Full wwPDB EM Validation Report (i)

Sep 10, 2026 – 10:13 pm BST

PDB ID	:	8CMO / pdb_00008cmo
EMDB ID	:	EMD-16732
Title	:	Cryo-EM structure of the Photosystem I - LHCI supercomplex from Coelastrella sp.
Authors	:	Fadeeva, M.; Klaiman, D.; Nelson, N.; Khozin-Goldberg, I.; Zorin, B.
Deposited on	:	2023-02-20
Resolution	:	2.81 Å(reported)

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

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

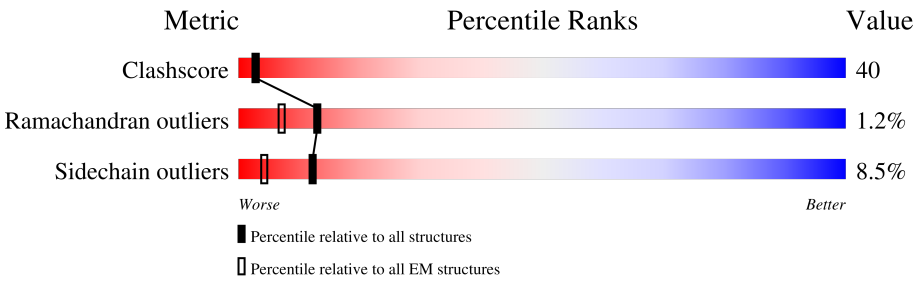
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

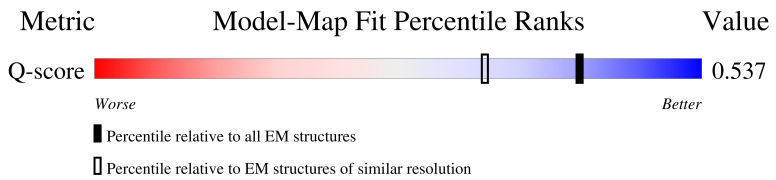
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

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	740	59% 39%
2	B	732	53% 44%
3	C	80	49% 50%
4	D	142	8% 55% 41%

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Mol	Chain	Length	Quality of chain
5	E	61	10% 57% 39%
6	F	165	50% 42% 8%
7	G	93	35% 38% 57% 5%
8	I	41	7% 44% 56%
9	J	40	50% 48%
10	K	89	6% 56% 37% 7%
11	L	123	13% 59% 37%
12	1	194	10% 58% 37% 5%
12	Z	194	41% 53% 44%
13	3	218	48% 46% 6%
14	7	220	55% 40%
15	8	214	49% 41% 9%
16	4	207	8% 50% 46%
17	5	226	53% 42%
18	6	226	46% 51%
19	9	184	23% 53% 41% 5%
20	2	70	63% 43% 51% 6%

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
22	CLA	3	312	-	-	X	-
22	CLA	3	313	-	-	X	-
22	CLA	5	307	-	-	X	-
22	CLA	5	308	-	-	X	-
22	CLA	6	309	-	-	X	-
22	CLA	8	305	-	-	X	-
22	CLA	A	812	-	-	X	-
22	CLA	A	814	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	816	-	-	X	-
22	CLA	A	821	-	-	X	-
22	CLA	A	822	-	-	X	-
22	CLA	A	823	-	-	X	-
22	CLA	B	811	-	-	X	-
22	CLA	B	812	X	-	-	-
22	CLA	B	815	-	-	X	-
22	CLA	B	825	-	-	X	-
22	CLA	B	827	-	-	X	-
22	CLA	B	842	-	-	X	-
22	CLA	F	304	-	-	X	-
22	CLA	Z	303	-	-	X	-
22	CLA	Z	309	-	-	X	-
22	CLA	Z	313	-	-	X	-
24	BCR	3	304	-	X	-	-
24	BCR	3	307	-	X	-	-
24	BCR	4	804	-	-	X	-
24	BCR	6	306	-	X	-	-
24	BCR	A	844	-	-	X	-
24	BCR	A	845	-	X	-	-
24	BCR	A	856	-	X	X	-
24	BCR	B	846	-	X	-	-
24	BCR	B	848	-	X	-	-
24	BCR	B	853	-	X	-	-
29	SF4	B	802	-	-	X	-
29	SF4	C	101	-	-	X	-
29	SF4	C	102	-	-	X	-
31	DGD	3	301	-	-	X	-
37	DAO	K	201	-	-	X	-
38	LUT	Z	301	-	-	X	-
39	CHL	4	816	-	-	X	-
39	CHL	6	315	-	-	X	-
39	CHL	8	315	-	-	X	-
39	CHL	9	312	-	-	X	-

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 50057 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	740	5819	3806	991	1000	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5800	3804	973	1005	18	0	0

- Molecule 3 is a protein called Photosystem I subunit VII PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	603	370	105	116	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	142	1129	724	196	204	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	61	484	309	83	92	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1265	813	219	230	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	93	690	440	116	131	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	41	308	210	44	53	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	40	319	217	47	54	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	89	617	390	110	115	2	0	0

- Molecule 11 is a protein called Photosystem I reaction centre subunit XI PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	123	897	580	148	165	4	0	0

- Molecule 12 is a protein called Light-harvesting protein of photosystem I Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1	194	1457	936	248	265	8	0	0
12	Z	194	1457	936	248	265	8	0	0

- Molecule 13 is a protein called Light-harvesting protein of photosystem I Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	3	218	1695	1107	272	309	7	0	0

- Molecule 14 is a protein called Light-harvesting protein of photosystem I Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	7	220	1705	1102	283	313	7	0	0

- Molecule 15 is a protein called Light-harvesting protein of photosystem I Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	8	214	1602	1032	269	291	10	0	0

- Molecule 16 is a protein called Light-harvesting protein of photosystem I Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	4	207	1598	1036	272	284	6	0	0

- Molecule 17 is a protein called Light-harvesting protein of photosystem I Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5	226	1764	1136	302	318	8	0	0

- Molecule 18 is a protein called Light-harvesting protein of photosystem I Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	6	226	1762	1162	289	303	8	0	0

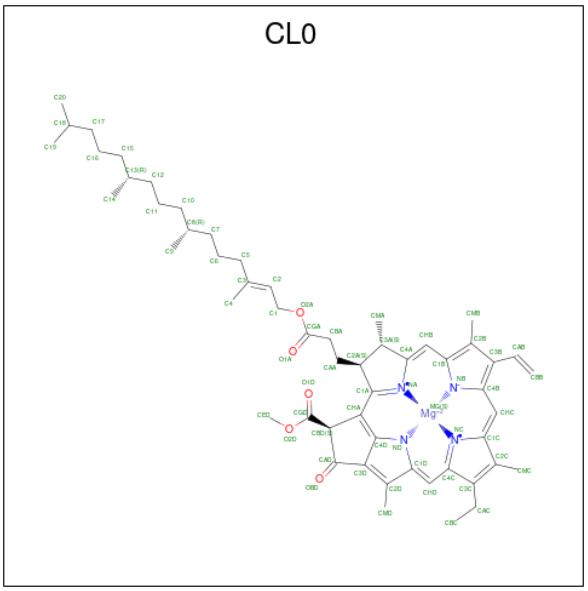
- Molecule 19 is a protein called Light-harvesting protein of photosystem I Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	9	184	1416	914	239	254	9	0	0

- Molecule 20 is a protein called Light-harvesting protein of photosystem I Lhca2 partial.

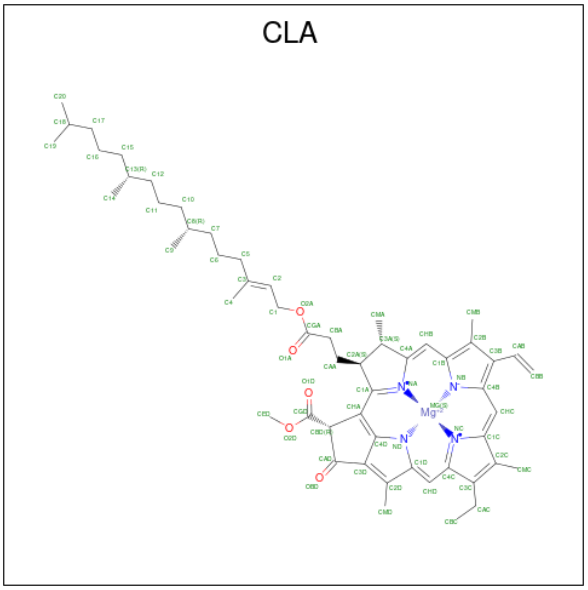
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	2	70	525	336	90	94	5	0	0

- Molecule 21 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	
21	A	1	65	55	1	4	5	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0

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

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	G	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	G	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	K	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	K	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	Z	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	Z	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	8	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	4	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	56	46	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	5	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0

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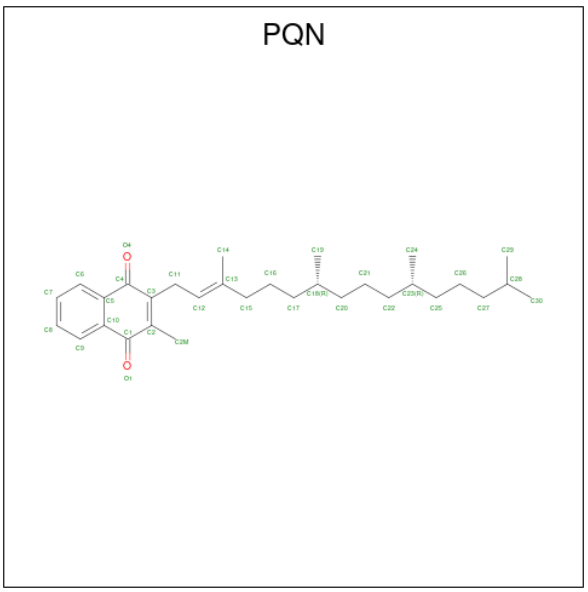
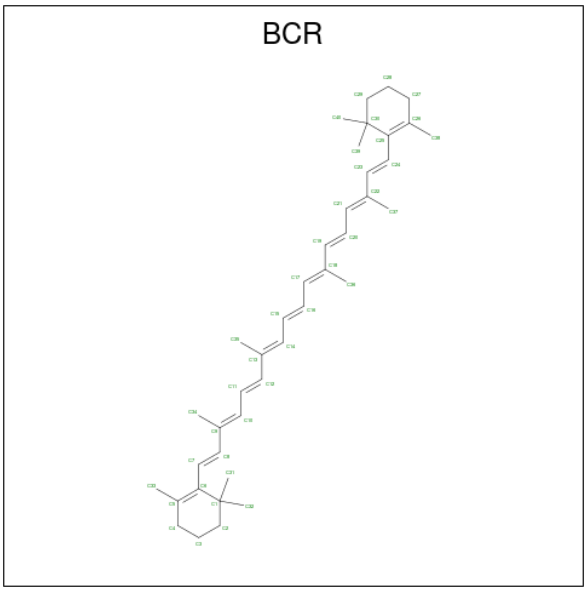
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	2	1	46	36	1	4	5	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms		AltConf
			Total	C	
24	A	1	40	40	0
			Total	C	
24	A	1	40	40	0
			Total	C	
24	A	1	40	40	0
			Total	C	
24	A	1	40	40	0
			Total	C	
24	A	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	B	1	40	40	0
			Total	C	
24	F	1	40	40	0
			Total	C	
24	G	1	40	40	0
			Total	C	
24	I	1	40	40	0
			Total	C	
24	J	1	40	40	0
			Total	C	
24	K	1	40	40	0
			Total	C	
24	L	1	40	40	0
			Total	C	
24	3	1	40	40	0
			Total	C	
24	3	1	40	40	0
			Total	C	
24	3	1	40	40	0

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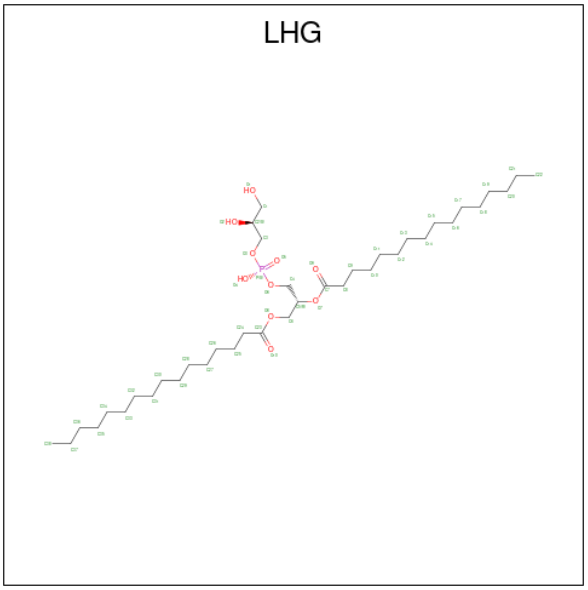
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
24	3	1	40	40	0
			Total	C	
24	7	1	40	40	0
			Total	C	
24	8	1	40	40	0
			Total	C	
24	4	1	40	40	0
			Total	C	
24	5	1	40	40	0
			Total	C	
24	5	1	40	40	0
			Total	C	
24	6	1	40	40	0
			Total	C	
24	6	1	40	40	0

- Molecule 25 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	
25	A	1	35	24	10	1	0
			Total	C	O	P	
25	A	1	49	38	10	1	0
			Total	C	O	P	
25	B	1	33	22	10	1	0

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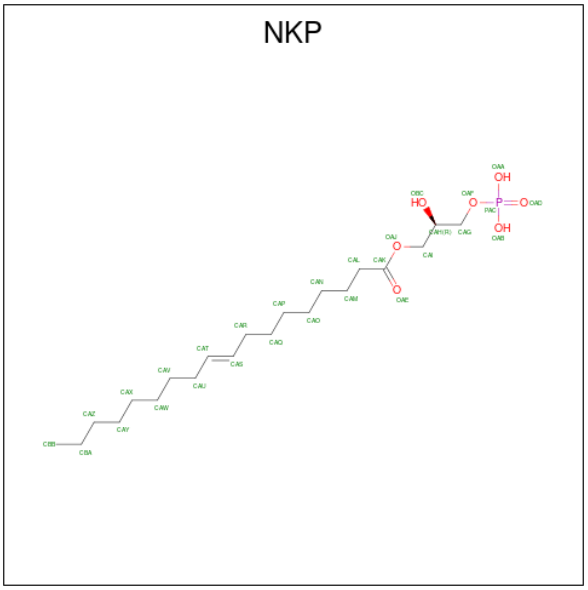
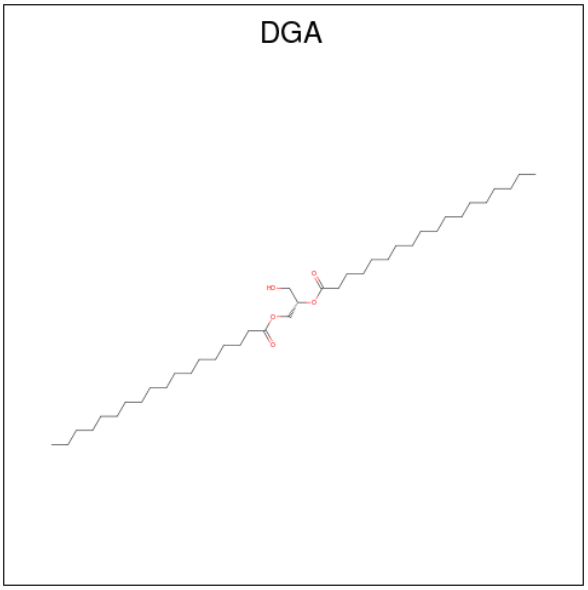
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	B	1	23	12	10	1	0
			Total	C	O	P	
25	B	1	20	9	10	1	0
			Total	C	O	P	
25	1	1	43	32	10	1	0
			Total	C	O	P	
25	Z	1	43	32	10	1	0
			Total	C	O	P	
25	3	1	20	9	10	1	0
			Total	C	O	P	
25	7	1	37	26	10	1	0
			Total	C	O	P	
25	8	1	38	27	10	1	0
			Total	C	O	P	
25	4	1	49	38	10	1	0
			Total	C	O	P	
25	4	1	32	21	10	1	0
			Total	C	O	P	
25	5	1	37	26	10	1	0
			Total	C	O	P	
25	6	1	49	38	10	1	0
			Total	C	O	P	
25	9	1	33	22	10	1	0

- Molecule 26 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: $C_{21}H_{41}O_7P$).



