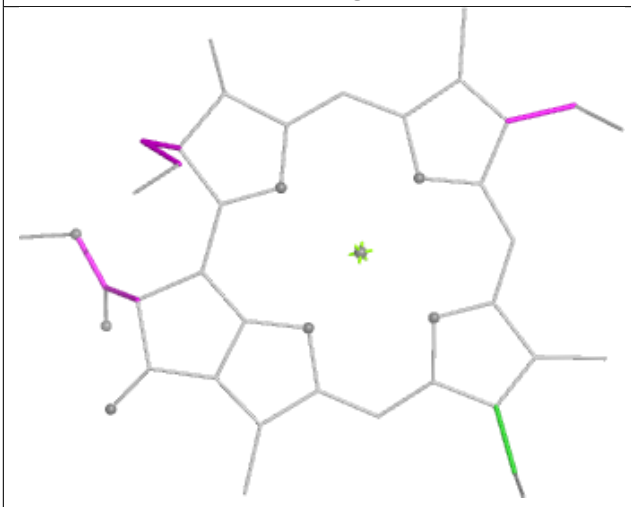
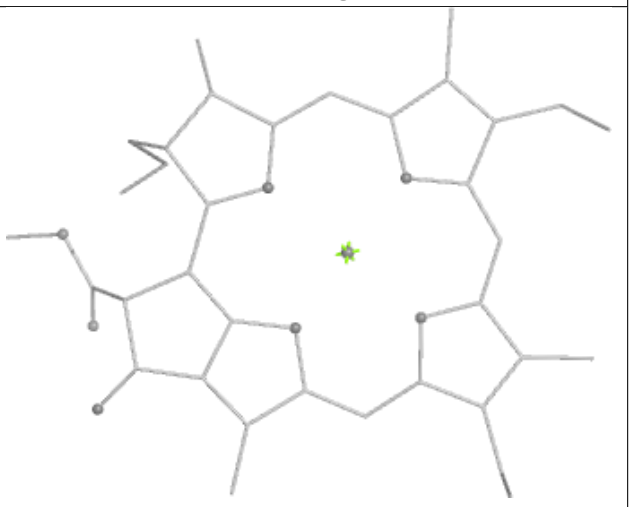
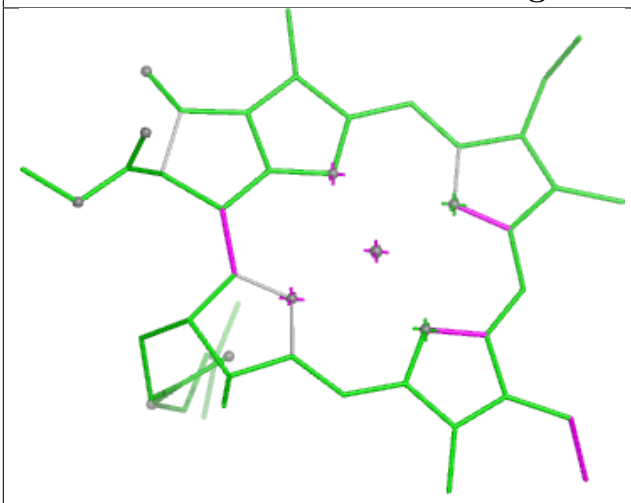
	
Torsions	**Rings**

Ligand CLA 4 612



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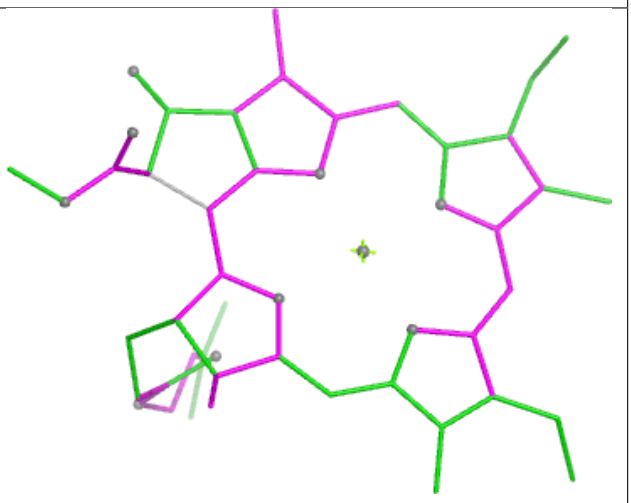
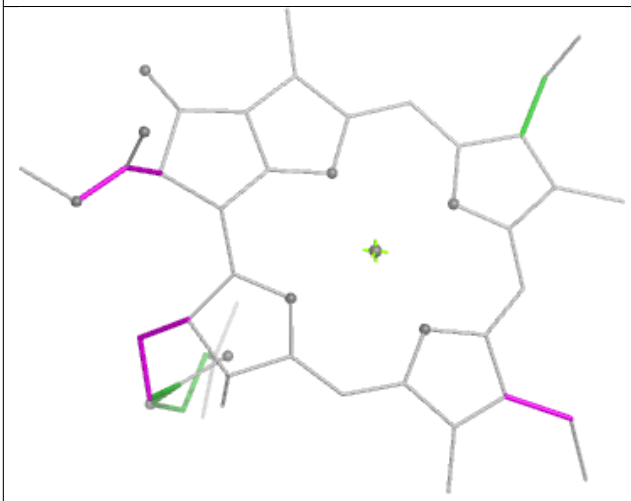


Bond angles



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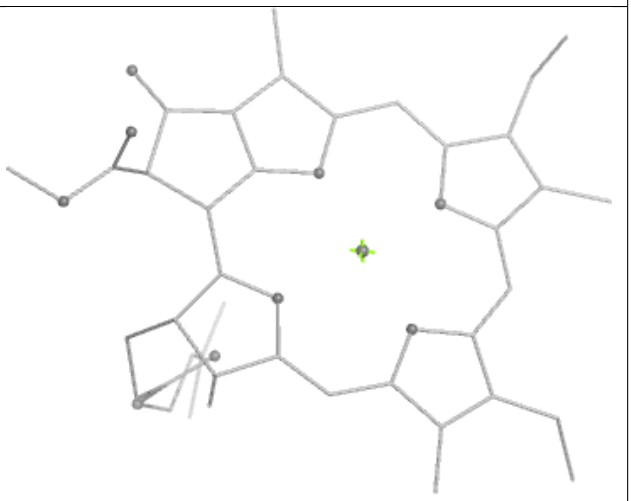
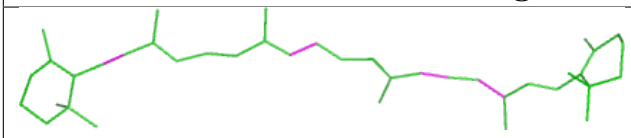


Rings

Ligand BCR A 4004



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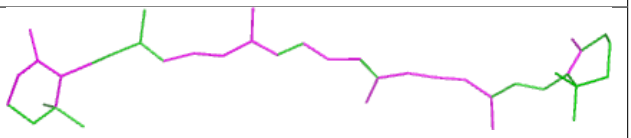

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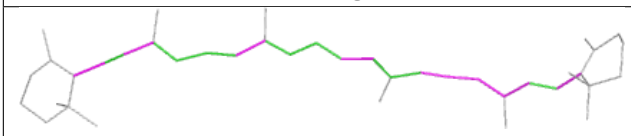

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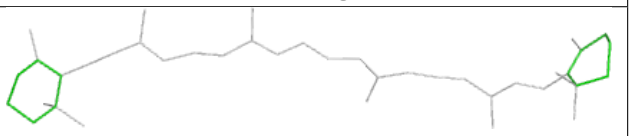
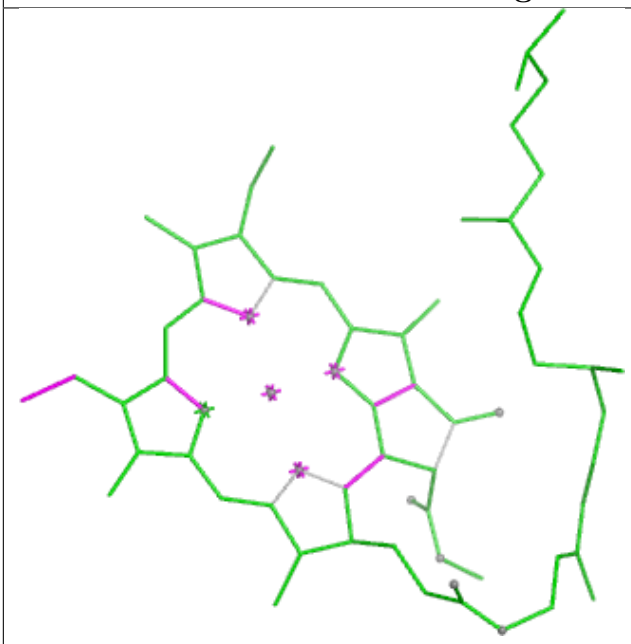


Rings

Ligand CLA A 1123



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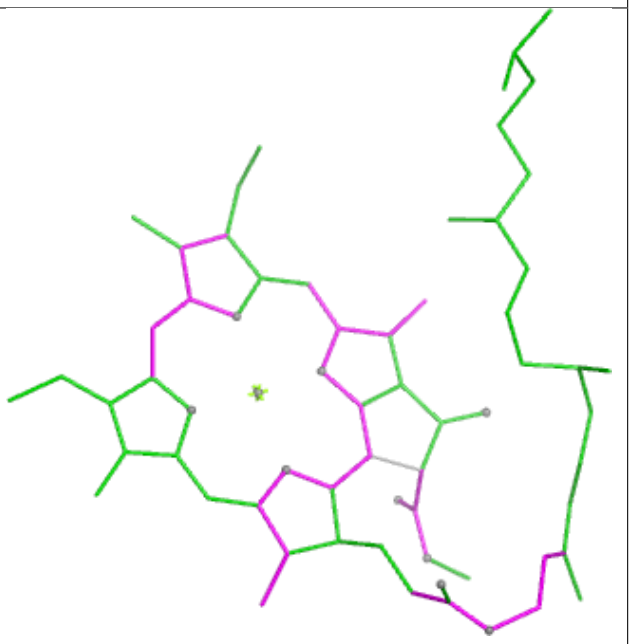
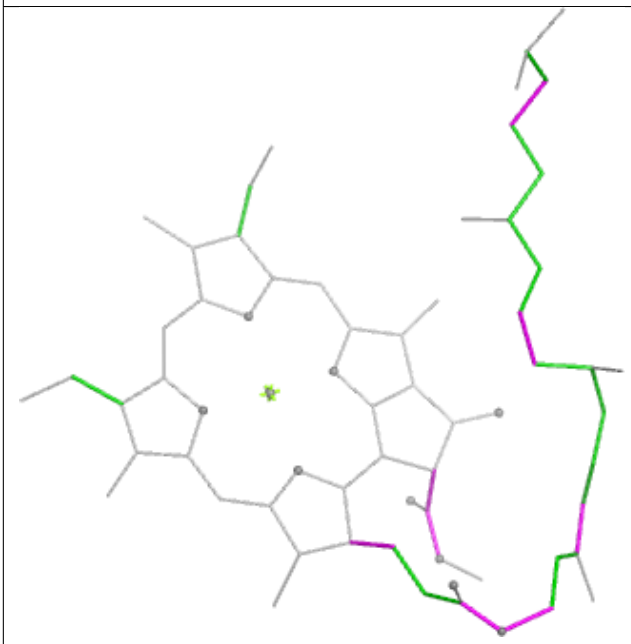


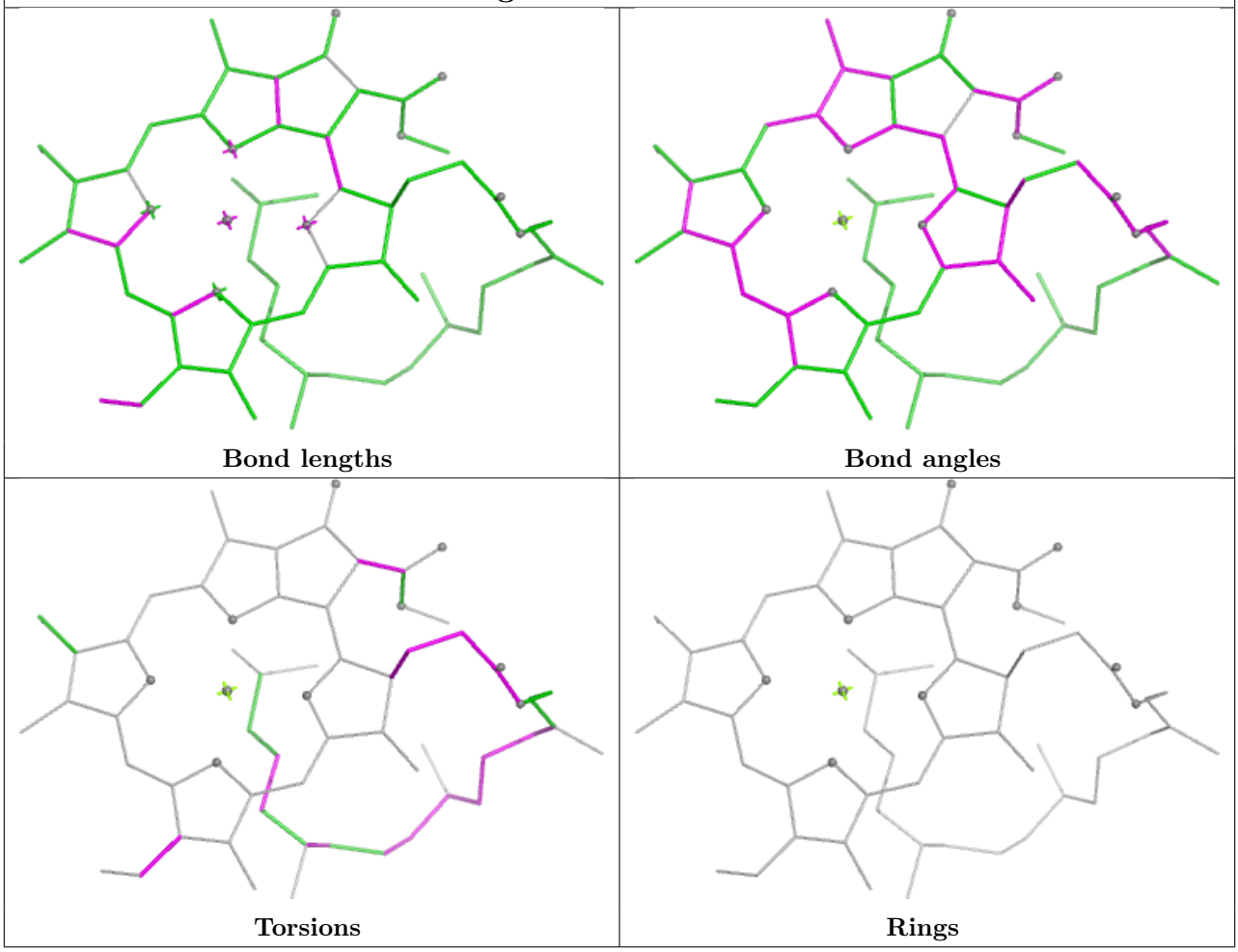
Bond angles



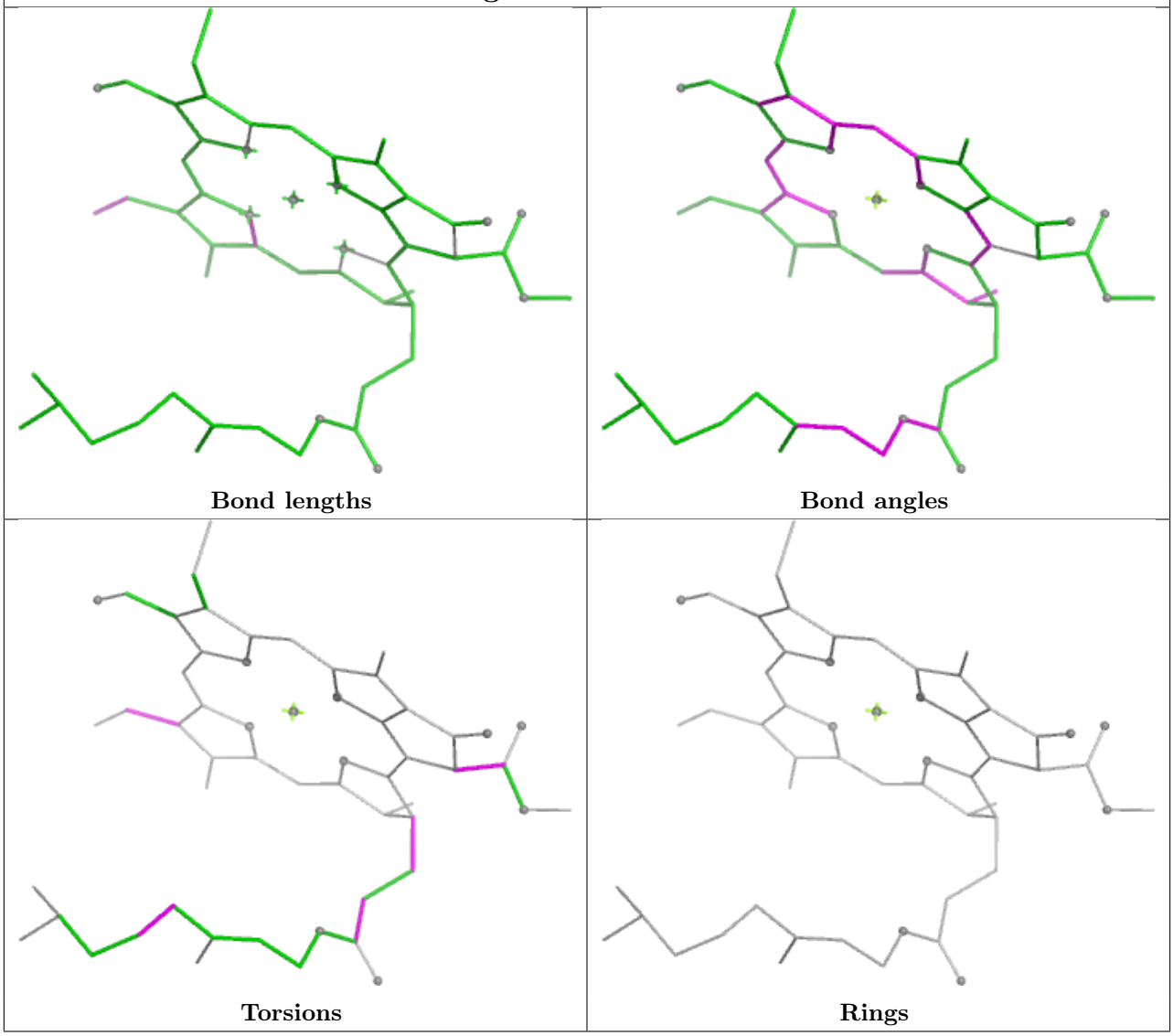
Torsions

Rings

Ligand CLA A 1104



Ligand CHL 6 610



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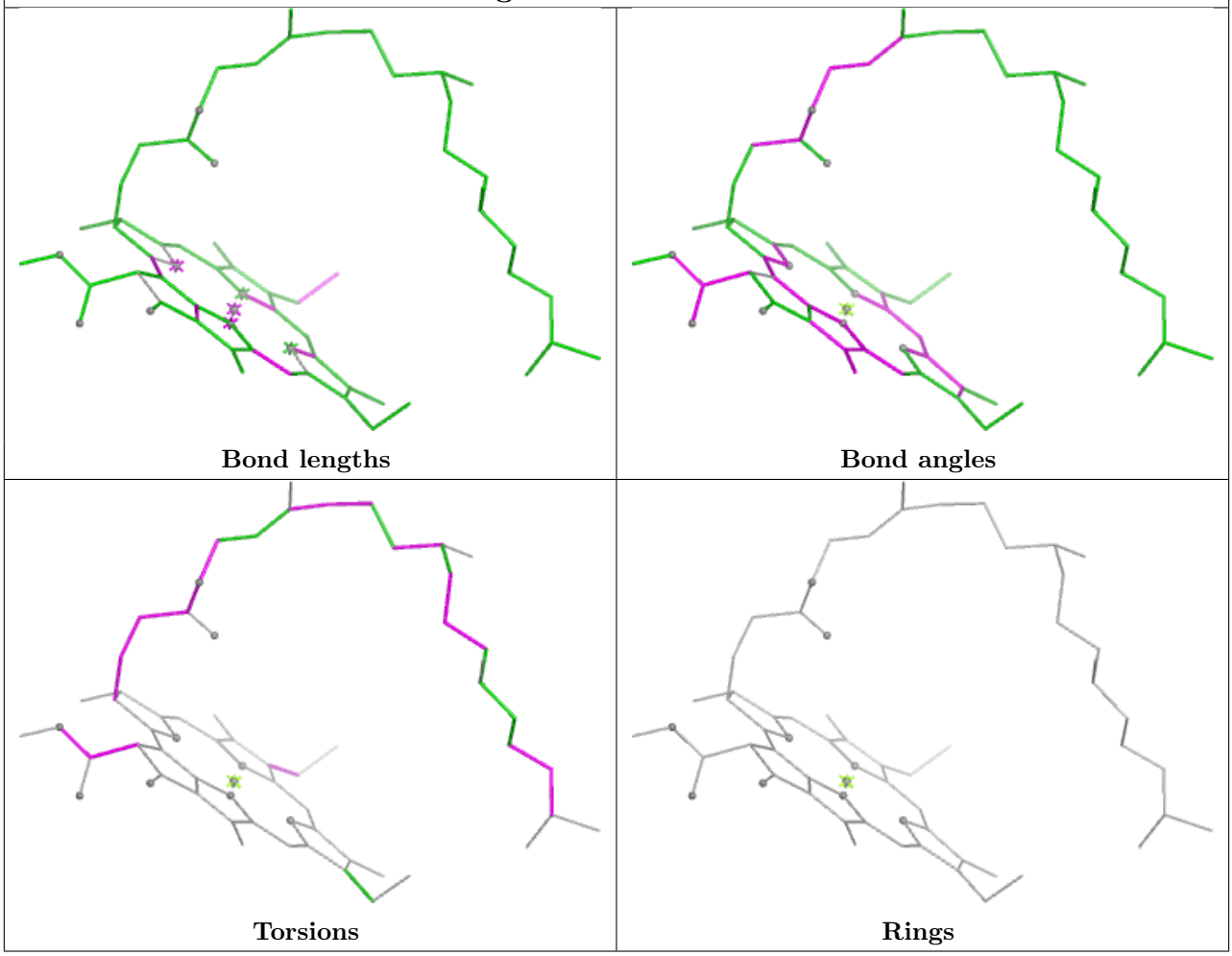

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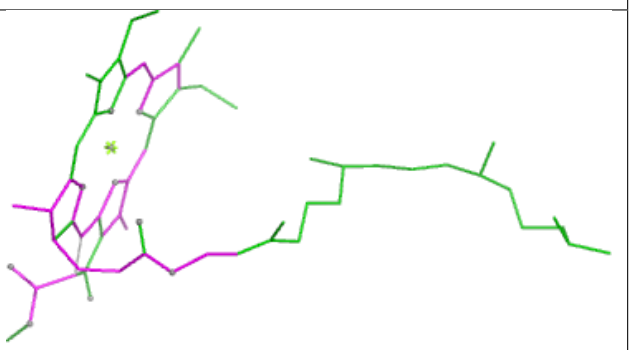
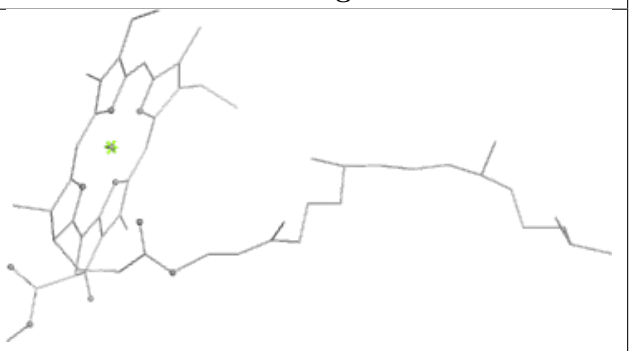
Bond lengths	 Bond angles
Torsions	 Rings

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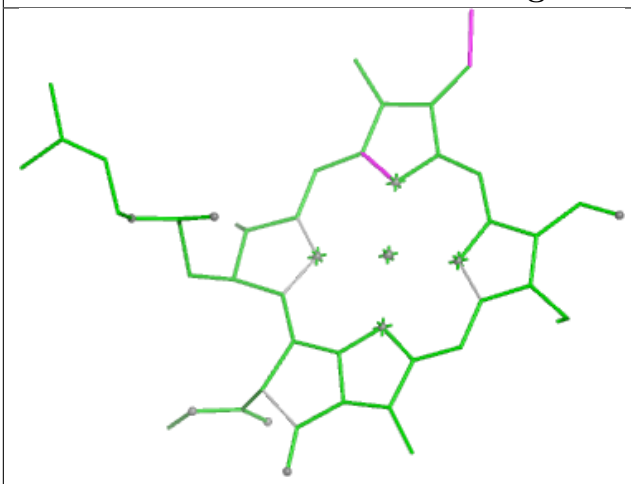

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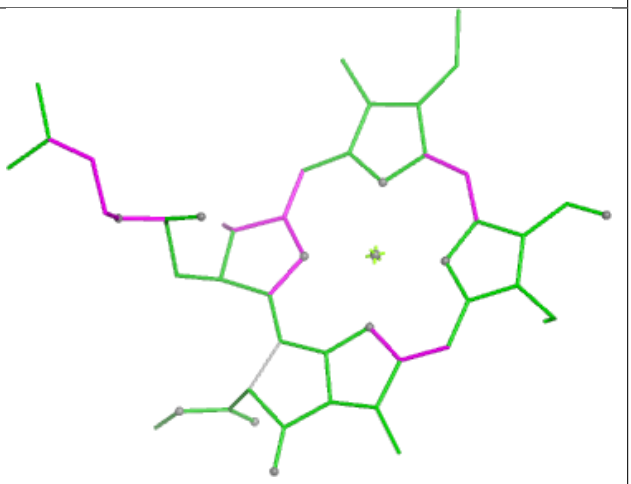

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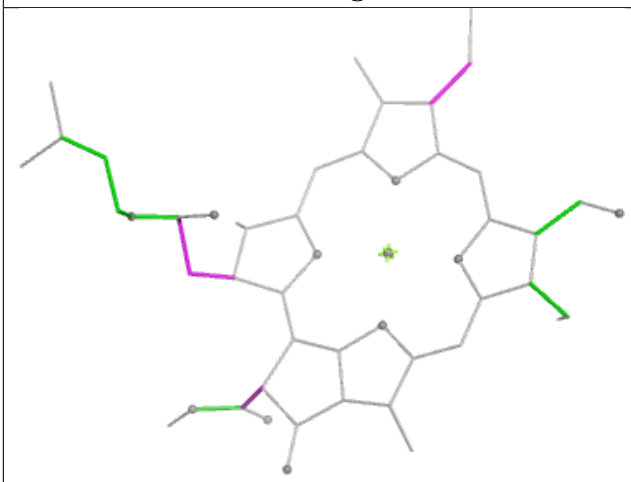

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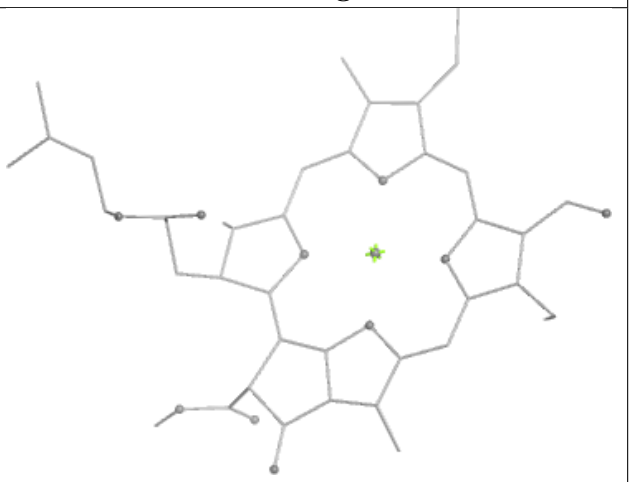
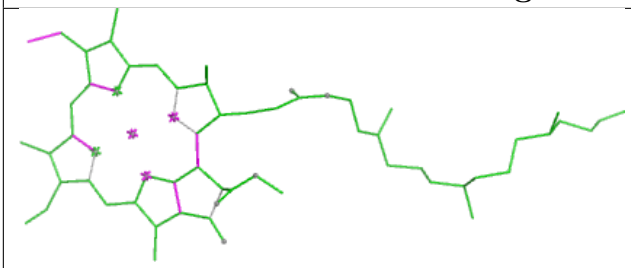


Rings

Ligand CLA A 1140



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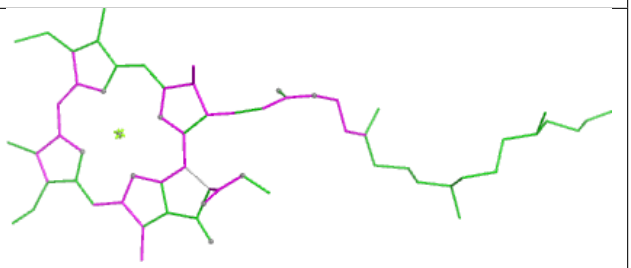

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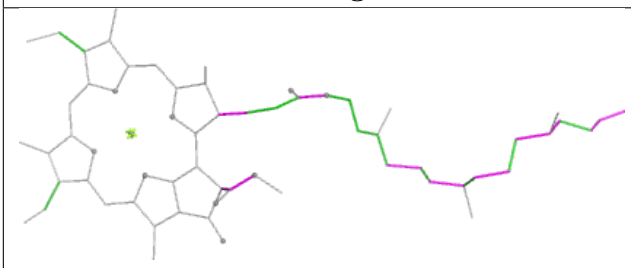

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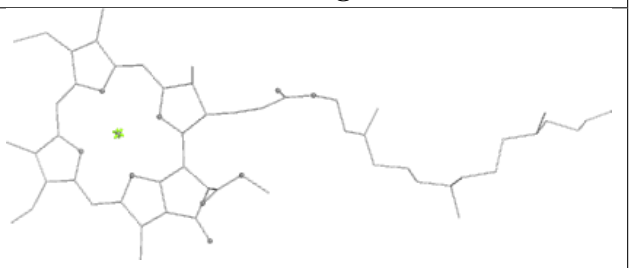
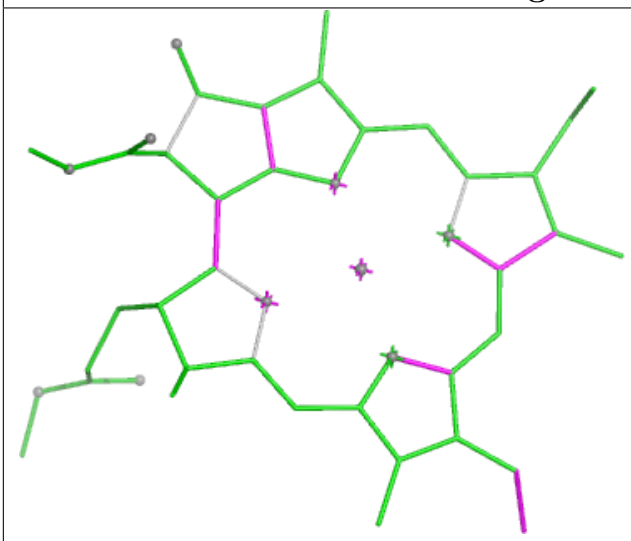


Rings

Ligand CLA 8 612



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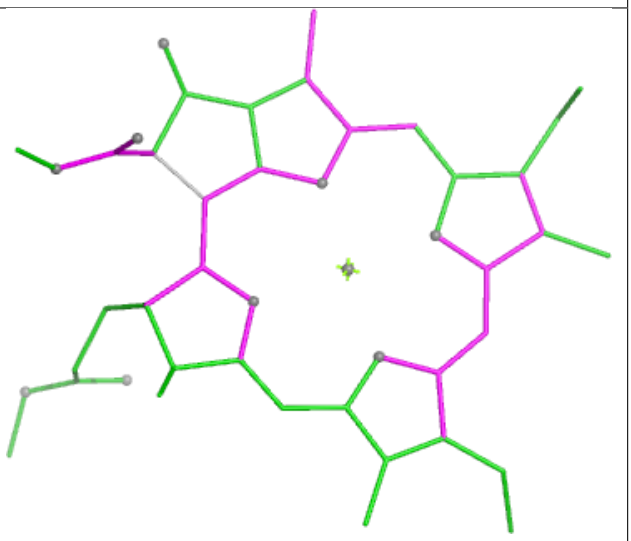
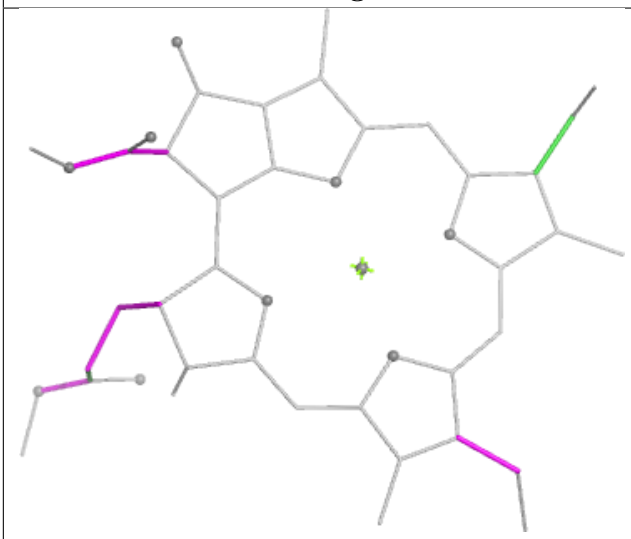


Bond angles



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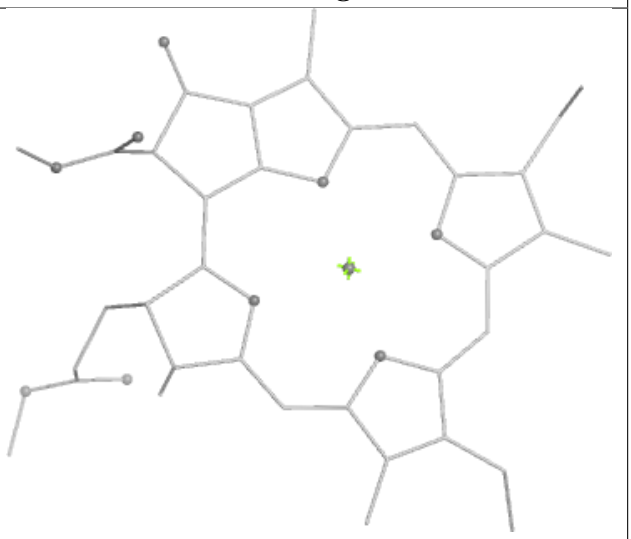
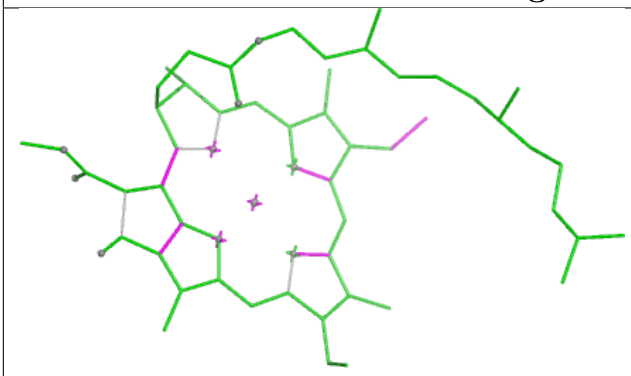


Rings

Ligand CLA 8 601



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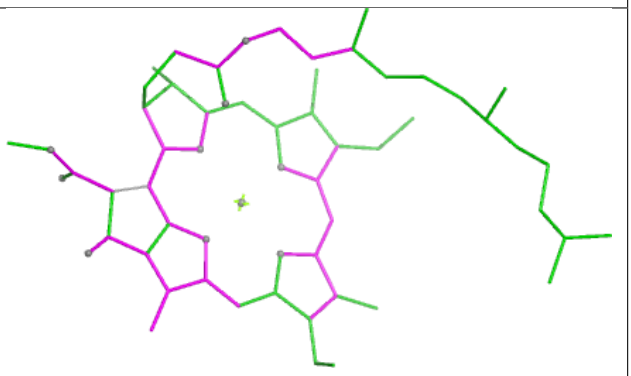
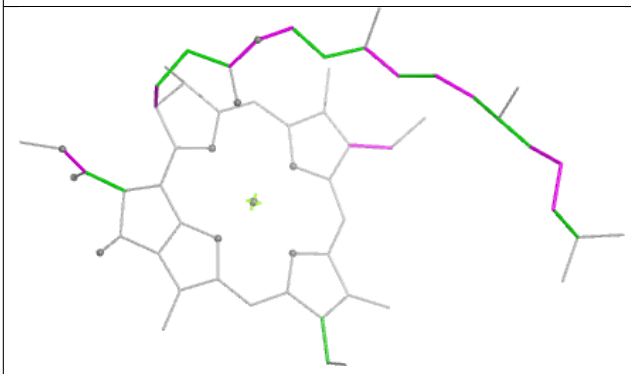


Bond angles



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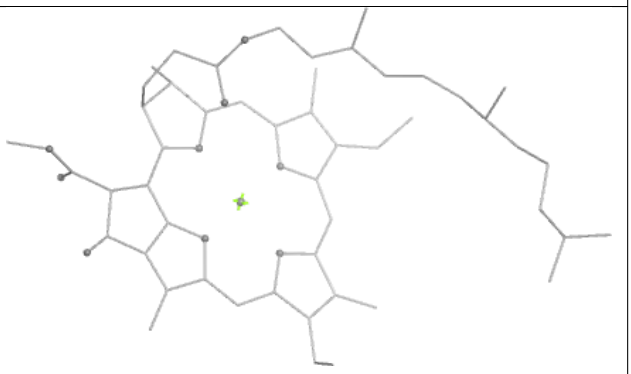
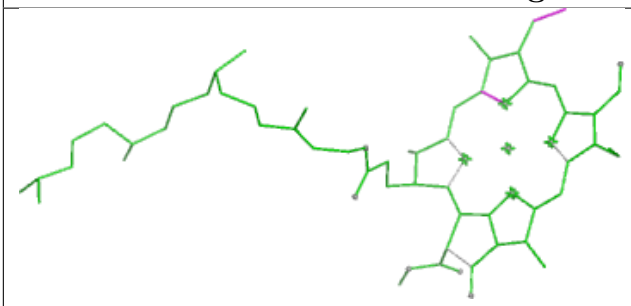


Rings

Ligand CHL 3 611



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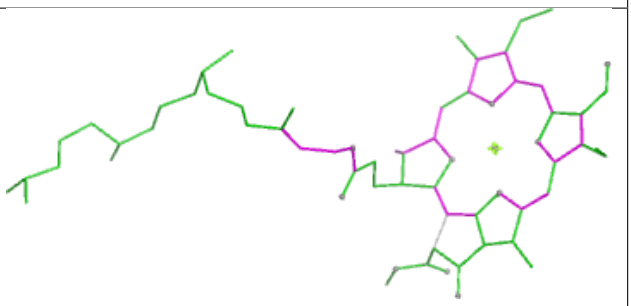
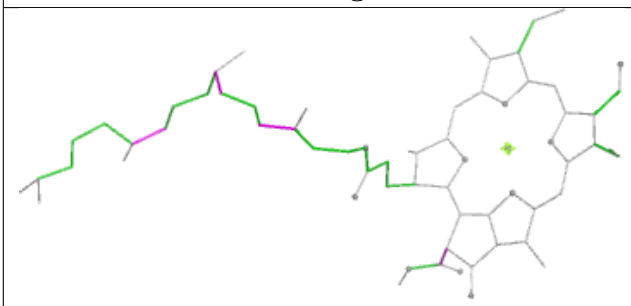
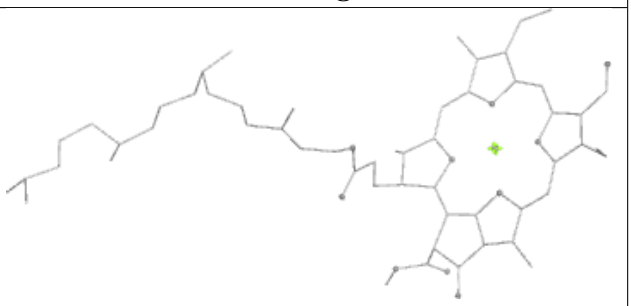


Bond angles



Torsions



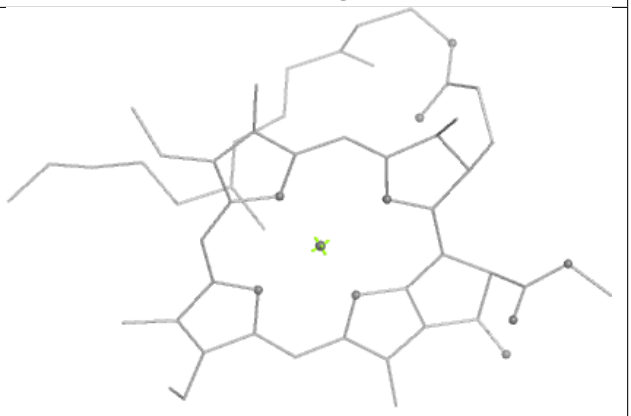
Rings

Ligand CLA B 1214

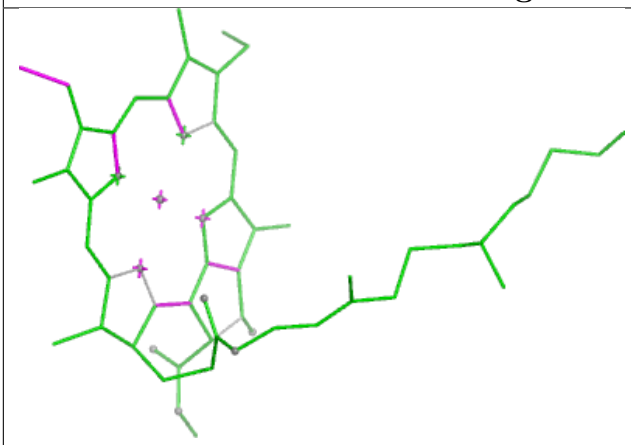
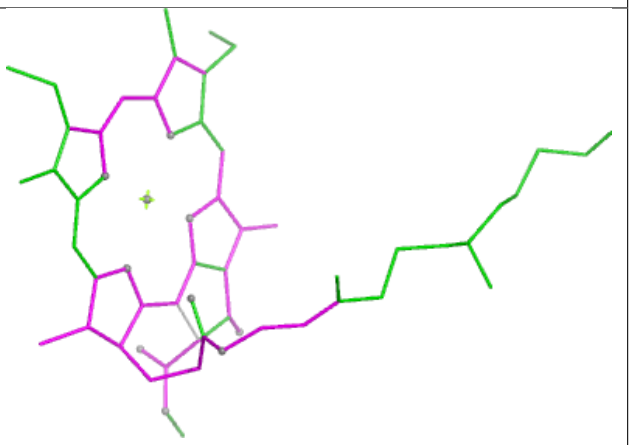
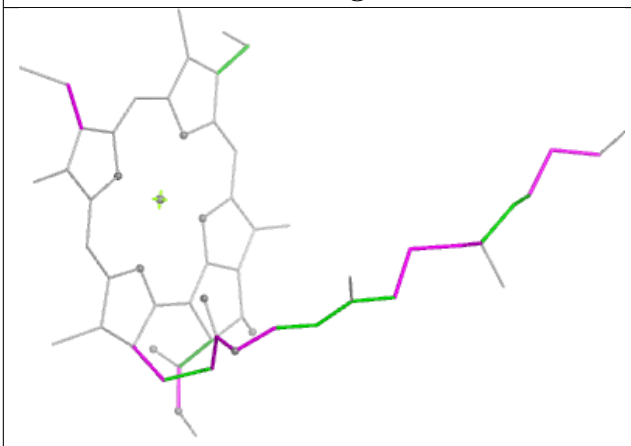
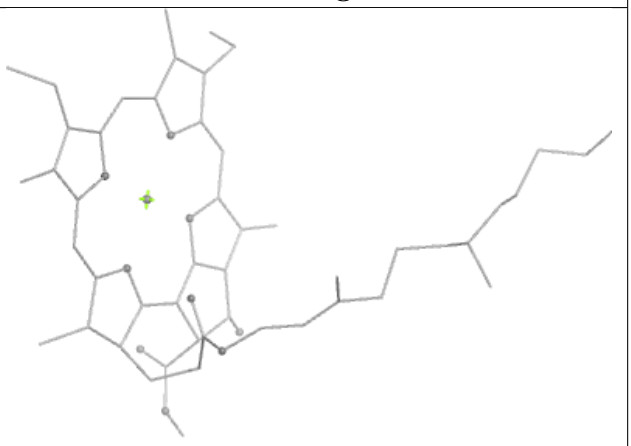
Bond lengths

Bond angles

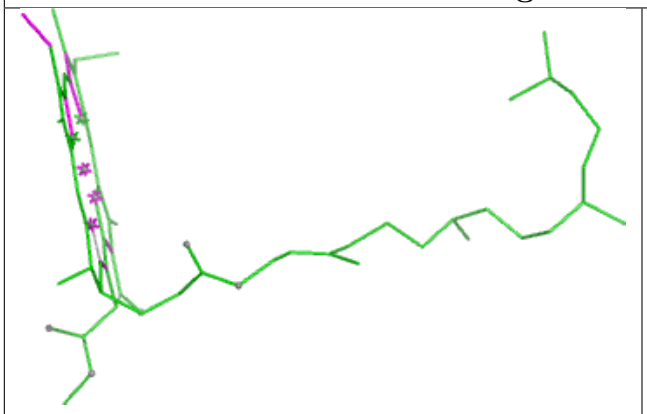
Torsions



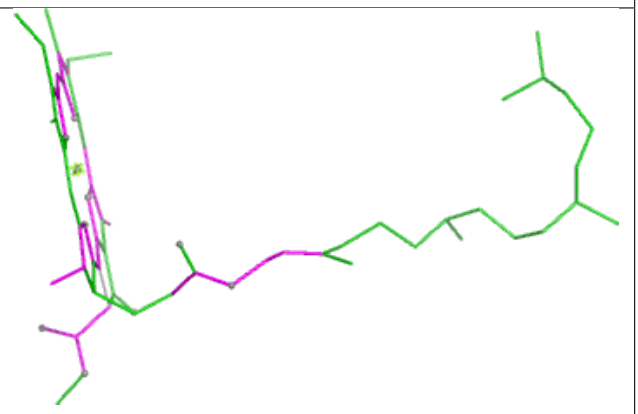
Rings

Ligand CLA B 1219	
 Bond lengths	 Bond angles
 Torsions	 Rings

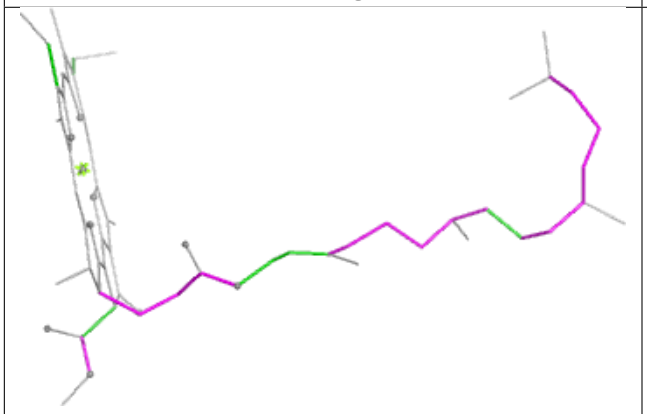
Ligand CLA B 1236



Bond lengths



Bond angles



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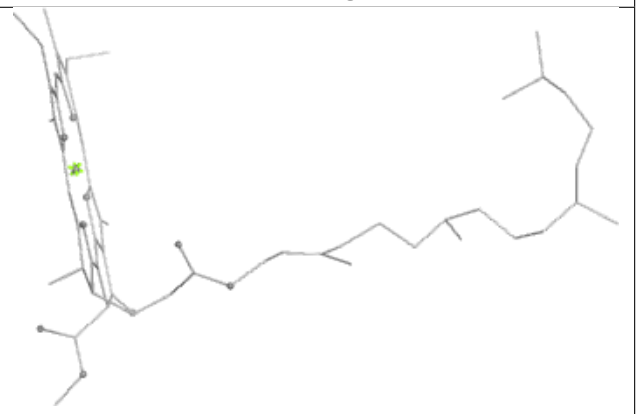
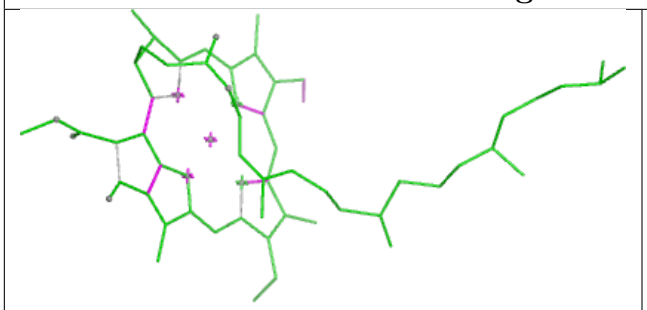


Rings

Ligand CLA A 1139



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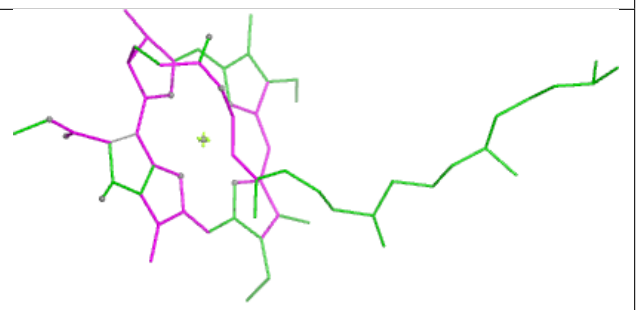
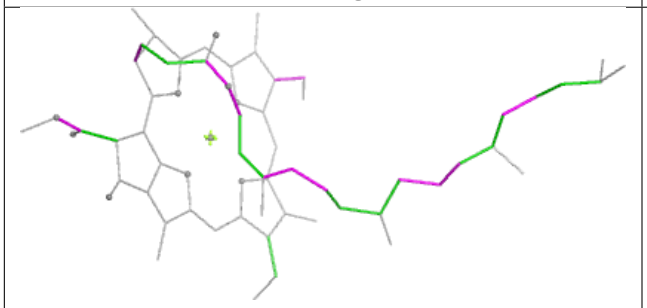
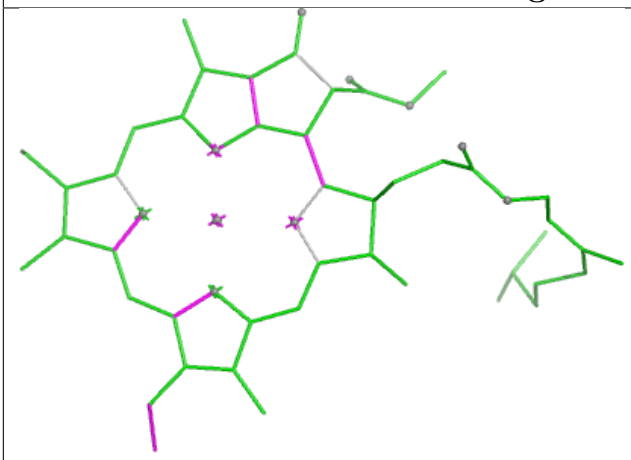
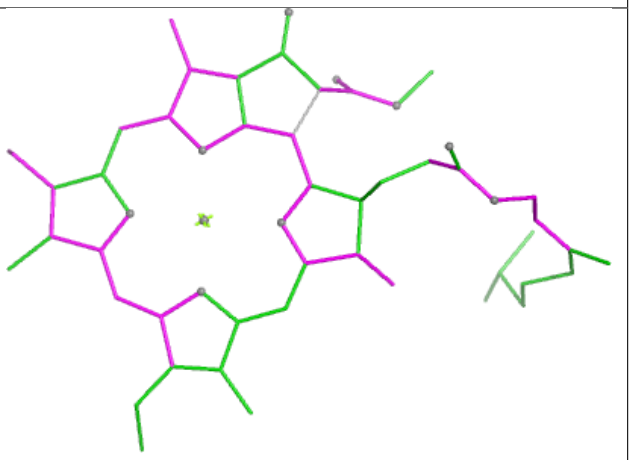
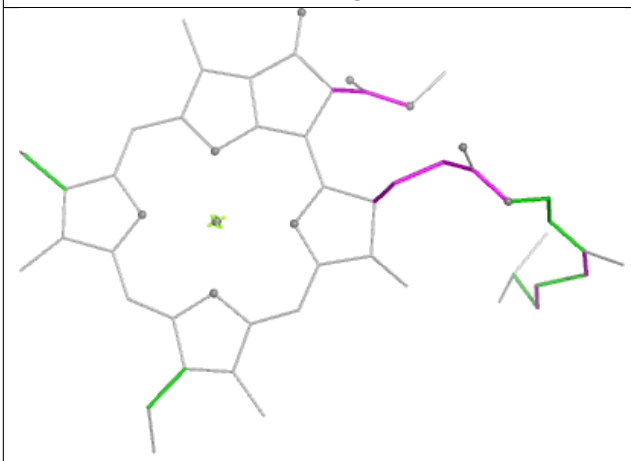
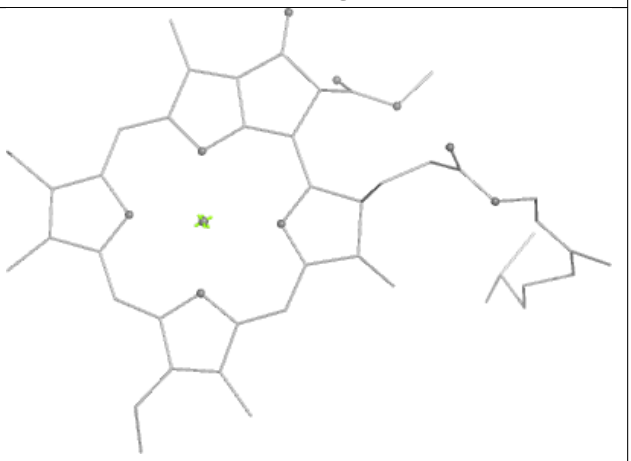


Bond angles

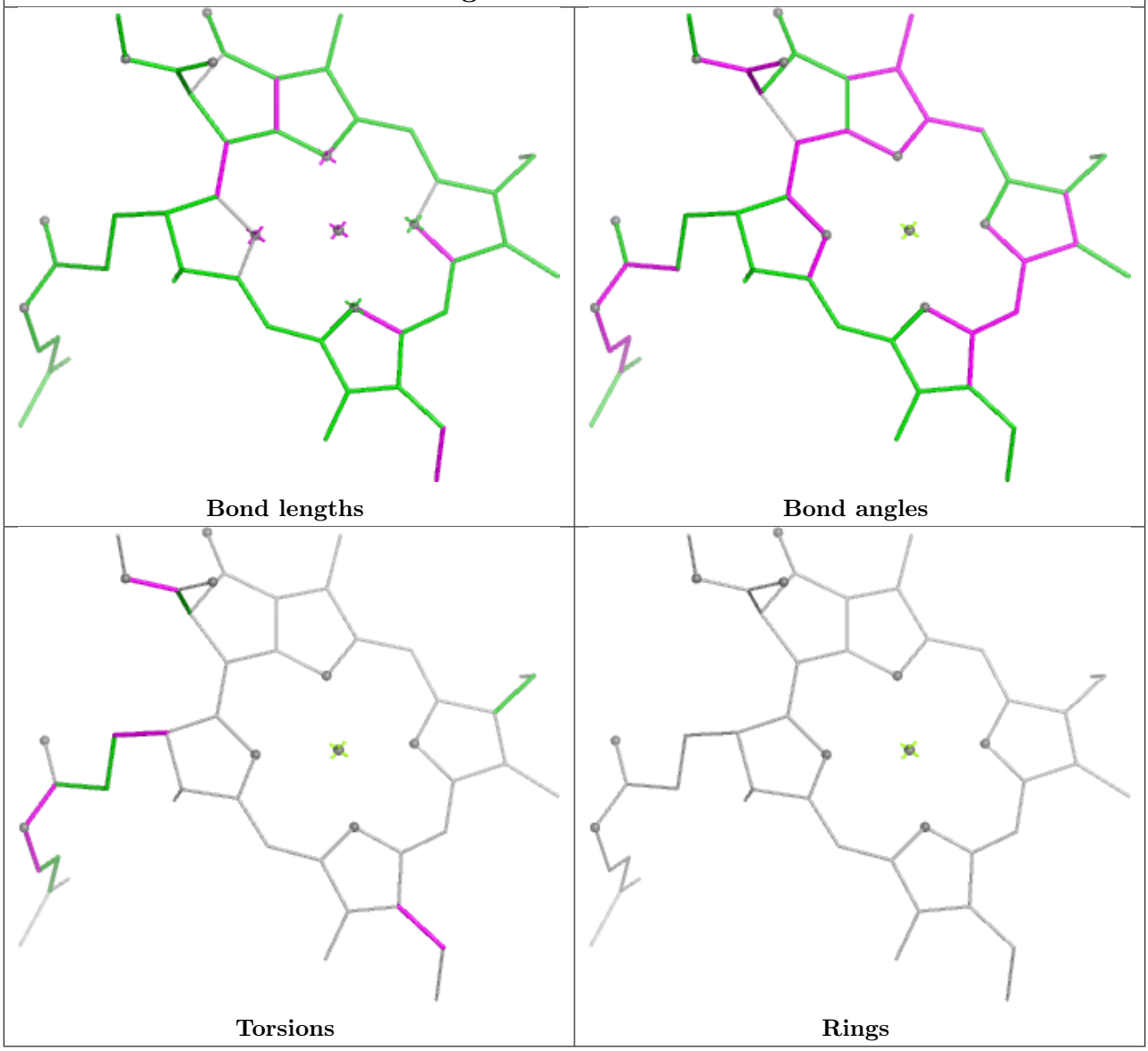


Torsions

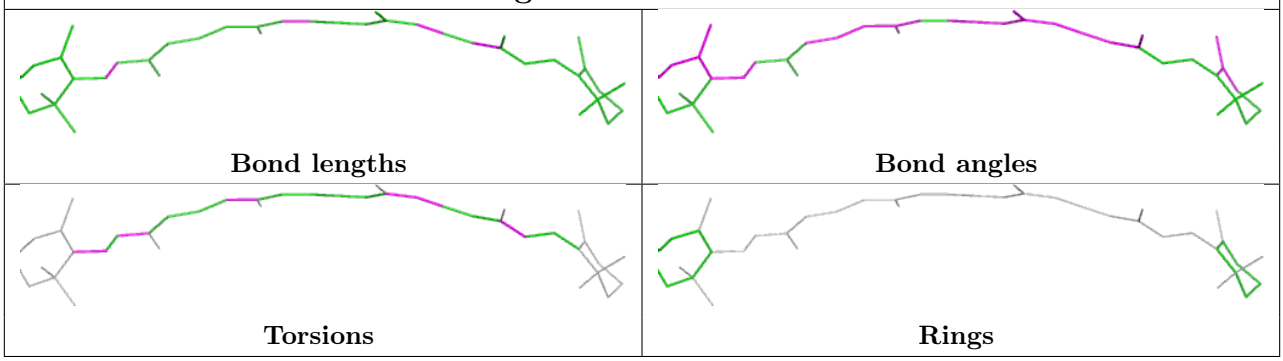
Rings

Ligand CLA 5 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1129



Ligand BCR B 4006



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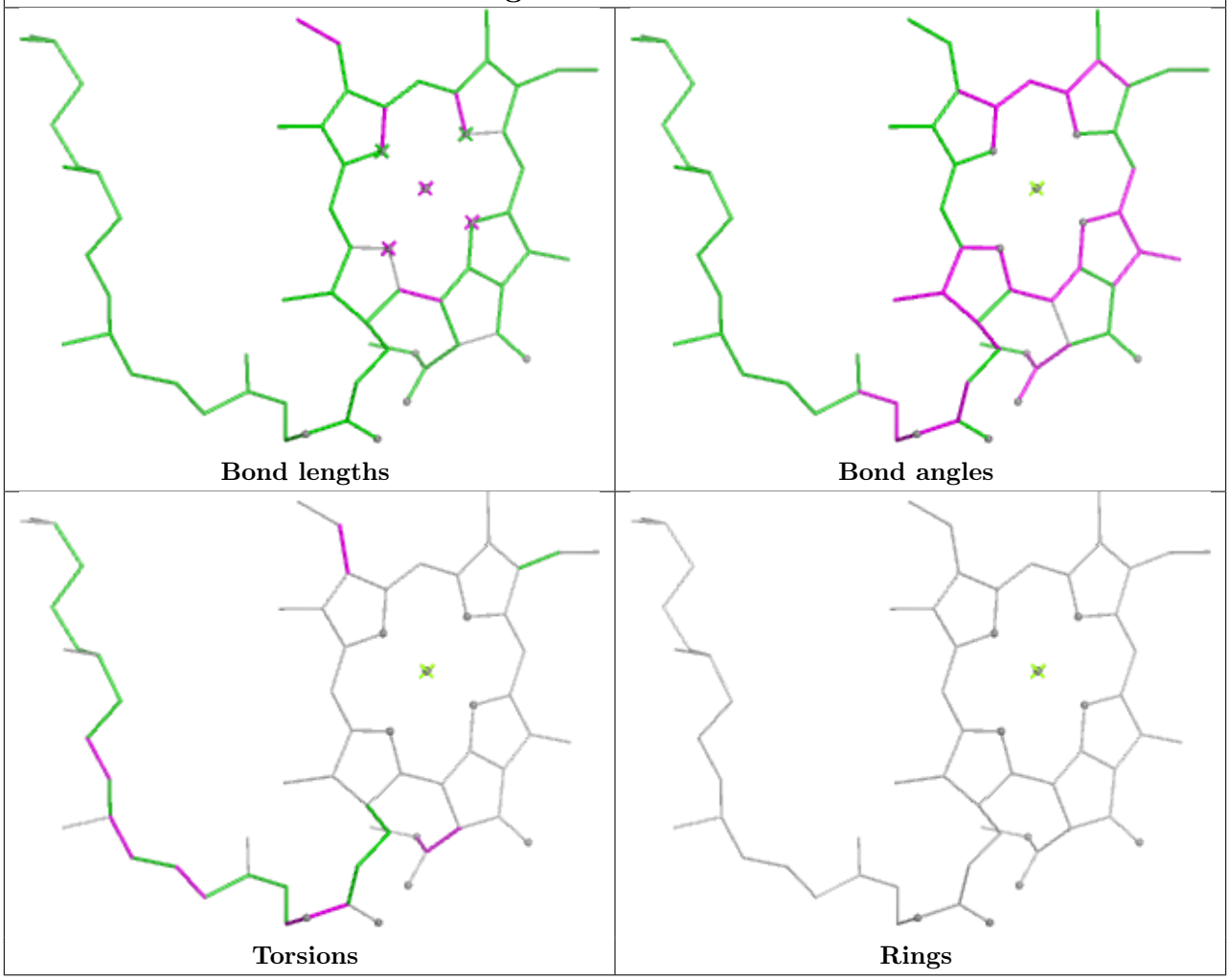

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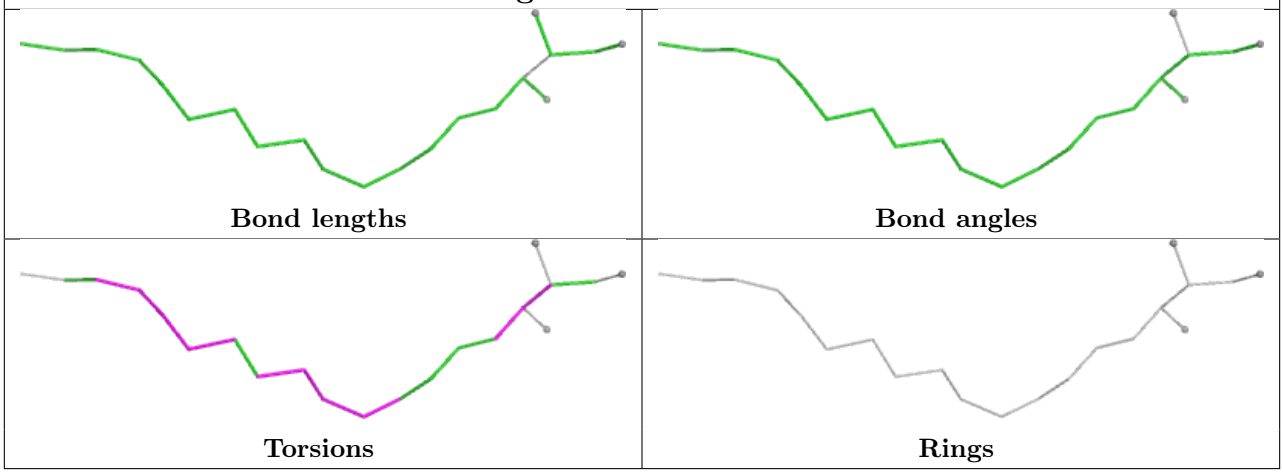

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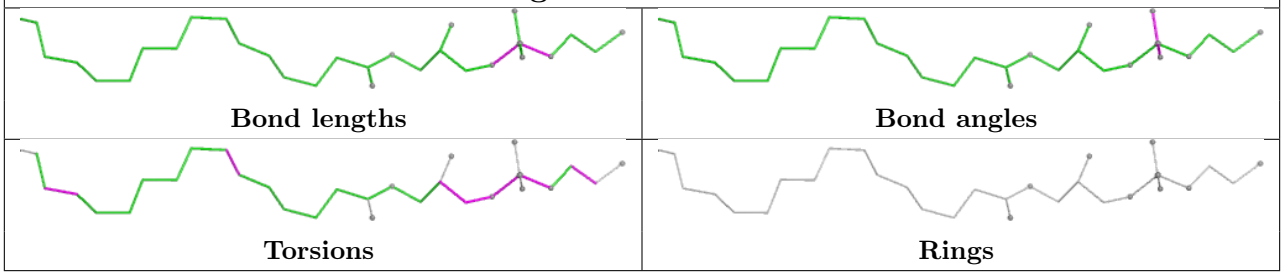

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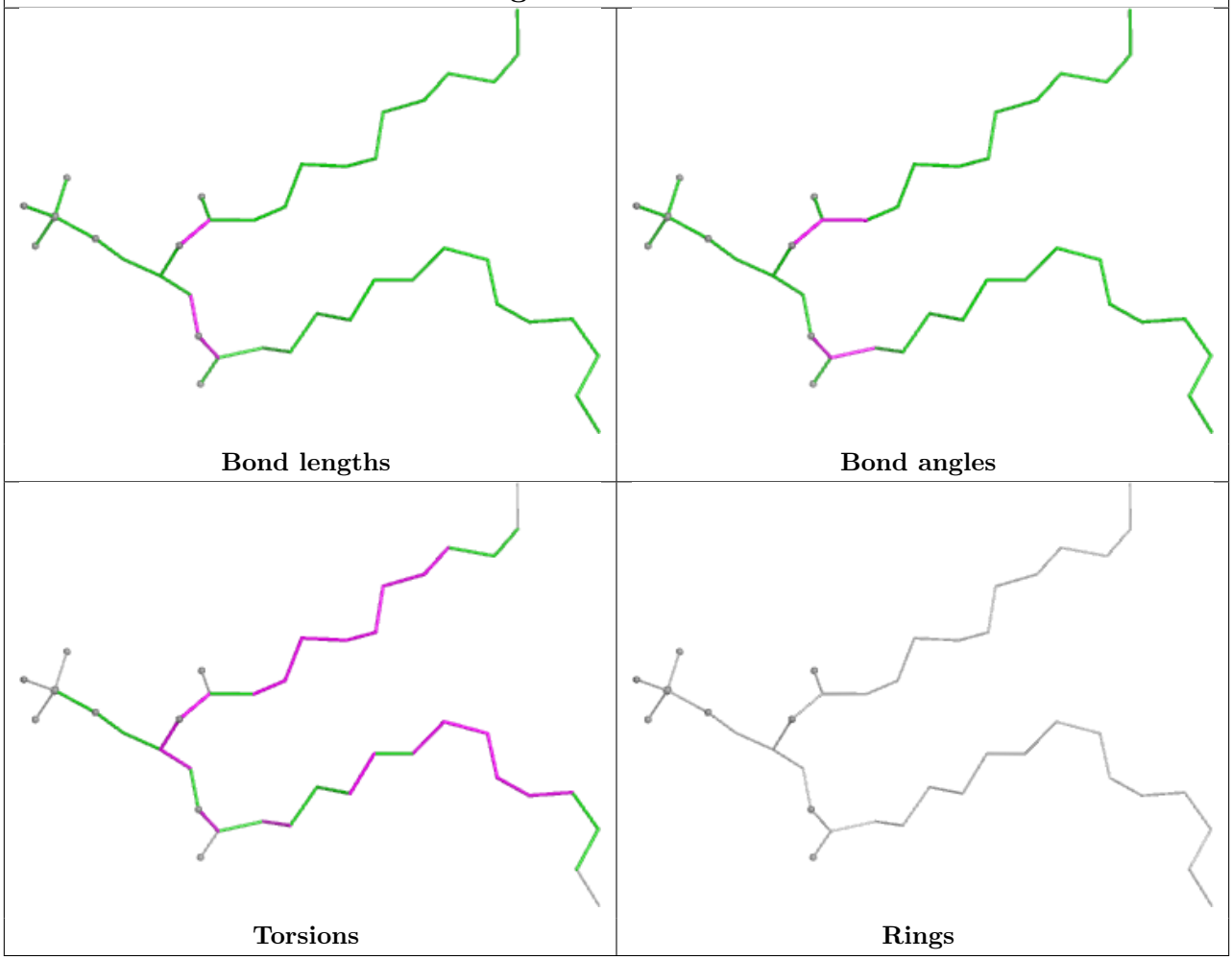