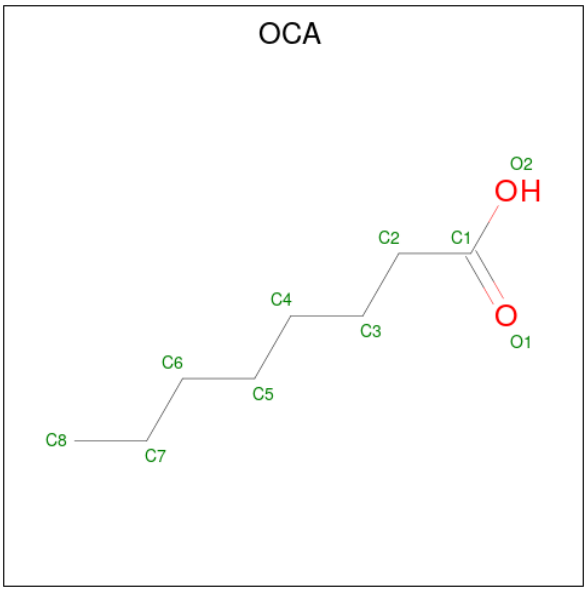
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			23	15	7	1	
26	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 27 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



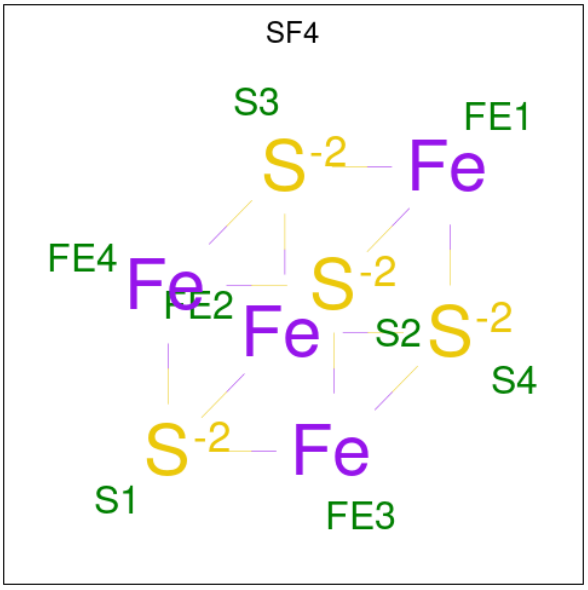
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			40	35	5	

- Molecule 28 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



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

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

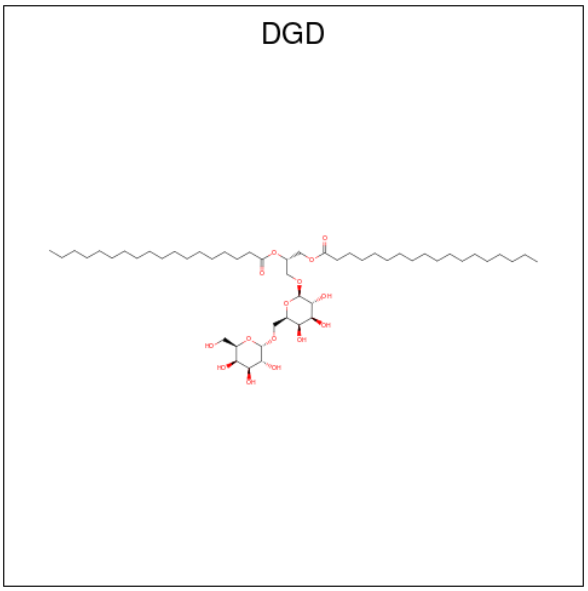


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
29	B	1	8	4	4	0
			Total	Fe	S	
29	C	1	8	4	4	0
			Total	Fe	S	
29	C	1	8	4	4	0

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

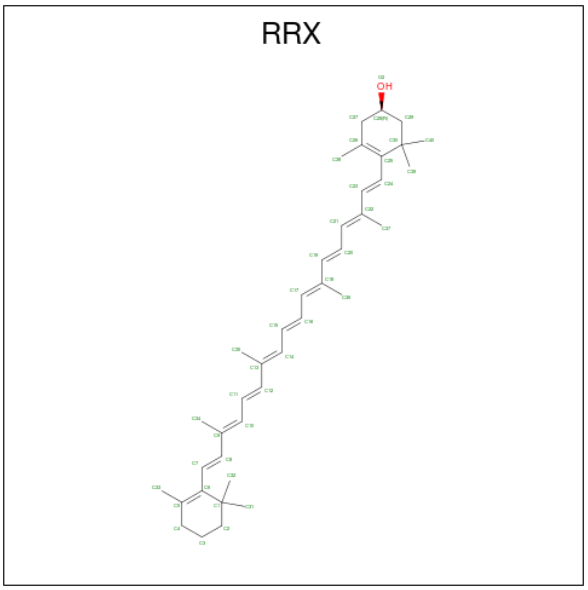
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
30	B	1	1	1	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



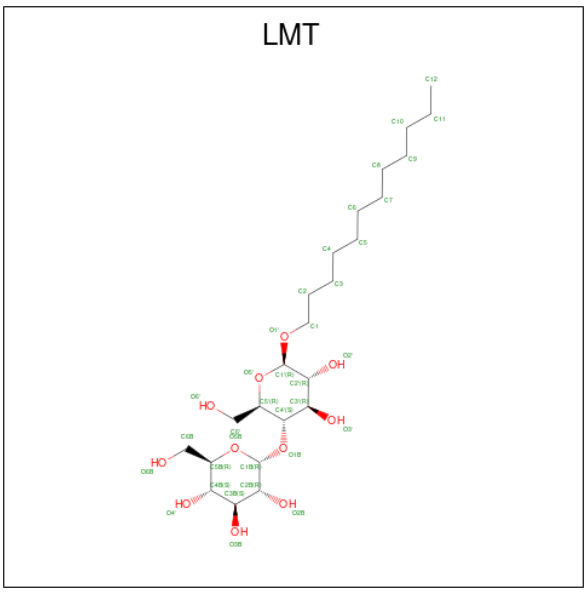
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			61	46	15	
31	1	1	Total	C	O	0
			51	36	15	
31	3	1	Total	C	O	0
			51	36	15	

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



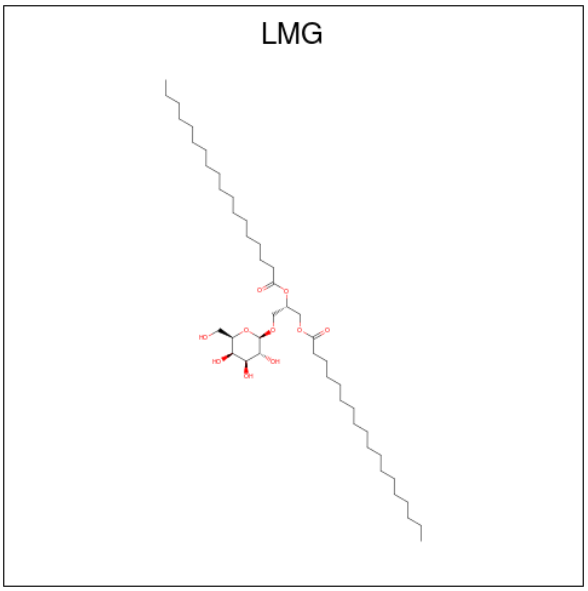
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			41	40	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



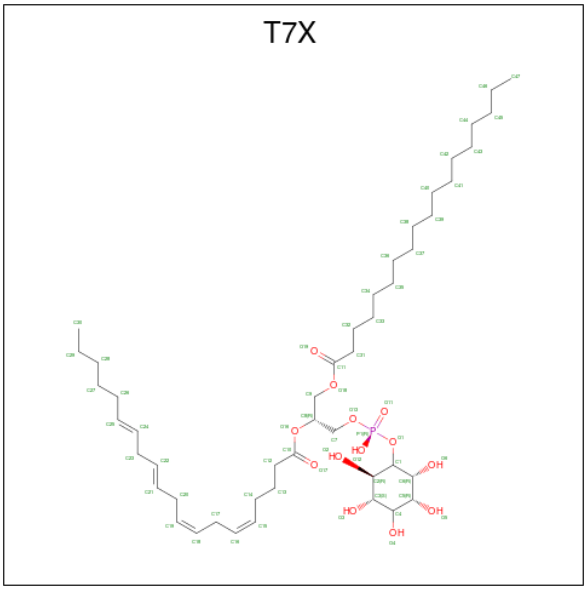
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	F	1	35	24	11	0
			Total	C	O	
33	G	1	35	24	11	0
			Total	C	O	
33	1	1	35	24	11	0
			Total	C	O	
33	4	1	35	24	11	0
			Total	C	O	
33	4	1	35	24	11	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

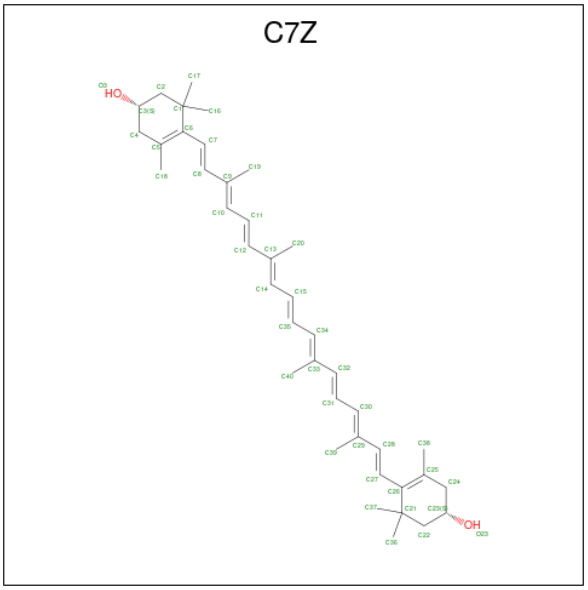
- Molecule 35 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
35	J	1	49	35	13	1	0

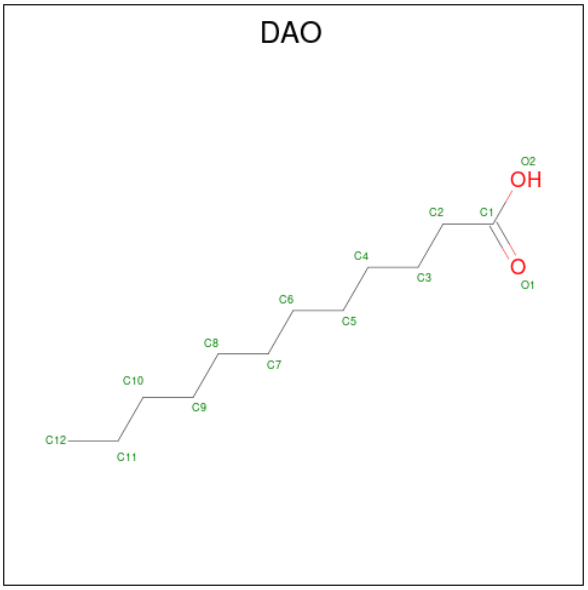
- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},

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: $C_{40}H_{56}O_2$).



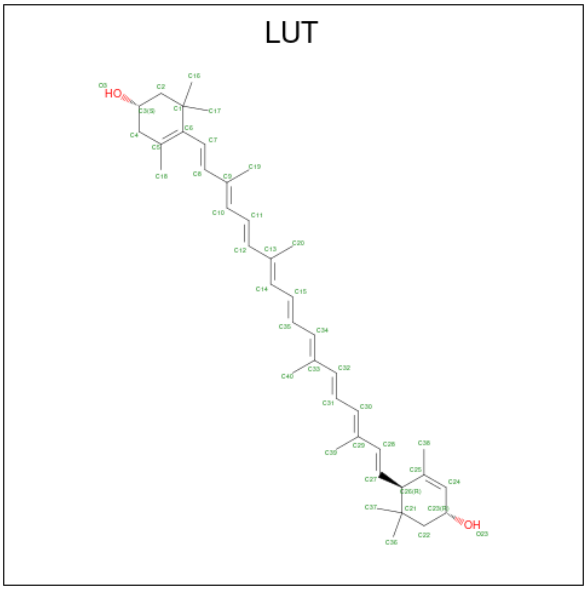
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	J	1	42	40	2	0
			Total	C	O	
36	5	1	42	40	2	0

- Molecule 37 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	K	1	14	12	2	0

- Molecule 38 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	
38	1	1	42	40	2	0
38	1	1	42	40	2	0
38	Z	1	42	40	2	0
38	Z	1	42	40	2	0
38	3	1	42	40	2	0
38	3	1	42	40	2	0
38	7	1	42	40	2	0
38	7	1	42	40	2	0
38	8	1	42	40	2	0
38	8	1	42	40	2	0

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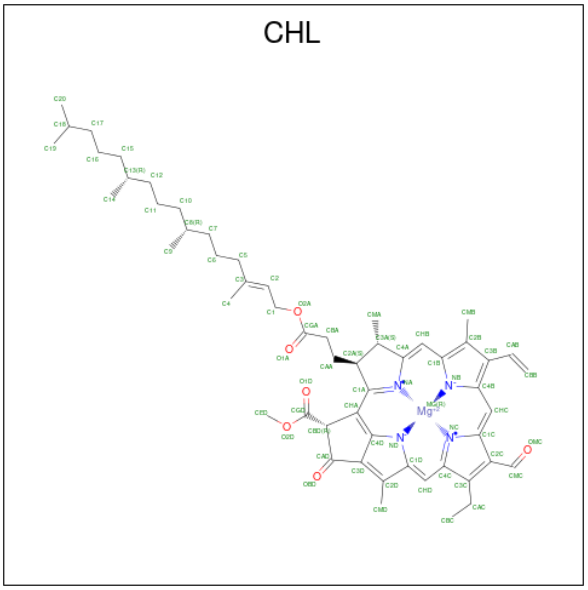
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	4	1	42	40	2	0
			Total	C	O	
38	4	1	42	40	2	0
			Total	C	O	
38	5	1	42	40	2	0
			Total	C	O	
38	5	1	42	40	2	0
			Total	C	O	
38	6	1	42	40	2	0
			Total	C	O	
38	6	1	42	40	2	0
			Total	C	O	
38	9	1	42	40	2	0
			Total	C	O	
38	9	1	42	40	2	0

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
39	1	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
39	Z	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
39	Z	1	48	37	1	4	6	0

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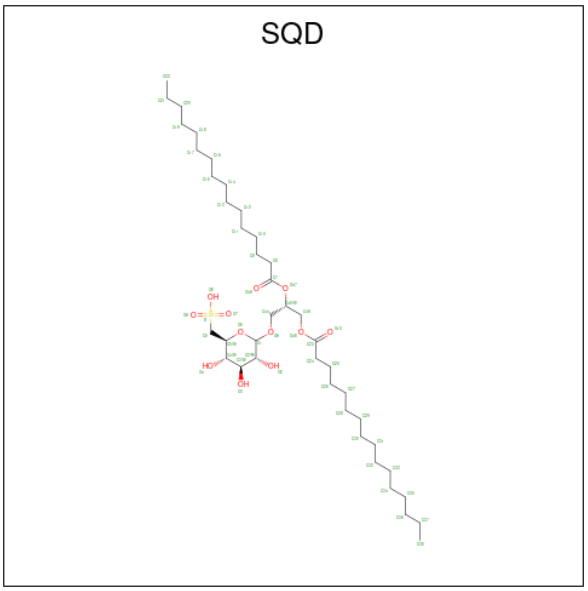
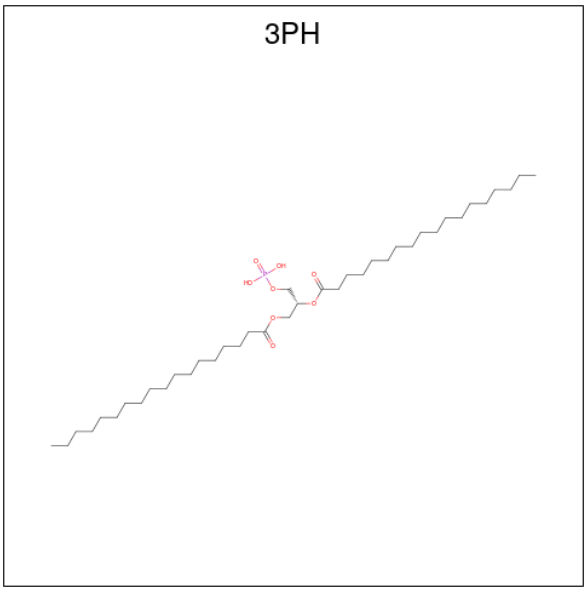
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
39	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
39	7	1	54	43	1	4	6	0
			Total	C	Mg	N	O	
39	8	1	58	47	1	4	6	0
			Total	C	Mg	N	O	
39	8	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
39	8	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
39	4	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
39	4	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
39	4	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
39	4	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
39	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
39	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
39	5	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
39	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
39	6	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
39	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
39	6	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
39	9	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
39	9	1	42	33	1	4	4	0
			Total	C	Mg	N	O	
39	2	1	51	40	1	4	6	0

- Molecule 40 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	
40	1	1	48	35	12	1	0

- Molecule 41 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	
41	7	1	39	30	8	1	0
			Total	C	O	P	
41	8	1	30	21	8	1	0

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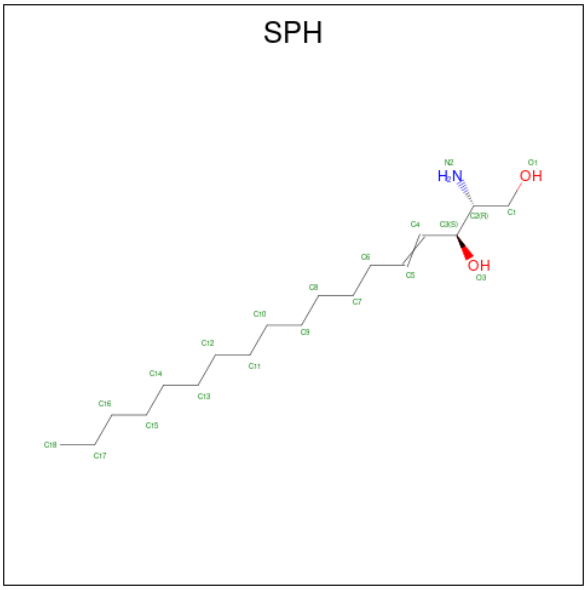
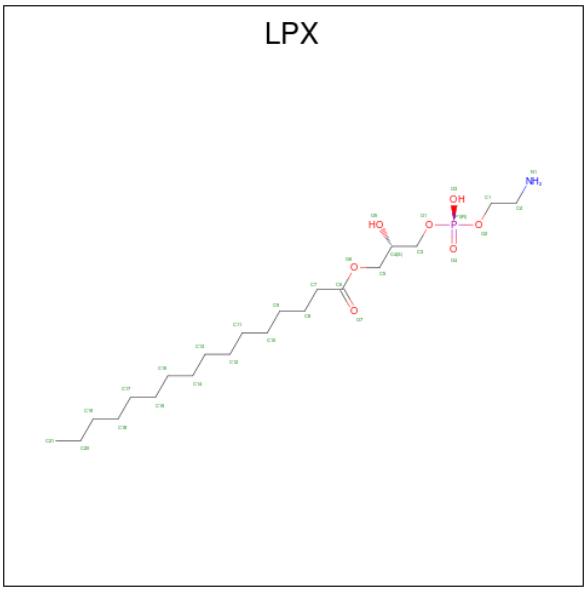
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	5	1	23	14	8	1	0
41	6	1	29	20	8	1	0

- Molecule 42 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	7	1	21	18	1	2	0
42	7	1	21	18	1	2	0

- Molecule 43 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
43	8	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	19	Total	O	0
			19	19	
44	B	17	Total	O	0
			17	17	
44	F	3	Total	O	0
			3	3	
44	I	1	Total	O	0
			1	1	
44	J	1	Total	O	0
			1	1	
44	K	1	Total	O	0
			1	1	
44	1	1	Total	O	0
			1	1	
44	Z	1	Total	O	0
			1	1	
44	3	2	Total	O	0
			2	2	
44	7	4	Total	O	0
			4	4	
44	8	4	Total	O	0
			4	4	

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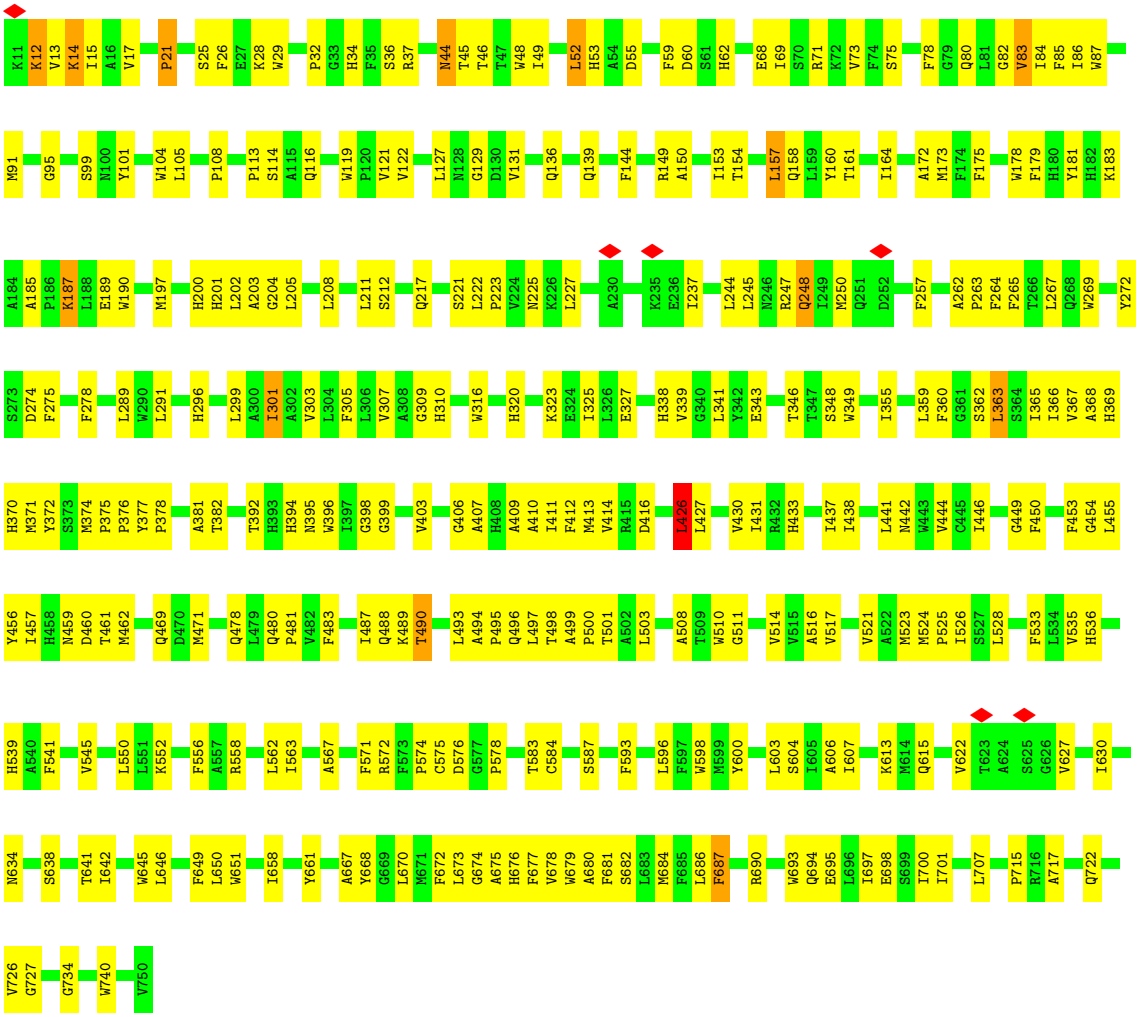
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
44	4	5	5	5	0
			Total	O	
44	5	5	5	5	0
			Total	O	
44	6	3	3	3	0
			Total	O	
44	2	1	1	1	0

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.

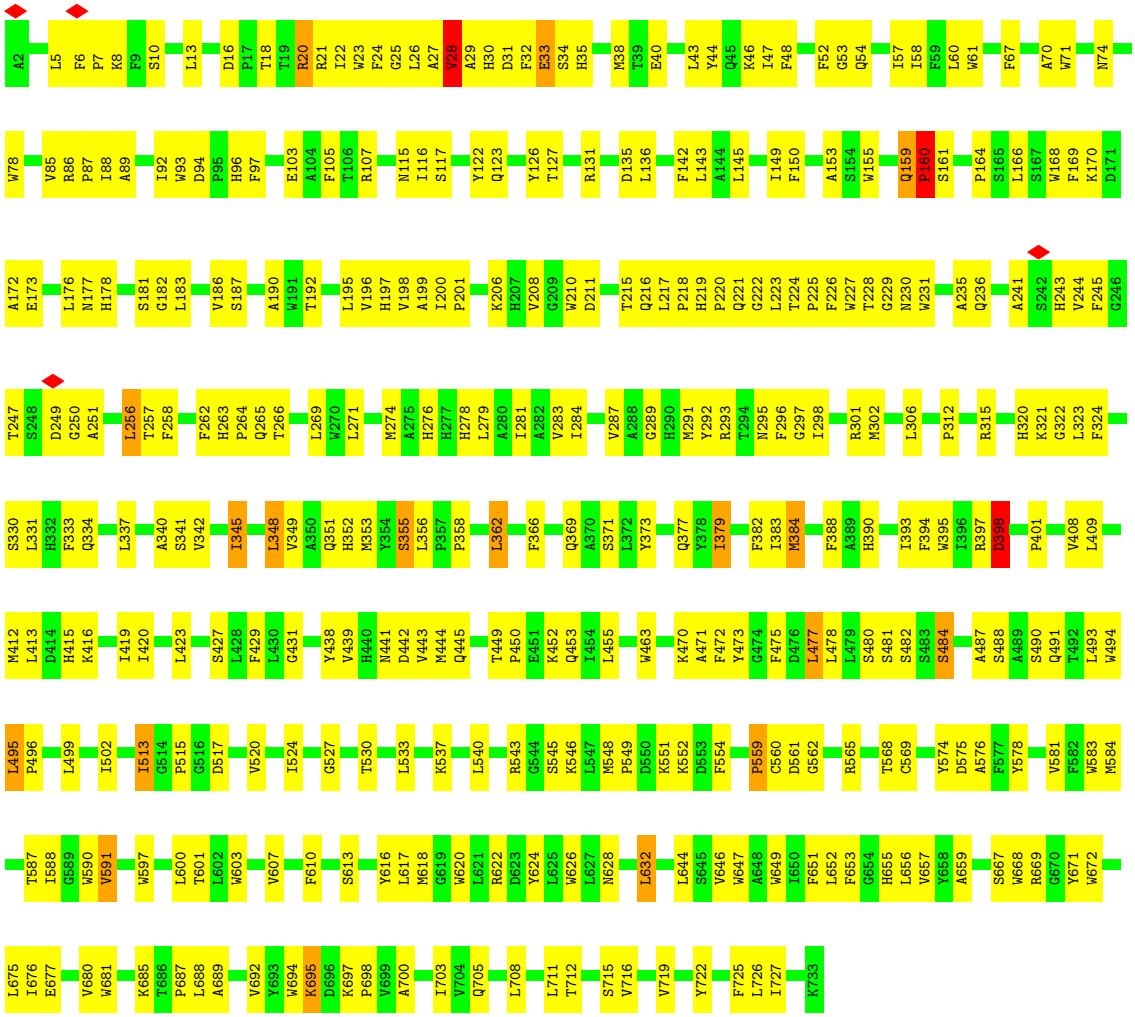
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 PsaA

Chain A: 59% 39%



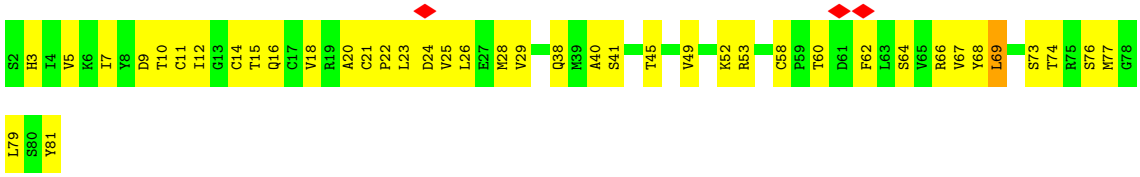
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 PsaB

Chain B: 53% 44%



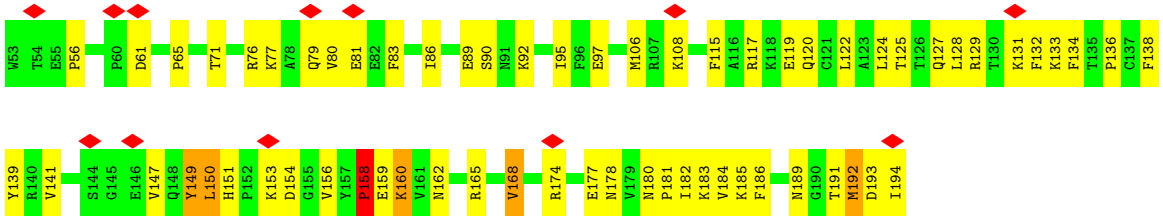
- Molecule 3: Photosystem I subunit VII PsaC

Chain C:



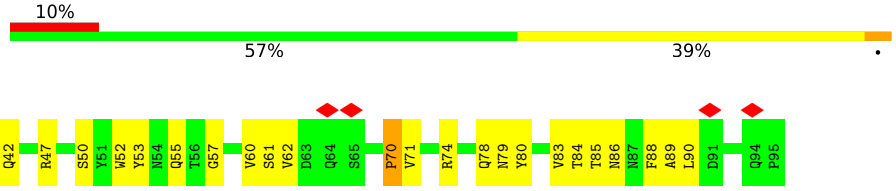
- Molecule 4: Photosystem I reaction center subunit II PsaD

Chain D:



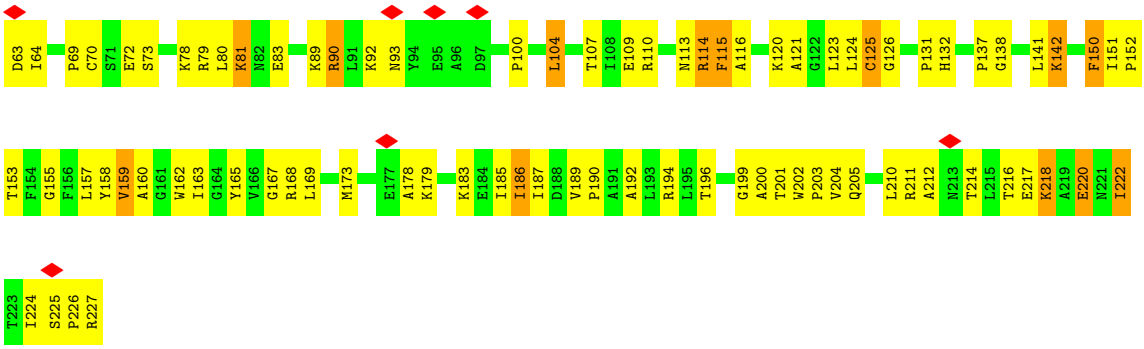
• Molecule 5: Photosystem I reaction center subunit IV PsaE

Chain E:



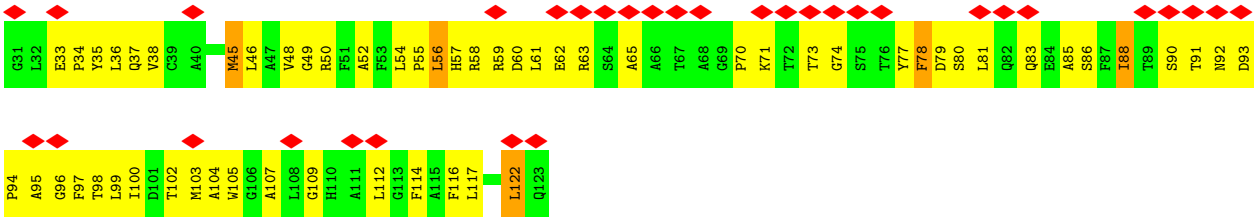
• Molecule 6: Photosystem I reaction center subunit III PsaF

Chain F:



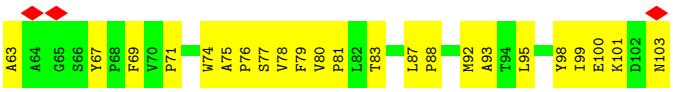
• Molecule 7: Photosystem I reaction center subunit V PsaG

Chain G:



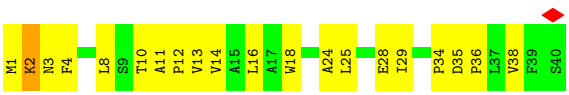
• Molecule 8: Photosystem I reaction center subunit VIII PsaI

Chain I:



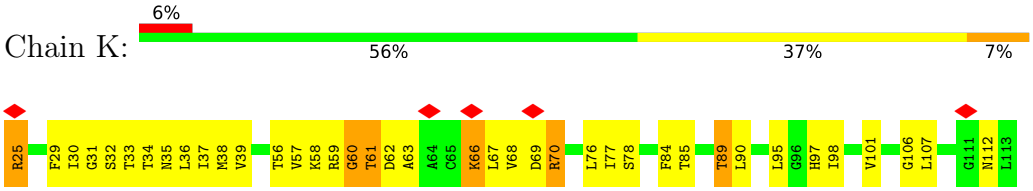
• Molecule 9: Photosystem I subunit IX PsaJ

Chain J:



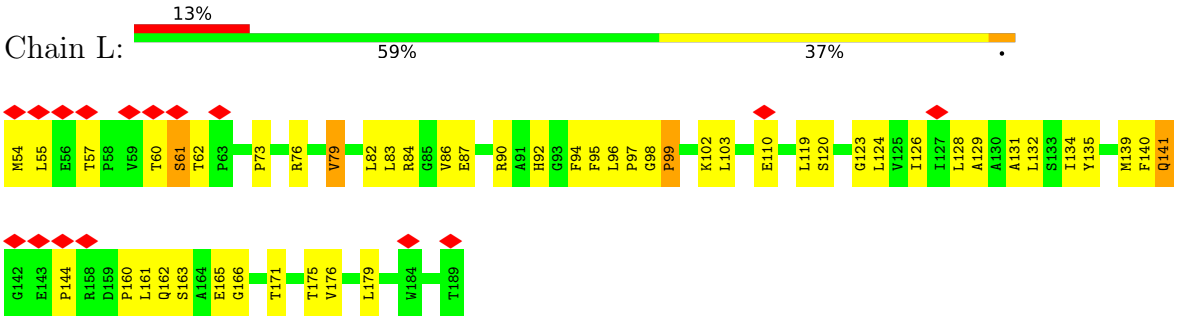
• Molecule 10: Photosystem I reaction center subunit X psaK

Chain K:



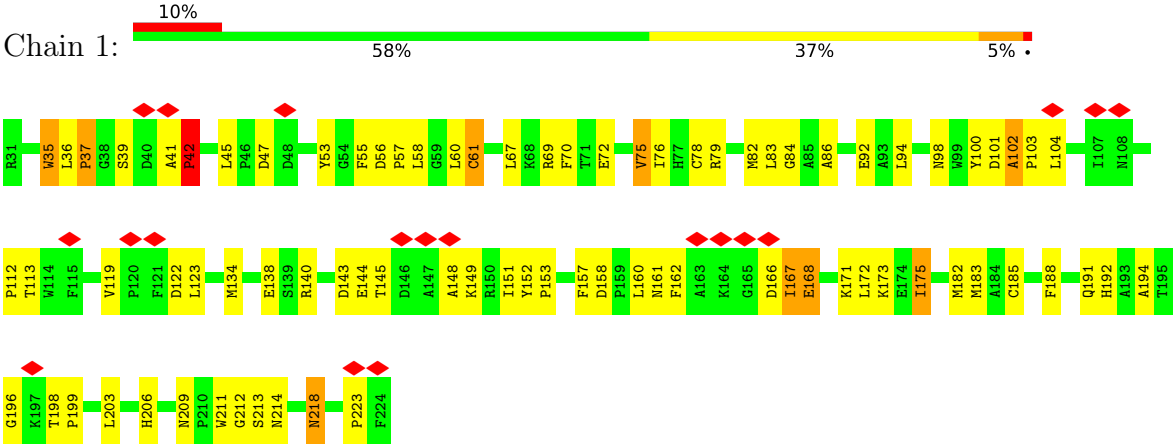
• Molecule 11: Photosystem I reaction centre subunit XI PsaL

Chain L:



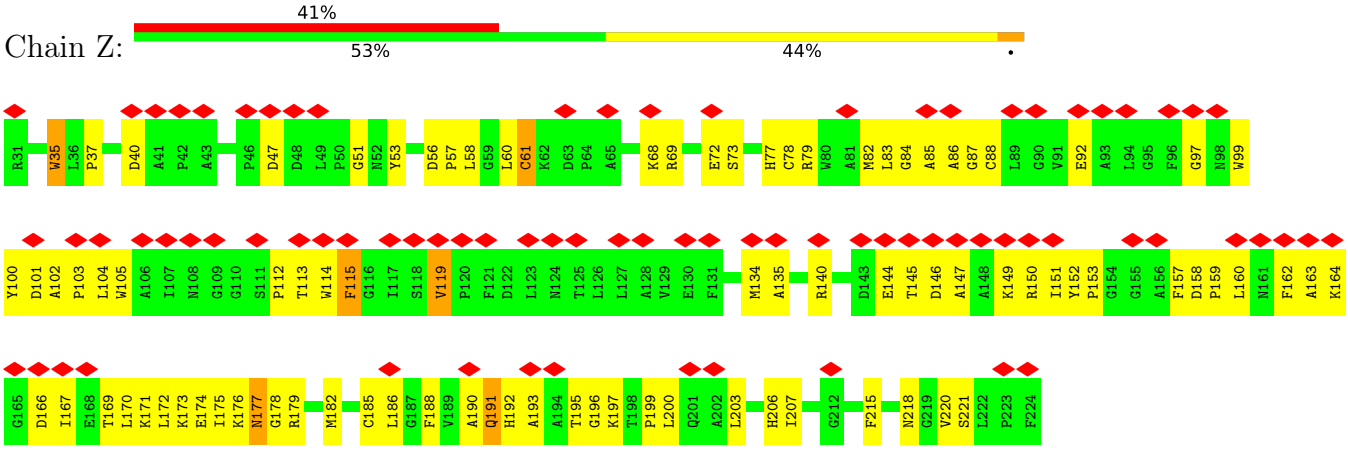
• Molecule 12: Light-harvesting protein of photosystem I Lhca1

Chain 1:



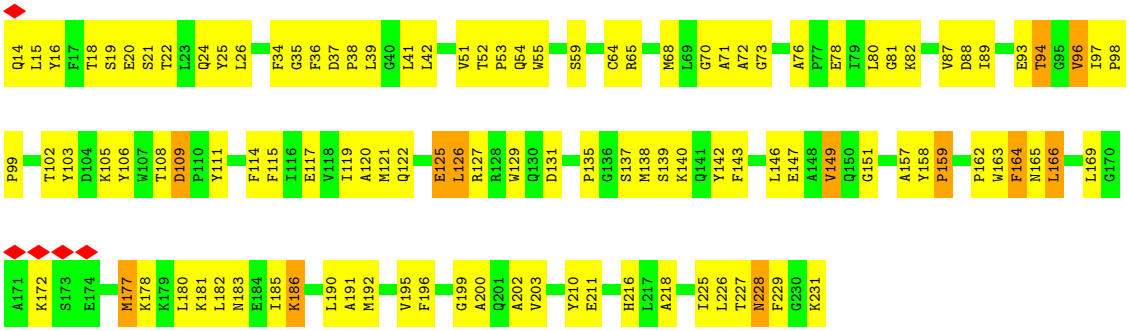
• Molecule 12: Light-harvesting protein of photosystem I Lhca1

Chain Z:



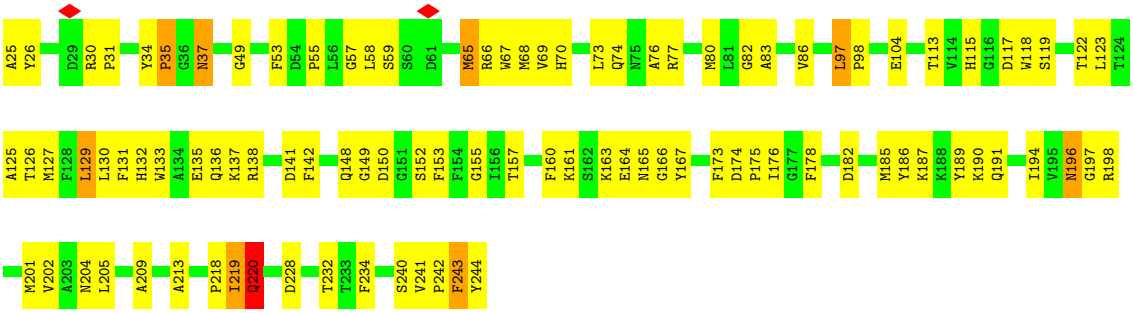
• Molecule 13: Light-harvesting protein of photosystem I Lhca3

Chain 3:



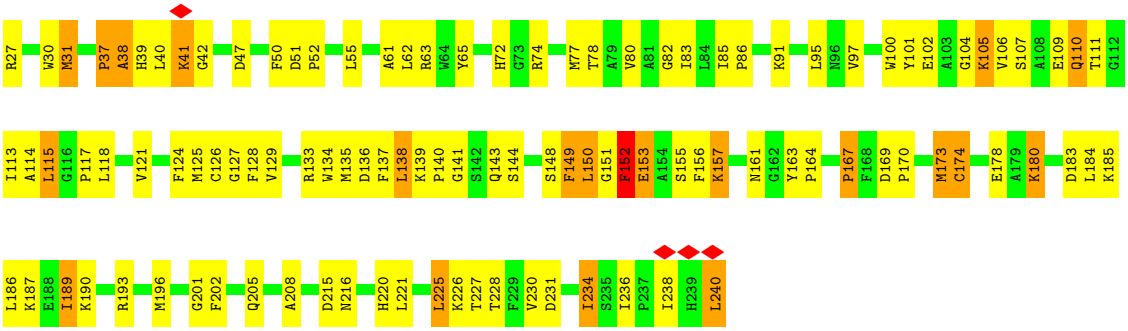
• Molecule 14: Light-harvesting protein of photosystem I Lhca7

Chain 7:



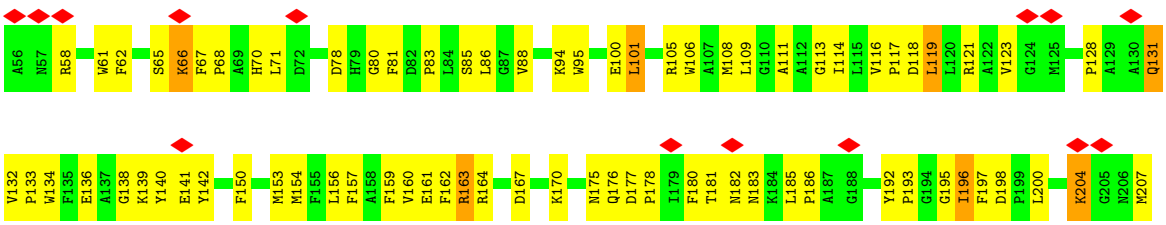
• Molecule 15: Light-harvesting protein of photosystem I Lhca8

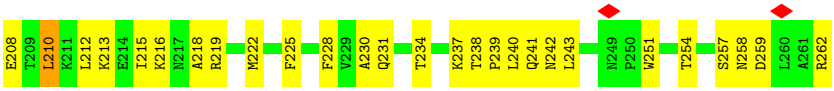
Chain 8:



• Molecule 16: Light-harvesting protein of photosystem I Lhca4

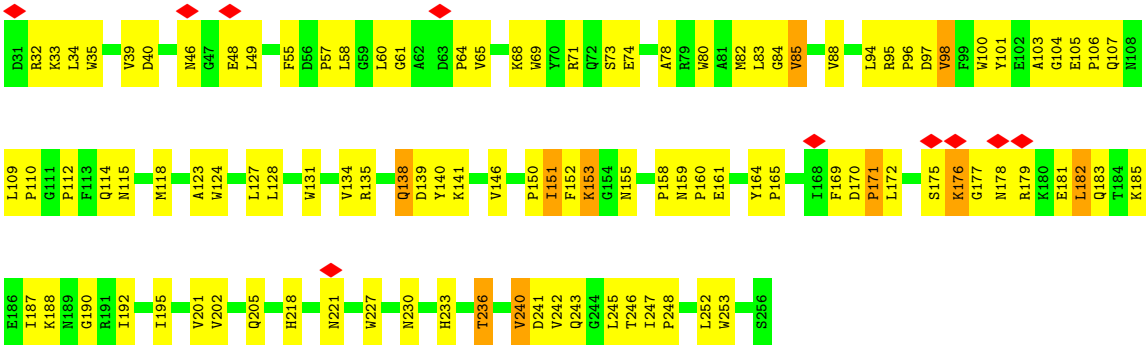
Chain 4:





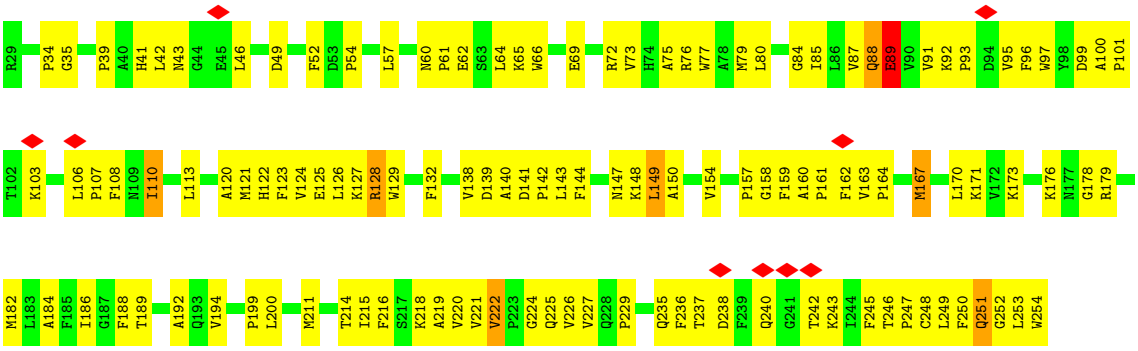
• Molecule 17: Light-harvesting protein of photosystem I Lhca5

Chain 5:



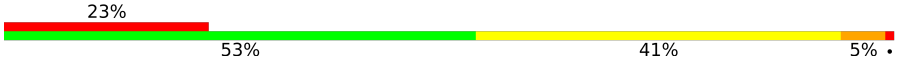
• Molecule 18: Light-harvesting protein of photosystem I Lhca6

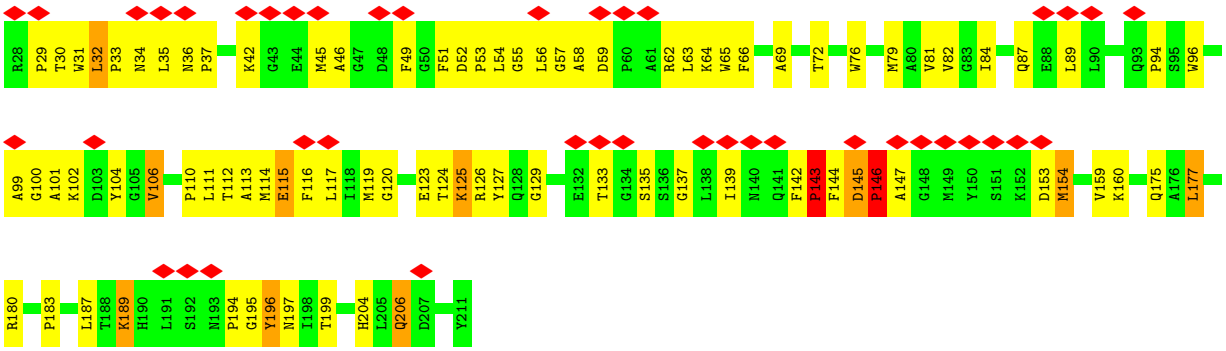
Chain 6:



• Molecule 19: Light-harvesting protein of photosystem I Lhca9

Chain 9:

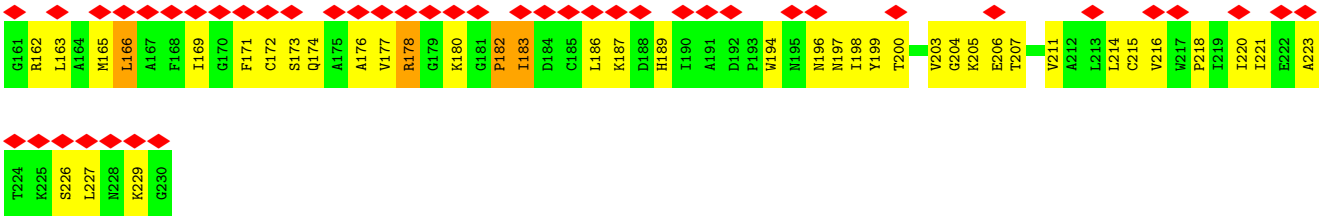




• Molecule 20: Light-harvesting protein of photosystem I Lhca2 partial

Chain 2:

63%
43%
51%
6%


G161 R162 L163 A164 M165 L166 A167 F168 I169 G170 F171 C172 S173 Q174 A175 A176 V177 R178 G179 K180 G181 P182 I183 D184 C185 L186 K187 D188 H189 I190 A191 D192 P193 W194 N195 N196 N197 I198 Y199 T200 V203 G204 K205 E206 T207 V211 A212 L213 L214 C215 V216 W217 P218 I219 I220 I221 E222 A223
T224 K225 S226 L227 N228 K229 G230

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	150	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	325.5, 325.5, 325.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.651, 0.651, 0.651	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: CL0, SQD, T7X, LHG, DAO, DGD, CA, LMG, SF4, OCA, RRX, CLA, CHL, 3PH, DGA, PQN, C7Z, LMT, LUT, LPX, BCR, SPH, NKP

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	0.91	0/6016	1.13	8/8200 (0.1%)
2	B	0.92	0/6010	1.13	3/8207 (0.0%)
3	C	0.98	0/613	1.15	0/830
4	D	0.89	0/1159	1.17	1/1569 (0.1%)
5	E	0.98	0/495	1.09	0/675
6	F	0.92	0/1292	1.25	3/1755 (0.2%)
7	G	0.95	0/706	1.20	1/960 (0.1%)
8	I	0.97	0/320	1.11	0/443
9	J	0.96	0/329	1.20	0/452
10	K	1.00	0/625	1.27	0/848
11	L	0.97	0/919	1.26	0/1253
12	1	0.91	0/1501	1.28	3/2045 (0.1%)
12	Z	0.78	0/1501	1.03	1/2045 (0.0%)
13	3	0.93	0/1747	1.21	2/2376 (0.1%)
14	7	0.93	0/1765	1.22	1/2407 (0.0%)
15	8	0.94	0/1643	1.24	2/2226 (0.1%)
16	4	0.92	0/1648	1.19	0/2240
17	5	0.92	0/1819	1.21	0/2480
18	6	0.92	0/1824	1.14	1/2488 (0.0%)
19	9	0.85	0/1456	1.30	5/1975 (0.3%)
20	2	0.96	0/535	1.24	0/726
All	All	0.92	0/33923	1.18	31/46200 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	9	143	PRO	CA-N-CD	-11.78	95.51	112.00
12	1	42	PRO	CA-N-CD	-9.96	98.06	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	9	189	LYS	N-CA-C	-7.90	105.61	114.62
19	9	143	PRO	CB-CA-C	7.80	124.43	111.56
19	9	146	PRO	CA-N-CD	-7.61	101.35	112.00
12	1	148	ALA	N-CA-C	-7.60	105.96	114.62
14	7	220	GLN	N-CA-C	-6.59	103.29	112.45
13	3	164	PHE	CB-CA-C	6.28	120.74	110.88
1	A	44	ASN	N-CA-C	-6.07	106.85	114.56
1	A	274	ASP	N-CA-C	-6.03	106.90	114.56
19	9	146	PRO	N-CA-CB	-6.03	96.92	103.25
15	8	167	PRO	N-CA-C	-5.96	105.24	113.53
1	A	157	LEU	N-CA-C	-5.90	106.21	113.41
12	1	42	PRO	CB-CA-C	5.85	121.21	111.56
7	G	78	PHE	N-CA-C	-5.58	107.05	112.97
15	8	180	LYS	N-CA-C	-5.56	105.23	112.23
2	B	576	ALA	N-CA-C	-5.55	104.86	111.69
6	F	89	LYS	N-CA-C	-5.53	106.89	113.97
1	A	687	PHE	CB-CA-C	-5.50	100.87	110.17
4	D	158	PRO	N-CA-CB	-5.50	97.48	103.25
1	A	426	LEU	N-CA-C	-5.44	106.72	113.19
1	A	469	GLN	N-CA-C	-5.27	106.89	113.38
1	A	433	HIS	CA-CB-CG	5.24	119.04	113.80
2	B	574	TYR	N-CA-C	-5.22	105.65	112.23
12	Z	97	GLY	CA-C-O	-5.16	118.15	122.33
2	B	398	ASP	CA-CB-CG	5.09	117.69	112.60
13	3	186	LYS	N-CA-C	-5.08	106.78	113.12
1	A	593	PHE	CA-CB-CG	5.07	118.87	113.80
6	F	90	ARG	N-CA-C	-5.07	107.10	113.28
18	6	89	GLU	N-CA-C	-5.06	107.78	114.31
6	F	186	ILE	CA-C-O	-5.04	118.24	122.63

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	5819	0	5666	295	0
2	B	5800	0	5556	371	0
3	C	603	0	587	41	0
4	D	1129	0	1127	46	0
5	E	484	0	477	25	0
6	F	1265	0	1292	75	0
7	G	690	0	671	69	0
8	I	308	0	310	31	0
9	J	319	0	327	23	0
10	K	617	0	635	54	0
11	L	897	0	891	48	0
12	1	1457	0	1406	79	0
12	Z	1457	0	1406	119	0
13	3	1695	0	1641	143	0
14	7	1705	0	1601	104	0
15	8	1602	0	1600	138	0
16	4	1598	0	1569	116	0
17	5	1764	0	1709	126	0
18	6	1762	0	1740	180	0
19	9	1416	0	1392	104	0
20	2	525	0	539	46	0
21	A	65	0	72	7	0
22	1	698	0	678	106	0
22	2	146	0	112	30	0
22	3	749	0	722	153	0
22	4	590	0	511	100	0
22	5	910	0	851	191	0
22	6	824	0	800	183	0
22	7	905	0	848	123	0
22	8	555	0	502	111	0
22	9	528	0	451	66	0
22	A	2640	0	2709	508	0
22	B	2340	0	2333	452	0
22	F	240	0	245	60	0
22	G	96	0	70	26	0
22	J	42	0	30	1	0
22	K	205	0	166	28	0
22	L	180	0	180	37	0
22	Z	679	0	631	147	0
23	A	33	0	46	10	0
23	B	33	0	46	5	0
24	3	160	0	224	59	0
24	4	40	0	56	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	5	80	0	112	30	0
24	6	80	0	112	35	0
24	7	40	0	56	14	0
24	8	40	0	56	14	0
24	A	240	0	336	98	0
24	B	280	0	392	103	0
24	F	40	0	56	14	0
24	G	40	0	56	12	0
24	I	40	0	56	12	0
24	J	40	0	56	18	0
24	K	40	0	55	12	0
24	L	40	0	56	17	0
25	1	43	0	56	8	0
25	3	20	0	12	1	0
25	4	81	0	108	19	0
25	5	37	0	44	7	0
25	6	49	0	74	11	0
25	7	37	0	44	10	0
25	8	38	0	46	7	0
25	9	33	0	36	2	0
25	A	84	0	114	13	0
25	B	76	0	64	15	0
25	Z	43	0	56	9	0
26	8	29	0	39	7	0
26	A	23	0	24	3	0
27	A	40	0	65	20	0
28	A	10	0	15	0	0
29	B	8	0	0	6	0
29	C	16	0	0	7	0
30	B	1	0	0	0	0
31	1	51	0	60	10	0
31	3	51	0	60	21	0
31	B	61	0	83	17	0
32	F	41	0	56	19	0
33	1	35	0	46	7	0
33	4	70	0	92	9	0
33	F	35	0	46	5	0
33	G	35	0	46	10	0
34	F	35	0	40	1	0
34	J	29	0	28	10	0
35	J	49	0	0	2	0
36	5	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	J	42	0	0	2	0
37	K	14	0	23	8	0
38	1	84	0	112	26	0
38	3	84	0	112	28	0
38	4	84	0	112	34	0
38	5	84	0	112	32	0
38	6	84	0	112	24	0
38	7	84	0	112	29	0
38	8	84	0	112	28	0
38	9	84	0	112	33	0
38	Z	84	0	112	36	0
39	1	48	0	32	8	0
39	2	51	0	36	8	0
39	3	66	0	69	14	0
39	4	192	0	130	42	0
39	5	160	0	134	31	0
39	6	206	0	156	51	0
39	7	54	0	42	9	0
39	8	180	0	165	44	0
39	9	108	0	95	35	0
39	Z	99	0	68	23	0
40	1	48	0	62	12	0
41	5	23	0	19	3	0
41	6	29	0	31	5	0
41	7	39	0	51	14	0
41	8	30	0	33	4	0
42	7	42	0	74	12	0
43	8	30	0	43	7	0
44	1	1	0	0	0	0
44	2	1	0	0	0	0
44	3	2	0	0	1	0
44	4	5	0	0	0	0
44	5	5	0	0	0	0
44	6	3	0	0	0	0
44	7	4	0	0	0	0
44	8	4	0	0	0	0
44	A	19	0	0	0	0
44	B	17	0	0	0	0
44	F	3	0	0	0	0
44	I	1	0	0	0	0
44	J	1	0	0	0	0
44	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Z	1	0	0	0	0
All	All	50057	0	49449	4003	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 40.