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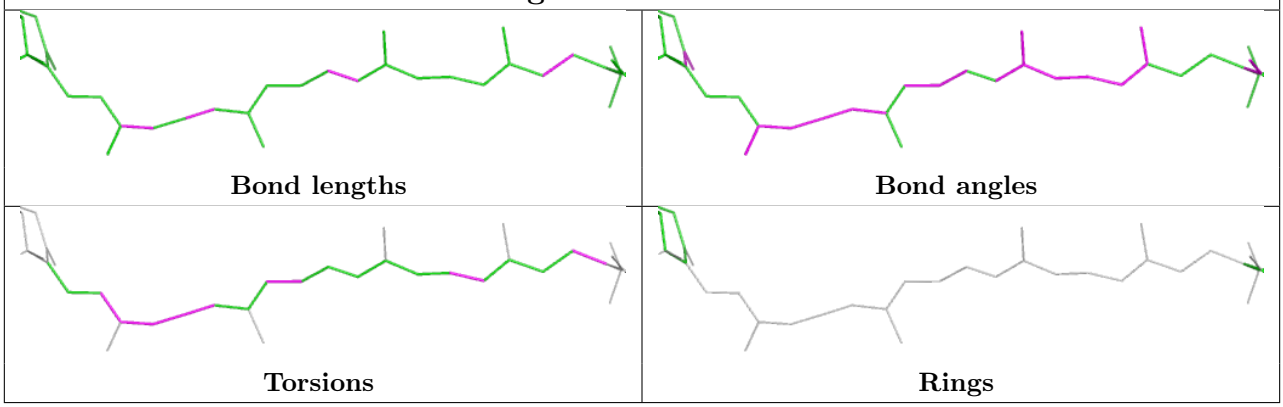

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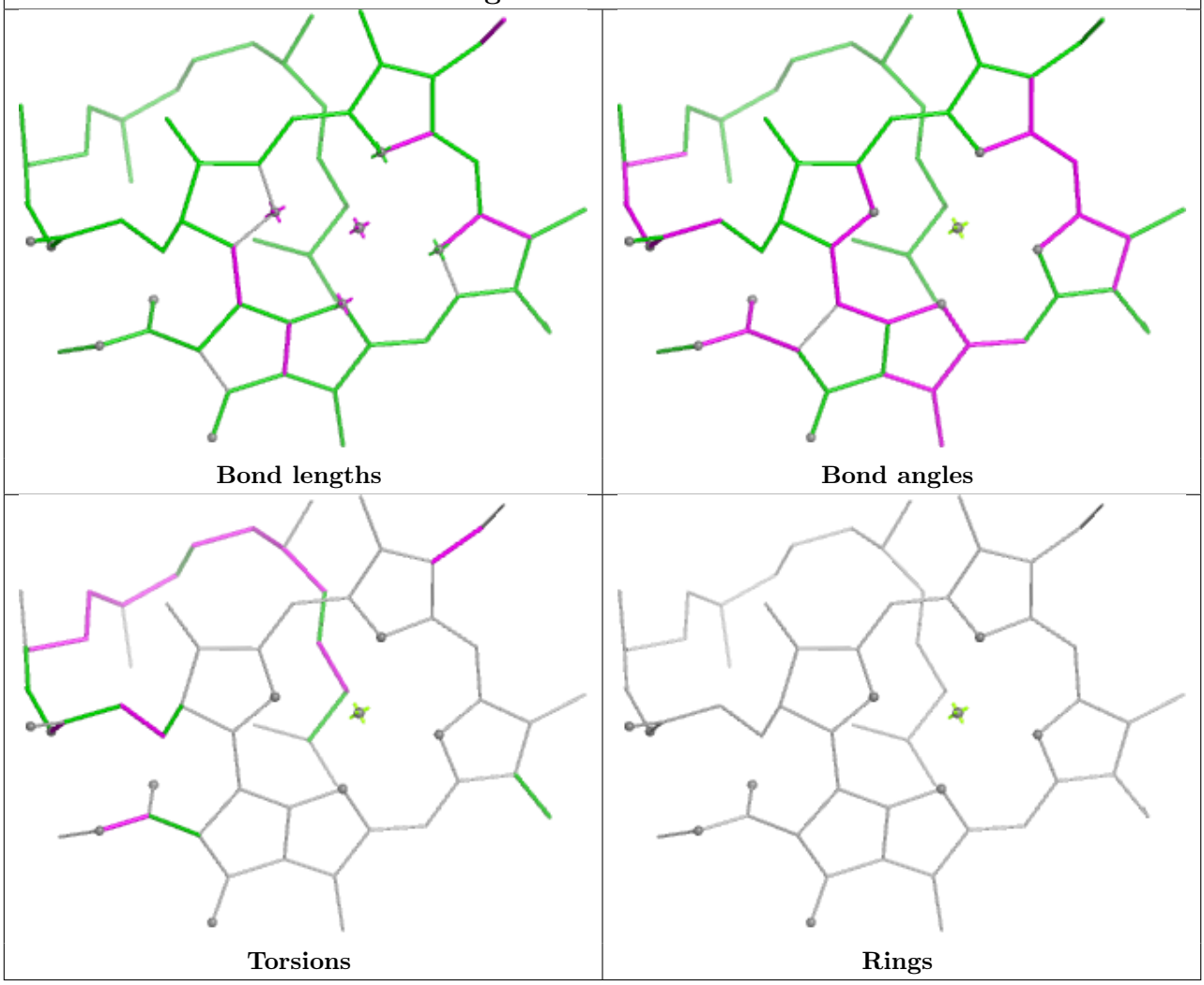

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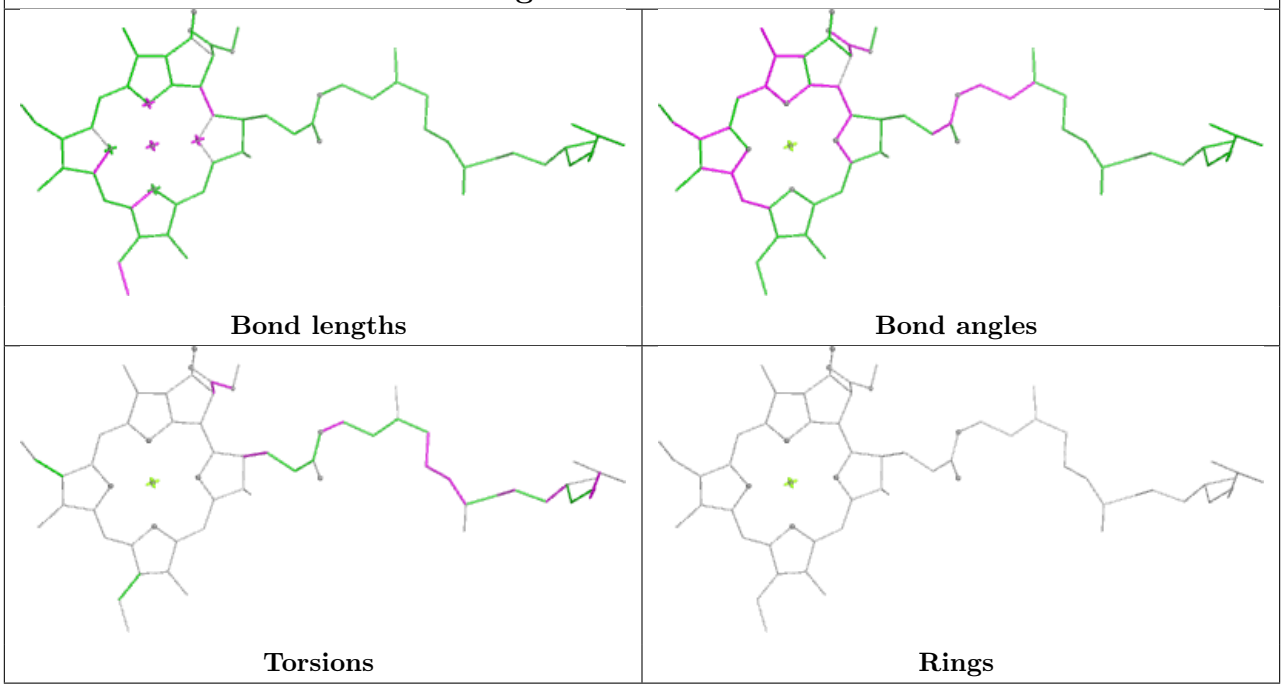

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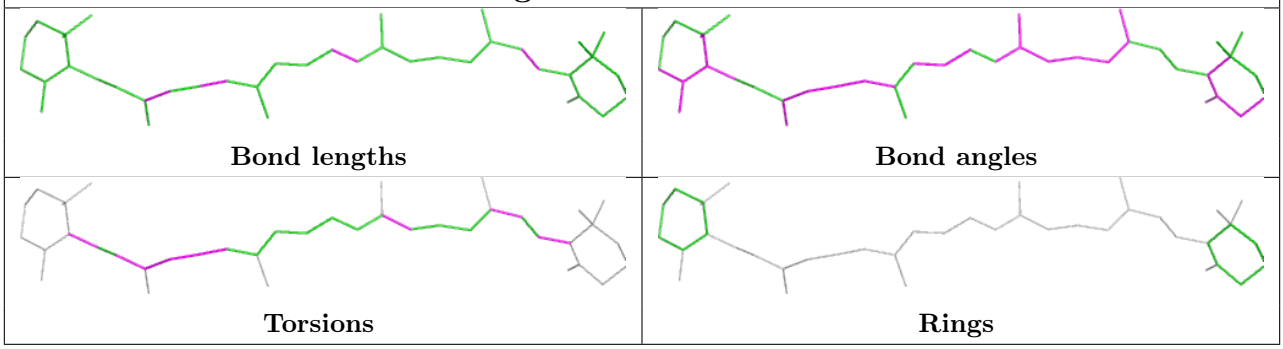

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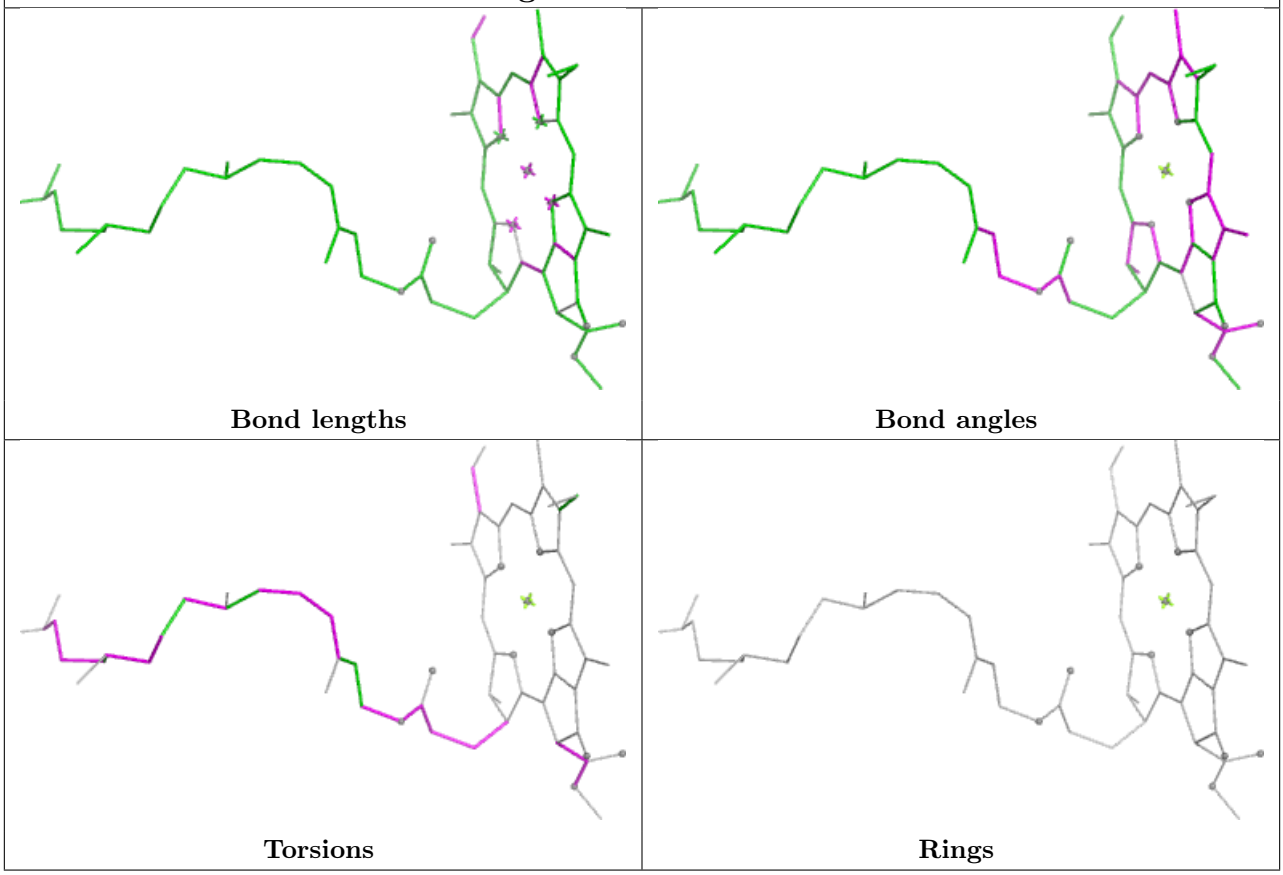

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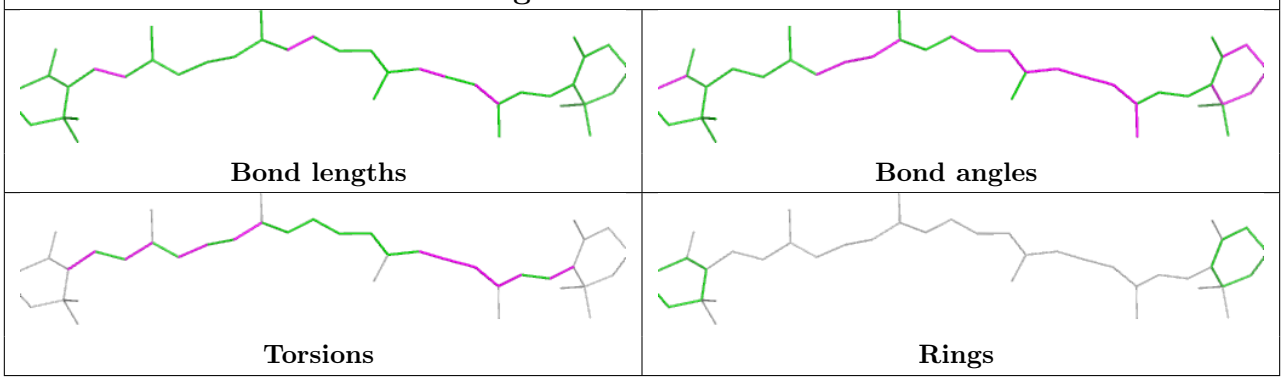

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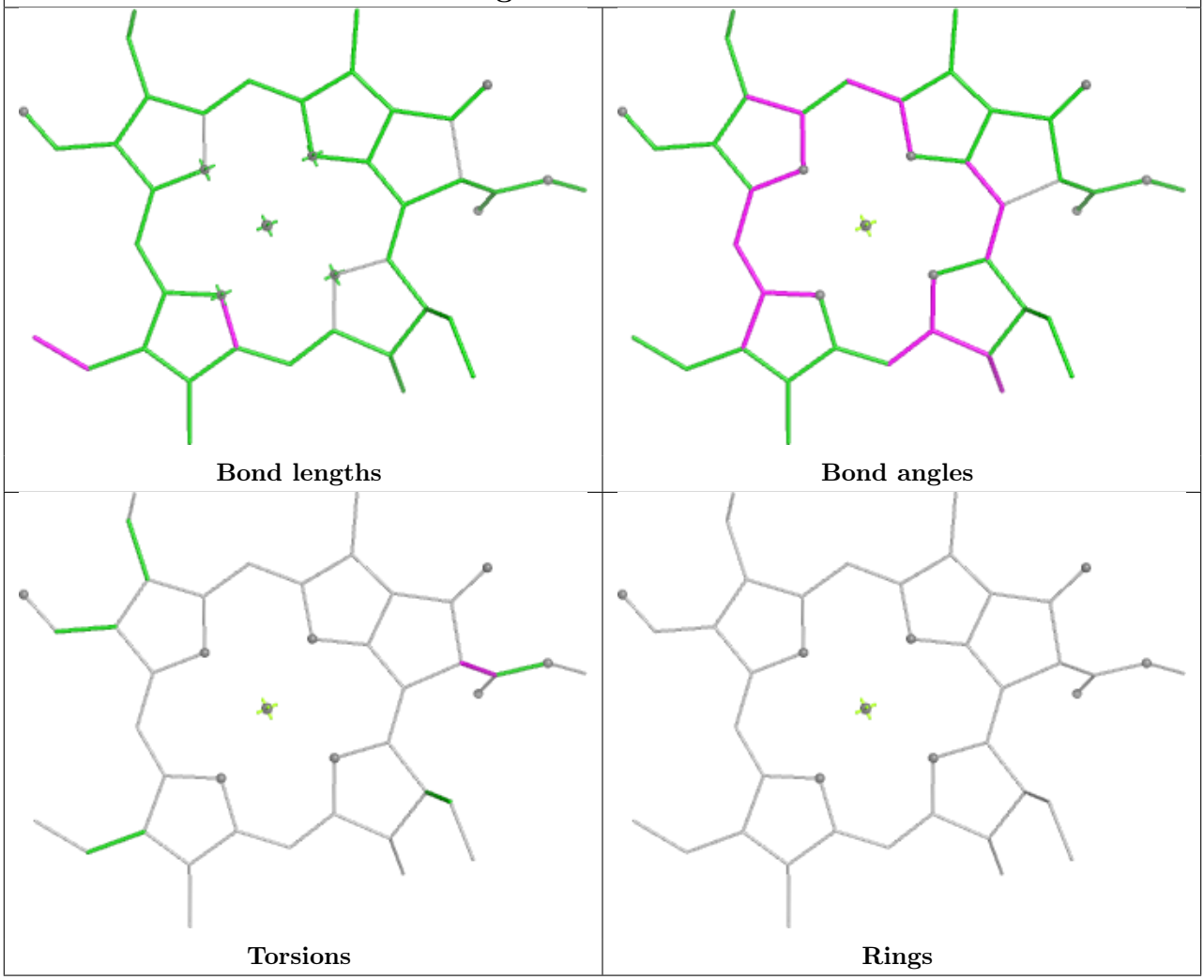

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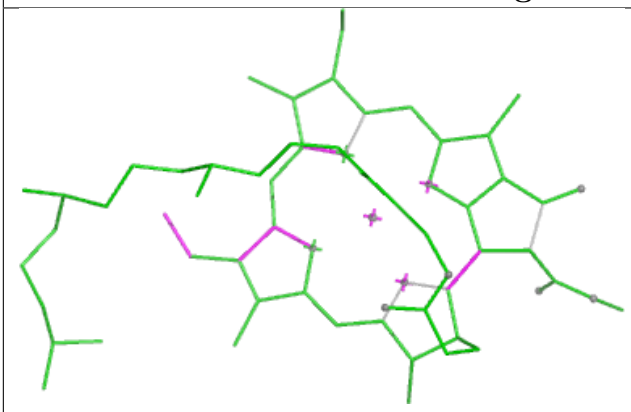
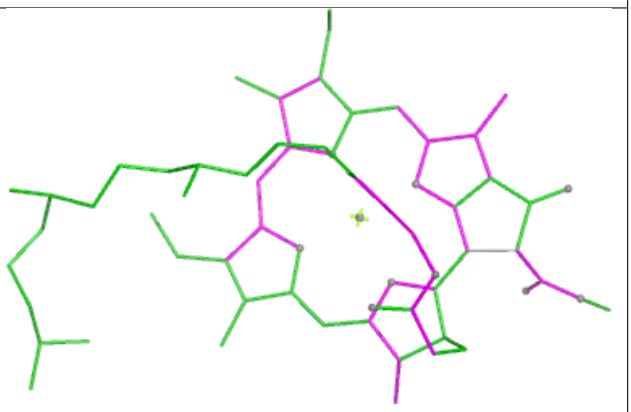
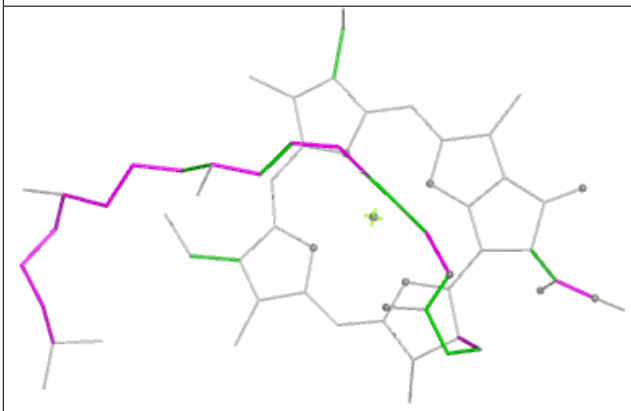
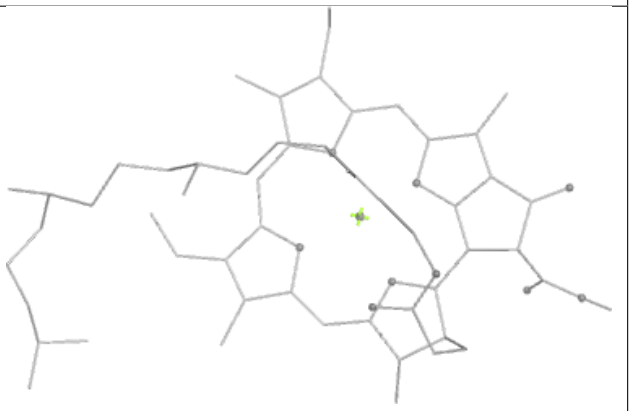
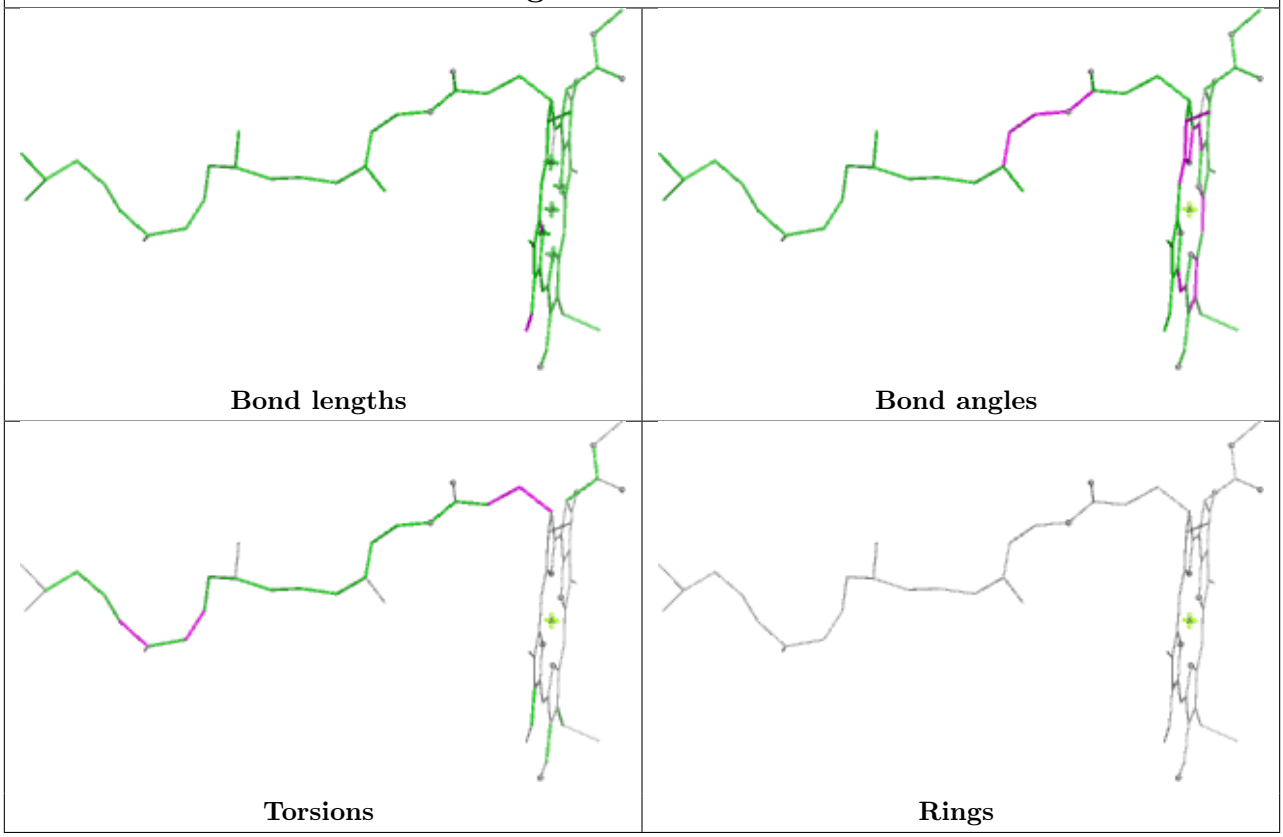
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Z 610



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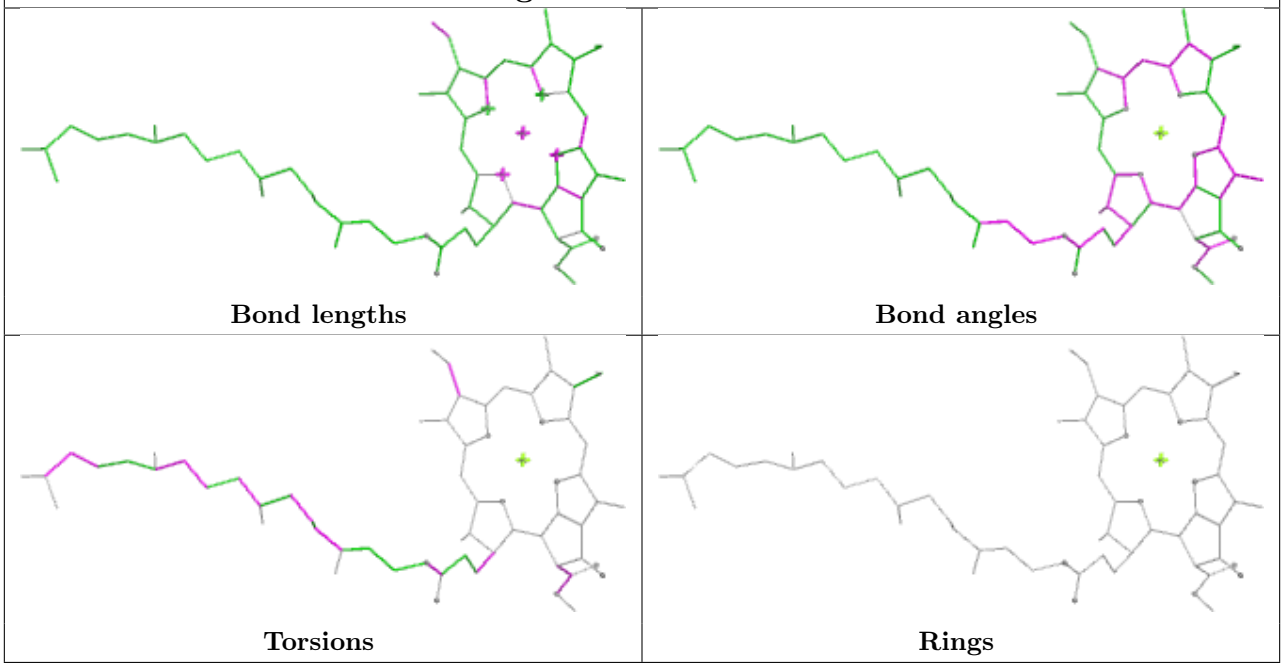
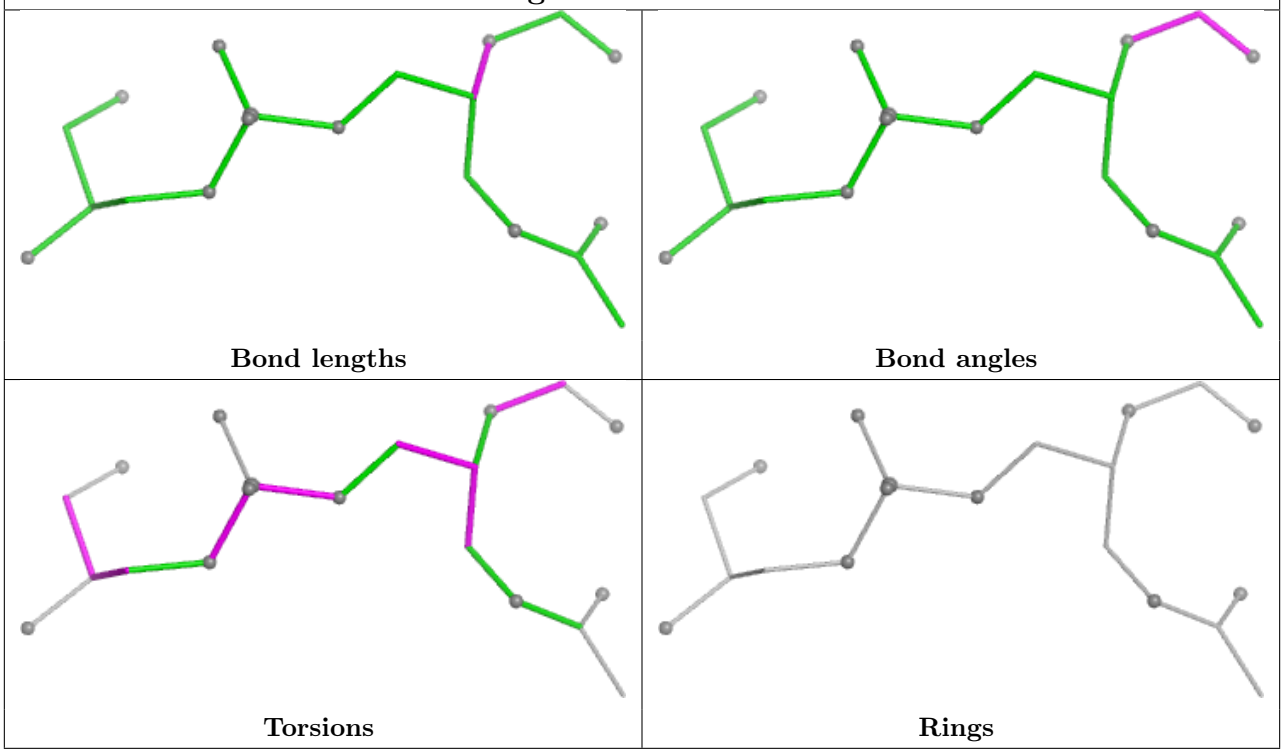
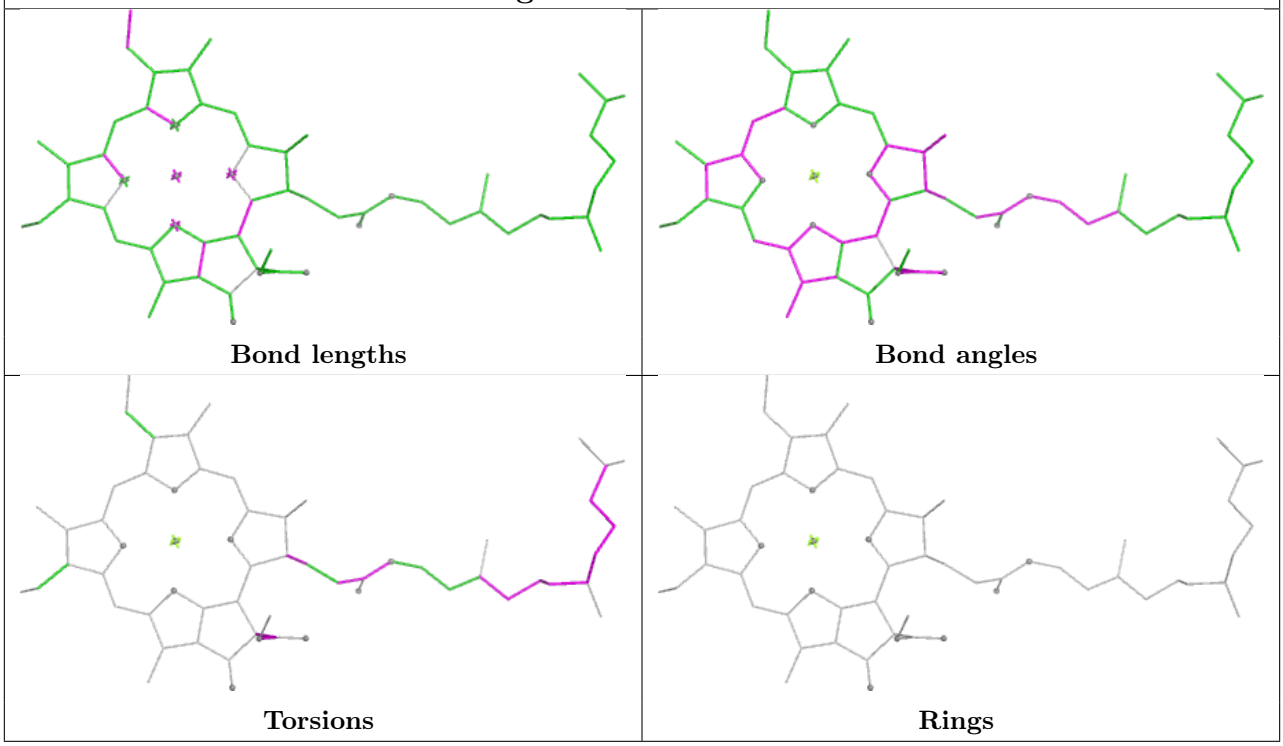


Ligand LHG 3 801



Ligand CLA B 1234



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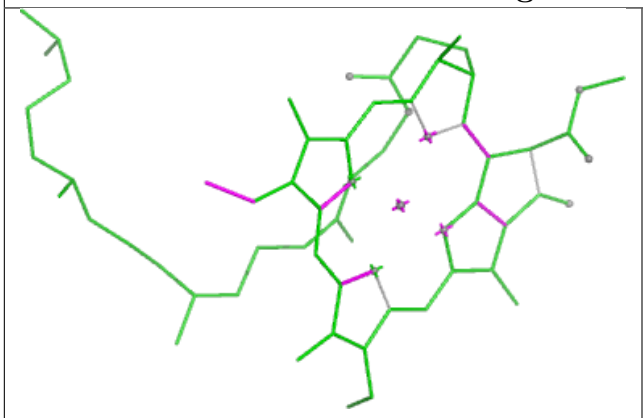
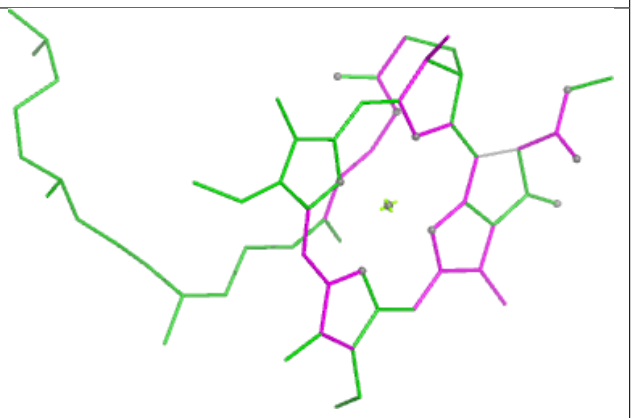
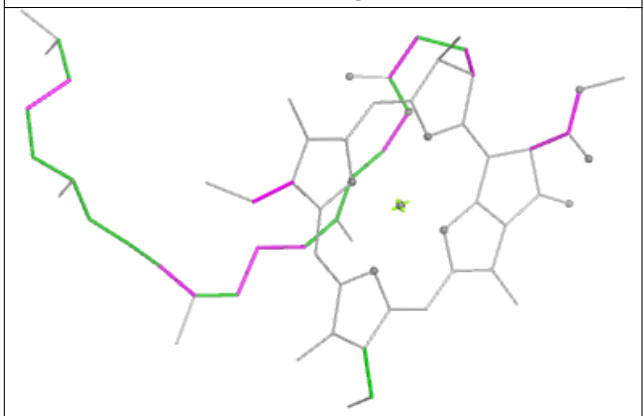
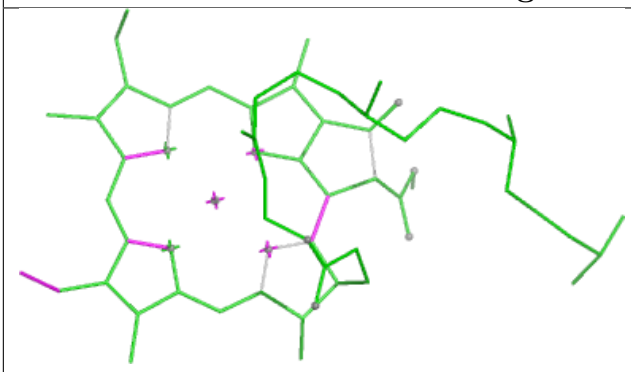
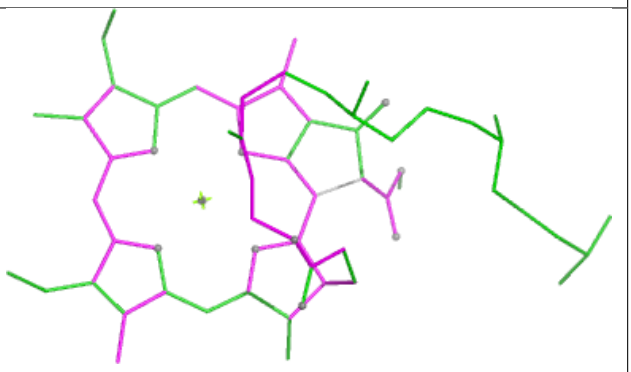
 Bond lengths	 Bond angles
 Torsions	Rings

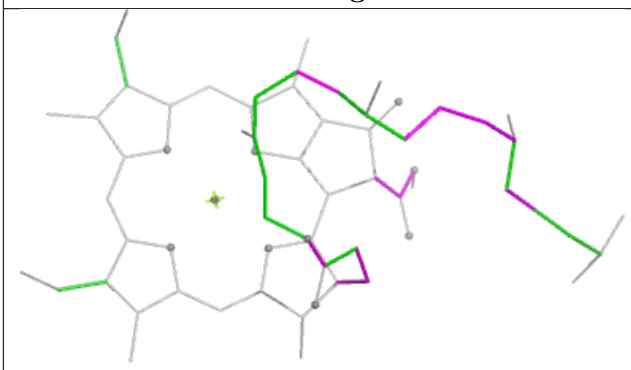
Ligand CLA F 1301



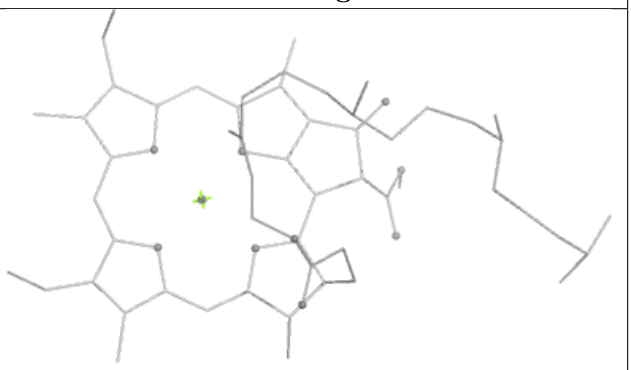
Bond lengths



Bond angles

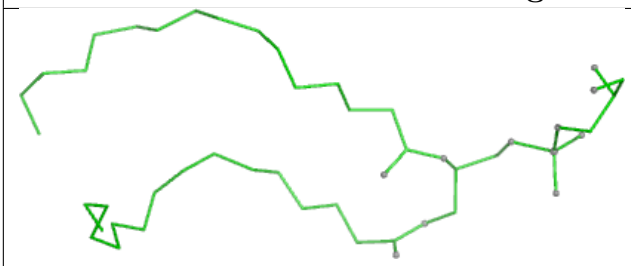


Torsions



Rings

Ligand LHG 4 801



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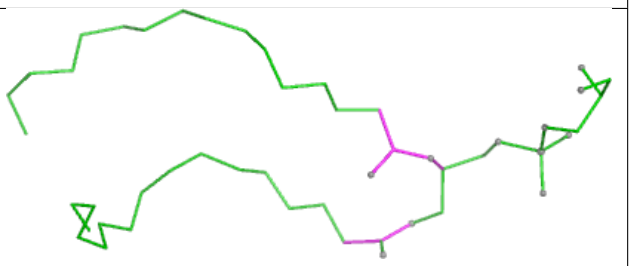
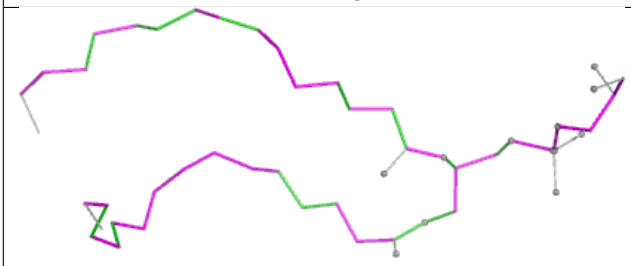


Bond angles



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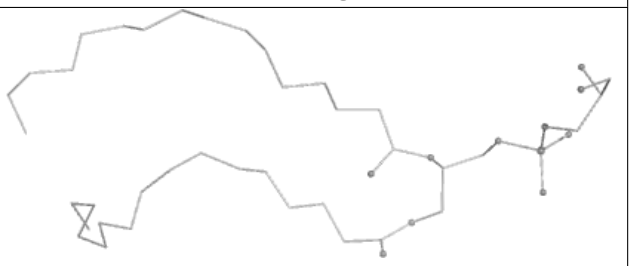
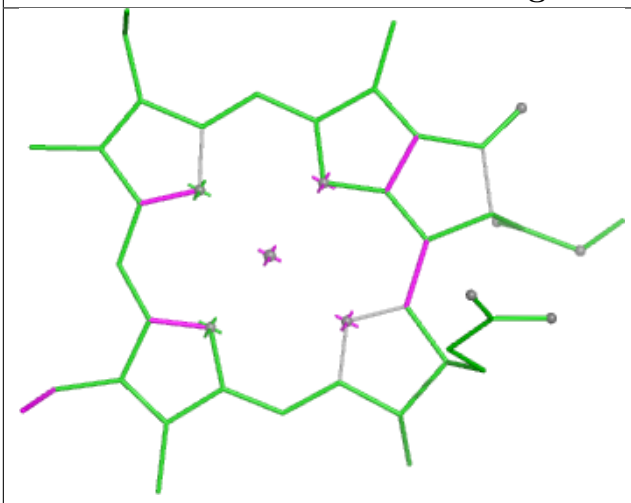
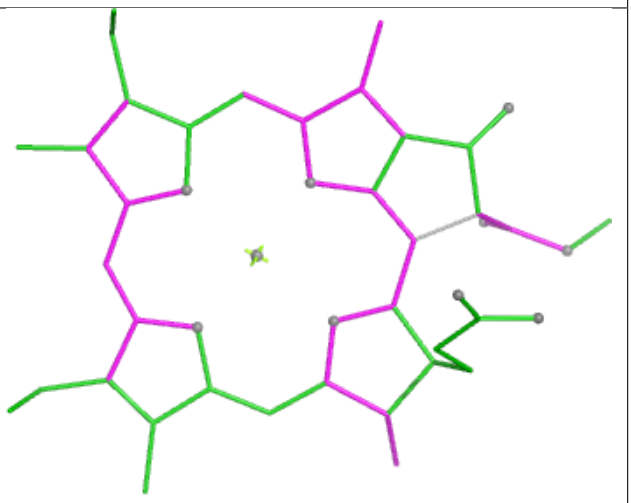
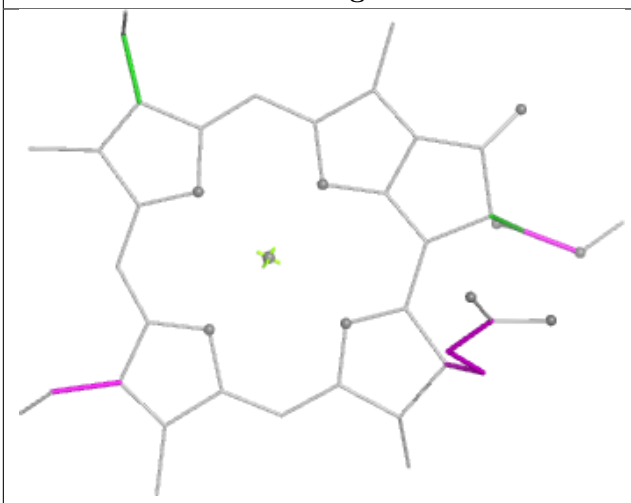
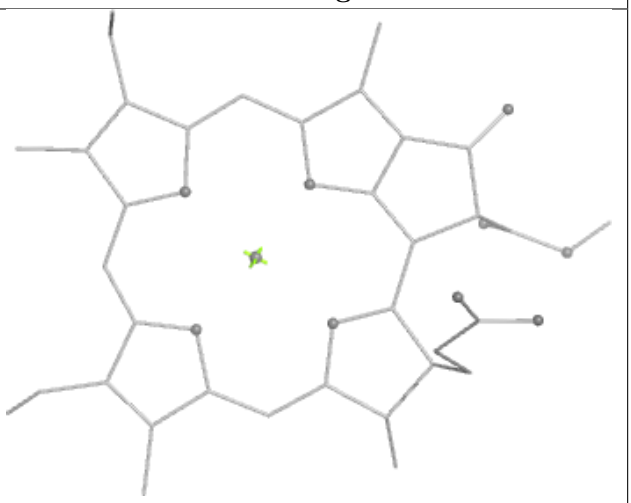
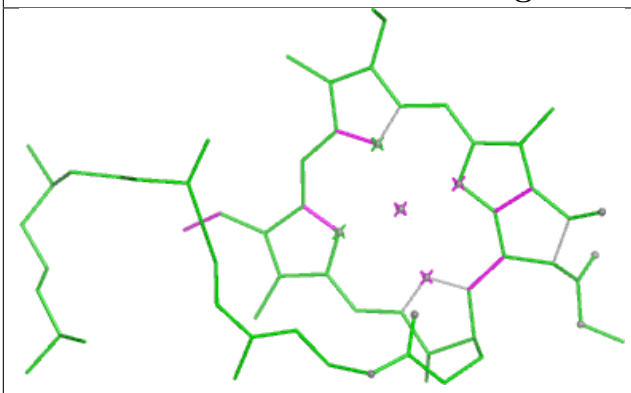


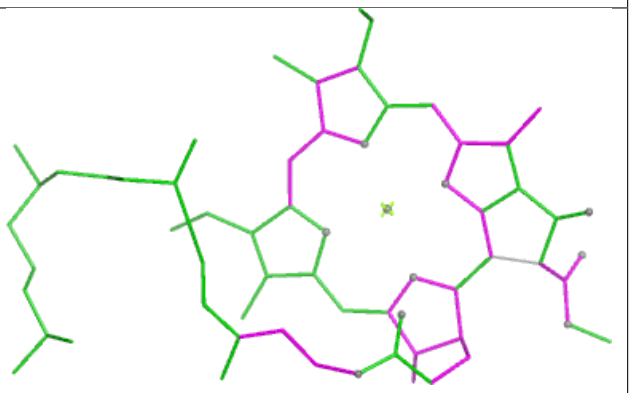
Rings

Ligand CLA 5 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

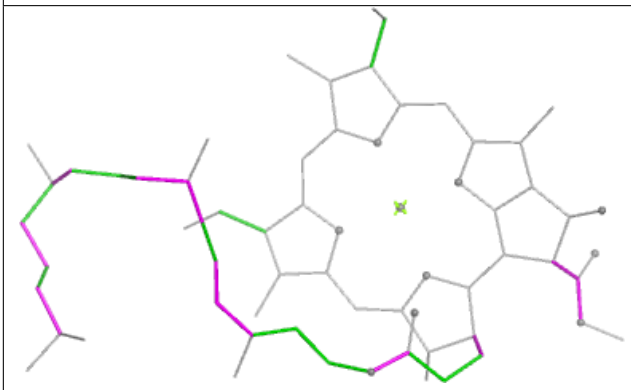
Ligand CLA A 1117



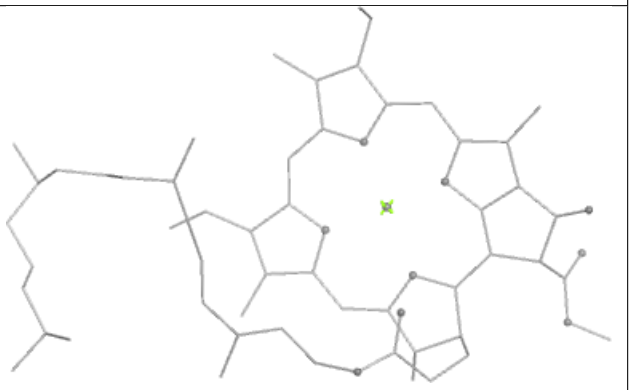
Bond lengths



Bond angles

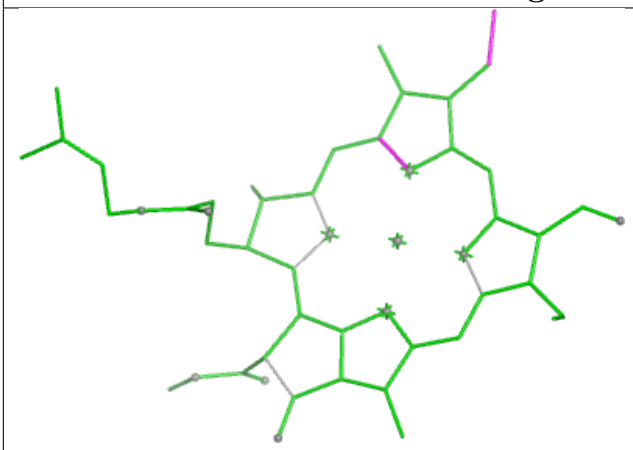


Torsions

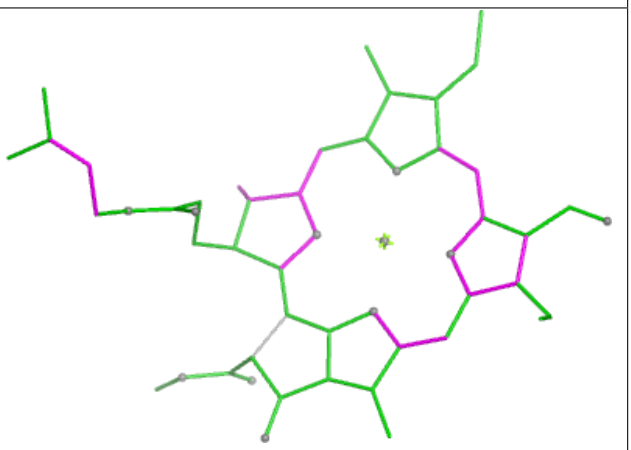


Rings

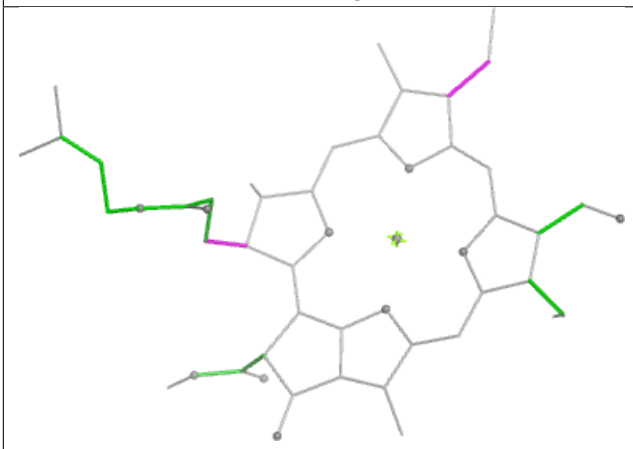
Ligand CHL 5 611



Bond lengths



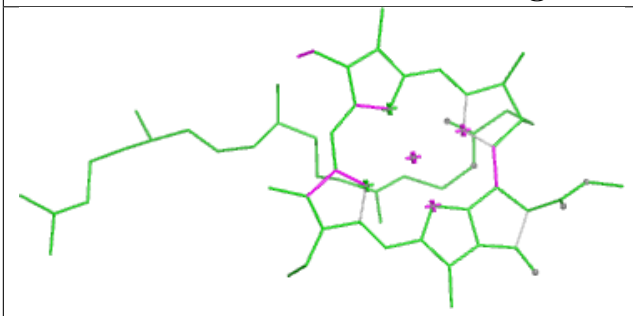
Bond angles



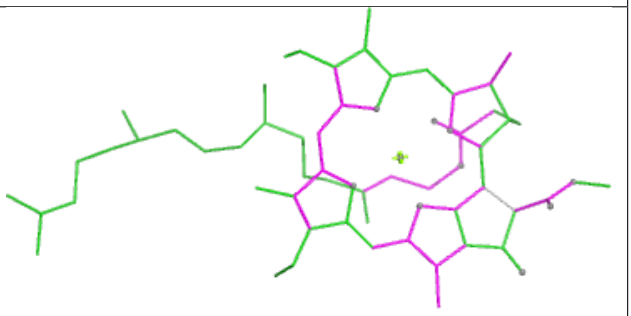
Torsions

Rings

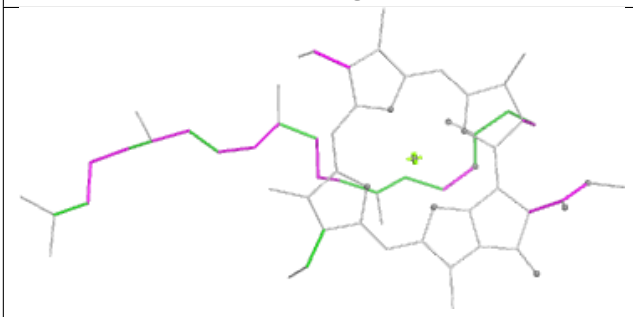
Ligand CLA 3 603



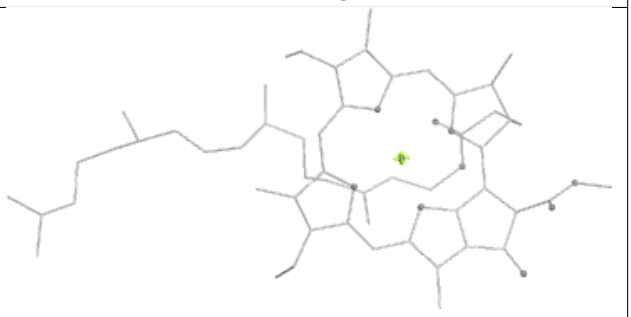
Bond lengths



Bond angles

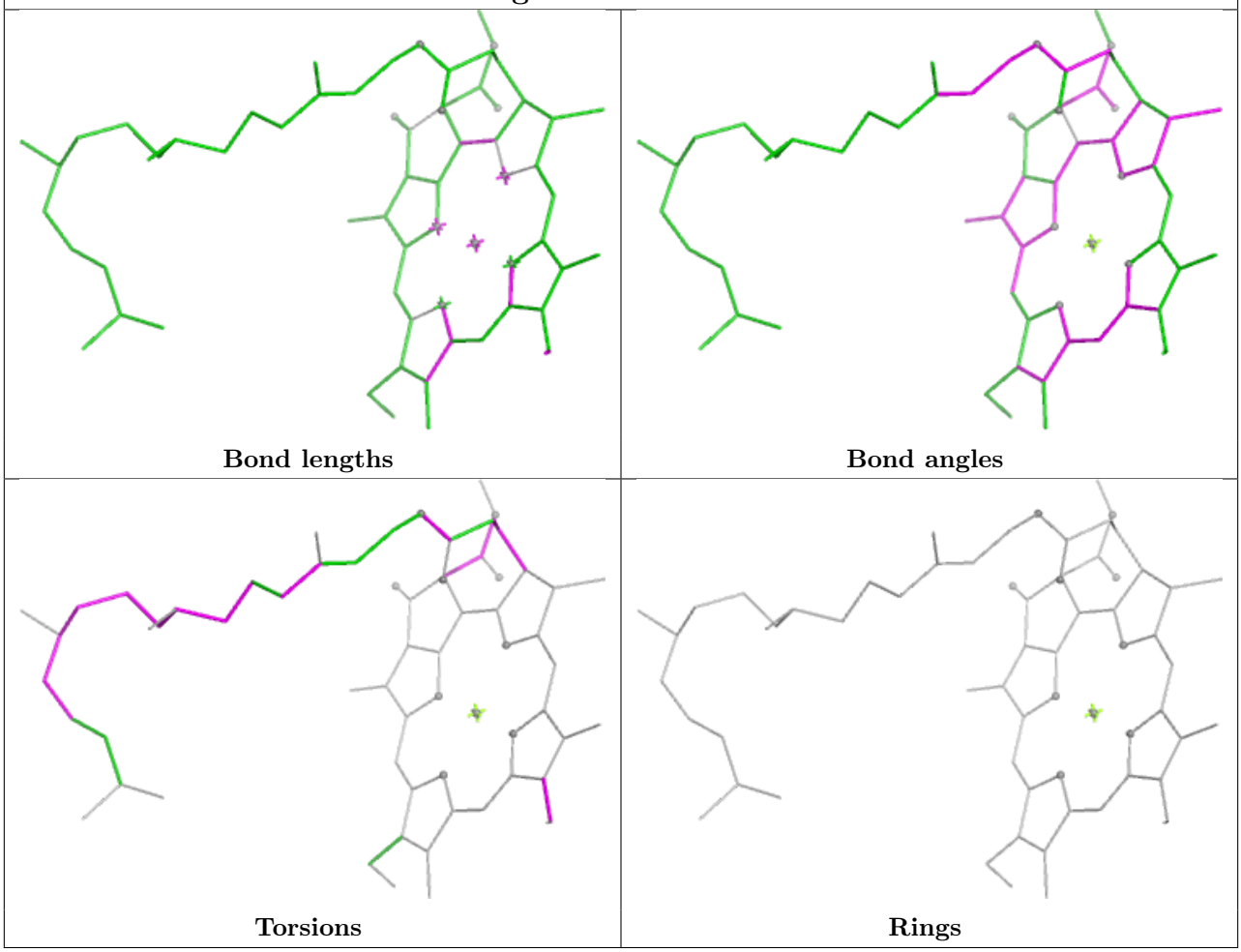


Torsions

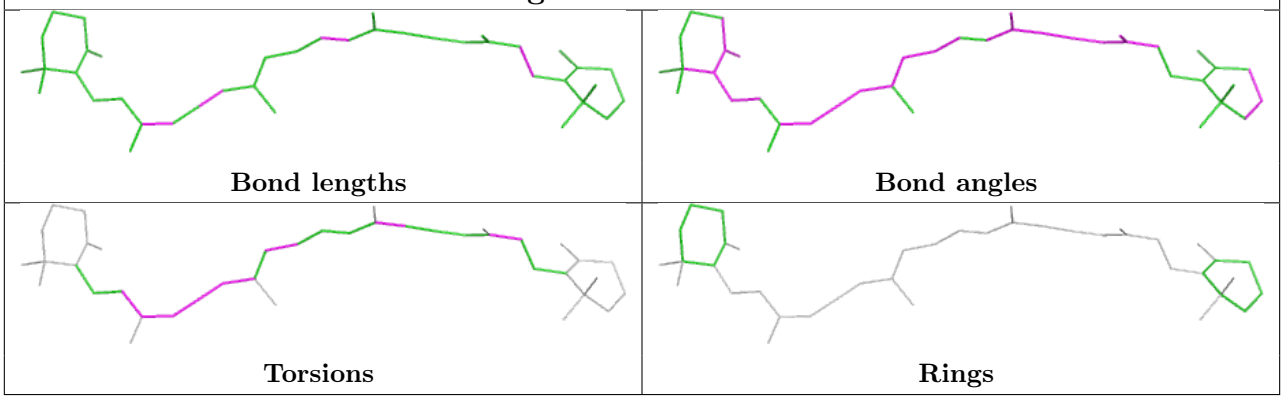


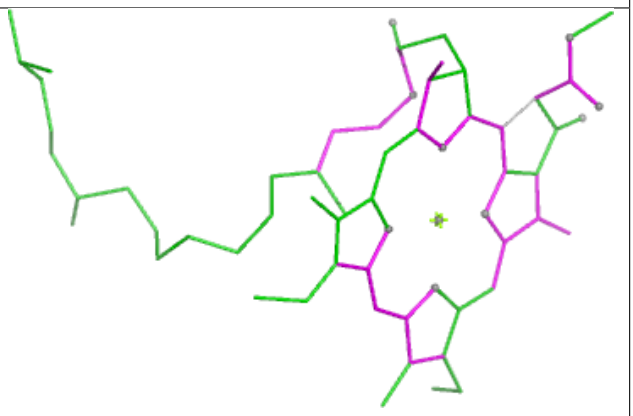
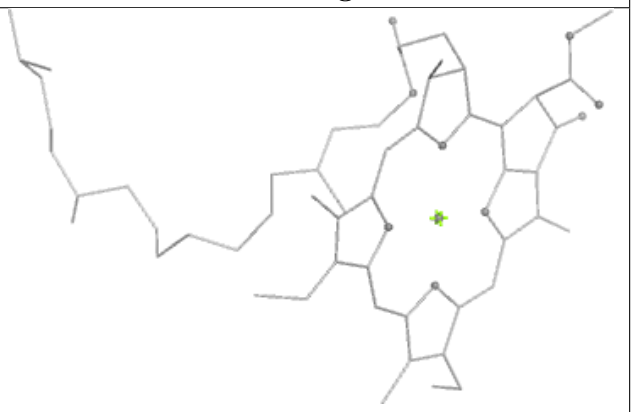
Rings