All (4003) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:238:ASP:HA	18:6:243:LYS:HA	1.26	1.13
24:3:306:BCR:H21C	22:3:318:CLA:H91	1.25	1.06
24:5:304:BCR:H19C	22:5:319:CLA:HBA2	1.40	1.04
19:9:53:PRO:HD2	38:9:302:LUT:H23	1.42	1.02
38:6:304:LUT:H28	22:6:310:CLA:H61	1.39	1.02
17:5:175:SER:HB3	22:5:307:CLA:HAA2	1.37	1.00
12:Z:72:GLU:HG2	12:Z:151:ILE:HG12	1.45	0.99
38:7:302:LUT:H32	22:7:307:CLA:HAB	1.44	0.98
18:6:127:LYS:HG3	22:6:302:CLA:HED3	1.43	0.98
2:B:560:CYS:HG	29:B:802:SF4:FE4	0.70	0.98
22:5:309:CLA:HBD	22:5:309:CLA:HBA1	1.46	0.97
22:A:817:CLA:HAB	24:K:206:BCR:HC32	1.42	0.97
22:B:810:CLA:H61	24:I:4001:BCR:HC31	1.45	0.97
15:8:52:PRO:HD2	38:8:303:LUT:H23	1.46	0.97
22:B:811:CLA:HHC	22:B:811:CLA:HBB1	1.47	0.96
16:4:198:ASP:HA	38:4:802:LUT:H24	1.47	0.95
22:B:840:CLA:H161	24:I:4001:BCR:H19C	1.49	0.95
1:A:307:VAL:HA	24:A:856:BCR:H17C	1.45	0.95
22:6:309:CLA:H71	25:6:323:LHG:H341	1.48	0.95
22:B:811:CLA:HBA2	22:B:829:CLA:HBD	1.45	0.95
22:3:310:CLA:HBD	22:3:310:CLA:HBA1	1.43	0.94
22:7:306:CLA:H91	22:7:306:CLA:H142	1.45	0.94
38:9:301:LUT:H30	22:9:303:CLA:H52	1.47	0.94
17:5:58:LEU:HD13	38:5:303:LUT:H222	1.49	0.93
22:7:306:CLA:HBD	22:7:306:CLA:HBA1	1.48	0.93
3:C:73:SER:H	3:C:76:SER:HB3	1.32	0.93
20:2:221:ILE:HG23	20:2:227:LEU:HD21	1.50	0.93
22:A:808:CLA:HHC	22:A:808:CLA:HBB1	1.51	0.93
22:5:311:CLA:H71	22:5:323:CLA:HAB	1.51	0.92
22:B:838:CLA:H202	32:F:306:RRX:H34	1.49	0.92
6:F:204:VAL:HG13	22:8:309:CLA:H2	1.49	0.92
12:1:158:ASP:HA	38:1:302:LUT:H24	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:CYS:HG	29:B:802:SF4:FE3	0.69	0.92
22:A:837:CLA:HHC	22:A:837:CLA:HBB1	1.50	0.92
22:1:310:CLA:HBB1	22:1:310:CLA:HHC	1.52	0.92
22:B:814:CLA:HAA1	7:G:81:LEU:HB3	1.52	0.92
1:A:212:SER:HB3	24:A:844:BCR:H363	1.52	0.91
22:B:823:CLA:HHC	22:B:823:CLA:HBB1	1.52	0.91
2:B:348:LEU:HD11	22:B:828:CLA:HAA2	1.50	0.91
22:F:302:CLA:HHC	22:F:302:CLA:HBB1	1.50	0.91
22:B:814:CLA:HBA1	19:9:54:LEU:HB3	1.51	0.91
22:4:809:CLA:HHC	22:4:809:CLA:HBB1	1.51	0.91
22:6:314:CLA:HHC	22:6:314:CLA:HBB1	1.53	0.90
22:8:306:CLA:HBB1	22:8:306:CLA:HHC	1.52	0.90
2:B:210:TRP:HB2	25:B:851:LHG:HC5	1.54	0.90
22:B:825:CLA:H92	22:B:825:CLA:H2	1.54	0.90
22:B:805:CLA:HBB1	22:B:805:CLA:HHC	1.55	0.89
5:E:78:GLN:HB3	5:E:84:THR:HG22	1.54	0.89
22:A:824:CLA:H2	22:A:835:CLA:H171	1.54	0.89
22:A:823:CLA:HBB1	22:A:823:CLA:HHC	1.54	0.89
22:B:827:CLA:H151	22:B:842:CLA:H161	1.55	0.89
2:B:382:PHE:HB3	22:B:809:CLA:H112	1.54	0.89
22:A:802:CLA:H13	22:A:828:CLA:H143	1.53	0.88
22:A:824:CLA:HMD3	22:A:825:CLA:HAB	1.56	0.88
24:B:844:BCR:H362	24:G:203:BCR:H312	1.56	0.88
22:1:305:CLA:HHC	22:1:305:CLA:HBB1	1.53	0.88
13:3:195:VAL:HG11	38:3:303:LUT:H12	1.56	0.88
22:B:833:CLA:H8	32:F:306:RRX:H27	1.56	0.88
22:6:317:CLA:HED2	22:6:317:CLA:H2A	1.52	0.88
12:Z:145:THR:HA	12:Z:150:ARG:HH21	1.39	0.87
24:3:304:BCR:H281	22:5:301:CLA:HAB	1.57	0.87
22:B:821:CLA:H151	22:B:826:CLA:H172	1.57	0.87
24:5:305:BCR:H321	24:5:305:BCR:HC8	1.56	0.87
14:7:205:LEU:HD13	22:7:308:CLA:HBB2	1.55	0.87
16:4:95:TRP:HZ2	22:4:815:CLA:HAA2	1.38	0.87
22:Z:316:CLA:HHC	22:Z:316:CLA:HBB1	1.55	0.87
22:7:312:CLA:HHC	22:7:312:CLA:HBB1	1.57	0.87
6:F:79:ARG:HG2	6:F:115:PHE:HZ	1.40	0.86
38:3:302:LUT:H361	22:3:308:CLA:H143	1.57	0.86
12:1:35:TRP:HH2	40:1:318:SQD:H2	1.40	0.86
13:3:55:TRP:HZ2	22:3:318:CLA:HAA2	1.40	0.86
18:6:247:PRO:HB2	22:6:301:CLA:H11	1.56	0.86
19:9:81:VAL:HG11	38:9:301:LUT:H12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:203:VAL:HG22	31:3:301:DGD:HB62	1.58	0.86
22:A:820:CLA:HHC	22:A:820:CLA:HBB1	1.56	0.86
22:A:836:CLA:H61	22:K:203:CLA:HBA2	1.58	0.86
22:B:810:CLA:HMB2	24:I:4001:BCR:H322	1.58	0.85
3:C:14:CYS:SG	29:C:102:SF4:FE3	1.68	0.85
12:Z:149:LYS:HB3	22:Z:313:CLA:HBC1	1.57	0.85
20:2:197:ASN:HA	22:2:301:CLA:HBA2	1.58	0.85
10:K:59:ARG:HA	10:K:69:ASP:HA	1.58	0.85
15:8:55:LEU:HD12	38:8:303:LUT:H221	1.57	0.85
22:4:807:CLA:HBD	22:4:807:CLA:HBA1	1.59	0.85
22:6:309:CLA:HBD	22:6:309:CLA:HBA1	1.56	0.85
22:A:835:CLA:H102	24:A:847:BCR:H20C	1.59	0.85
22:B:840:CLA:H2	22:B:841:CLA:H121	1.59	0.85
22:A:803:CLA:HHC	22:A:803:CLA:HBB1	1.58	0.84
22:B:808:CLA:HBA1	22:B:815:CLA:HBA1	1.57	0.84
15:8:169:ASP:HB2	22:8:305:CLA:HBD	1.57	0.84
24:A:856:BCR:HC41	31:3:301:DGD:HAT1	1.58	0.84
2:B:345:ILE:HD11	22:B:820:CLA:H122	1.59	0.84
24:B:853:BCR:HC21	22:L:202:CLA:H62	1.60	0.84
22:8:307:CLA:HBD	22:8:307:CLA:HBA1	1.59	0.84
24:B:853:BCR:H11C	22:L:202:CLA:HAB	1.58	0.84
11:L:131:ALA:HB1	24:L:204:BCR:H19C	1.57	0.84
22:L:201:CLA:HHC	22:L:201:CLA:HBB1	1.57	0.84
17:5:227:TRP:HB3	22:5:309:CLA:H2	1.58	0.84
17:5:109:LEU:HD21	22:5:319:CLA:HAC1	1.57	0.84
22:G:201:CLA:HBB1	22:G:201:CLA:HHC	1.57	0.83
22:B:827:CLA:H8	22:B:839:CLA:HMD2	1.58	0.83
38:9:302:LUT:H28	22:9:306:CLA:H52	1.58	0.83
39:9:312:CHL:HBC2	39:9:312:CHL:HMC	1.60	0.83
1:A:496:GLN:HG3	1:A:497:LEU:HG	1.59	0.83
6:F:204:VAL:HG22	22:8:309:CLA:H72	1.60	0.83
12:Z:73:SER:HB2	22:Z:314:CLA:HED3	1.61	0.83
22:A:825:CLA:H193	22:A:825:CLA:H13	1.61	0.83
22:3:320:CLA:HMD1	41:7:319:3PH:H342	1.58	0.83
18:6:110:ILE:HD13	24:6:306:BCR:HC8	1.59	0.83
13:3:82:LYS:HZ2	13:3:210:TYR:HB3	1.42	0.83
18:6:54:PRO:HD2	38:6:304:LUT:H23	1.59	0.83
18:6:249:LEU:HG	24:6:306:BCR:H291	1.61	0.82
17:5:170:ASP:HA	38:5:302:LUT:H24	1.59	0.82
38:5:303:LUT:H28	22:5:310:CLA:H52	1.61	0.82
22:6:301:CLA:H122	39:6:315:CHL:H43	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TRP:HE1	22:A:811:CLA:CHB	1.93	0.82
22:B:814:CLA:HHC	22:B:814:CLA:HBB1	1.59	0.82
22:A:829:CLA:H2	24:A:845:BCR:HC7	1.59	0.81
18:6:222:VAL:HG12	18:6:225:GLN:H	1.45	0.81
1:A:338:HIS:HE1	25:A:849:LHG:HC12	1.45	0.81
22:A:812:CLA:HBB1	22:A:812:CLA:HHC	1.62	0.81
22:B:841:CLA:HAC2	24:B:849:BCR:H24C	1.62	0.81
12:Z:215:PHE:HB3	22:Z:305:CLA:H11	1.60	0.81
22:1:314:CLA:H172	22:1:314:CLA:H91	1.62	0.81
3:C:14:CYS:HG	29:C:102:SF4:FE3	0.96	0.81
22:A:821:CLA:H101	24:A:847:BCR:H10C	1.63	0.81
24:A:844:BCR:H362	24:A:845:BCR:H21C	1.62	0.80
15:8:163:TYR:HB3	22:8:305:CLA:HED3	1.63	0.80
22:3:316:CLA:HHC	22:3:316:CLA:HBB1	1.61	0.80
11:L:119:LEU:O	22:L:201:CLA:H112	1.80	0.80
40:1:318:SQD:H192	39:8:301:CHL:HMA1	1.64	0.80
22:B:819:CLA:H92	22:B:828:CLA:HAB	1.63	0.80
17:5:57:PRO:HD2	38:5:303:LUT:H23	1.63	0.80
22:A:807:CLA:HMB3	22:A:808:CLA:HHB	1.64	0.80
2:B:560:CYS:SG	29:B:802:SF4:FE4	1.74	0.80
22:B:813:CLA:HMB3	22:B:813:CLA:HBB1	1.64	0.79
22:B:830:CLA:HHC	22:B:830:CLA:HBB1	1.62	0.79
15:8:127:GLY:HA3	39:8:301:CHL:H12	1.63	0.79
16:4:83:PRO:HD2	38:4:803:LUT:H23	1.63	0.79
19:9:56:LEU:HD11	38:9:302:LUT:H221	1.64	0.79
14:7:104:GLU:HA	39:7:313:CHL:HED3	1.64	0.79
22:A:840:CLA:HBC2	24:F:303:BCR:H21C	1.63	0.79
1:A:338:HIS:HA	1:A:426:LEU:HD11	1.62	0.79
12:1:36:LEU:HD11	40:1:318:SQD:H172	1.65	0.79
22:B:840:CLA:H172	22:B:841:CLA:H91	1.65	0.79
12:1:86:ALA:HB1	22:1:304:CLA:H172	1.64	0.78
24:3:305:BCR:H21C	22:3:313:CLA:HAC1	1.63	0.78
14:7:115:HIS:HB2	15:8:225:LEU:HD11	1.66	0.78
22:Z:308:CLA:H61	22:Z:315:CLA:HAA2	1.65	0.78
15:8:128:PHE:CE1	24:8:304:BCR:H10C	2.18	0.78
16:4:154:MET:HA	16:4:154:MET:HE2	1.66	0.78
24:A:844:BCR:H23C	24:3:306:BCR:H333	1.63	0.78
24:6:306:BCR:H382	22:6:319:CLA:H112	1.65	0.78
22:B:820:CLA:HBB1	22:B:820:CLA:HMB3	1.64	0.78
22:A:814:CLA:H121	22:A:816:CLA:CAB	2.13	0.78
19:9:142:PHE:HB3	19:9:143:PRO:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:802:LUT:H30	22:4:805:CLA:H52	1.65	0.78
22:A:822:CLA:HMB1	22:A:822:CLA:HBB1	1.66	0.78
22:A:832:CLA:H18	22:L:202:CLA:H18	1.65	0.78
22:A:841:CLA:HBA2	25:A:850:LHG:H161	1.64	0.78
25:1:317:LHG:H101	24:8:304:BCR:H313	1.65	0.77
22:A:823:CLA:H111	24:A:856:BCR:H401	1.66	0.77
22:B:828:CLA:HBB1	22:B:828:CLA:HHC	1.66	0.77
7:G:94:PRO:HG2	22:G:202:CLA:HBC2	1.65	0.77
22:4:810:CLA:HMA2	39:4:816:CHL:C3C	2.14	0.77
22:A:814:CLA:H121	22:A:816:CLA:HAB	1.65	0.77
2:B:543:ARG:HB2	2:B:552:LYS:HB3	1.65	0.77
24:3:307:BCR:H311	22:3:315:CLA:HHB	1.66	0.77
38:7:302:LUT:H28	22:7:307:CLA:H61	1.65	0.77
6:F:142:LYS:HG3	33:F:307:LMT:H2'	1.66	0.77
14:7:133:TRP:CD1	24:7:303:BCR:H12C	2.18	0.77
22:B:813:CLA:H11	22:9:307:CLA:H61	1.67	0.77
12:Z:153:PRO:HD3	22:Z:313:CLA:HMD1	1.65	0.77
12:Z:206:HIS:HB2	22:Z:305:CLA:HAA2	1.65	0.77
22:7:309:CLA:H52	22:7:316:CLA:HBD	1.65	0.77
12:Z:173:LYS:HD3	22:Z:304:CLA:HAA2	1.67	0.77
2:B:284:ILE:HA	22:B:818:CLA:H172	1.67	0.77
24:3:307:BCR:H312	22:3:315:CLA:HMB3	1.67	0.77
16:4:133:PRO:HG2	16:4:136:GLU:HB2	1.66	0.77
2:B:227:TRP:HH2	22:B:817:CLA:H71	1.50	0.77
17:5:218:HIS:CG	22:5:309:CLA:HAA1	2.19	0.77
24:6:306:BCR:H16C	39:6:315:CHL:CHD	2.14	0.77
22:6:307:CLA:HBB1	22:6:308:CLA:HAA1	1.65	0.77
38:Z:301:LUT:H28	22:Z:303:CLA:H2	1.65	0.77
24:B:844:BCR:H272	24:B:846:BCR:HC31	1.67	0.76
16:4:108:MET:HE2	16:4:218:ALA:HB2	1.67	0.76
22:5:322:CLA:HMB1	22:5:322:CLA:HBB1	1.66	0.76
22:A:840:CLA:H111	22:A:840:CLA:HAB	1.66	0.76
7:G:59:ARG:HG2	7:G:63:ARG:HE	1.48	0.76
25:4:820:LHG:H191	22:6:321:CLA:HBA2	1.65	0.76
38:6:303:LUT:H403	22:6:307:CLA:H122	1.66	0.76
22:B:814:CLA:C4D	22:B:814:CLA:H2	2.15	0.76
22:5:322:CLA:H61	22:6:310:CLA:H193	1.66	0.76
39:9:312:CHL:HHC	39:9:312:CHL:HBB1	1.67	0.76
22:A:854:CLA:H152	22:L:201:CLA:HBC1	1.65	0.76
22:B:836:CLA:HBC2	31:1:319:DGD:HA32	1.68	0.76
23:B:843:PQN:H221	24:B:849:BCR:H17C	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:35:TRP:CH2	40:1:318:SQD:H2	2.20	0.76
22:3:309:CLA:HBB1	22:3:309:CLA:HMB3	1.67	0.76
39:6:316:CHL:CHB	39:6:318:CHL:H71	2.16	0.76
24:A:848:BCR:H372	2:B:439:VAL:HG21	1.65	0.76
22:B:841:CLA:HBD	23:B:843:PQN:H302	1.68	0.76
22:6:317:CLA:HBB1	22:6:317:CLA:HMB3	1.66	0.76
19:9:79:MET:HG2	22:9:308:CLA:HAB	1.67	0.76
8:I:83:THR:HG21	24:I:4001:BCR:HC42	1.68	0.76
12:1:152:TYR:HB3	22:1:304:CLA:HED2	1.66	0.76
18:6:75:ALA:HB1	18:6:178:GLY:HA3	1.67	0.76
20:2:177:VAL:HG21	22:2:304:CLA:CMD	2.16	0.76
22:B:834:CLA:HBA2	24:J:104:BCR:H272	1.68	0.76
12:Z:203:LEU:HB2	38:Z:301:LUT:H22	1.68	0.76
31:3:301:DGD:HAE2	24:3:306:BCR:H10C	1.66	0.76
22:7:309:CLA:HBB1	22:7:309:CLA:HMB3	1.68	0.76
6:F:204:VAL:HA	22:8:309:CLA:H51	1.68	0.76
13:3:55:TRP:CZ2	22:3:318:CLA:HAA2	2.19	0.76
18:6:46:LEU:H	18:6:46:LEU:HD12	1.50	0.76
22:A:804:CLA:HBA2	22:A:811:CLA:H92	1.66	0.75
11:L:132:LEU:HB3	11:L:171:THR:HG22	1.68	0.75
15:8:80:VAL:HG11	38:8:302:LUT:H12	1.68	0.75
11:L:132:LEU:HD21	24:L:204:BCR:H383	1.68	0.75
16:4:136:GLU:HA	39:4:813:CHL:HED2	1.67	0.75
17:5:241:ASP:HA	17:5:246:THR:HA	1.69	0.75