Ligand CLA 1 612

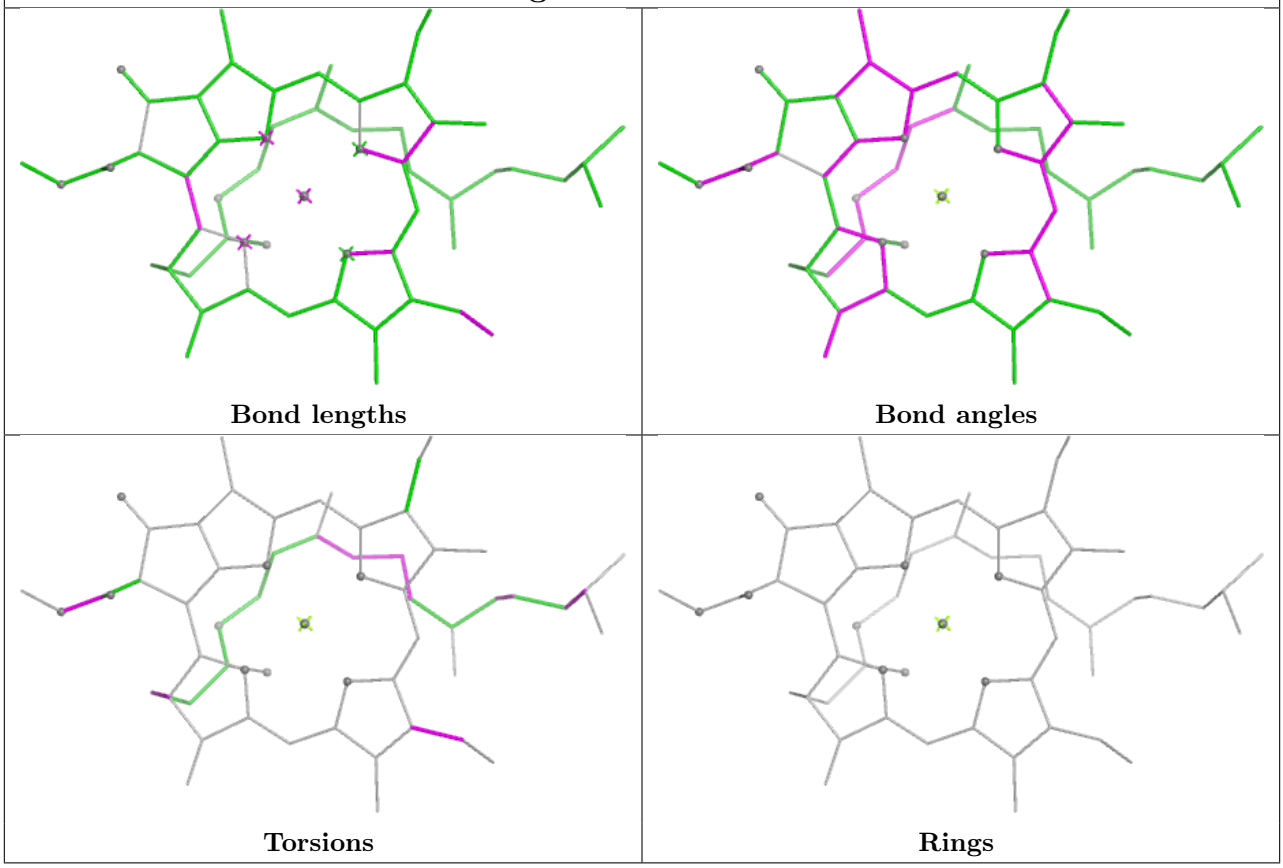


Ligand BCR 7 504

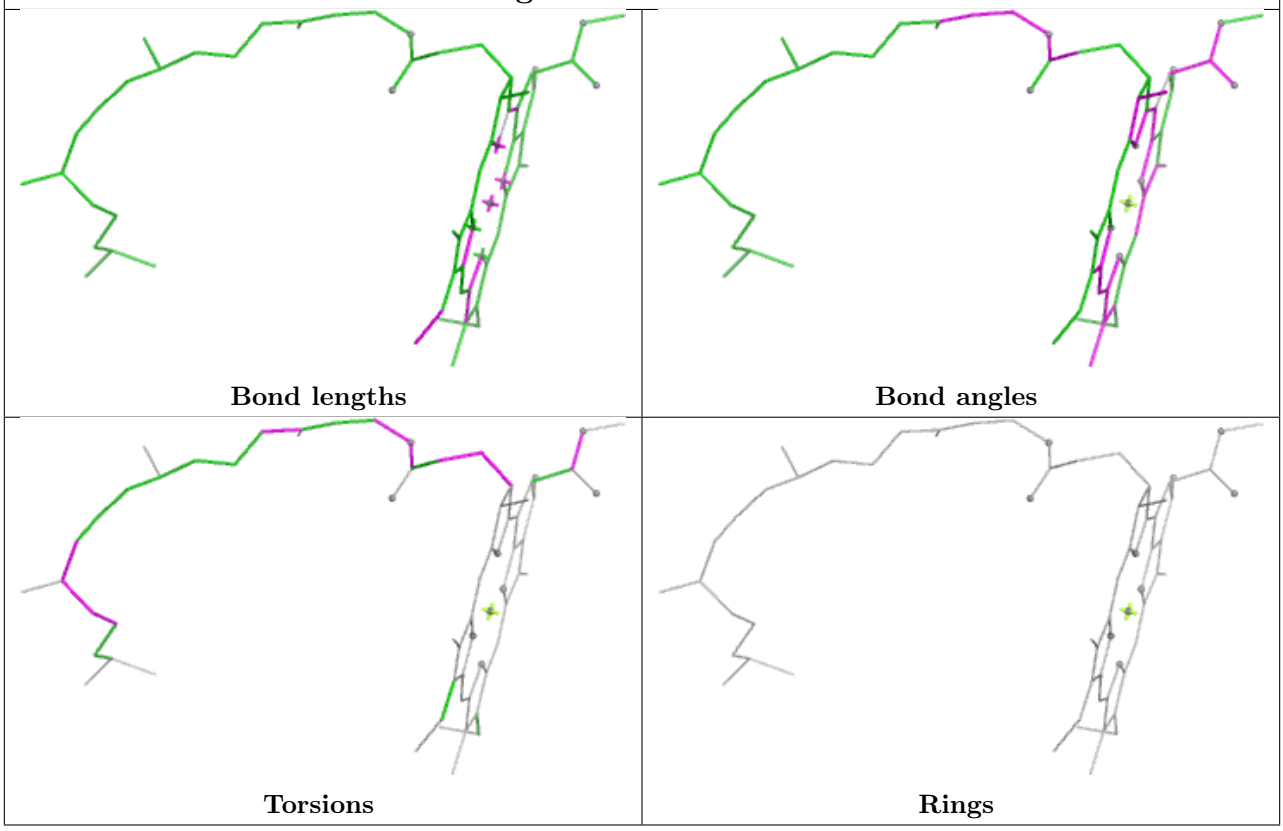


Ligand CLA B 1237	
Bond lengths	 Bond angles
Torsions	 Rings

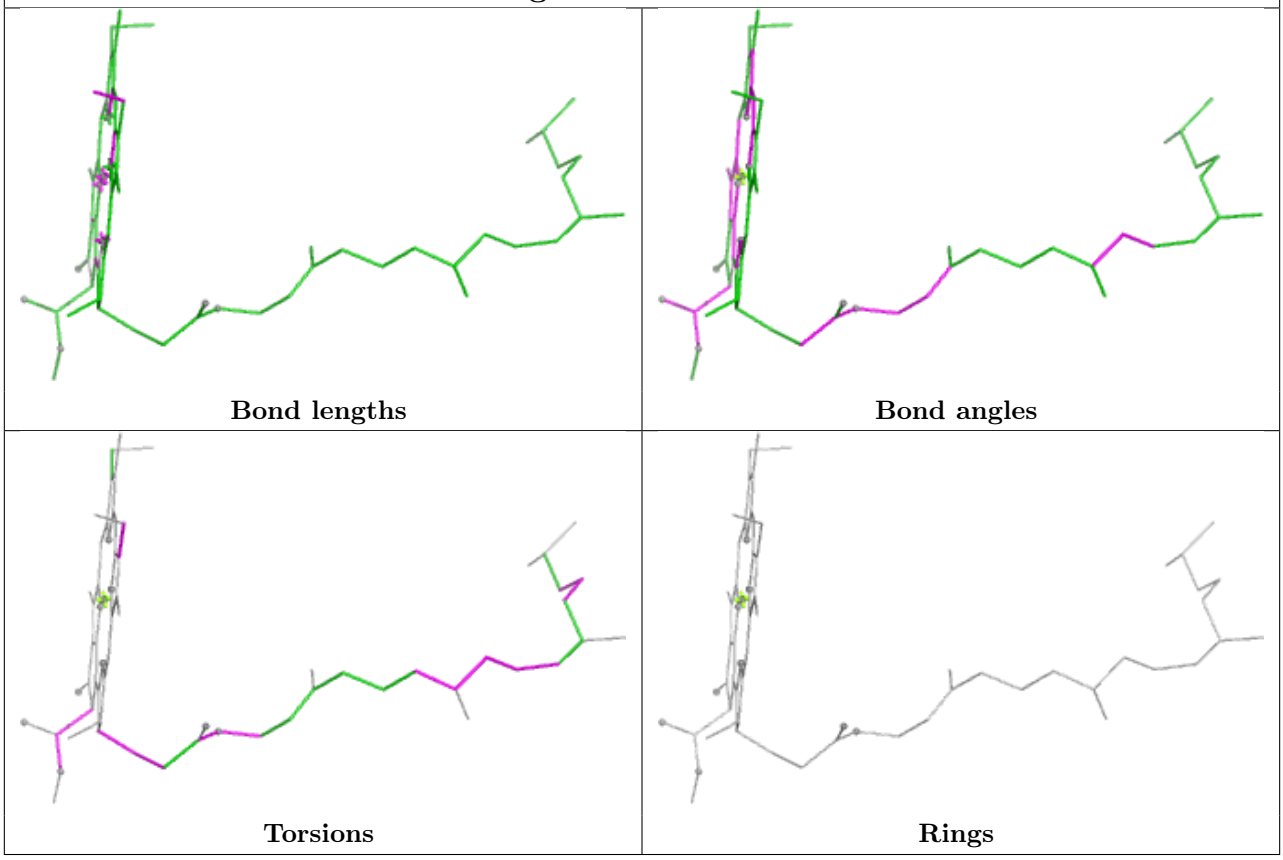
Ligand CLA 7 616



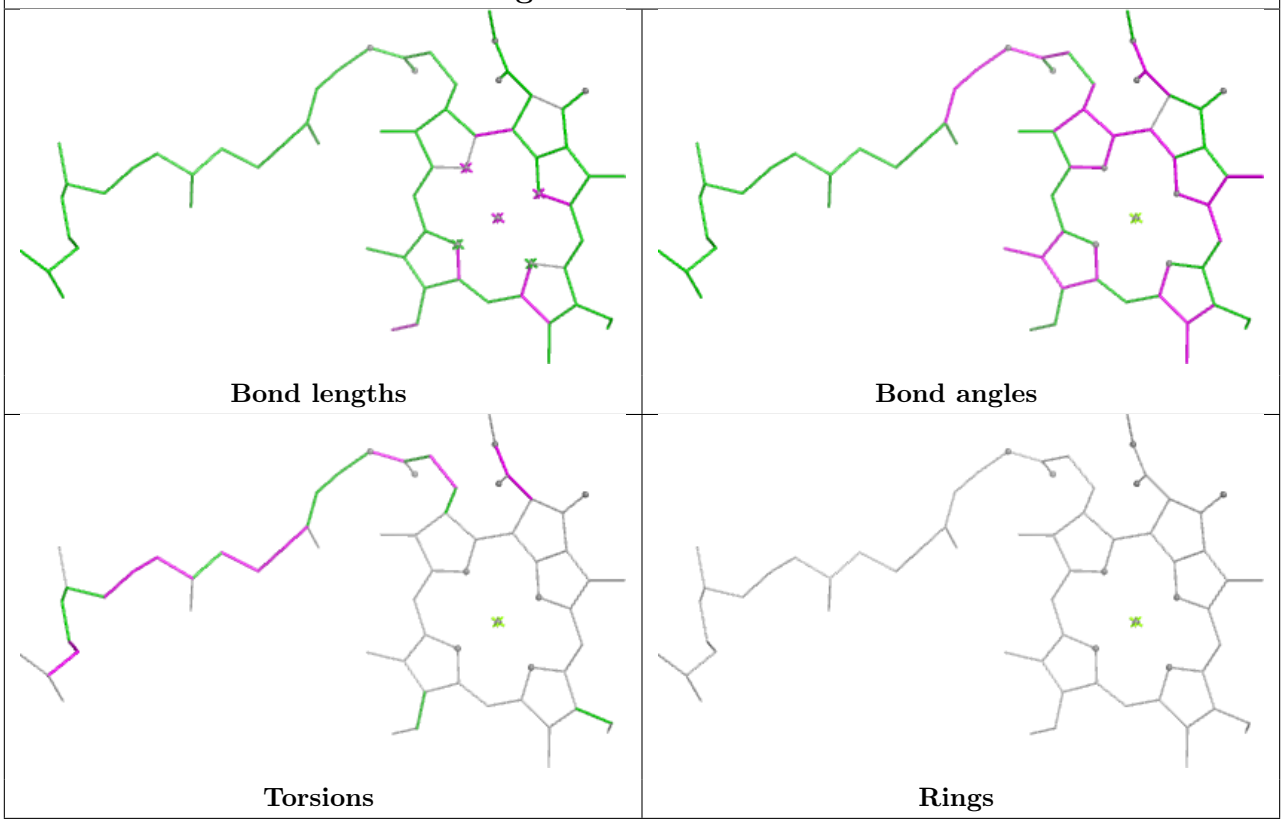
Ligand CLA A 1105



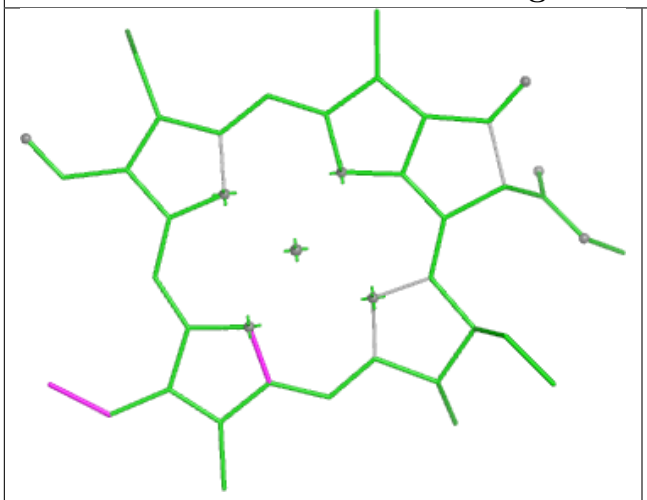
Ligand CLA 3 606



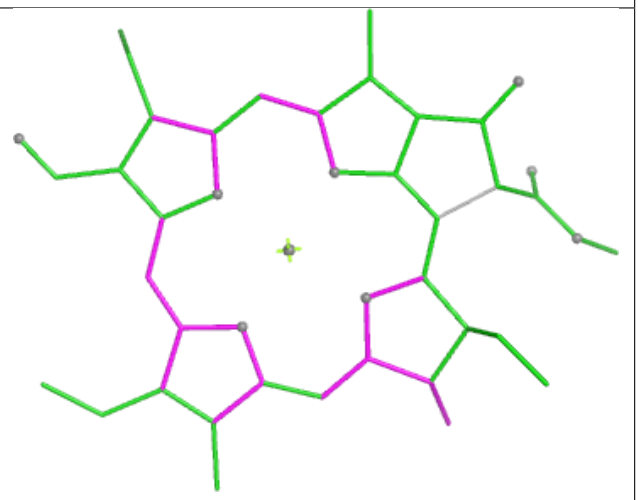
Ligand CLA A 1013



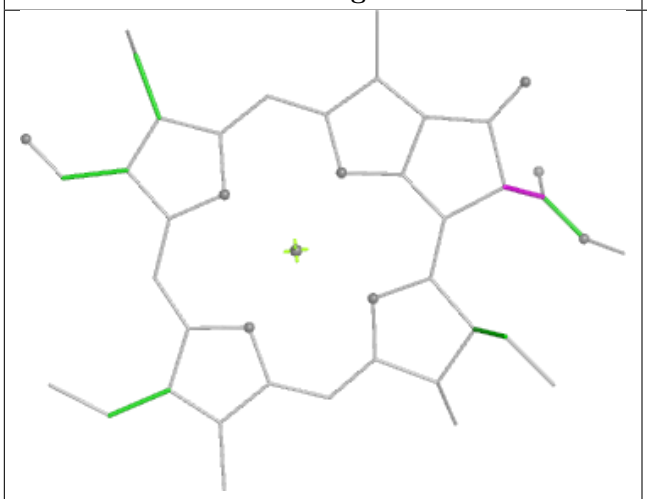
Ligand CHL 6 617



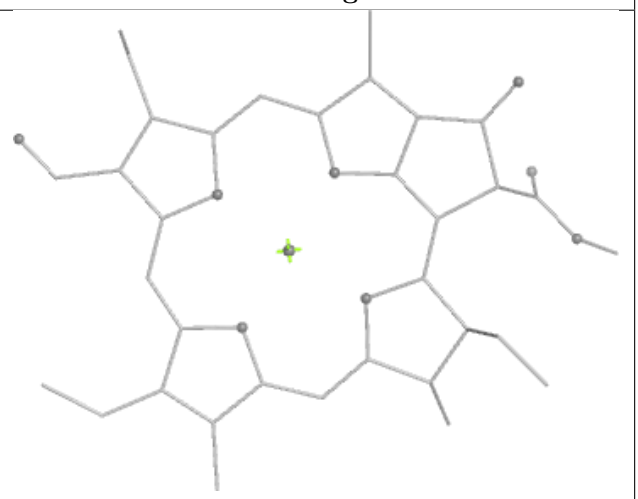
Bond lengths



Bond angles

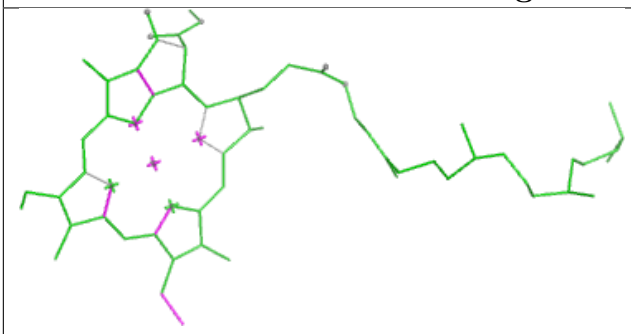


Torsions

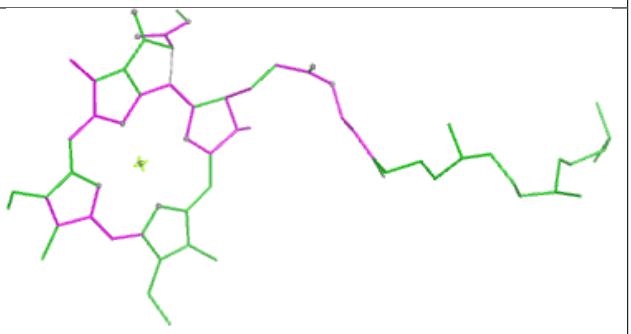


Rings

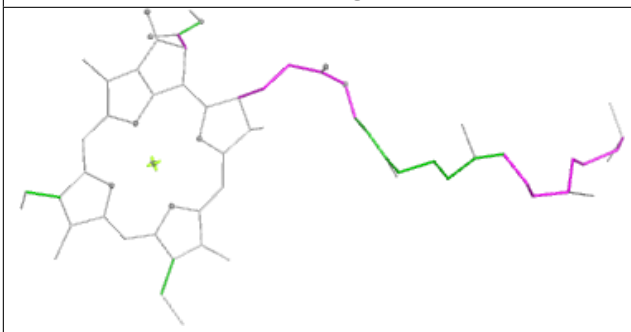
Ligand CLA B 1210



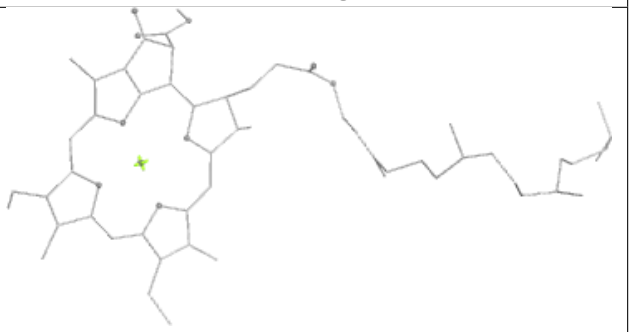
Bond lengths



Bond angles

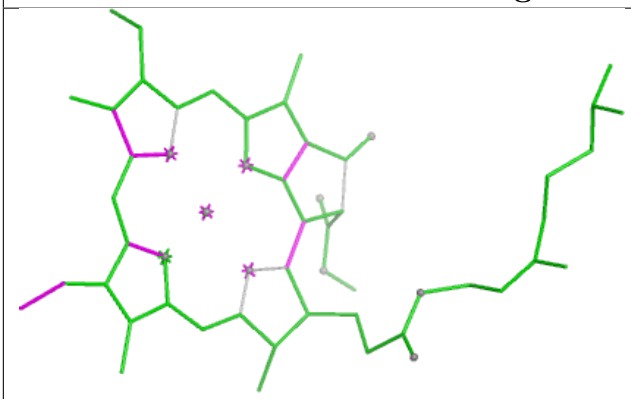


Torsions

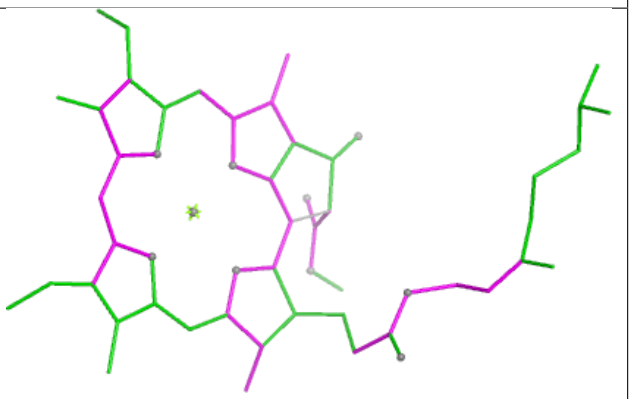


Rings

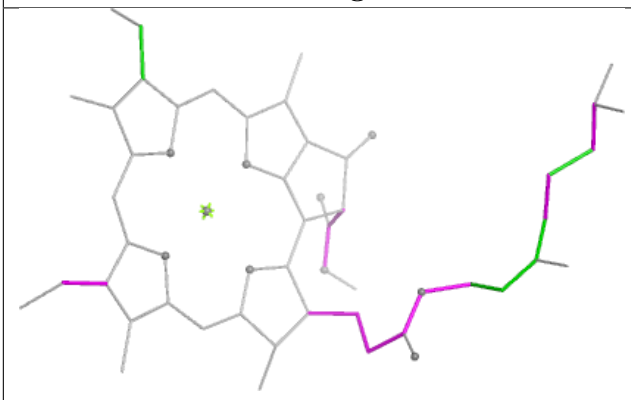
Ligand CLA K 1402



Bond lengths



Bond angles



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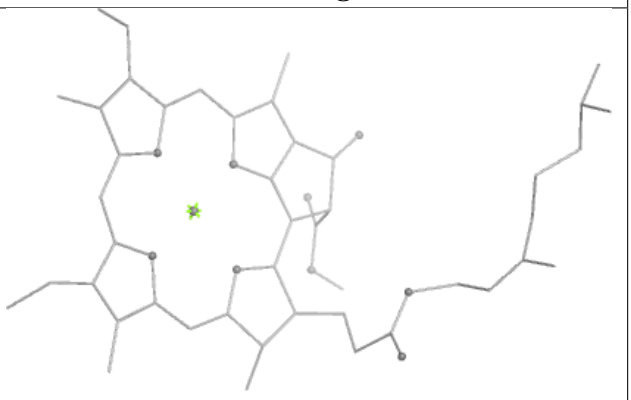
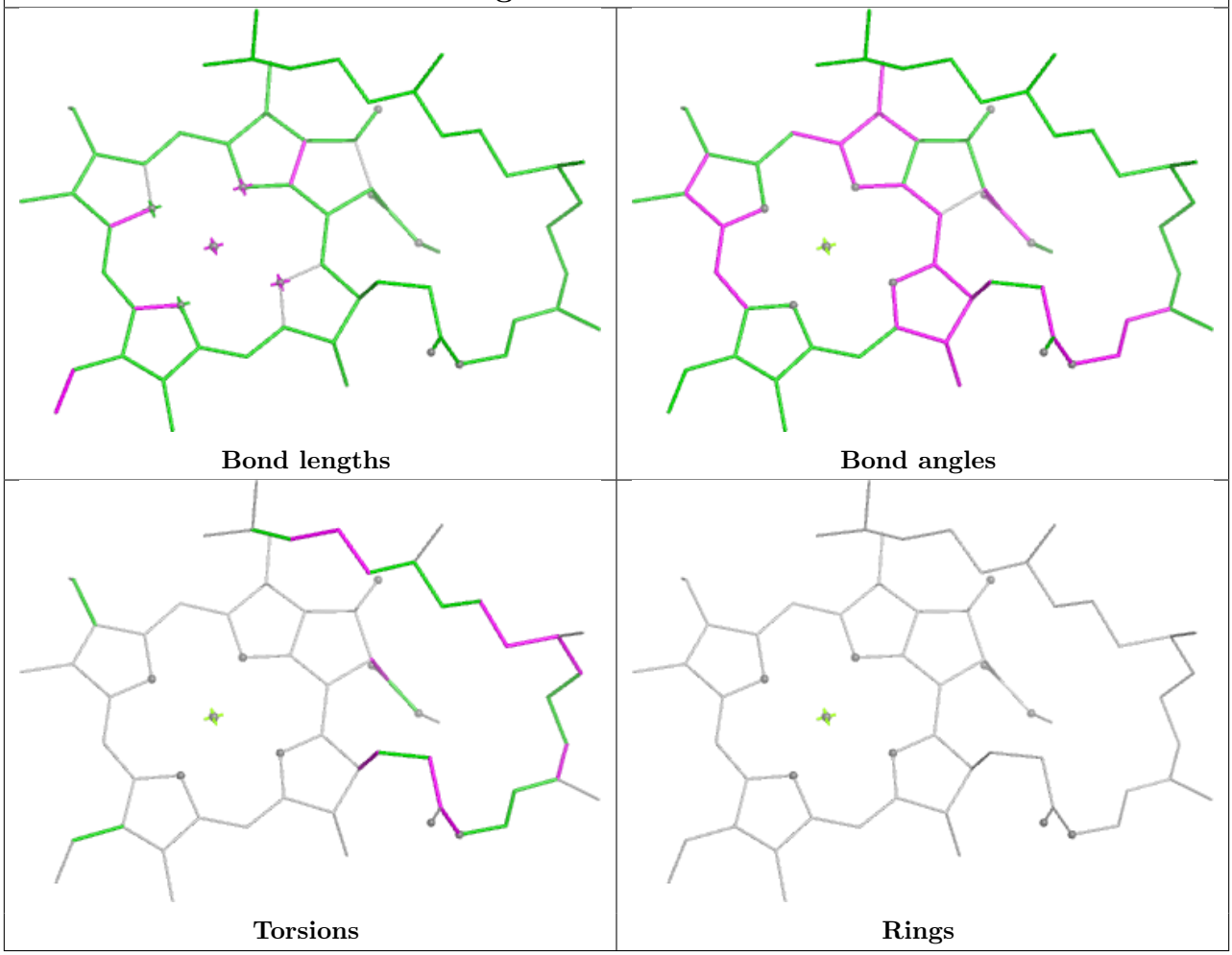
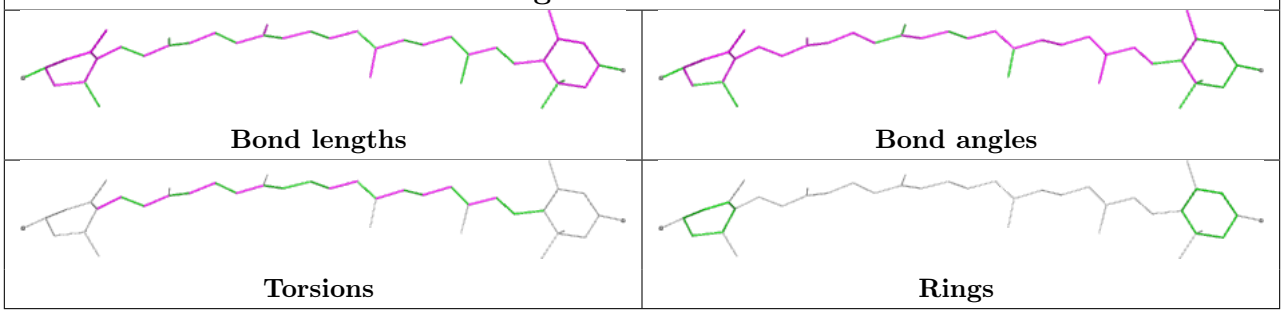


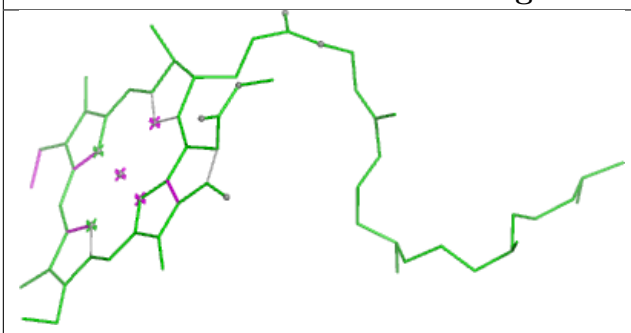
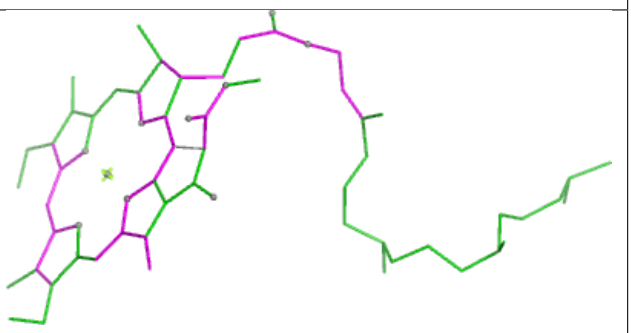
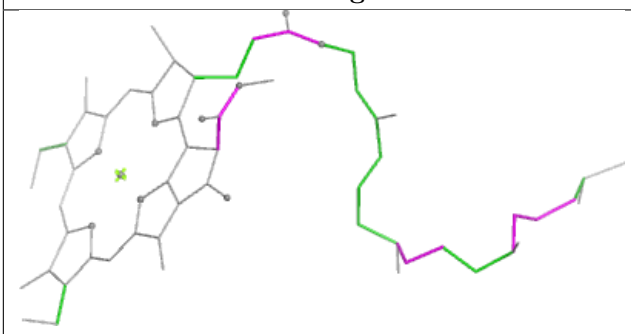
Rings

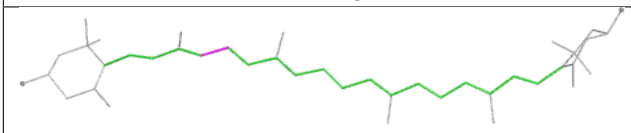
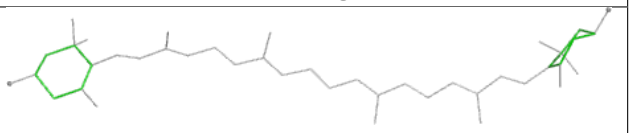
Ligand CLA B 1202



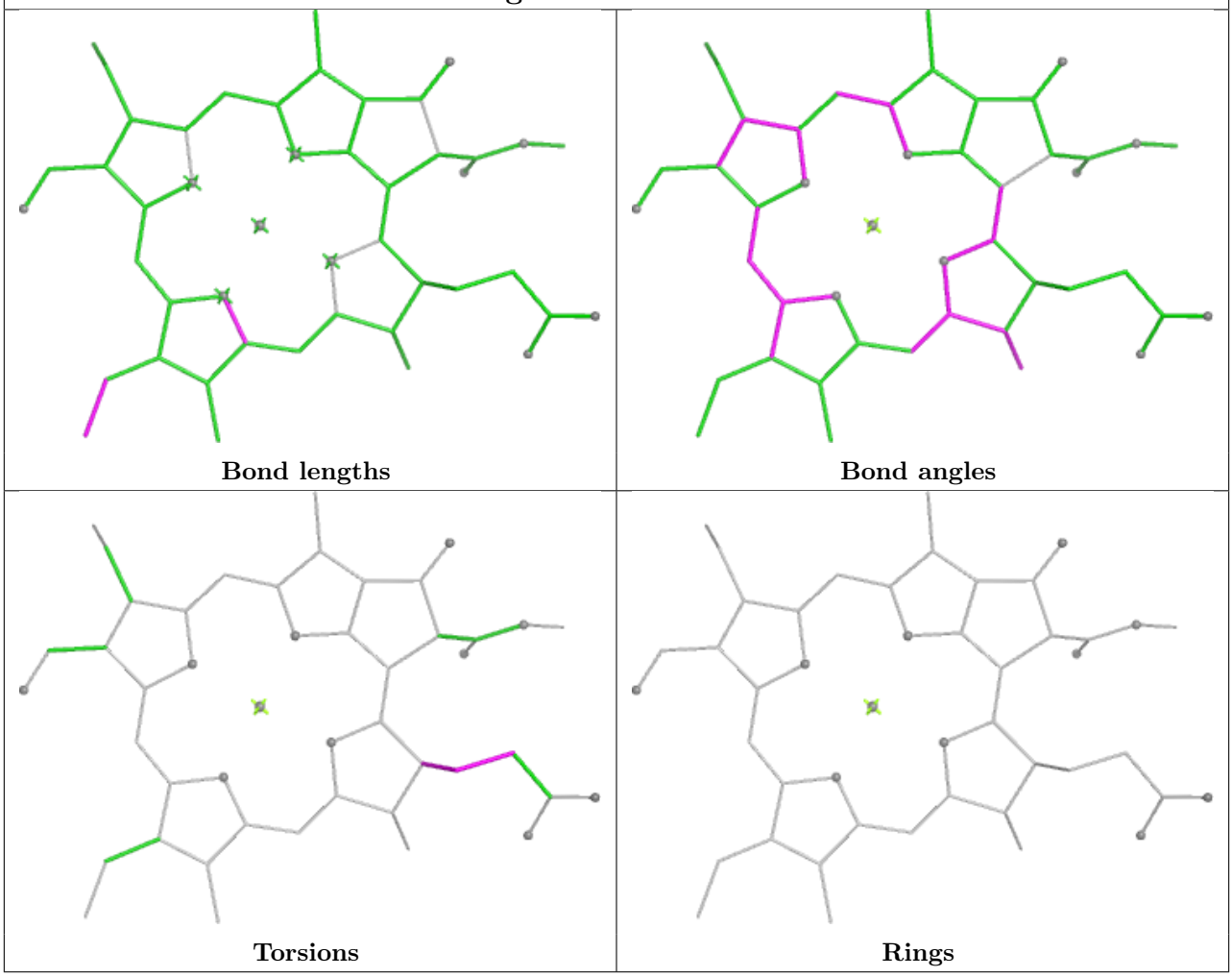
Ligand C7Z 5 505



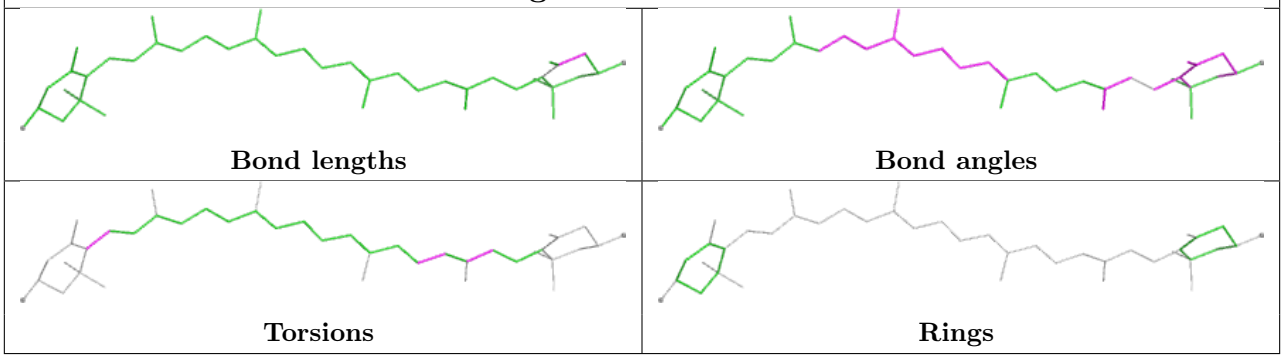
Ligand CLA B 1021	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LUT Z 502	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand CHL Z 613



Ligand LUT 1 501



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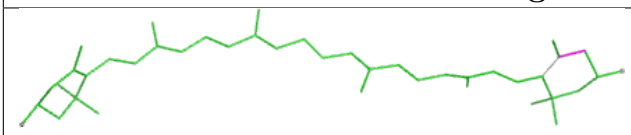
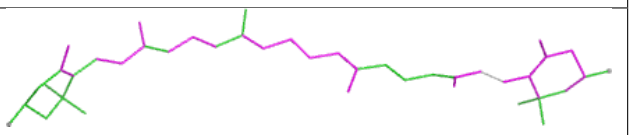
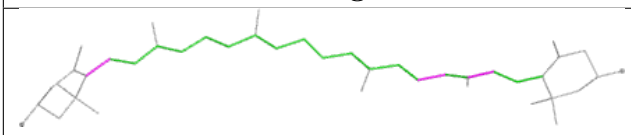


Bond lengths



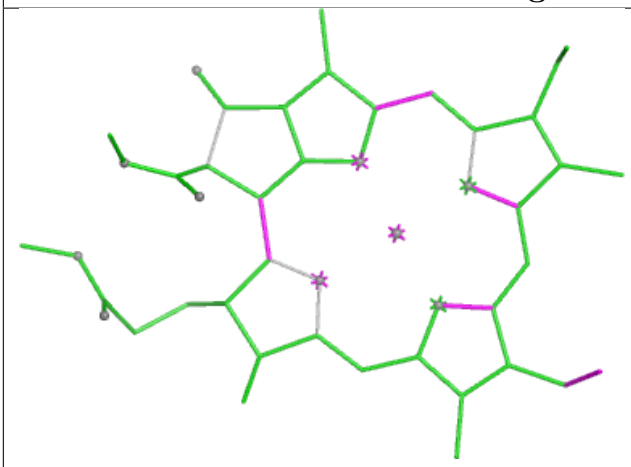
Bond angles



Torsions

Rings

Ligand CLA 5 622



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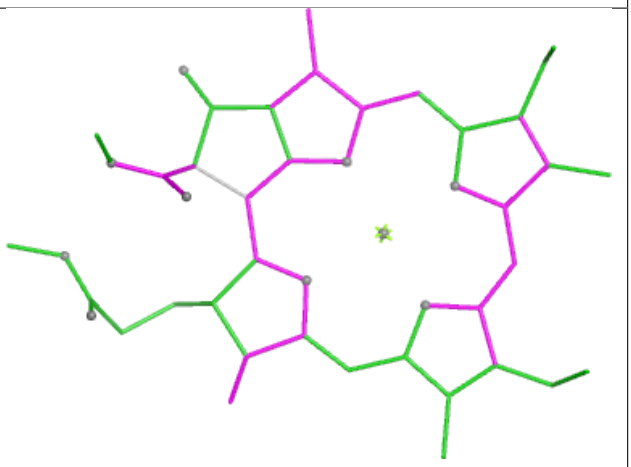
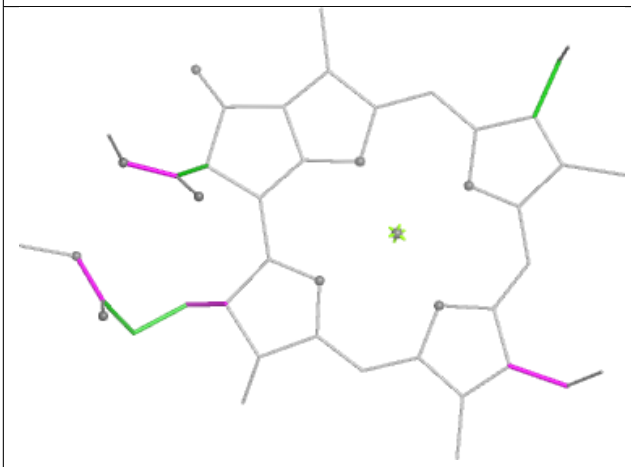