19:9:32:LEU:HD22	19:9:33:PRO:HD2	1.69	0.75
12:Z:190:ALA:HB2	22:Z:316:CLA:H61	1.68	0.75
38:Z:301:LUT:H30	22:Z:303:CLA:H52	1.67	0.75
22:3:313:CLA:H43	22:5:320:CLA:HED2	1.68	0.75
22:B:827:CLA:H143	22:B:842:CLA:H18	1.67	0.75
39:5:316:CHL:HMC	22:5:319:CLA:HAB	1.66	0.75
22:A:842:CLA:HMB1	24:A:846:BCR:H12C	1.69	0.75
2:B:86:ARG:NH2	2:B:107:ARG:HB2	2.02	0.75
24:B:847:BCR:H323	33:1:301:LMT:H102	1.67	0.75
22:F:305:CLA:HMB3	22:F:305:CLA:HBB1	1.69	0.75
17:5:159:ASN:HA	17:5:165:PRO:HA	1.69	0.75
2:B:351:GLN:HG3	22:B:827:CLA:HED2	1.68	0.75
11:L:120:SER:HA	22:L:201:CLA:H71	1.69	0.74
22:1:306:CLA:H152	25:1:317:LHG:HC92	1.69	0.74
13:3:37:ASP:HA	38:3:303:LUT:H24	1.70	0.74
22:B:825:CLA:HBB2	22:B:842:CLA:H61	1.70	0.74
39:1:312:CHL:HAA2	31:1:319:DGD:HG31	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:820:CLA:H102	22:A:820:CLA:H142	1.69	0.74
22:B:833:CLA:HBC2	22:B:839:CLA:HMC3	1.69	0.74
12:Z:51:GLY:HA3	12:Z:175:ILE:HD13	1.69	0.74
39:Z:311:CHL:HBC3	39:Z:311:CHL:HHD	1.68	0.74
1:A:575:CYS:SG	29:B:802:SF4:FE3	1.79	0.74
2:B:86:ARG:HH21	2:B:107:ARG:HB2	1.52	0.74
13:3:165:ASN:HA	38:3:302:LUT:H24	1.69	0.74
14:7:205:LEU:HD11	22:7:307:CLA:H202	1.69	0.74
22:8:313:CLA:HMA2	39:8:315:CHL:H52	1.68	0.74
22:A:854:CLA:HBB2	2:B:659:ALA:HB3	1.70	0.74
22:3:310:CLA:HBA1	22:3:310:CLA:CBD	2.17	0.74
22:A:802:CLA:HAB	2:B:583:TRP:CH2	2.23	0.74
22:B:838:CLA:H171	32:F:306:RRX:H38	1.68	0.74
12:Z:68:LYS:HD2	12:Z:147:ALA:HB1	1.69	0.74
1:A:363:LEU:HD11	22:A:819:CLA:H111	1.68	0.74
34:J:101:LMG:HC91	34:J:101:LMG:H121	1.70	0.74
1:A:676:HIS:HB2	22:A:802:CLA:HBA1	1.70	0.73
22:A:822:CLA:HBA2	22:A:823:CLA:H72	1.70	0.73
22:A:836:CLA:HMB1	24:A:847:BCR:H281	1.70	0.73
11:L:140:PHE:HA	11:L:144:PRO:HD2	1.70	0.73
12:Z:162:PHE:HB2	22:Z:303:CLA:CGA	2.18	0.73
22:A:838:CLA:HBB1	22:A:838:CLA:HMB3	1.70	0.73
22:A:840:CLA:H121	22:F:305:CLA:HAC1	1.70	0.73
22:Z:304:CLA:NA	22:Z:309:CLA:H71	2.03	0.73
14:7:68:MET:HE1	22:7:308:CLA:H2	1.70	0.73
22:5:320:CLA:HAC2	41:5:325:3PH:H232	1.70	0.73
22:4:807:CLA:H102	25:4:820:LHG:H162	1.68	0.73
22:6:314:CLA:H92	25:6:323:LHG:H152	1.71	0.73
22:5:322:CLA:H143	22:6:310:CLA:H101	1.71	0.73
22:3:320:CLA:HMA3	22:3:322:CLA:H112	1.69	0.73
22:4:818:CLA:H2	22:4:818:CLA:HBA1	1.71	0.73
22:B:825:CLA:HBA2	24:B:847:BCR:H14C	1.71	0.73
39:4:816:CHL:HMB1	39:4:816:CHL:HBB1	1.70	0.73
2:B:26:LEU:HD21	24:L:204:BCR:H332	1.71	0.73
10:K:59:ARG:CA	10:K:69:ASP:HA	2.19	0.73
31:3:301:DGD:HB21	31:3:301:DGD:HG31	1.71	0.73
14:7:174:ASP:HA	38:7:301:LUT:H24	1.70	0.73
24:5:304:BCR:H353	39:5:317:CHL:HBB1	1.69	0.73
39:6:320:CHL:HHC	39:6:320:CHL:HBB1	1.70	0.73
19:9:100:GLY:HA2	39:9:314:CHL:HAC2	1.70	0.73
22:A:840:CLA:H91	22:F:305:CLA:HAC2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:305:BCR:H321	24:3:305:BCR:HC8	1.69	0.72
22:7:322:CLA:H61	22:7:323:CLA:H72	1.70	0.72
15:8:125:MET:HE2	24:8:304:BCR:H15C	1.71	0.72
24:4:804:BCR:H272	22:4:810:CLA:H2	1.69	0.72
22:A:823:CLA:H191	10:K:98:ILE:HD12	1.71	0.72
12:Z:182:MET:HE3	22:Z:306:CLA:HMC2	1.71	0.72
22:B:815:CLA:HMB3	22:B:815:CLA:HBB1	1.72	0.72
20:2:177:VAL:HG21	22:2:304:CLA:HMD2	1.71	0.72
22:A:815:CLA:H161	13:3:195:VAL:HG12	1.70	0.72
24:6:305:BCR:H16C	39:6:316:CHL:HMB2	1.70	0.72
22:A:818:CLA:H62	22:A:818:CLA:C4C	2.19	0.72
14:7:167:TYR:HB3	22:7:304:CLA:HED3	1.70	0.72
16:4:121:ARG:HH22	16:4:133:PRO:HA	1.55	0.72
22:A:822:CLA:HED1	10:K:70:ARG:HE	1.54	0.72
2:B:296:PHE:O	7:G:88:ILE:HG13	1.89	0.72
22:B:834:CLA:H51	24:F:303:BCR:HC22	1.72	0.72
22:B:827:CLA:H192	22:B:842:CLA:H91	1.70	0.72
22:5:308:CLA:HMD2	22:5:313:CLA:H43	1.70	0.72
1:A:615:GLN:HG2	1:A:630:ILE:HD12	1.70	0.72
22:A:806:CLA:HHC	22:A:806:CLA:HBB1	1.70	0.72
22:B:840:CLA:H8	22:B:841:CLA:H142	1.70	0.72
13:3:70:GLY:HA2	38:3:303:LUT:H181	1.71	0.72
15:8:187:LYS:HG3	22:8:311:CLA:HED2	1.69	0.72
22:B:823:CLA:H71	22:B:824:CLA:H112	1.71	0.71
22:8:305:CLA:H71	22:8:306:CLA:HMA2	1.72	0.71
14:7:133:TRP:CZ2	24:7:303:BCR:HC8	2.24	0.71
22:B:828:CLA:H112	24:B:847:BCR:H373	1.71	0.71
6:F:202:TRP:CG	6:F:203:PRO:HD3	2.25	0.71
22:A:827:CLA:H192	22:A:835:CLA:H91	1.70	0.71
24:F:303:BCR:H321	24:F:303:BCR:HC8	1.72	0.71
22:7:306:CLA:NC	22:7:306:CLA:H52	2.05	0.71
39:4:819:CHL:HBB1	39:4:819:CHL:HHC	1.73	0.71
22:A:822:CLA:H2	22:A:823:CLA:H92	1.73	0.71
18:6:250:PHE:H	22:6:301:CLA:H43	1.55	0.71
22:A:822:CLA:HMD1	24:A:856:BCR:H23C	1.72	0.71
7:G:38:VAL:HG11	22:G:201:CLA:C4D	2.21	0.71
13:3:120:ALA:HB1	24:3:304:BCR:H363	1.72	0.71
22:B:827:CLA:CAB	24:B:848:BCR:H19C	2.21	0.71
10:K:31:GLY:H	10:K:35:ASN:HD22	1.37	0.71
6:F:202:TRP:CD1	6:F:203:PRO:HD3	2.25	0.71
39:4:813:CHL:HAB	39:4:816:CHL:HBB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:126:LEU:HD12	22:6:302:CLA:HBA1	1.72	0.71
22:B:815:CLA:H152	22:B:830:CLA:HMD3	1.72	0.71
12:1:45:LEU:HD21	22:1:307:CLA:HAA2	1.71	0.71
15:8:85:ILE:HB	15:8:86:PRO:HD3	1.72	0.71
22:F:302:CLA:H193	32:F:306:RRX:H21	1.73	0.71
22:1:308:CLA:HHC	22:1:308:CLA:HBB1	1.73	0.71
6:F:201:THR:HA	22:8:309:CLA:H152	1.72	0.70
38:1:302:LUT:H30	22:1:304:CLA:H52	1.73	0.70
12:1:92:GLU:HG2	12:1:98:ASN:HA	1.72	0.70
12:Z:78:CYS:HB3	12:Z:178:GLY:HA3	1.73	0.70
19:9:129:GLY:HA3	19:9:142:PHE:CZ	2.26	0.70
1:A:316:TRP:HD1	10:K:76:LEU:HD21	1.55	0.70
22:B:824:CLA:HAB	24:B:847:BCR:C10	2.20	0.70
22:7:306:CLA:HBA1	22:7:306:CLA:CBD	2.21	0.70
25:4:820:LHG:HC82	24:6:305:BCR:HC42	1.73	0.70
22:A:820:CLA:HBB2	24:A:844:BCR:H402	1.73	0.70
2:B:549:PRO:HB3	6:F:226:PRO:HG2	1.72	0.70
2:B:719:VAL:HG21	31:B:852:DGD:HBV1	1.73	0.70
16:4:200:LEU:HD12	38:4:802:LUT:H222	1.74	0.70
22:Z:308:CLA:H151	22:Z:313:CLA:HAA2	1.73	0.70
22:A:810:CLA:HMD1	22:3:312:CLA:H102	1.74	0.70
22:A:816:CLA:HBB1	22:A:816:CLA:HMB3	1.74	0.70
22:A:831:CLA:HMA2	11:L:57:THR:HG21	1.72	0.70
2:B:620:TRP:O	2:B:624:TYR:HB3	1.91	0.70
22:Z:304:CLA:HHC	22:Z:304:CLA:HBB1	1.72	0.70
38:6:303:LUT:H371	22:6:307:CLA:H92	1.73	0.70
2:B:618:MET:HG3	2:B:622:ARG:HH12	1.55	0.70
22:B:815:CLA:H51	22:B:820:CLA:HBC3	1.70	0.70
8:I:88:PRO:HG3	24:I:4001:BCR:H12C	1.72	0.70
22:4:815:CLA:HED2	22:4:815:CLA:H2A	1.72	0.70
17:5:106:PRO:HB2	17:5:115:ASN:HA	1.74	0.70
39:5:316:CHL:H122	39:5:316:CHL:H91	1.74	0.70
1:A:45:THR:HG23	5:E:78:GLN:HE21	1.55	0.70
13:3:96:VAL:HG11	38:3:303:LUT:H172	1.71	0.70
22:3:308:CLA:H152	39:3:317:CHL:H72	1.73	0.70
22:3:312:CLA:HHC	22:3:312:CLA:HBB1	1.74	0.70
22:5:311:CLA:C7	22:5:323:CLA:HAB	2.22	0.70
24:B:853:BCR:H271	22:L:201:CLA:HED1	1.73	0.70
18:6:247:PRO:HG3	22:6:301:CLA:H111	1.73	0.70
22:6:312:CLA:HBC3	22:6:312:CLA:H122	1.74	0.70
22:B:817:CLA:HMA2	24:B:846:BCR:H343	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:203:VAL:HG13	31:3:301:DGD:HG32	1.74	0.69
1:A:205:LEU:HA	24:A:845:BCR:H363	1.74	0.69
22:F:304:CLA:HBB1	32:F:306:RRX:H51	1.74	0.69
24:3:304:BCR:H281	22:5:301:CLA:CAB	2.22	0.69
39:3:317:CHL:HHC	39:3:317:CHL:HBB1	1.74	0.69
22:6:308:CLA:HMB3	22:6:308:CLA:HBB1	1.73	0.69
33:G:204:LMT:H4'	22:1:314:CLA:HMA2	1.73	0.69
22:1:307:CLA:HBB1	22:1:307:CLA:HMB3	1.74	0.69
38:Z:301:LUT:H403	22:Z:303:CLA:H141	1.73	0.69
39:6:316:CHL:HHC	39:6:316:CHL:HBB1	1.73	0.69
13:3:103:TYR:HB3	13:3:106:TYR:CE2	2.26	0.69
14:7:53:PHE:HB3	22:7:307:CLA:CAD	2.23	0.69
14:7:178:PHE:HE2	38:7:301:LUT:H221	1.56	0.69
15:8:104:GLY:HA2	39:8:315:CHL:HAC2	1.75	0.69
22:A:809:CLA:HHC	22:A:809:CLA:HBB1	1.74	0.69
22:A:830:CLA:HMB3	22:A:830:CLA:HBB1	1.73	0.69
12:Z:84:GLY:HA2	38:Z:302:LUT:H181	1.75	0.69
22:A:813:CLA:HBA1	22:A:825:CLA:H41	1.74	0.69
22:B:809:CLA:H41	31:B:852:DGD:HB61	1.75	0.69
38:8:302:LUT:H11	22:8:306:CLA:HMC1	1.75	0.69
18:6:123:PHE:CZ	39:6:320:CHL:HBB2	2.28	0.69
39:2:303:CHL:HHC	39:2:303:CHL:HBB1	1.73	0.69
22:A:822:CLA:HAA2	10:K:61:THR:HG21	1.75	0.69
13:3:203:VAL:HA	31:3:301:DGD:HB42	1.73	0.69
39:5:321:CHL:HBB1	39:5:321:CHL:HHC	1.74	0.69
22:1:305:CLA:HBC3	22:1:310:CLA:H143	1.74	0.69
17:5:185:LYS:HD3	22:5:308:CLA:HAA2	1.75	0.69
22:A:823:CLA:HAA2	10:K:63:ALA:O	1.93	0.68
6:F:153:THR:HA	22:F:302:CLA:HAC2	1.75	0.68
19:9:115:GLU:HA	39:9:314:CHL:HMA3	1.75	0.68
1:A:157:LEU:HD11	27:A:852:DGA:HA81	1.75	0.68
22:A:812:CLA:HBA1	22:A:812:CLA:CHA	2.23	0.68
22:A:841:CLA:H12	22:A:841:CLA:NA	2.08	0.68
22:B:824:CLA:HAB	24:B:847:BCR:C9	2.24	0.68
22:A:855:CLA:H122	22:B:841:CLA:H141	1.76	0.68
13:3:73:GLY:HA3	38:3:303:LUT:H182	1.76	0.68
18:6:142:PRO:HB2	22:6:302:CLA:HMD3	1.75	0.68
1:A:59:PHE:CD2	22:A:805:CLA:HMC2	2.28	0.68
2:B:283:VAL:HG13	24:B:844:BCR:H363	1.74	0.68
12:Z:152:TYR:HB3	22:Z:303:CLA:HED3	1.74	0.68
39:9:314:CHL:HBB1	39:9:314:CHL:HHC	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:808:CLA:HBB2	22:A:828:CLA:H171	1.74	0.68
22:F:301:CLA:H152	9:J:18:TRP:HE3	1.58	0.68
24:4:804:BCR:H373	39:4:816:CHL:HHB	1.76	0.68
18:6:64:LEU:HD12	22:6:310:CLA:HMA2	1.76	0.68
22:A:807:CLA:HHB	22:A:808:CLA:HMB3	1.76	0.68
22:A:807:CLA:H8	22:A:809:CLA:H61	1.73	0.68
22:A:823:CLA:H152	24:A:856:BCR:H401	1.73	0.68
22:B:835:CLA:HMB3	22:B:835:CLA:HBB1	1.75	0.68
11:L:141:GLN:HE21	11:L:141:GLN:H	1.41	0.68
22:B:817:CLA:H51	24:B:844:BCR:H282	1.75	0.68
22:3:313:CLA:HMB1	22:3:313:CLA:HBB1	1.75	0.68
22:A:818:CLA:H8	22:A:836:CLA:HMA3	1.74	0.68
2:B:687:PRO:HG2	22:L:202:CLA:H52	1.76	0.68
18:6:99:ASP:HA	39:6:315:CHL:O1D	1.94	0.68
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.76	0.67
6:F:79:ARG:HG2	6:F:115:PHE:CZ	2.26	0.67
13:3:82:LYS:HZ1	13:3:211:GLU:HG2	1.59	0.67
22:5:322:CLA:H152	22:6:319:CLA:H71	1.77	0.67
24:A:856:BCR:H24C	10:K:95:LEU:HD21	1.76	0.67
2:B:197:HIS:O	2:B:201:PRO:HG2	1.95	0.67
22:B:836:CLA:HMB1	22:B:836:CLA:HBB1	1.77	0.67
22:G:201:CLA:CAB	24:G:203:BCR:H352	2.24	0.67
10:K:39:VAL:HG22	22:K:202:CLA:HBA1	1.75	0.67
12:1:168:GLU:CD	12:1:168:GLU:H	2.02	0.67
22:3:309:CLA:HMD2	22:3:314:CLA:H43	1.77	0.67
39:6:315:CHL:H51	39:6:315:CHL:H92	1.77	0.67
22:9:306:CLA:H71	22:9:307:CLA:HMA3	1.76	0.67
22:Z:313:CLA:H101	22:Z:313:CLA:HBA1	1.76	0.67
22:9:306:CLA:HMB1	22:9:306:CLA:HBB1	1.76	0.67
22:A:840:CLA:H111	22:A:840:CLA:CAB	2.25	0.67
22:B:833:CLA:C8	32:F:306:RRX:H27	2.24	0.67
13:3:89:ILE:HD13	13:3:94:THR:HG22	1.76	0.67
18:6:149:LEU:HD11	18:6:158:GLY:HA3	1.75	0.67
22:A:815:CLA:HBB1	22:A:815:CLA:HMB1	1.76	0.67
16:4:67:PHE:HD1	16:4:80:GLY:HA3	1.60	0.67
16:4:121:ARG:HG3	16:4:131:GLN:HA	1.75	0.67
23:B:843:PQN:H201	24:B:849:BCR:H21C	1.76	0.67
22:Z:306:CLA:H71	22:Z:307:CLA:HMA1	1.76	0.67
14:7:26:TYR:HE2	14:7:191:GLN:HB2	1.59	0.67
22:9:313:CLA:HHC	22:9:313:CLA:HBB1	1.76	0.67