Bond angles



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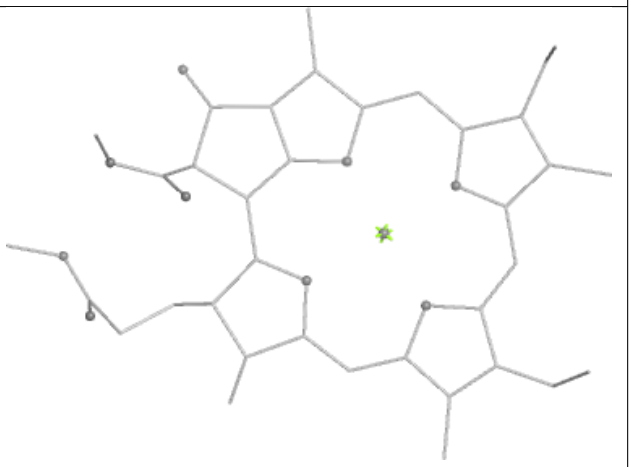
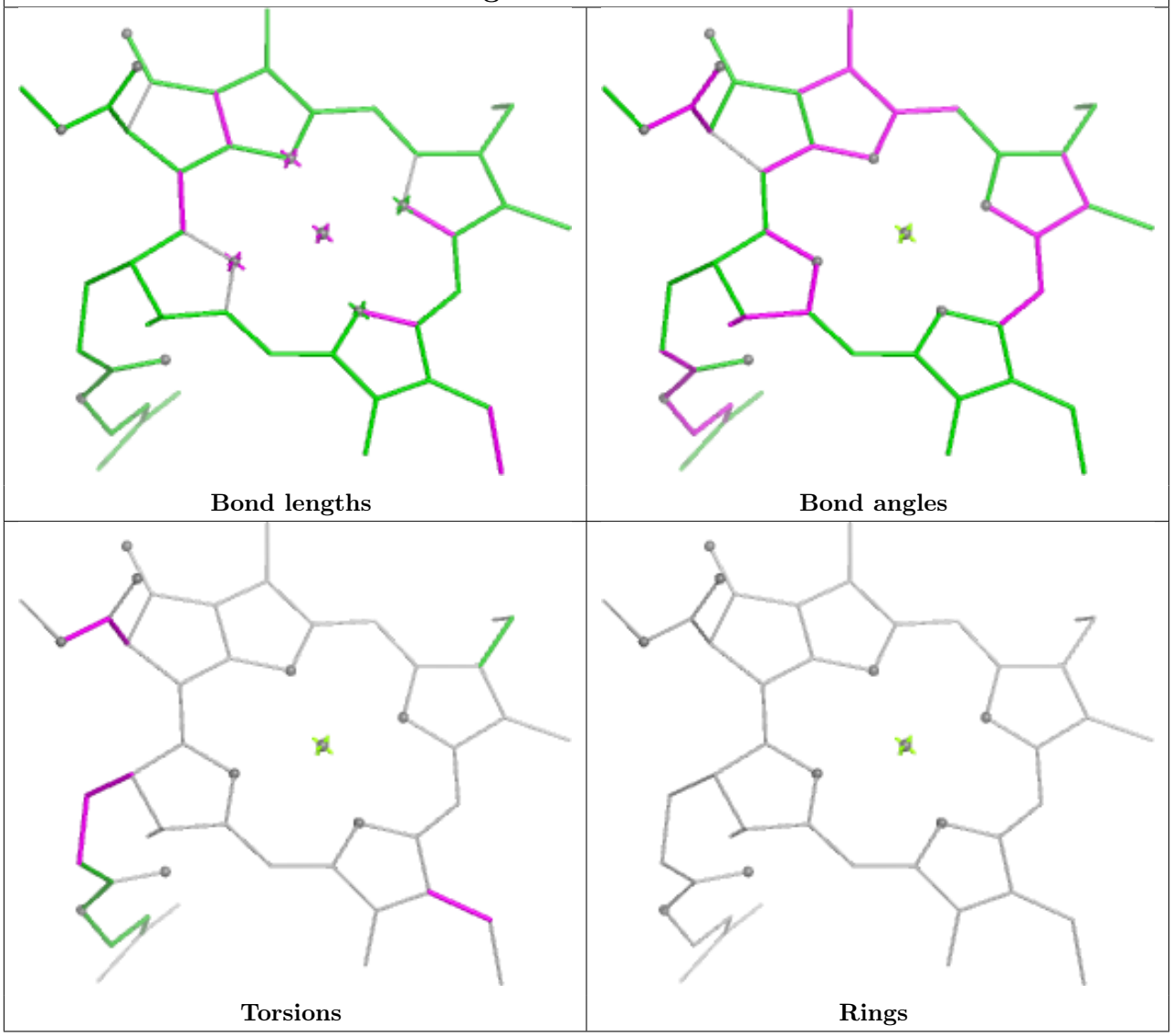
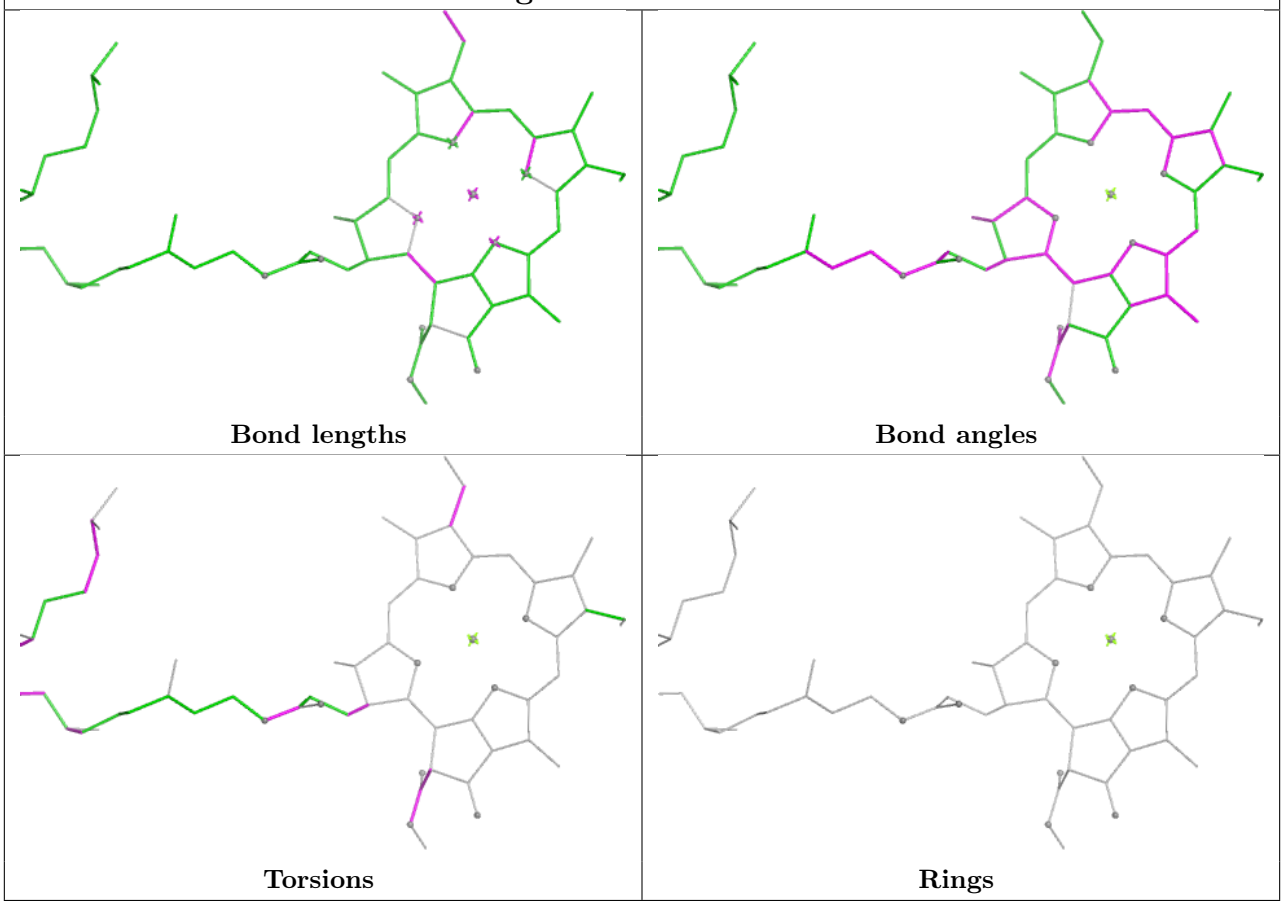


Rings

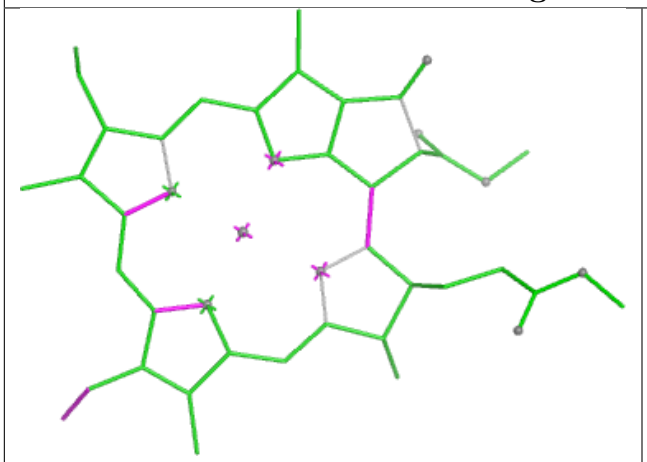
Ligand CLA 6 612



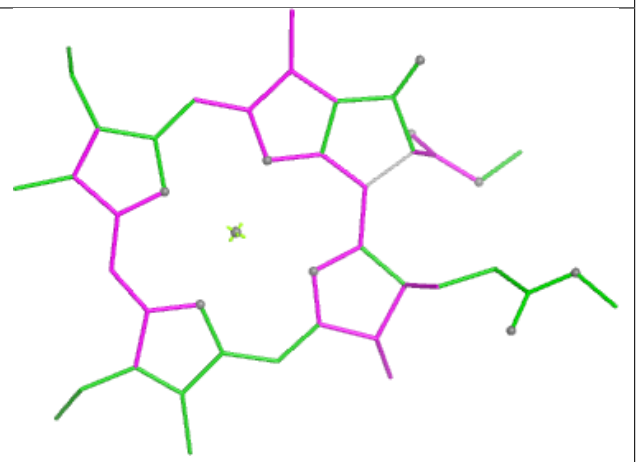
Ligand CLA A 1124



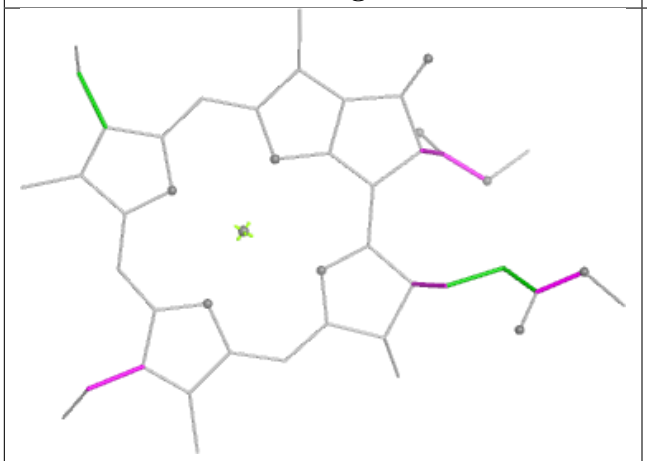
Ligand CLA 6 618



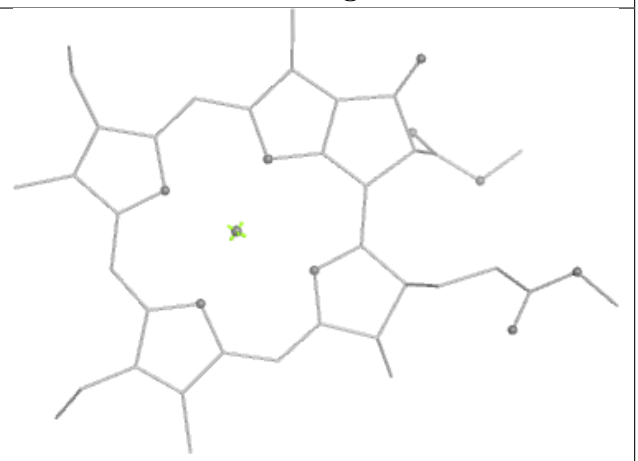
Bond lengths



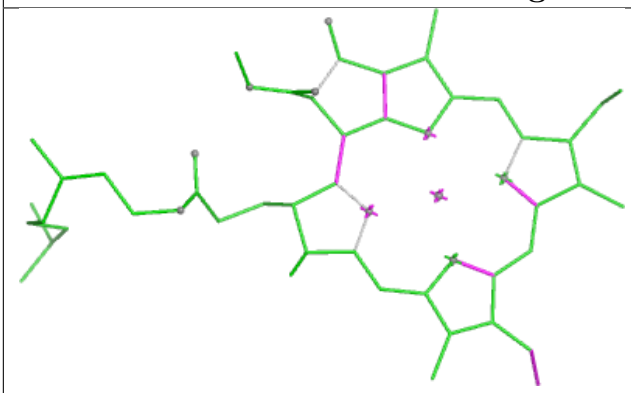
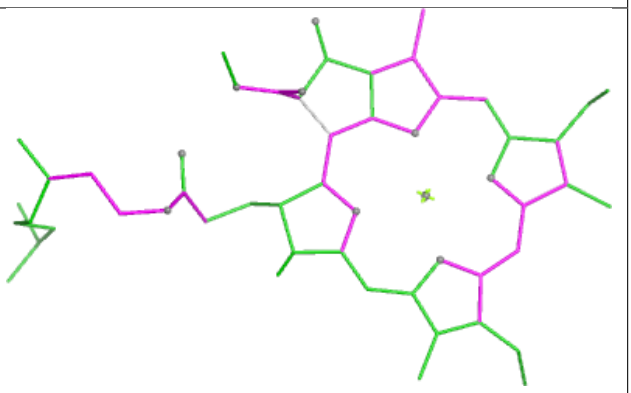
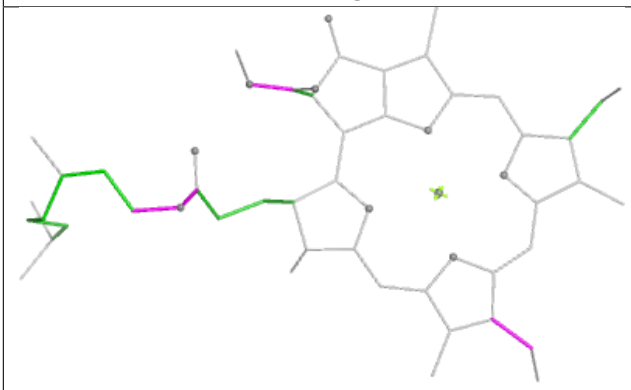
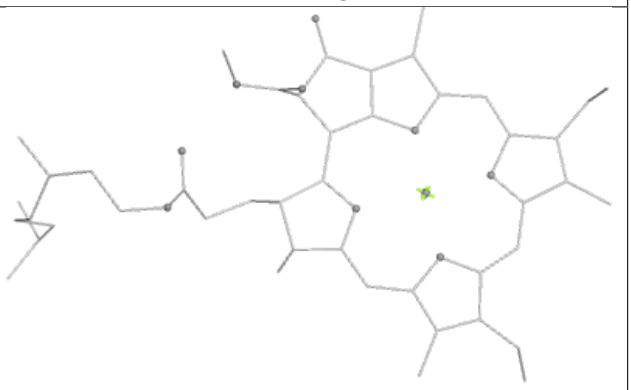
Bond angles



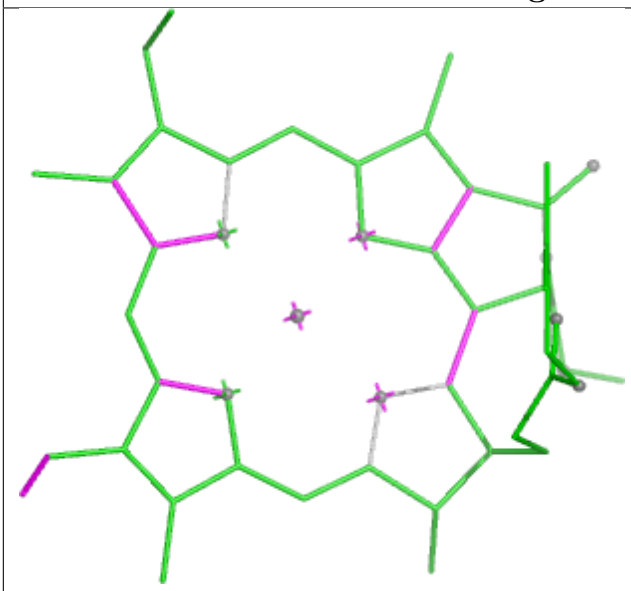
Torsions



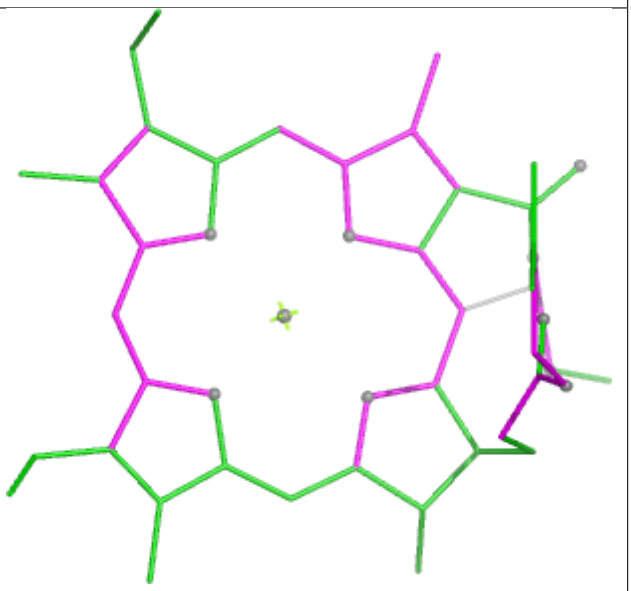
Rings

Ligand CLA 3 613	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

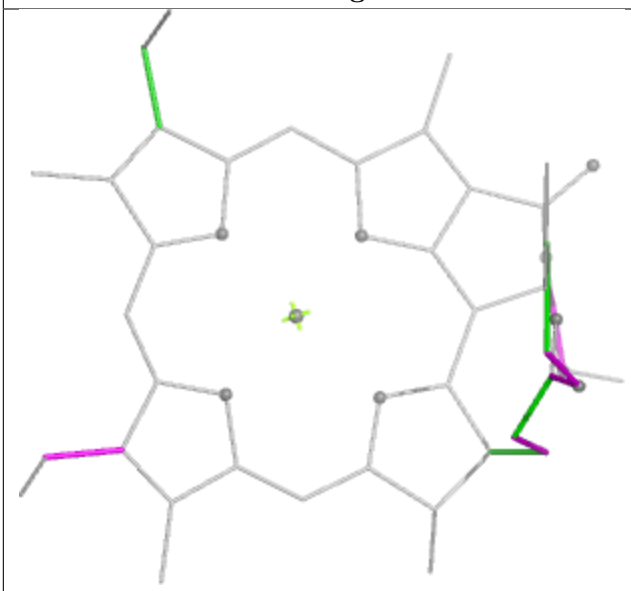
Ligand CLA 4 606



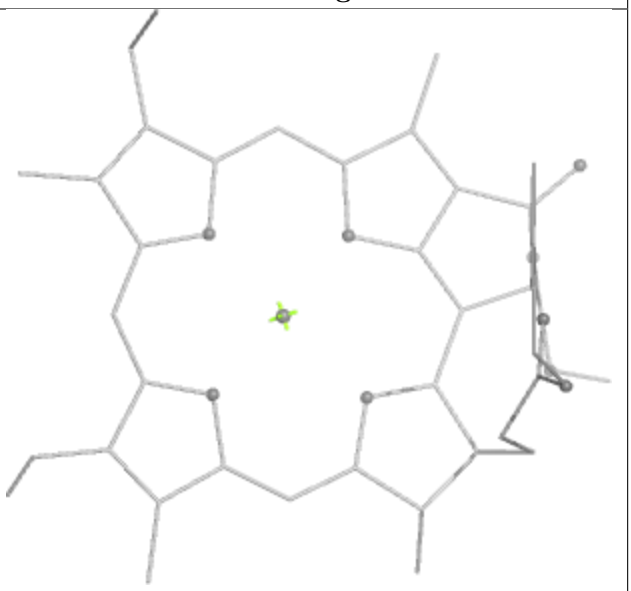
Bond lengths



Bond angles

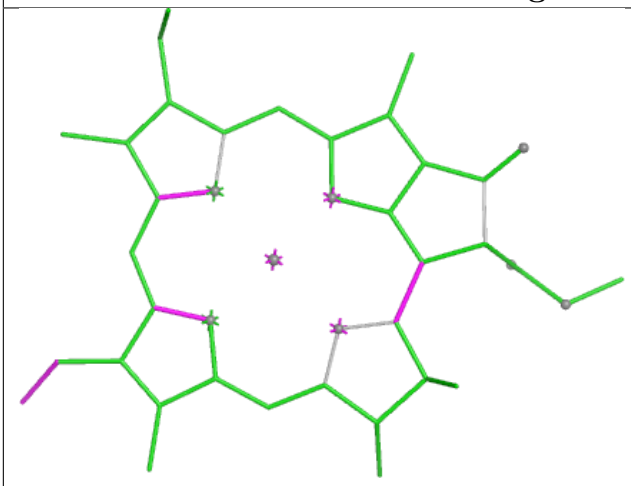


Torsions

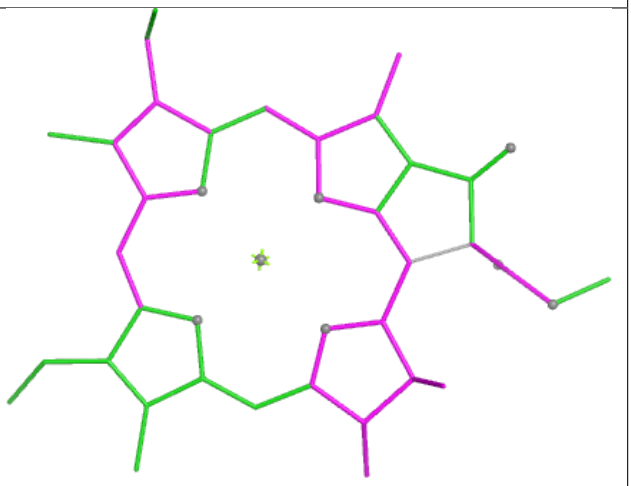


Rings

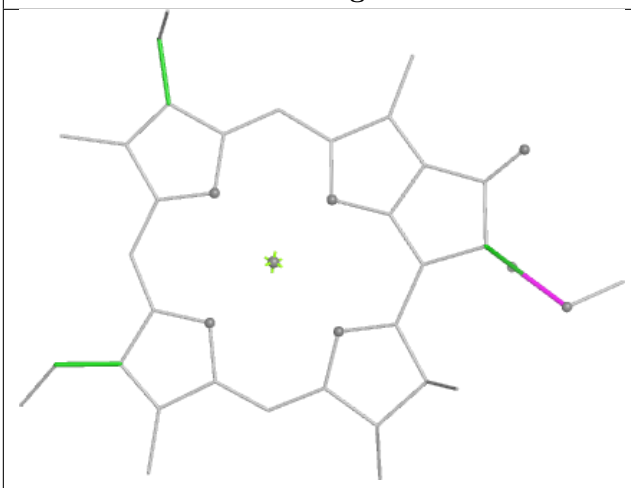
Ligand CLA 4 615



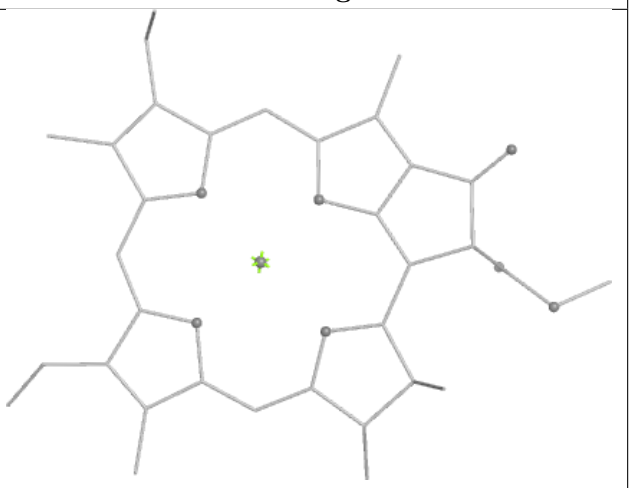
Bond lengths



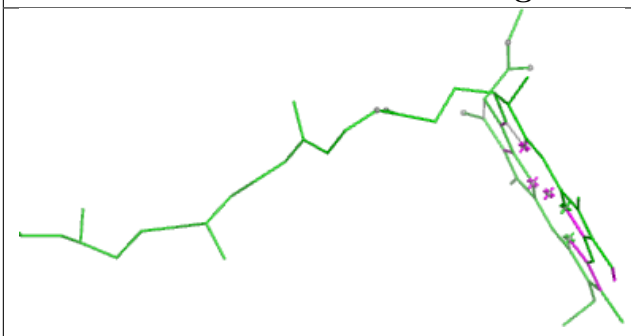
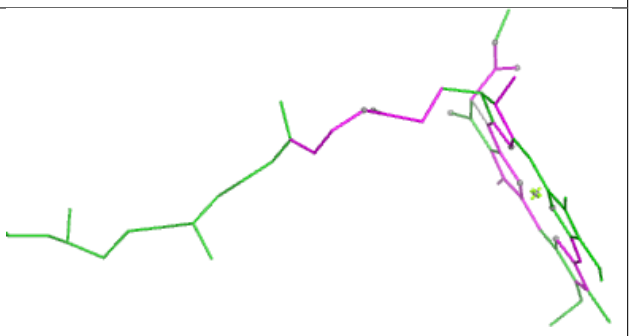
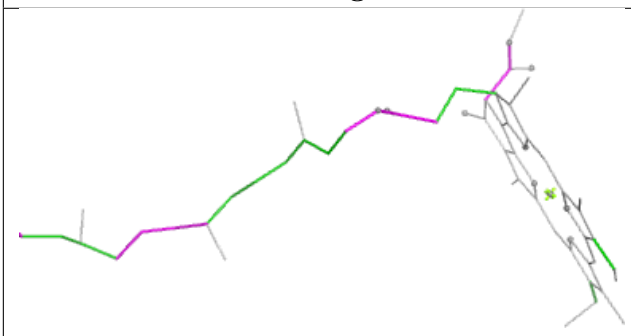
Bond angles



Torsions

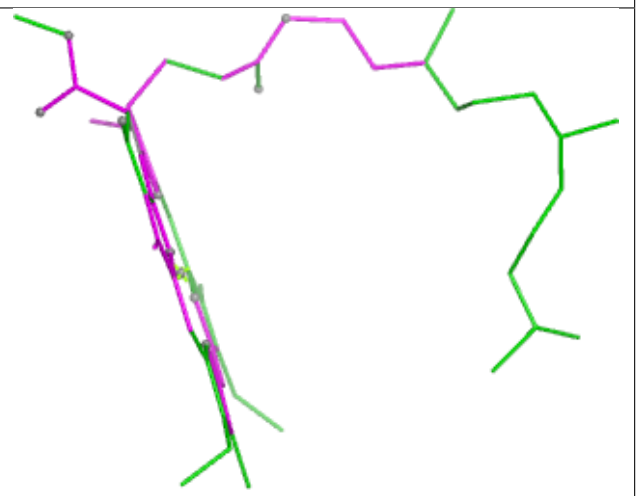


Rings

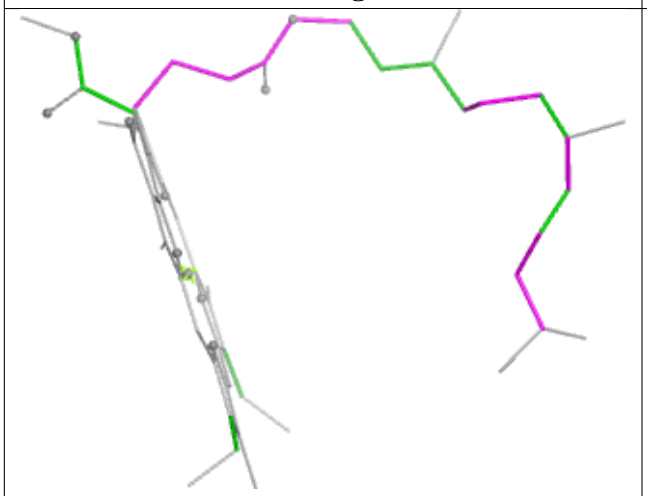
Ligand CLA A 1137	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 3 610

Bond lengths



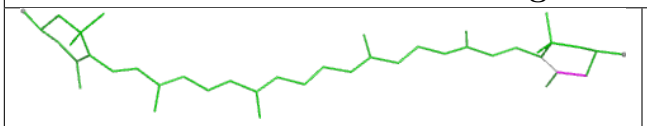
Bond angles



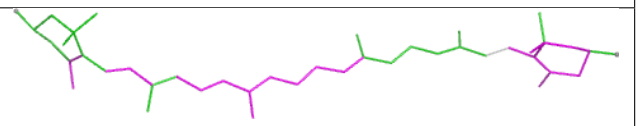
Torsions

Rings

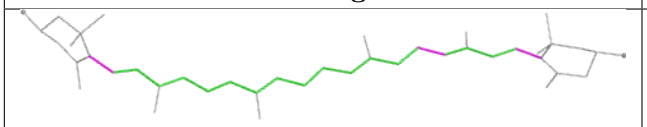
Ligand LUT 7 501



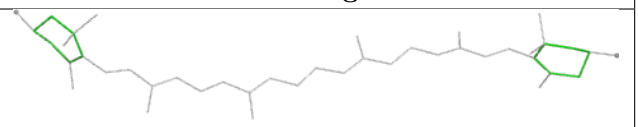
Bond lengths



Bond angles

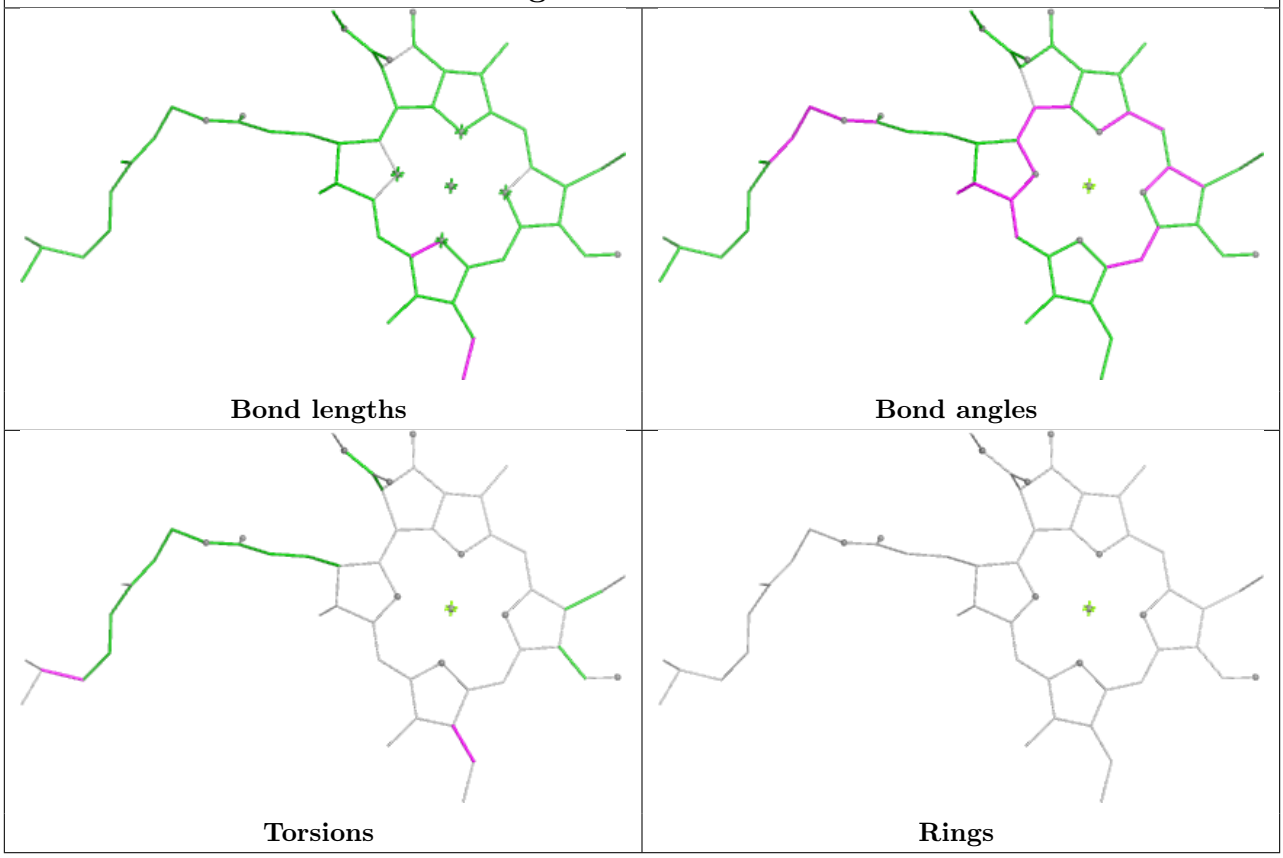


Torsions



Rings

Ligand CHL 6 613



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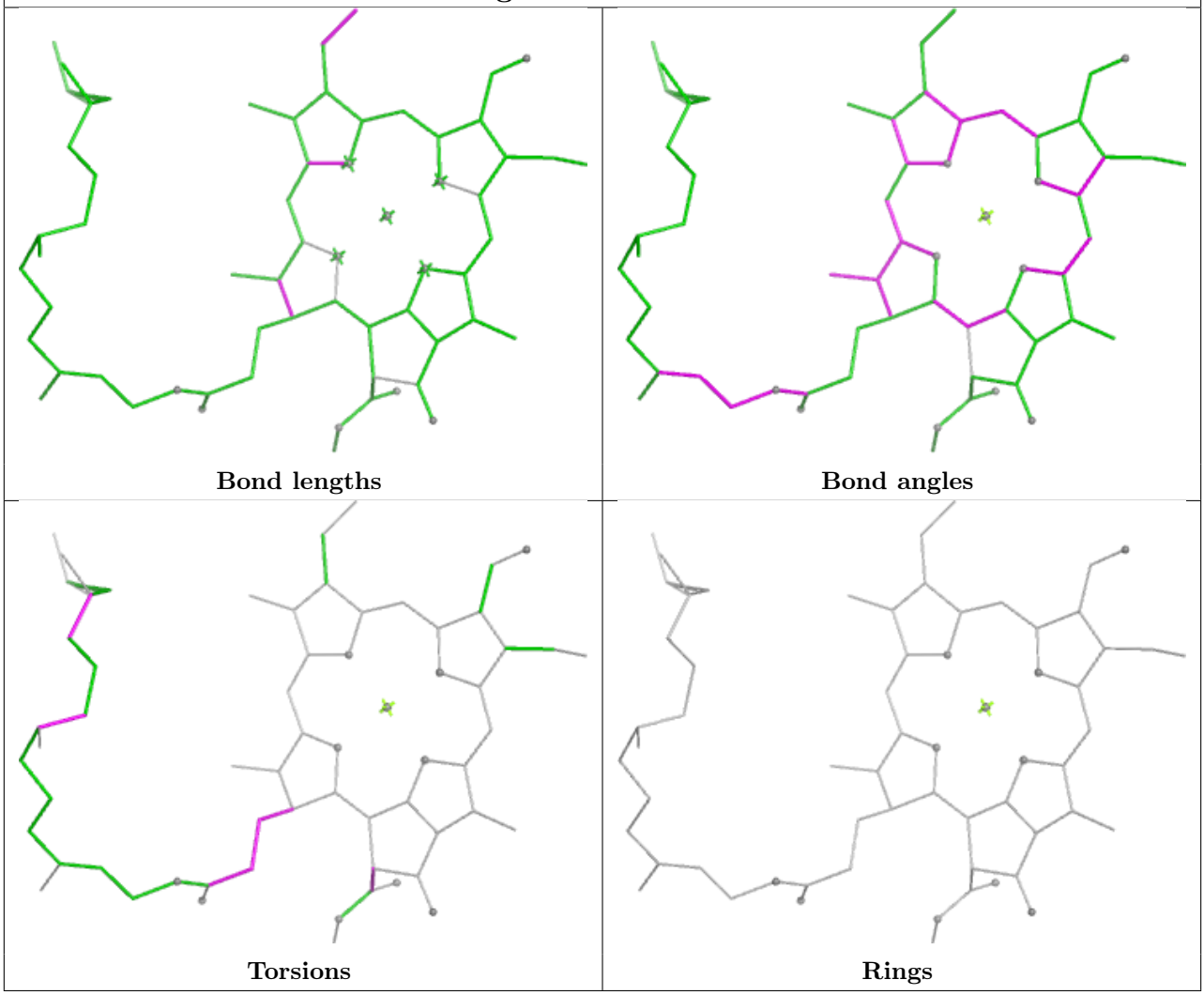
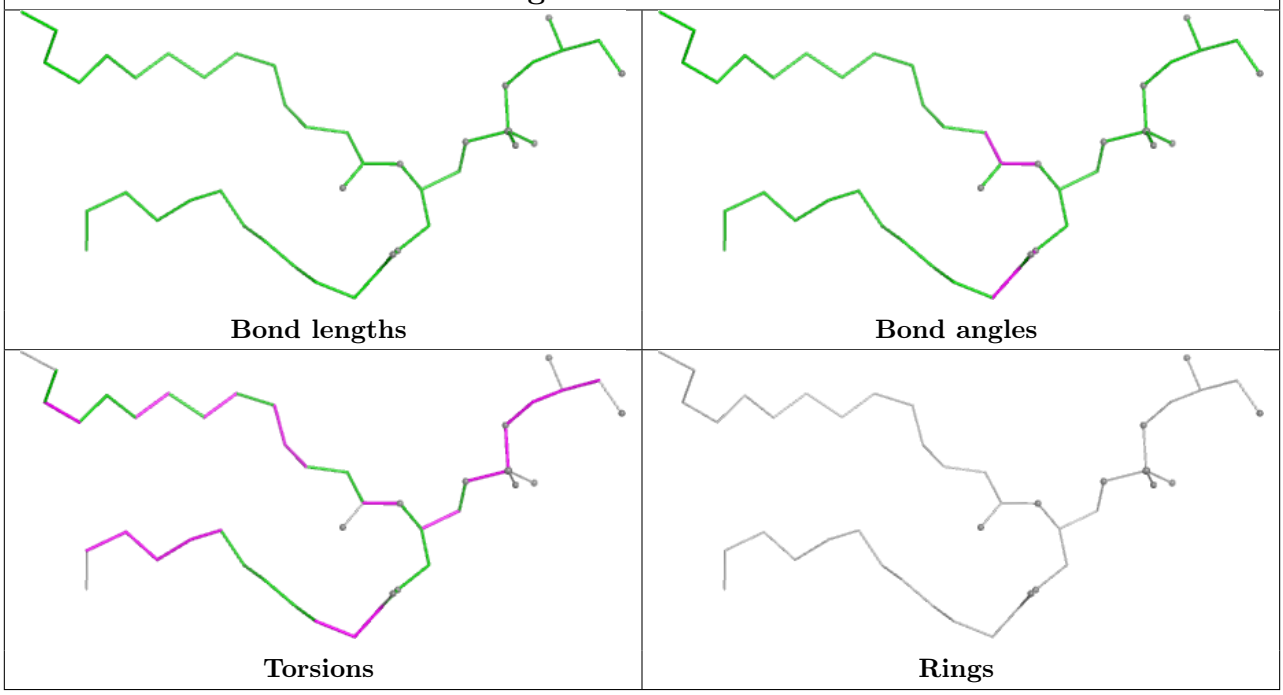
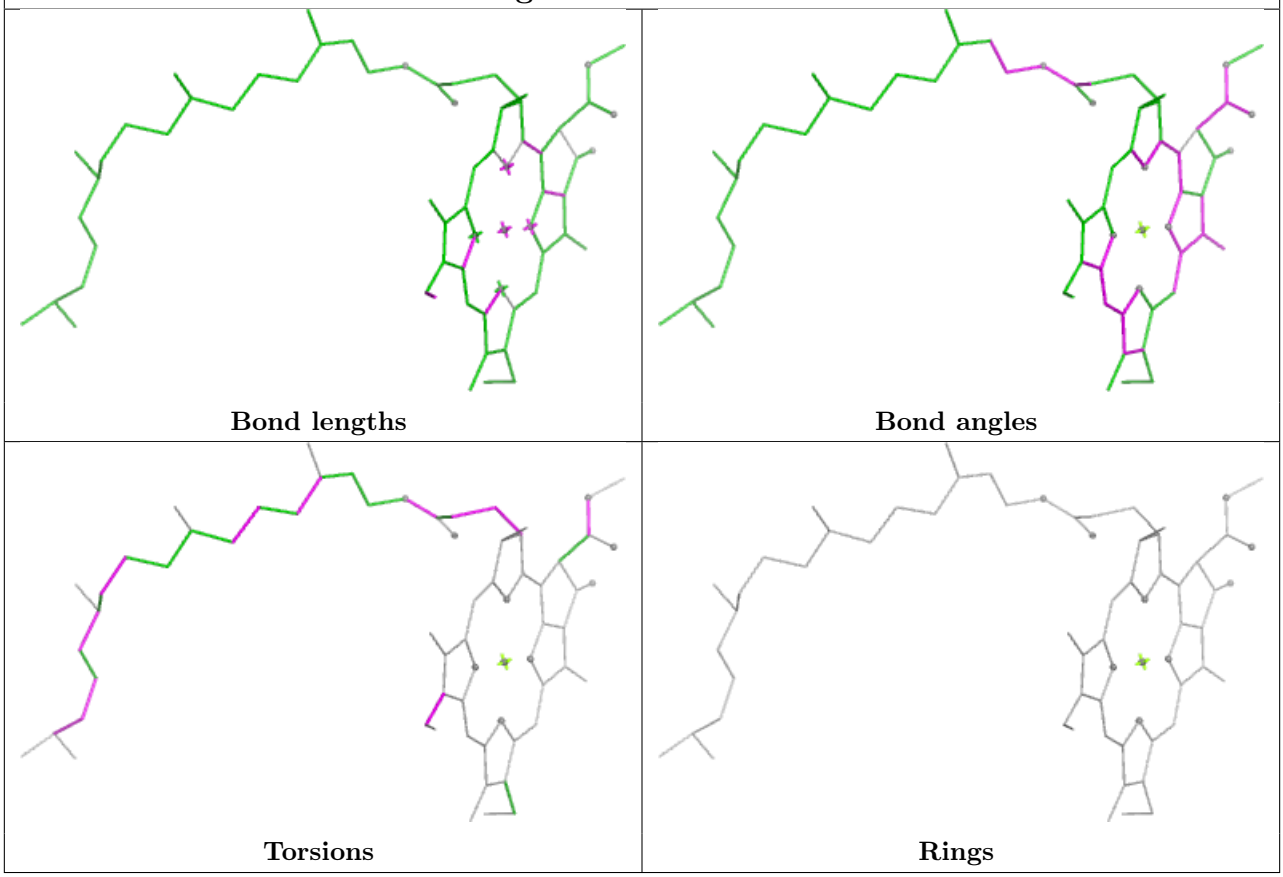


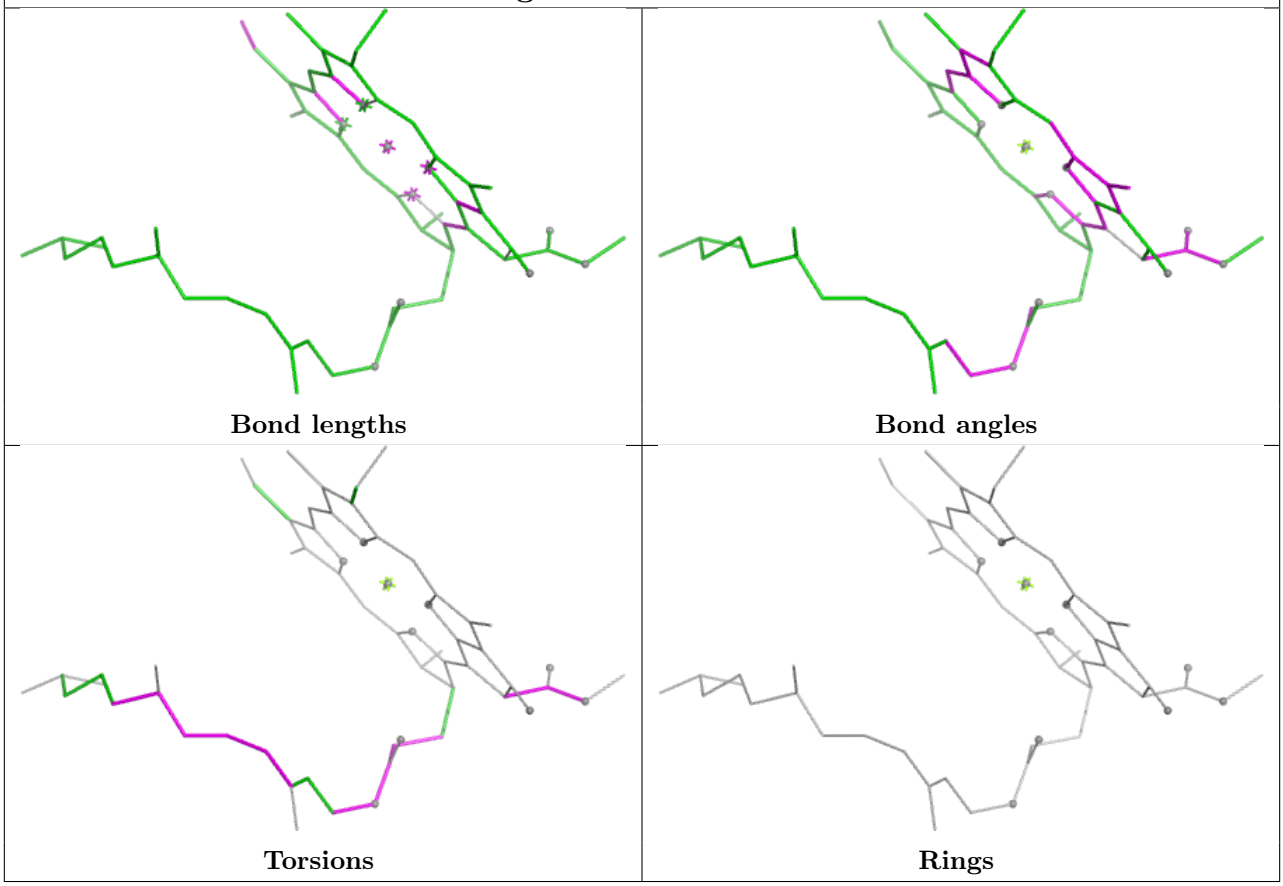
Ligand LHG 1 801



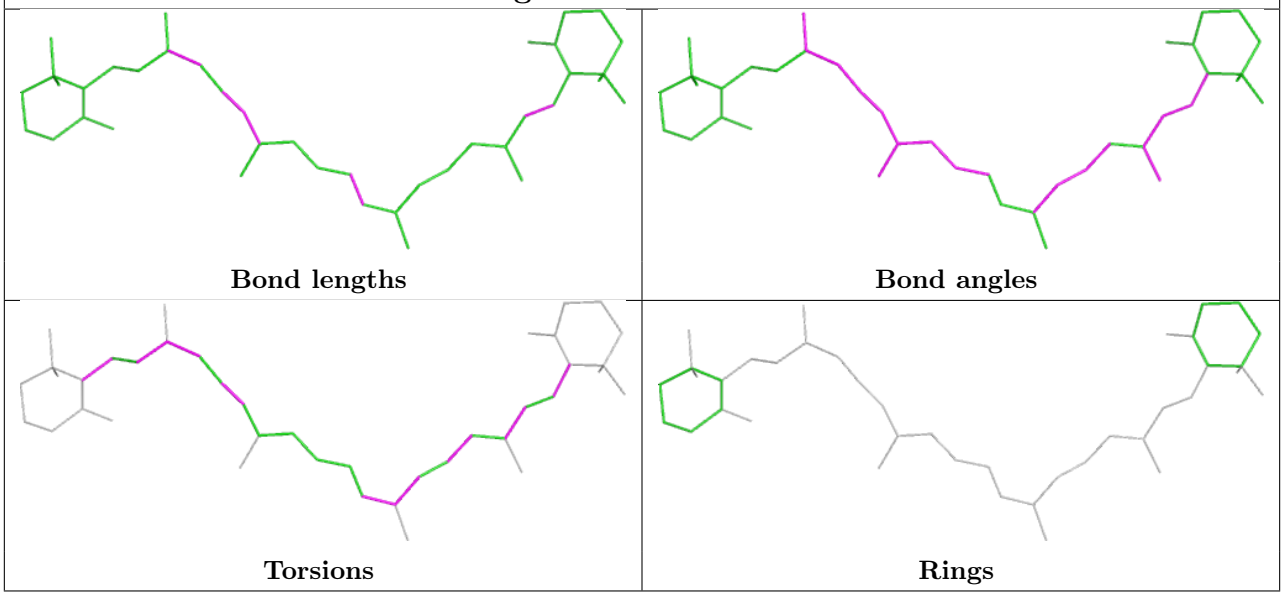
Ligand CLA A 1133

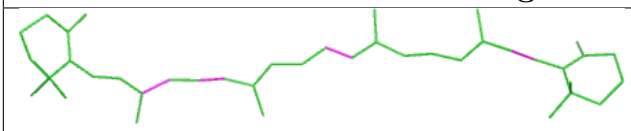
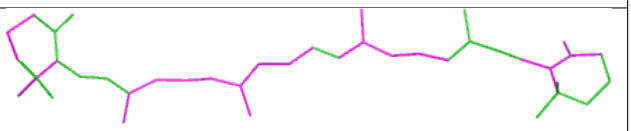
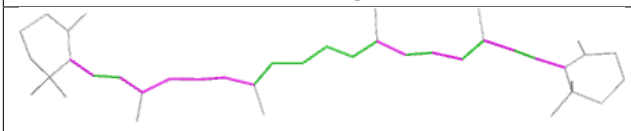
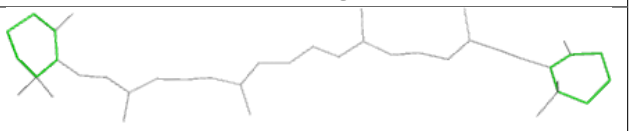


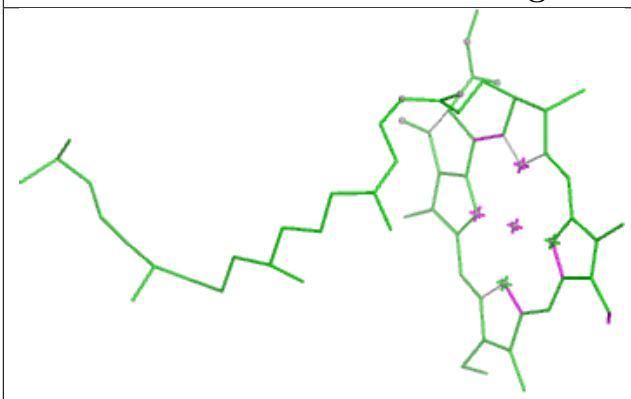
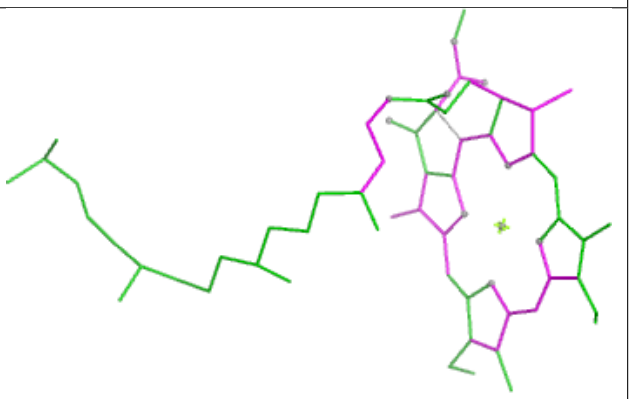
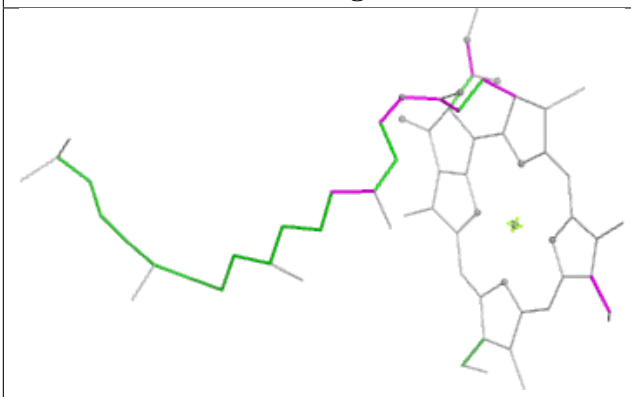
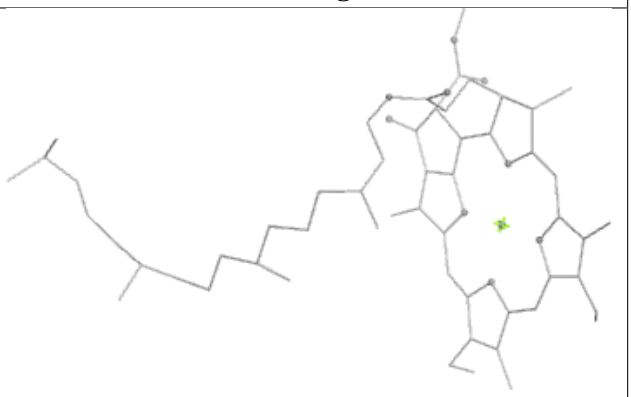
Ligand CLA B 1211



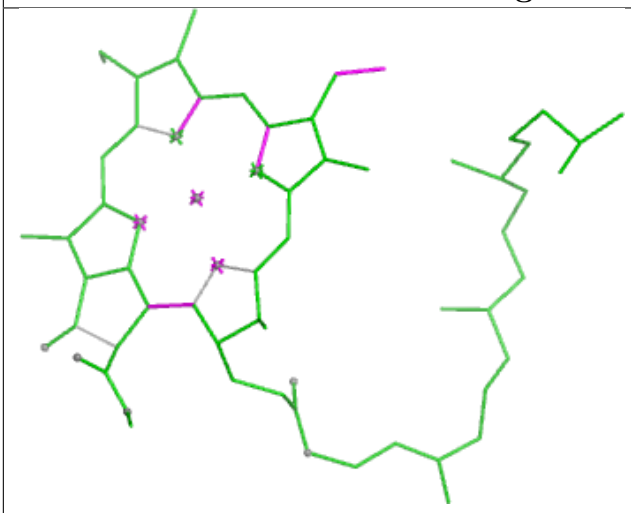
Ligand BCR A 4005



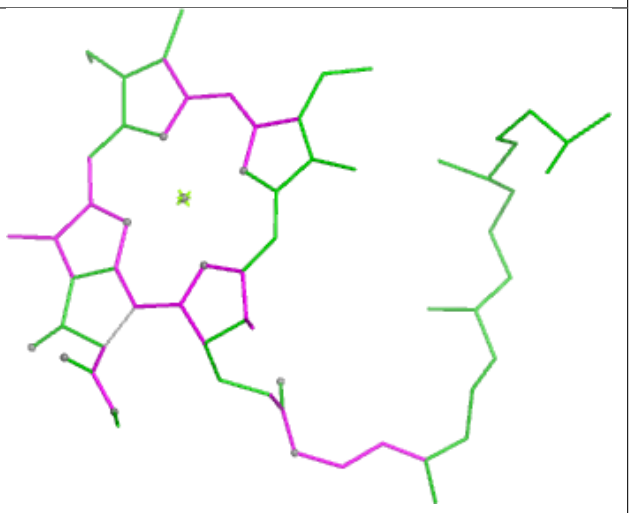
Ligand BCR J 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

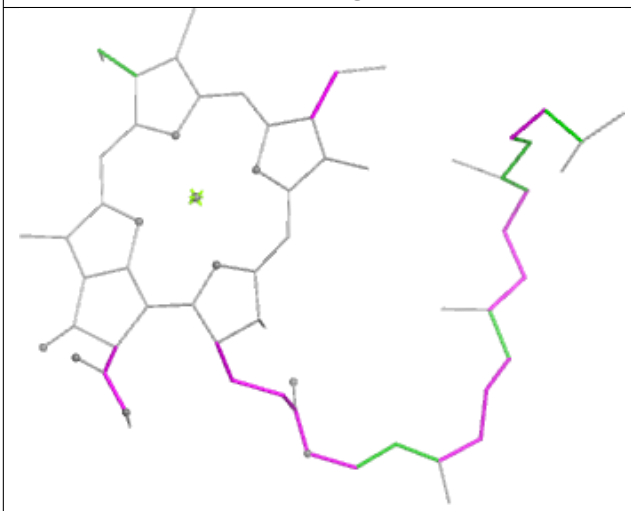
Ligand CLA B 1220



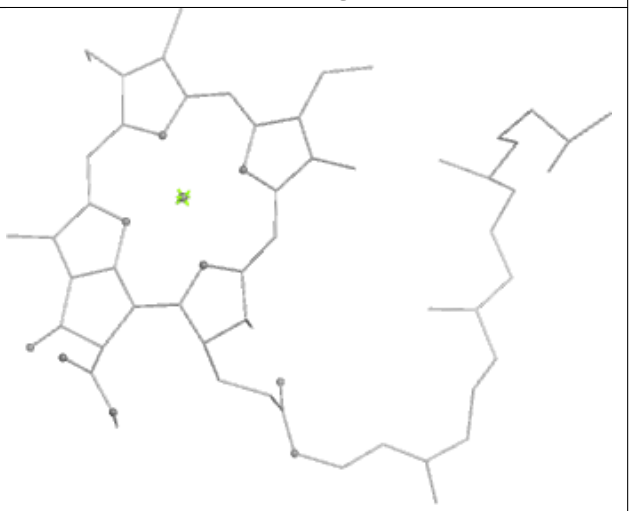
Bond lengths



Bond angles

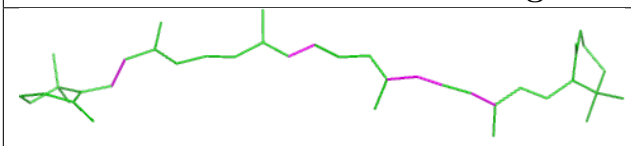


Torsions

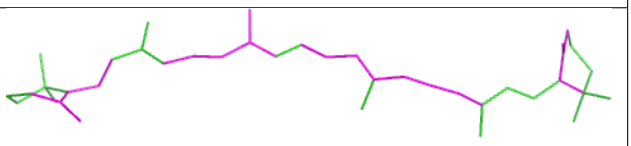


Rings

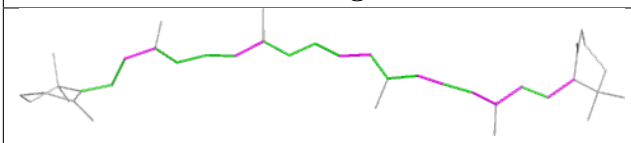
Ligand BCR 3 504



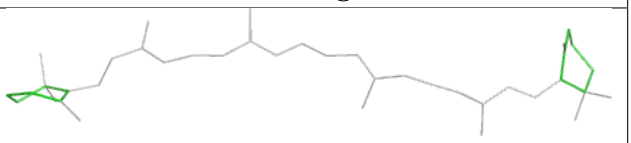
Bond lengths



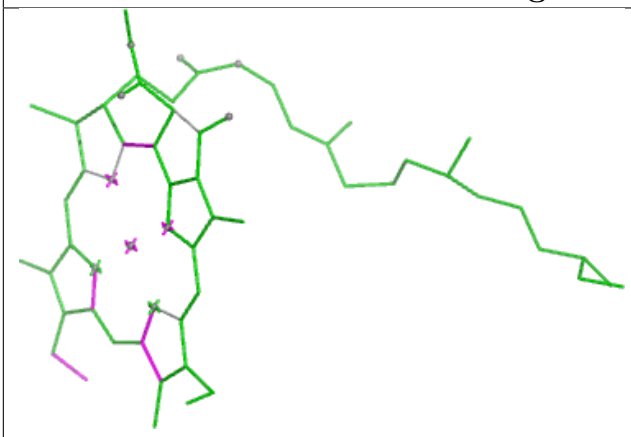
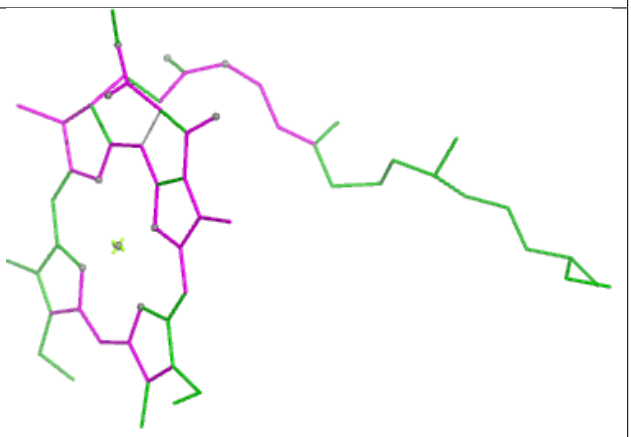
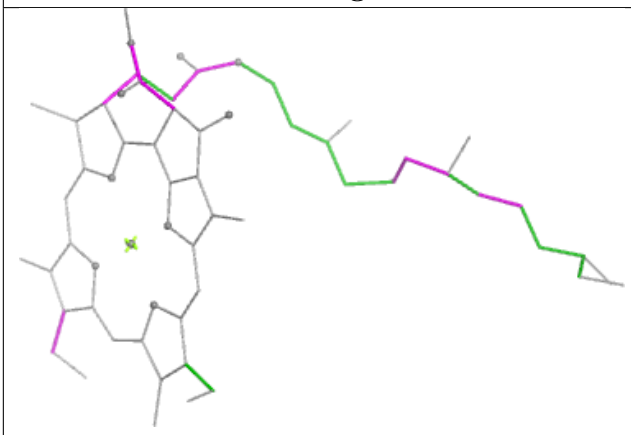
Bond angles



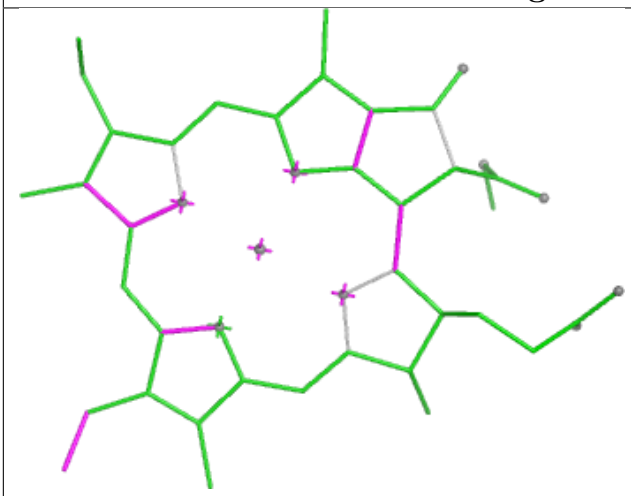
Torsions



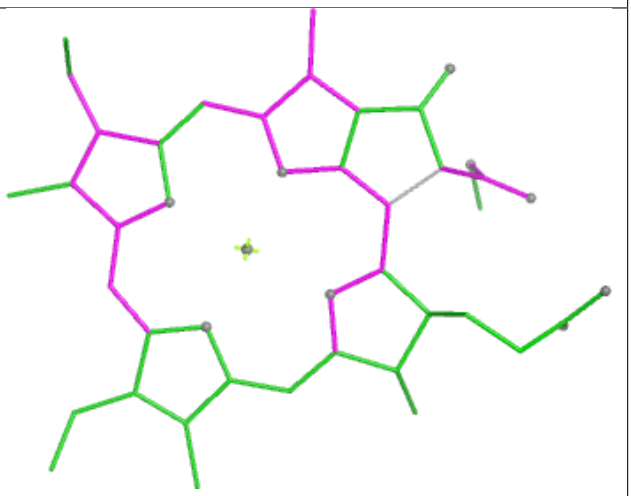
Rings

Ligand CLA 5 607	
 Bond lengths	 Bond angles
 Torsions	Rings

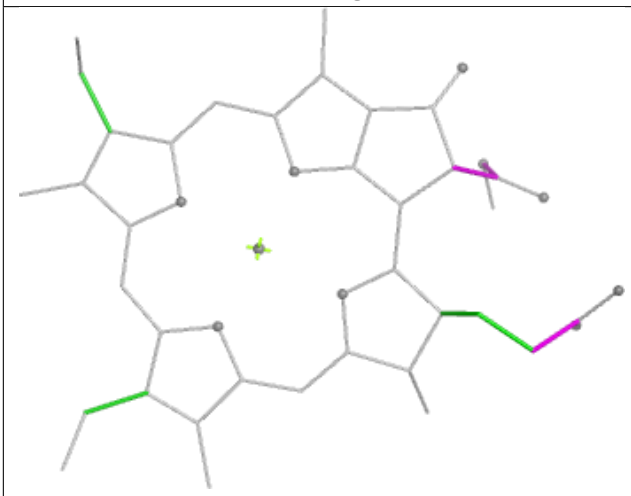
Ligand CLA 1 602



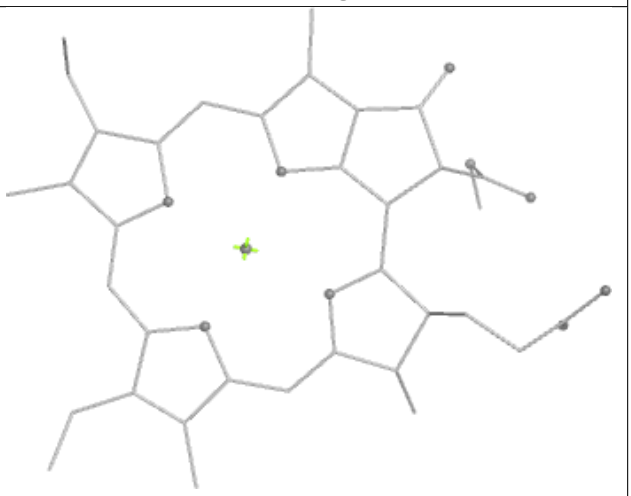
Bond lengths



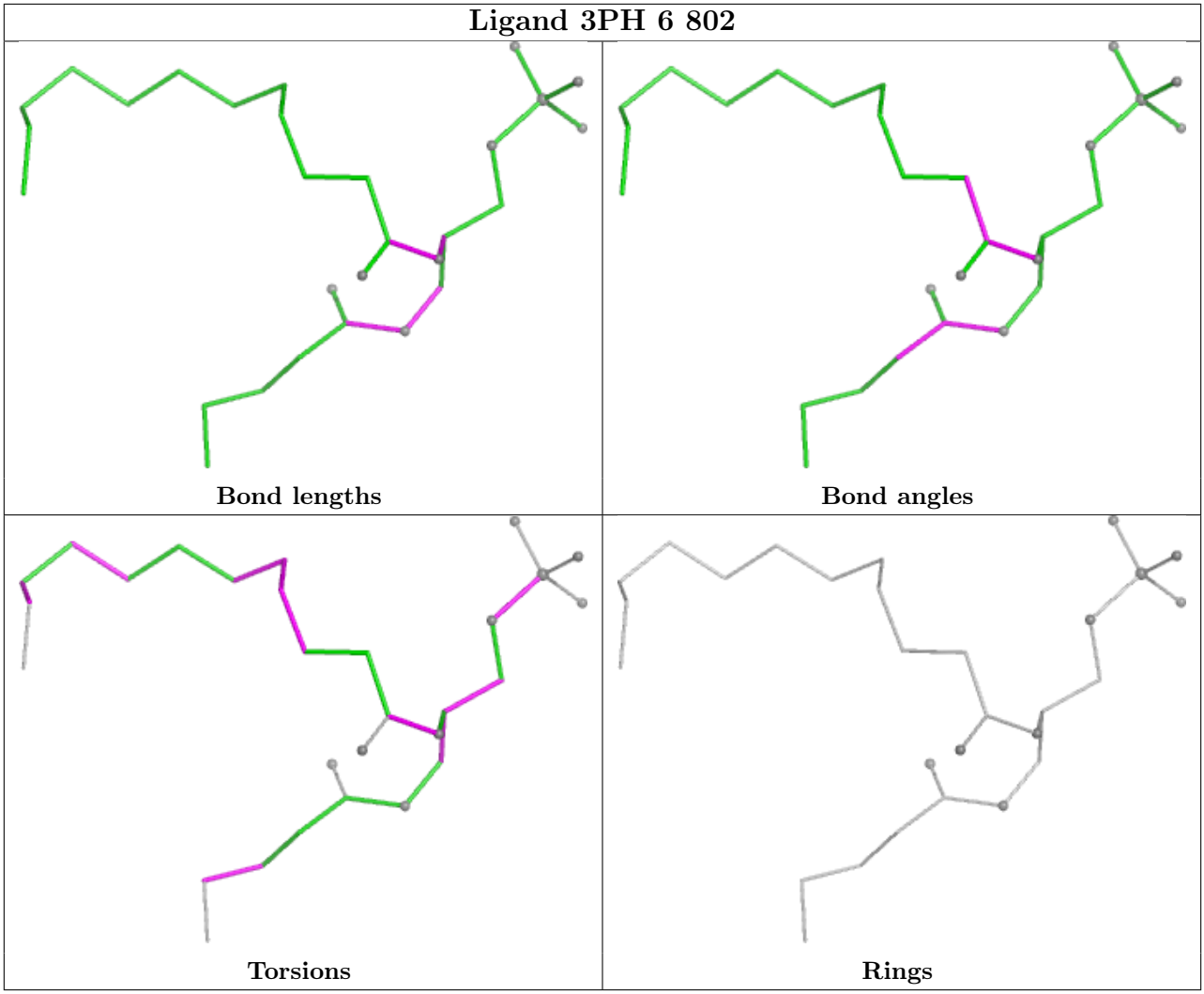
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	143:THR	C	156:VAL	N	16.29

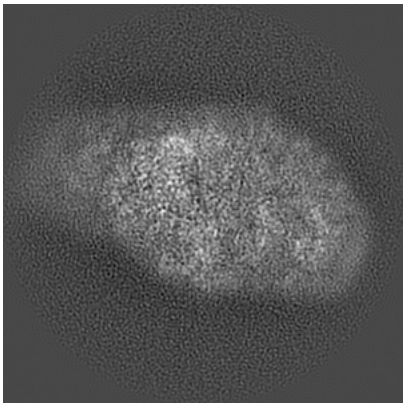
6 Map visualisation (i)

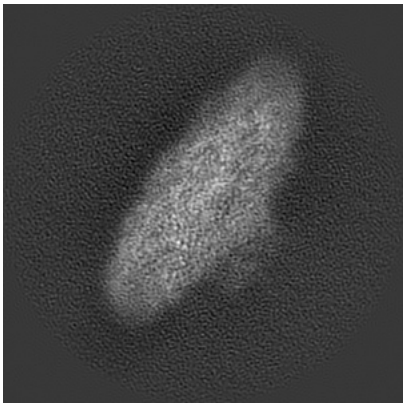
This section contains visualisations of the EMDB entry EMD-12227. These allow visual inspection of the internal detail of the map and identification of artifacts.

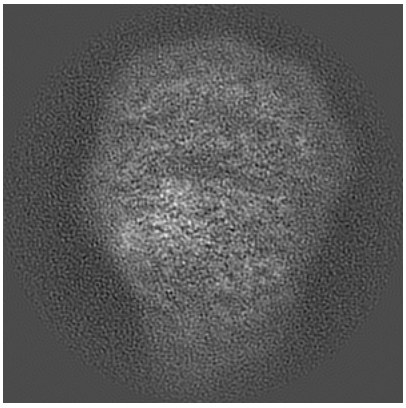
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

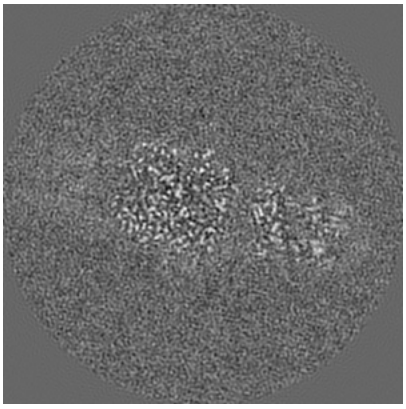

Y

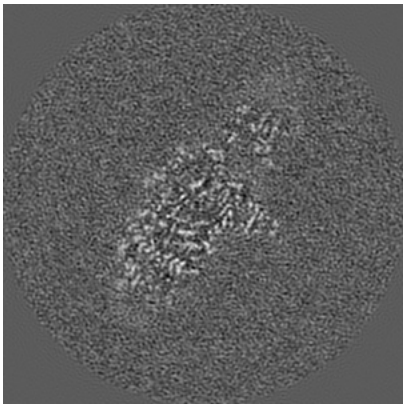

Z

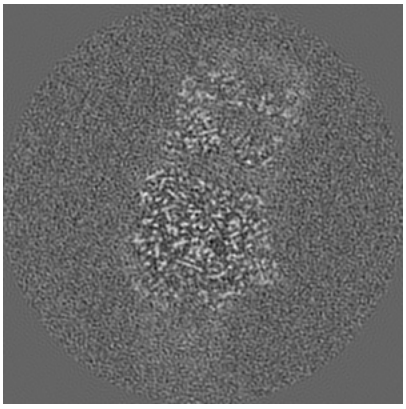
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 160

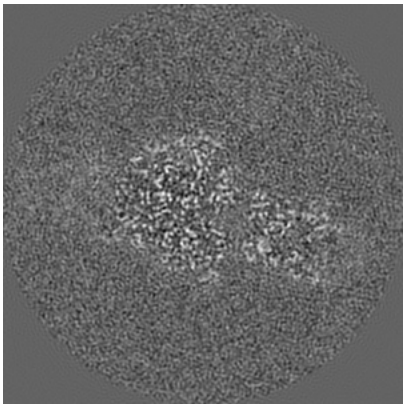

Y Index: 160

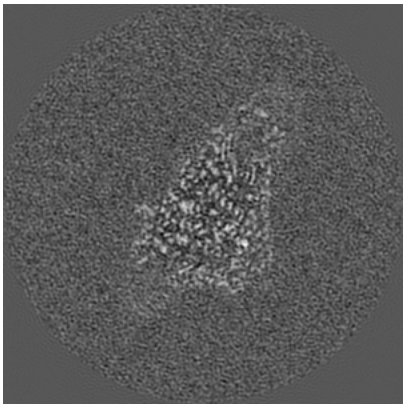

Z Index: 160

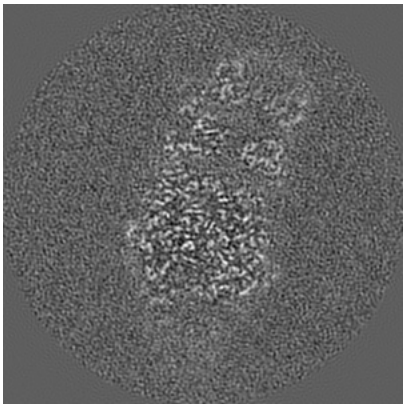
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 147

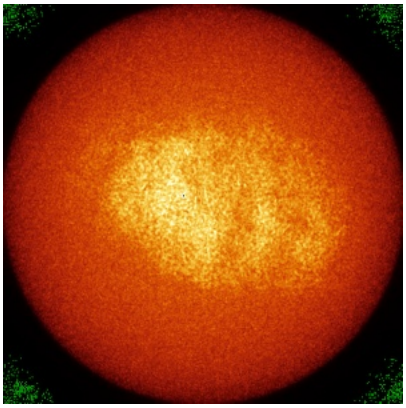

Y Index: 135

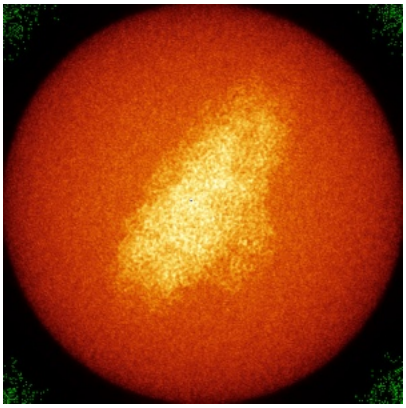

Z Index: 163

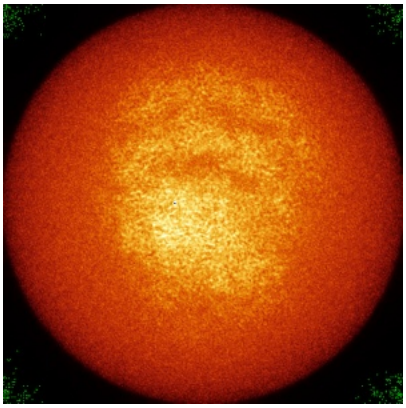
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

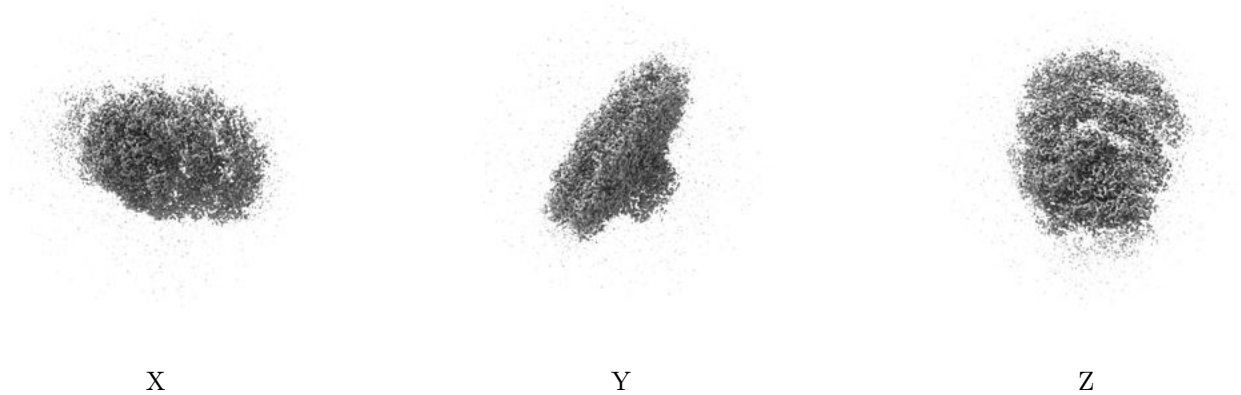

Y


Z

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 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

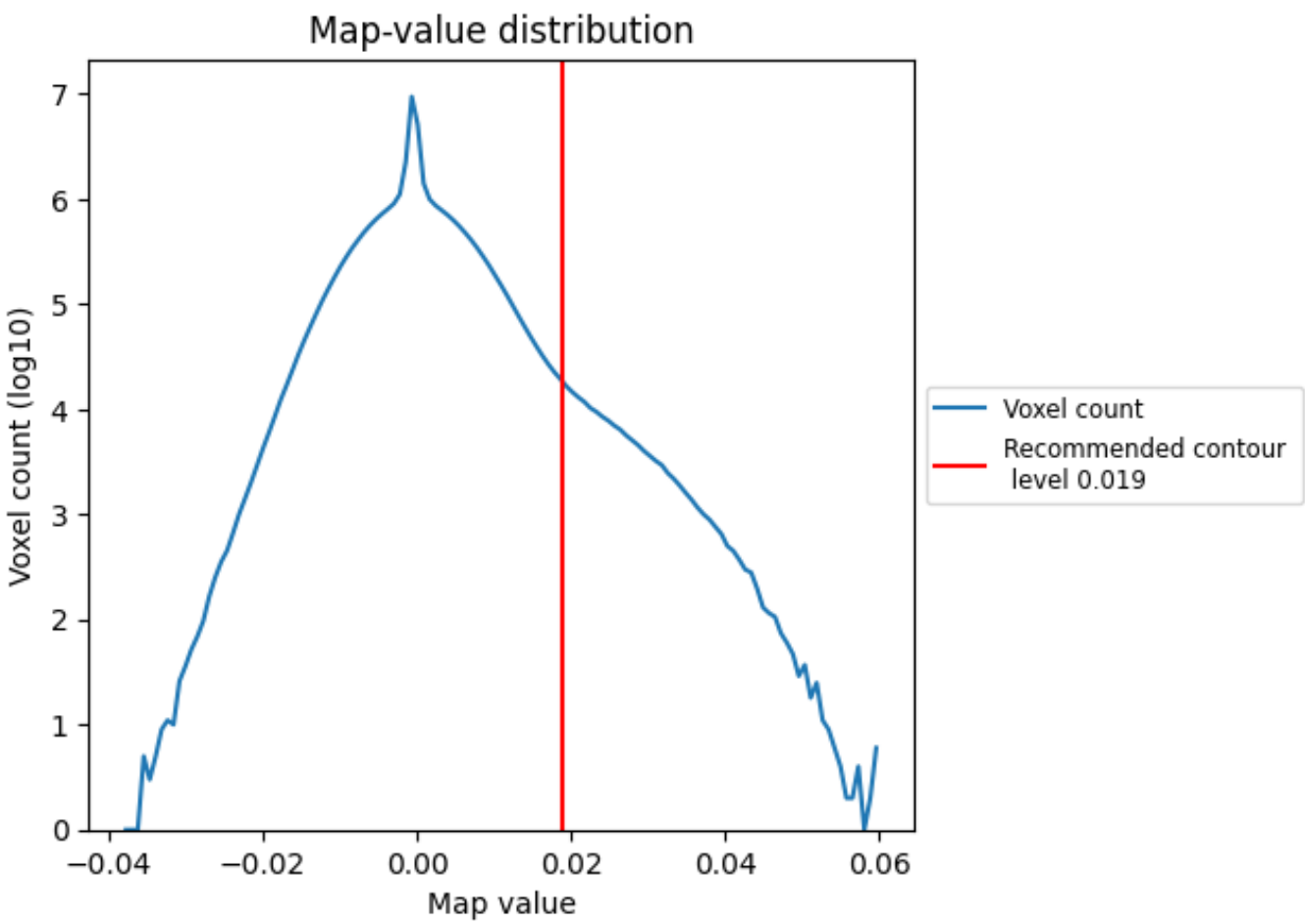
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

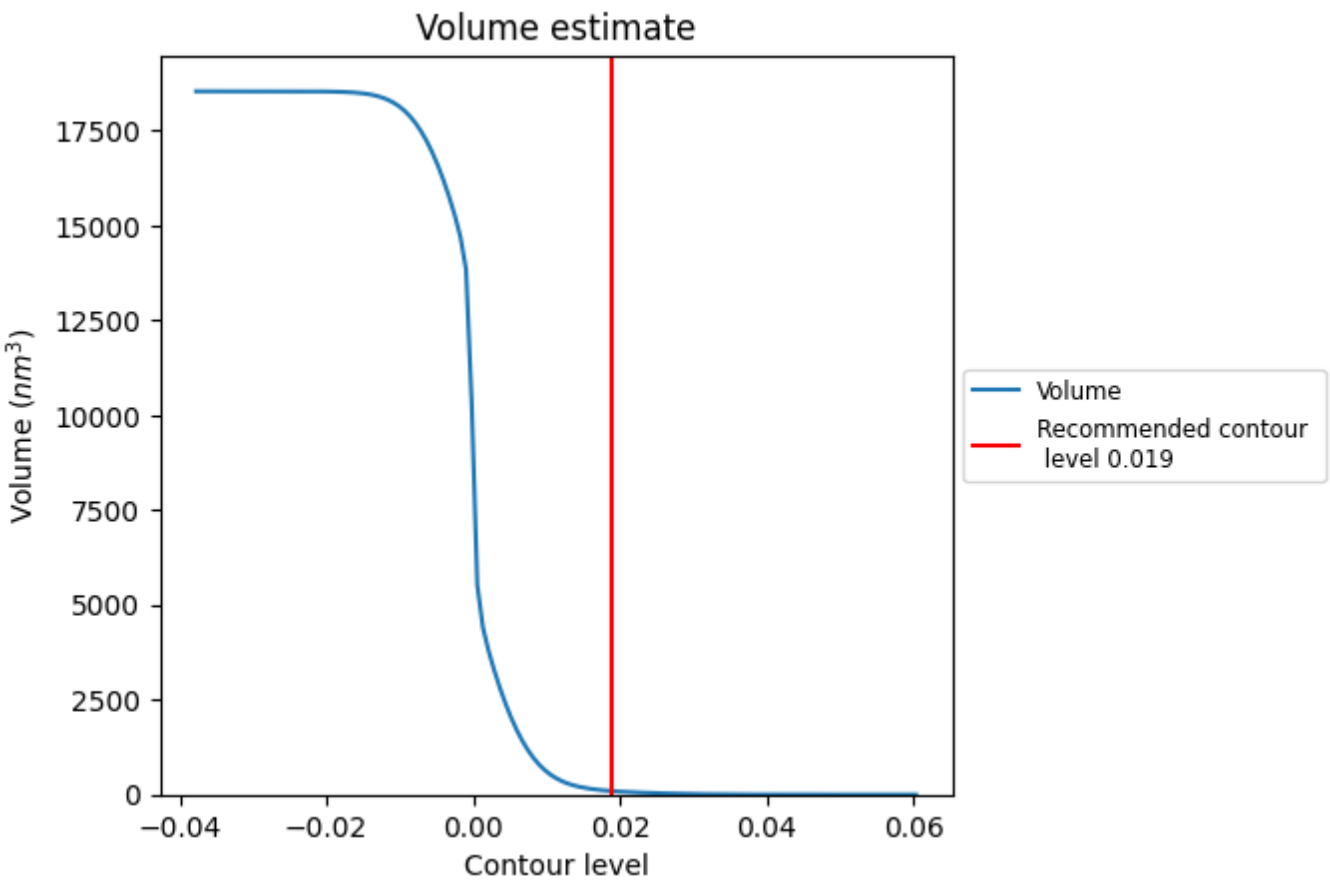
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

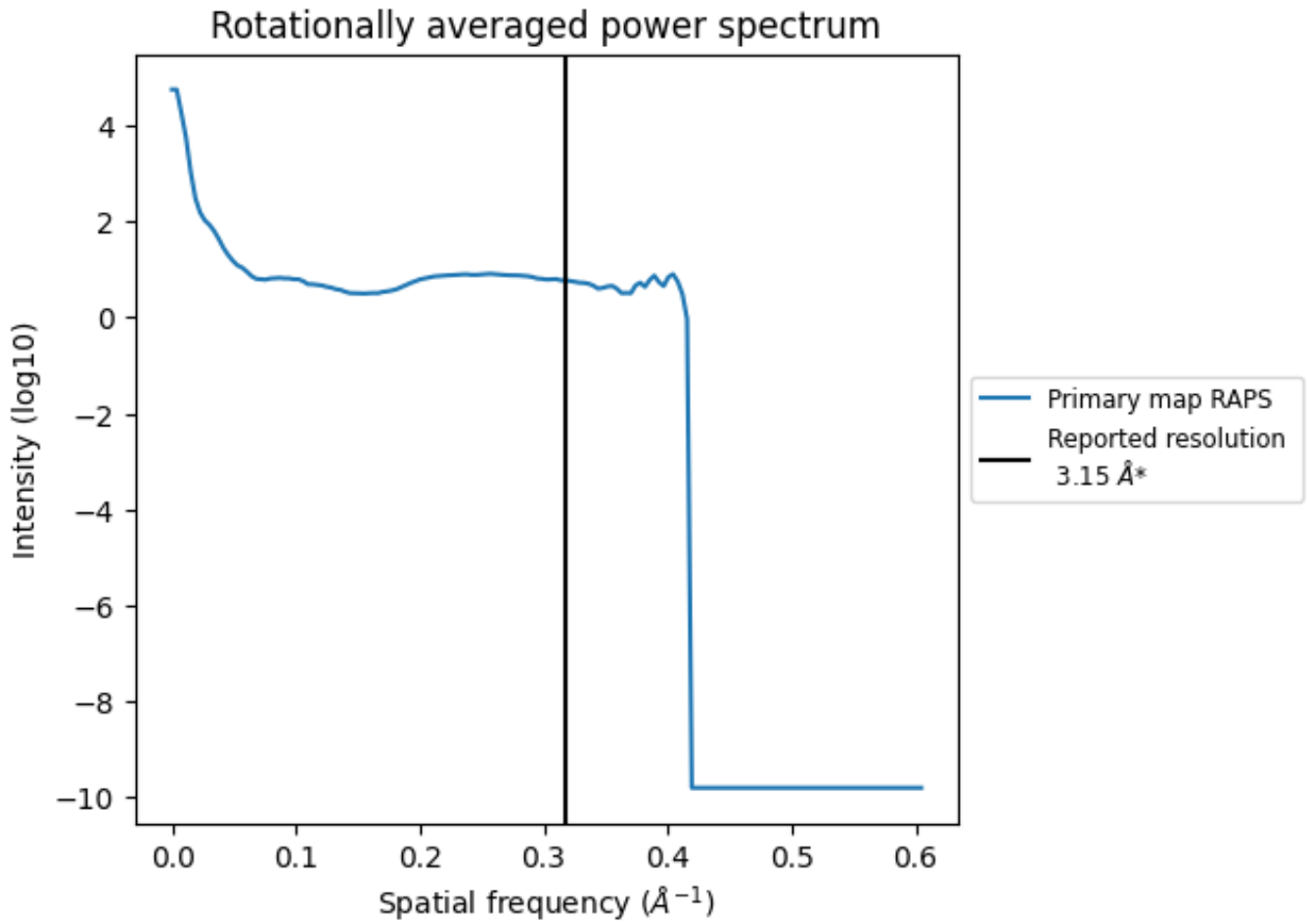
7.2 Volume estimate (i)



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 83 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)

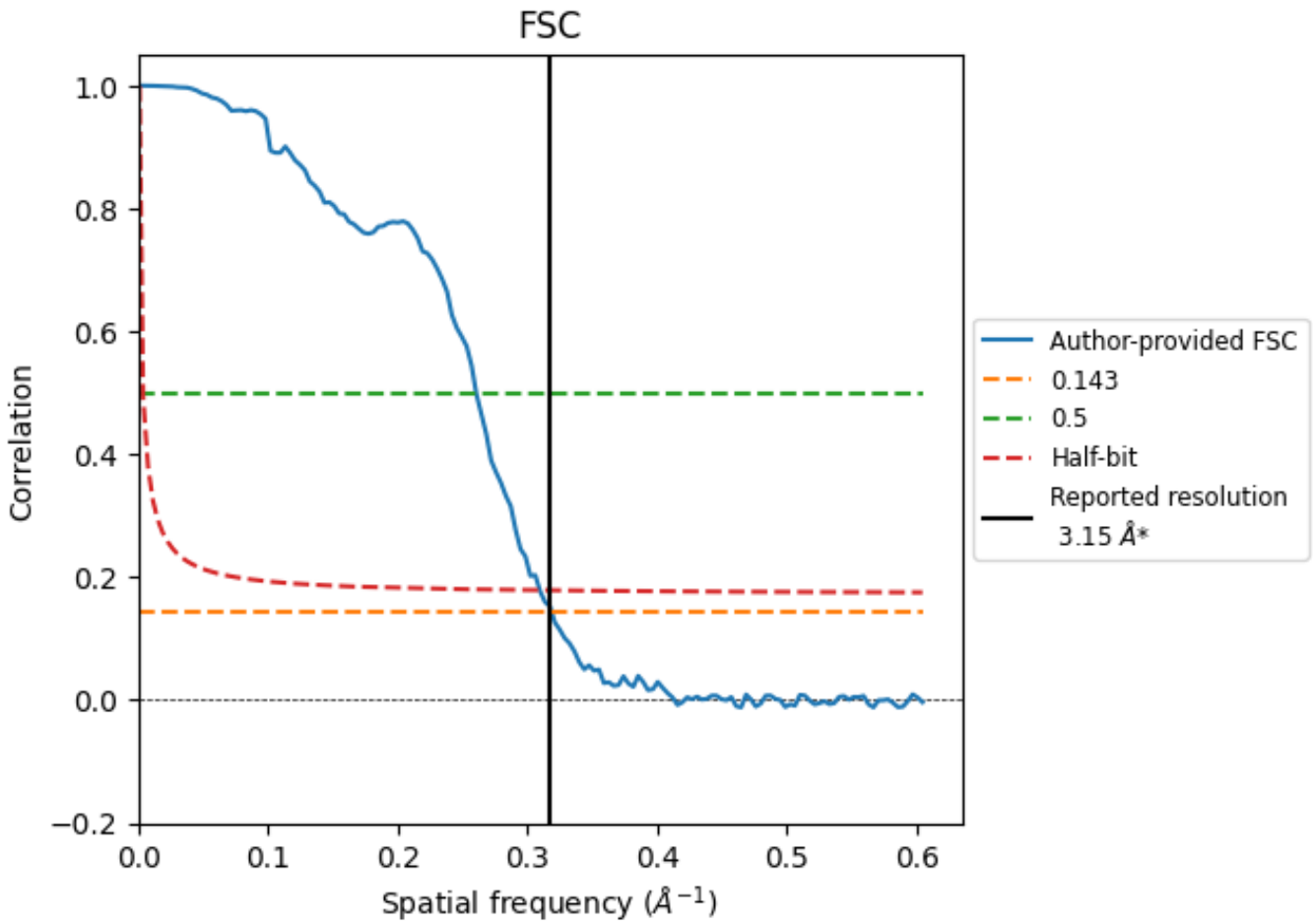


*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8.2 Resolution estimates (i)

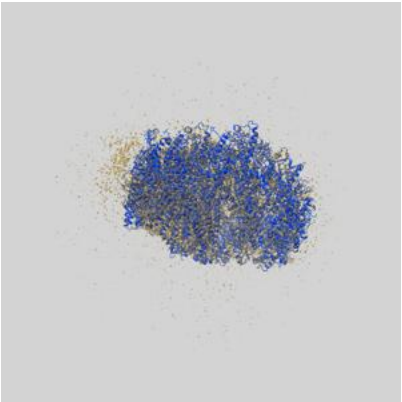
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.14	3.84	3.23
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

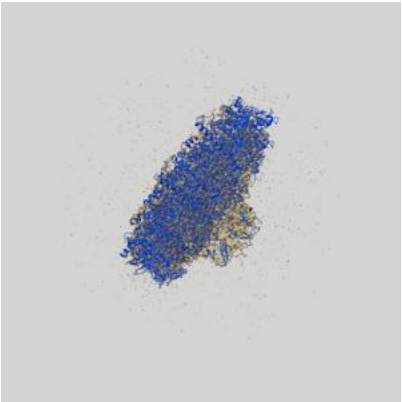
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12227 and PDB model 7BLX. Per-residue inclusion information can be found in section 3 on page 39.

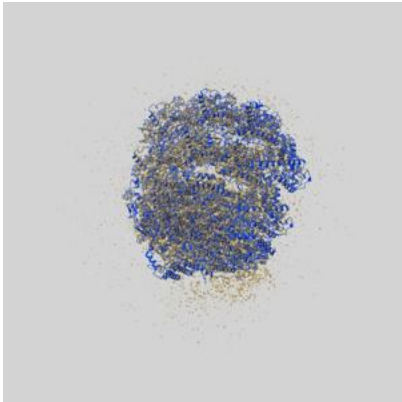
9.1 Map-model overlay (i)



X



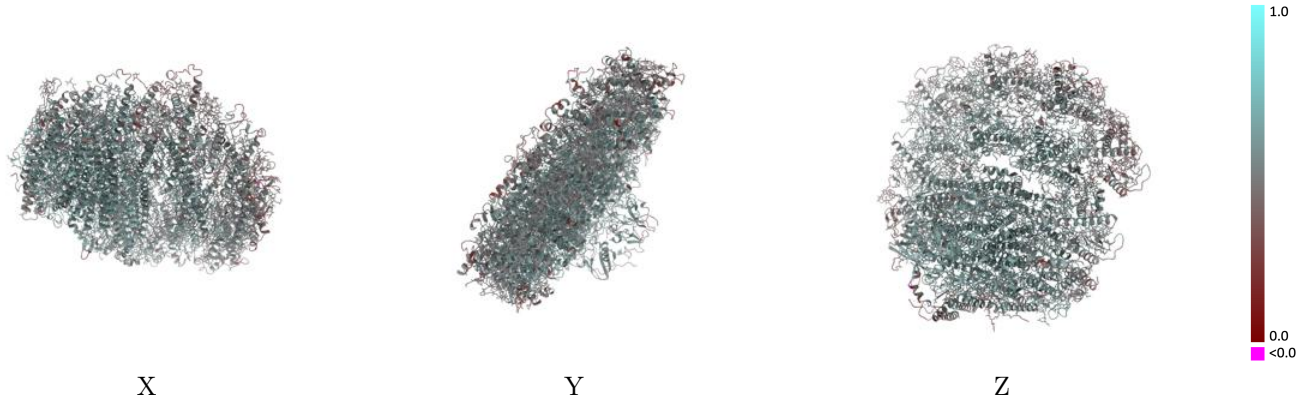
Y



Z

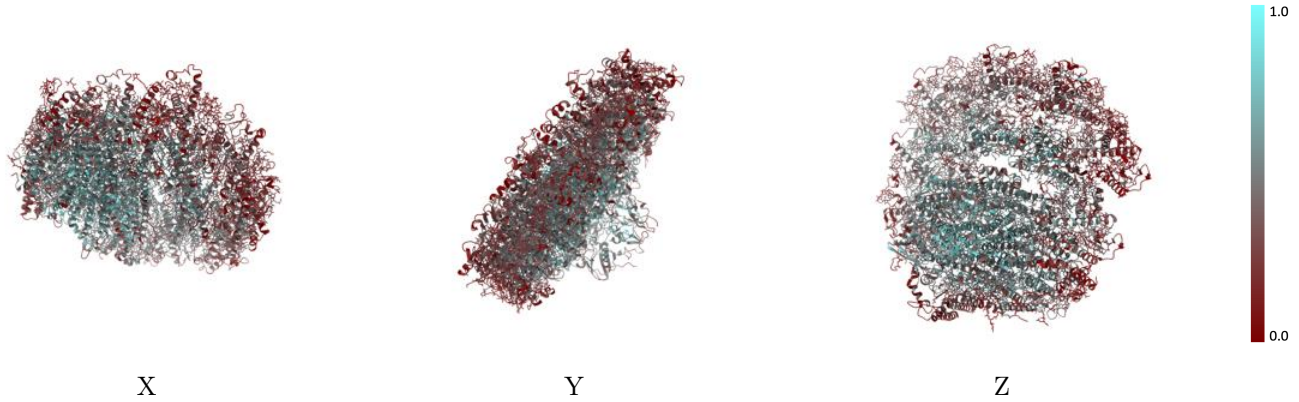
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



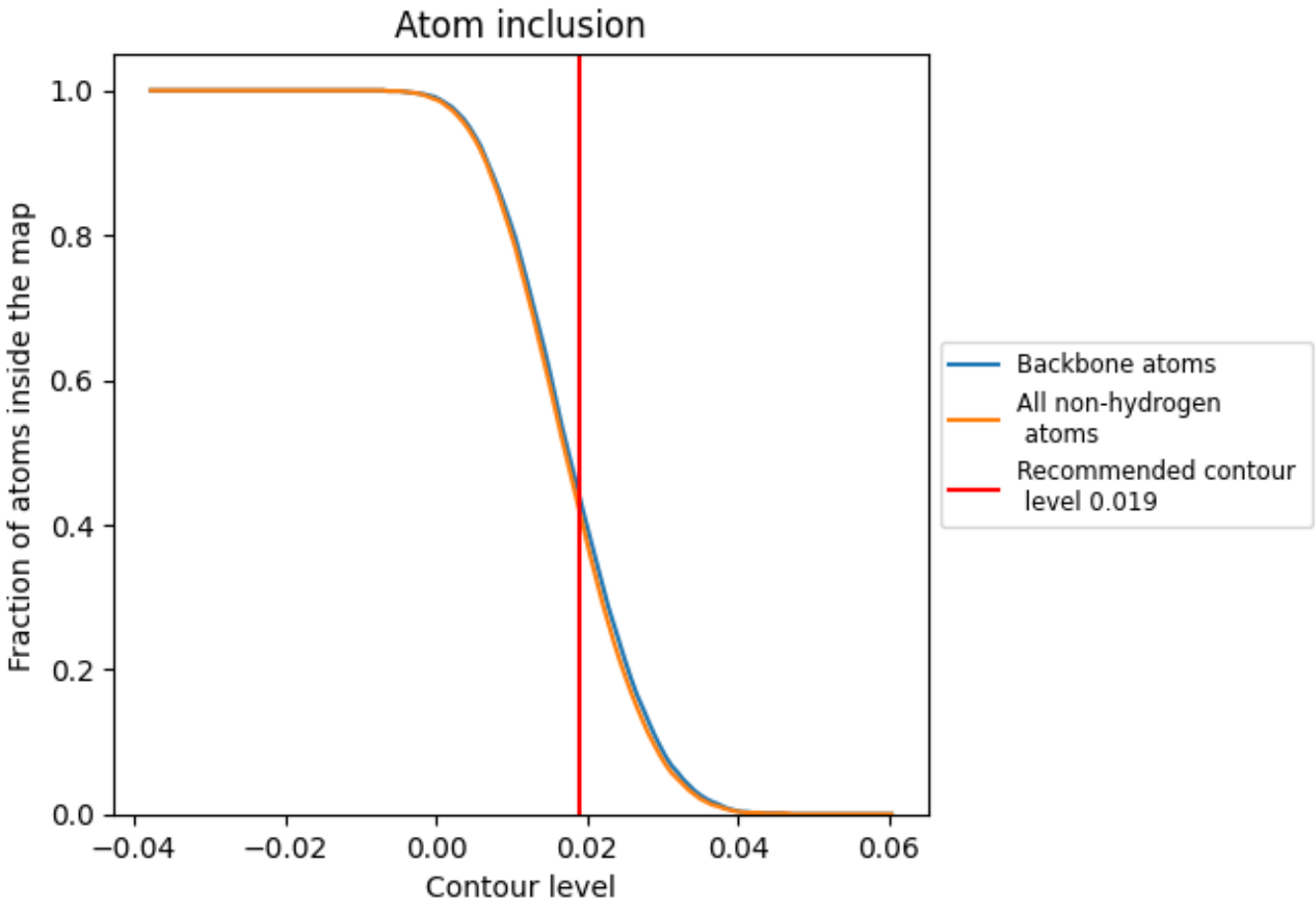
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4190	0.5360
1	0.3530	0.5190
3	0.3980	0.5260
4	0.2400	0.4710
5	0.2730	0.4920
6	0.2620	0.4830
7	0.4720	0.5520
8	0.4530	0.5500
A	0.5670	0.5860
B	0.5320	0.5780
C	0.5820	0.5690
D	0.4130	0.5350
E	0.4900	0.5270
F	0.4540	0.5500
G	0.1450	0.4470
I	0.2720	0.5160
J	0.4710	0.5680
K	0.1890	0.4500
L	0.1900	0.4460
Z	0.1980	0.4510