1:A:446:ILE:HA	22:A:854:CLA:CGA	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:815:CLA:H43	24:3:306:BCR:HC21	1.77	0.67
2:B:453:GLN:HE21	2:B:455:LEU:HD11	1.58	0.67
39:5:316:CHL:HHC	39:5:316:CHL:HBB1	1.76	0.67
18:6:108:PHE:HD2	18:6:113:LEU:HD21	1.60	0.67
22:A:804:CLA:HAB	22:A:806:CLA:CAD	2.24	0.67
7:G:91:THR:HG21	7:G:98:THR:HA	1.77	0.67
7:G:99:LEU:HD12	7:G:99:LEU:H	1.60	0.67
13:3:146:LEU:HD22	24:3:305:BCR:HC32	1.76	0.67
22:5:309:CLA:H12	22:5:309:CLA:NA	2.09	0.67
22:B:827:CLA:H2	22:B:839:CLA:HBD	1.76	0.67
7:G:77:TYR:HD2	7:G:79:ASP:HB3	1.59	0.67
9:J:1:MET:H2	34:J:101:LMG:HC2	1.60	0.67
40:1:318:SQD:C7	40:1:318:SQD:H121	2.25	0.67
17:5:85:VAL:HG11	38:5:302:LUT:H12	1.77	0.67
19:9:145:ASP:H	19:9:146:PRO:HD2	1.59	0.67
22:B:811:CLA:CBA	22:B:829:CLA:HBD	2.24	0.66
4:D:178:ASN:HB3	4:D:191:THR:HG22	1.77	0.66
12:Z:79:ARG:HA	12:Z:82:MET:HE3	1.76	0.66
38:3:302:LUT:C30	22:3:308:CLA:H72	2.24	0.66
22:A:822:CLA:HMB2	22:A:823:CLA:H2	1.77	0.66
38:1:303:LUT:H8	22:1:309:CLA:HBB1	1.78	0.66
38:Z:301:LUT:H26	22:Z:303:CLA:H2	1.76	0.66
14:7:209:ALA:HB2	22:7:317:CLA:H8	1.77	0.66
39:8:301:CHL:HHC	39:8:301:CHL:HBB1	1.76	0.66
39:6:318:CHL:HBB1	39:6:318:CHL:HMB3	1.77	0.66
22:A:810:CLA:H161	24:A:845:BCR:H372	1.77	0.66
22:B:808:CLA:HBB1	22:B:808:CLA:HMB1	1.76	0.66
4:D:189:ASN:HD22	4:D:194:ILE:HD13	1.59	0.66
38:7:302:LUT:H28	22:7:307:CLA:C6	2.25	0.66
15:8:156:PHE:CE1	22:8:313:CLA:HAB	2.30	0.66
24:5:304:BCR:HC8	22:5:326:CLA:H72	1.77	0.66
22:B:813:CLA:HBB1	22:B:813:CLA:CMB	2.24	0.66
22:B:820:CLA:HBB1	22:B:820:CLA:CMB	2.25	0.66
22:3:310:CLA:H52	22:3:310:CLA:NC	2.10	0.66
18:6:62:GLU:HA	18:6:65:LYS:HD3	1.76	0.66
2:B:475:PHE:HB3	22:F:304:CLA:H191	1.77	0.66
22:B:831:CLA:H52	31:B:852:DGD:HB52	1.77	0.66
16:4:95:TRP:CZ2	22:4:815:CLA:HAA2	2.27	0.66
1:A:114:SER:HB2	1:A:131:VAL:HG11	1.77	0.66
22:K:202:CLA:HBB1	22:K:202:CLA:HMB3	1.75	0.66
22:5:326:CLA:H71	22:6:314:CLA:H72	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLN:HA	25:A:850:LHG:HC5	1.78	0.66
33:G:204:LMT:H51	22:1:314:CLA:H2	1.78	0.66
23:A:843:PQN:H193	24:F:303:BCR:H23C	1.76	0.66
2:B:89:ALA:HB2	2:B:117:SER:HB3	1.77	0.66
12:1:60:LEU:HD13	22:1:307:CLA:H42	1.76	0.66
22:Z:303:CLA:HBB1	22:Z:303:CLA:HMB1	1.78	0.66
18:6:99:ASP:HB3	39:6:315:CHL:HED3	1.77	0.66
2:B:657:VAL:HG22	22:B:841:CLA:HMB3	1.77	0.66
12:1:57:PRO:HD2	38:1:303:LUT:H23	1.77	0.66
15:8:63:ARG:HG2	15:8:137:PHE:CE2	2.31	0.66
17:5:205:GLN:HG3	17:5:253:TRP:HZ3	1.61	0.66
38:9:301:LUT:H26	22:9:303:CLA:O1A	1.95	0.66
22:5:309:CLA:HBA1	22:5:309:CLA:CBD	2.24	0.65
1:A:680:ALA:HB3	22:B:801:CLA:HBB2	1.77	0.65
22:A:824:CLA:HBB1	22:A:824:CLA:HHC	1.78	0.65
13:3:89:ILE:HG12	22:3:313:CLA:HED2	1.78	0.65
14:7:49:GLY:H	14:7:191:GLN:HE22	1.44	0.65
17:5:230:ASN:HA	17:5:233:HIS:NE2	2.12	0.65
39:9:312:CHL:HBC3	39:9:312:CHL:H151	1.77	0.65
38:3:302:LUT:H383	39:3:317:CHL:H11	1.79	0.65
22:3:312:CLA:O1D	22:3:318:CLA:H62	1.96	0.65
22:7:304:CLA:H101	22:7:310:CLA:H18	1.78	0.65
1:A:316:TRP:CD1	10:K:76:LEU:HD21	2.31	0.65
22:8:311:CLA:HHC	22:8:311:CLA:HBB1	1.79	0.65
19:9:117:LEU:HD21	39:2:303:CHL:H2	1.77	0.65
1:A:449:GLY:HA3	22:A:854:CLA:O1A	1.95	0.65
22:A:814:CLA:HBA2	22:A:816:CLA:HHB	1.78	0.65
24:F:303:BCR:H12C	22:F:305:CLA:CAB	2.27	0.65
15:8:41:LYS:H	15:8:41:LYS:HD2	1.61	0.65
6:F:160:ALA:HB1	22:F:302:CLA:H8	1.79	0.65
24:3:307:BCR:H392	22:3:314:CLA:HAC2	1.78	0.65
16:4:67:PHE:CD1	16:4:80:GLY:HA3	2.31	0.65
1:A:80:GLN:HG2	22:A:805:CLA:HMA1	1.78	0.65
22:A:822:CLA:H71	22:K:204:CLA:HAB	1.79	0.65
5:E:36:GLY:HA3	5:E:62:VAL:HG11	1.78	0.65
12:Z:158:ASP:HA	38:Z:301:LUT:H24	1.79	0.65
13:3:82:LYS:NZ	13:3:211:GLU:HG2	2.11	0.65
2:B:463:TRP:CD1	22:F:304:CLA:H193	2.32	0.65
2:B:487:ALA:O	2:B:491:GLN:HG3	1.97	0.65
22:B:814:CLA:H12	19:9:56:LEU:HD22	1.79	0.65
13:3:146:LEU:HD11	22:5:315:CLA:H171	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:322:CLA:HBB2	22:7:307:CLA:HHD	1.79	0.65
39:7:313:CHL:HHC	39:7:313:CHL:HBB1	1.77	0.65
17:5:182:LEU:HB3	22:5:307:CLA:CMA	2.26	0.65
39:5:316:CHL:H162	22:6:322:CLA:H193	1.78	0.65
22:B:838:CLA:H171	32:F:306:RRX:C35	2.26	0.65
15:8:55:LEU:CD1	38:8:303:LUT:H221	2.25	0.65
15:8:125:MET:HB3	24:8:304:BCR:H15C	1.78	0.65
22:5:326:CLA:HBD	22:5:326:CLA:HBA1	1.79	0.65
22:A:814:CLA:H112	24:A:844:BCR:H353	1.79	0.64
22:A:833:CLA:HAB	22:A:834:CLA:HHB	1.77	0.64
22:A:833:CLA:NC	22:A:834:CLA:H101	2.12	0.64
39:Z:311:CHL:HHC	39:Z:311:CHL:HBB1	1.78	0.64
38:4:802:LUT:H383	39:4:814:CHL:H12	1.78	0.64
17:5:131:TRP:CE3	22:6:314:CLA:HBA2	2.32	0.64
18:6:125:GLU:HG2	22:6:317:CLA:C1B	2.26	0.64
20:2:189:HIS:CG	22:2:301:CLA:HAA2	2.33	0.64
24:A:856:BCR:H323	24:3:306:BCR:HC41	1.78	0.64
22:B:810:CLA:H62	22:B:810:CLA:NC	2.11	0.64
22:3:320:CLA:CMA	22:3:322:CLA:H112	2.28	0.64
24:8:304:BCR:H292	22:8:310:CLA:HBA1	1.80	0.64
22:5:326:CLA:HMD2	22:6:309:CLA:H2	1.80	0.64
7:G:57:HIS:CE1	7:G:61:LEU:HD11	2.33	0.64
12:Z:61:CYS:HB2	22:Z:306:CLA:HBA1	1.80	0.64
12:Z:134:MET:HG3	22:Z:314:CLA:HMC3	1.79	0.64
13:3:122:GLN:O	13:3:126:LEU:HB2	1.97	0.64
19:9:102:LYS:HB3	19:9:104:TYR:CE2	2.32	0.64
22:B:830:CLA:H151	24:B:845:BCR:H15C	1.78	0.64
6:F:224:ILE:HB	6:F:227:ARG:HH22	1.61	0.64
7:G:35:TYR:HB3	22:G:201:CLA:HED2	1.80	0.64
38:Z:301:LUT:H382	22:Z:303:CLA:C4D	2.27	0.64
15:8:135:MET:HB3	15:8:143:GLN:NE2	2.13	0.64
22:8:309:CLA:HED2	22:8:309:CLA:H2A	1.80	0.64
38:4:802:LUT:H28	22:4:805:CLA:H2	1.78	0.64
24:4:804:BCR:H19C	39:4:816:CHL:O1A	1.98	0.64
22:A:821:CLA:H72	24:A:846:BCR:H361	1.80	0.64
22:B:816:CLA:H61	24:B:846:BCR:H362	1.79	0.64
22:B:833:CLA:HBC2	22:B:839:CLA:CMC	2.27	0.64
10:K:57:VAL:HG11	10:K:76:LEU:HD12	1.78	0.64
12:1:53:TYR:HB2	22:1:307:CLA:HMD1	1.80	0.64
38:7:301:LUT:C30	22:7:304:CLA:H72	2.27	0.64
22:A:855:CLA:HAB	2:B:692:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:98:PRO:HD2	22:3:316:CLA:C1B	2.28	0.64
39:4:813:CHL:HBB1	39:4:813:CHL:HMB3	1.78	0.64
38:5:303:LUT:H28	22:5:310:CLA:H72	1.78	0.64
1:A:80:GLN:HG2	22:A:805:CLA:CMA	2.28	0.64
24:3:306:BCR:H19C	22:3:312:CLA:C2C	2.28	0.64
17:5:57:PRO:HG2	22:5:315:CLA:H12	1.78	0.64
18:6:123:PHE:CD1	24:6:305:BCR:H10C	2.33	0.64
18:6:247:PRO:HG2	24:6:306:BCR:H272	1.79	0.64
22:A:832:CLA:H112	22:L:202:CLA:H171	1.80	0.64
2:B:394:PHE:CD2	24:B:848:BCR:H281	2.32	0.64
14:7:178:PHE:CE2	38:7:301:LUT:H221	2.32	0.64
22:4:815:CLA:HBB1	22:4:815:CLA:HMB1	1.78	0.64
38:6:304:LUT:H393	22:6:310:CLA:H141	1.80	0.64
22:A:806:CLA:H43	25:A:850:LHG:H262	1.79	0.63
22:A:825:CLA:H143	22:A:825:CLA:HMD2	1.79	0.63
2:B:283:VAL:HG13	24:B:844:BCR:C36	2.28	0.63
22:1:313:CLA:HBA1	22:1:313:CLA:H101	1.78	0.63
39:6:315:CHL:HBB1	39:6:315:CHL:HMB1	1.80	0.63
7:G:78:PHE:CE1	7:G:81:LEU:HD21	2.32	0.63
7:G:78:PHE:CZ	7:G:81:LEU:HD21	2.33	0.63
12:1:223:PRO:HG3	22:1:316:CLA:HAB	1.79	0.63
13:3:22:THR:HA	13:3:25:TYR:CE2	2.34	0.63
16:4:228:PHE:CD1	16:4:239:PRO:HB3	2.33	0.63
38:5:302:LUT:H11	22:5:308:CLA:HMC1	1.80	0.63
18:6:88:GLN:HE22	38:6:304:LUT:H42	1.62	0.63
22:A:810:CLA:H71	22:3:312:CLA:H51	1.80	0.63
22:A:814:CLA:HBB1	22:A:814:CLA:HMB3	1.80	0.63
24:B:847:BCR:H331	24:B:847:BCR:HC8	1.80	0.63
24:B:853:BCR:H403	24:I:4001:BCR:H372	1.80	0.63
22:F:302:CLA:C2B	24:F:303:BCR:H10C	2.28	0.63
13:3:195:VAL:HG11	38:3:303:LUT:C12	2.28	0.63
24:3:307:BCR:H403	24:3:307:BCR:H23C	1.78	0.63
22:7:322:CLA:HMB1	22:7:322:CLA:HBB1	1.80	0.63
39:8:315:CHL:HBB1	39:8:315:CHL:HMB1	1.81	0.63
22:A:838:CLA:H52	22:A:838:CLA:C1C	2.29	0.63
2:B:271:LEU:HD23	2:B:274:MET:HE3	1.80	0.63
10:K:57:VAL:O	10:K:58:LYS:HB3	1.97	0.63
12:1:194:ALA:HB1	12:1:218:ASN:HD21	1.64	0.63
13:3:42:LEU:HB2	22:3:311:CLA:HBA1	1.78	0.63
1:A:514:VAL:HG22	1:A:524:MET:HG3	1.79	0.63
2:B:420:ILE:HD13	2:B:537:LYS:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:809:CLA:H43	22:B:831:CLA:H2	1.78	0.63
22:B:816:CLA:HMA2	24:B:846:BCR:H282	1.81	0.63
11:L:87:GLU:HA	11:L:90:ARG:NH2	2.13	0.63
1:A:690:ARG:HG3	1:A:717:ALA:HB3	1.80	0.63
22:A:816:CLA:CBB	24:A:844:BCR:H12C	2.28	0.63
22:A:827:CLA:H193	22:A:827:CLA:H152	1.79	0.63
2:B:27:ALA:HB1	31:B:852:DGD:HG2	1.79	0.63
31:1:319:DGD:HG11	31:1:319:DGD:HB21	1.79	0.63
18:6:88:GLN:HG2	22:6:312:CLA:C4D	2.29	0.63
22:A:822:CLA:HBB1	37:K:201:DAO:H112	1.79	0.63
22:B:811:CLA:HBA2	22:B:829:CLA:CBD	2.27	0.63
38:1:303:LUT:H373	22:1:307:CLA:H91	1.78	0.63
13:3:71:ALA:HB1	38:3:302:LUT:H12	1.81	0.63
1:A:598:TRP:CH2	22:B:806:CLA:HAB	2.34	0.63
22:B:827:CLA:HBA2	22:B:839:CLA:HAA1	1.81	0.63
6:F:69:PRO:HG2	6:F:72:GLU:HB2	1.81	0.63
14:7:70:HIS:O	14:7:74:GLN:HG2	1.99	0.63
22:7:322:CLA:H2	22:7:323:CLA:H101	1.80	0.63
22:A:822:CLA:H62	22:A:823:CLA:H92	1.81	0.63
22:A:855:CLA:H152	24:B:853:BCR:H17C	1.81	0.63
2:B:258:PHE:HZ	22:B:819:CLA:H111	1.63	0.63
17:5:155:ASN:HB3	39:5:321:CHL:C3D	2.27	0.63
22:A:810:CLA:H43	22:A:812:CLA:H42	1.81	0.62
22:A:833:CLA:HBA1	22:A:855:CLA:H2	1.81	0.62
12:1:153:PRO:HB3	22:1:313:CLA:HBC2	1.80	0.62
22:8:314:CLA:C4B	26:8:318:NKP:HAY	2.29	0.62
16:4:66:LYS:HD3	25:4:821:LHG:HC31	1.81	0.62
18:6:96:PHE:HB3	18:6:99:ASP:OD1	1.99	0.62
18:6:143:LEU:HD22	39:6:320:CHL:HMB3	1.80	0.62
14:7:228:ASP:HB3	14:7:232:THR:HG23	1.81	0.62
18:6:238:ASP:CA	18:6:243:LYS:HA	2.17	0.62
23:A:843:PQN:H212	22:F:301:CLA:C3B	2.29	0.62
22:B:831:CLA:HBB1	22:B:831:CLA:HMB1	1.80	0.62
4:D:115:PHE:HB3	4:D:120:GLN:HE21	1.63	0.62
12:Z:203:LEU:HA	22:Z:305:CLA:HMA1	1.82	0.62
14:7:133:TRP:CH2	24:7:303:BCR:HC8	2.34	0.62
39:9:312:CHL:HED1	39:9:312:CHL:H93	1.80	0.62
7:G:93:ASP:HB2	22:G:202:CLA:CHA	2.29	0.62
14:7:175:PRO:HD2	38:7:301:LUT:H23	1.80	0.62
15:8:78:THR:HG23	22:8:305:CLA:CMC	2.30	0.62
15:8:135:MET:HB3	15:8:143:GLN:HE22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:8:303:LUT:H371	22:8:308:CLA:H142	1.81	0.62
39:8:312:CHL:HBB1	39:8:312:CHL:HMB1	1.81	0.62
22:2:304:CLA:HBB1	22:2:304:CLA:HHC	1.82	0.62
2:B:491:GLN:HA	2:B:495:LEU:HD12	1.82	0.62
22:1:310:CLA:HBA1	22:1:310:CLA:CHA	2.28	0.62
12:Z:103:PRO:HG2	39:Z:312:CHL:HED1	1.80	0.62
16:4:86:LEU:HD23	33:4:801:LMT:H2'	1.81	0.62
17:5:171:PRO:HD2	38:5:302:LUT:H23	1.82	0.62
19:9:101:ALA:HB2	39:9:312:CHL:HBA2	1.81	0.62
22:A:815:CLA:H41	24:3:306:BCR:HC8	1.81	0.62
22:B:834:CLA:NC	24:J:104:BCR:H292	2.15	0.62
1:A:59:PHE:HA	1:A:62:HIS:ND1	2.15	0.62
22:A:823:CLA:HBC2	22:A:824:CLA:HAA1	1.81	0.62
38:3:303:LUT:H26	22:3:311:CLA:H2	1.82	0.62
11:L:135:TYR:HB2	24:L:204:BCR:H361	1.81	0.62
12:Z:53:TYR:HB2	22:Z:306:CLA:HMD1	1.80	0.62
13:3:26:LEU:HD13	13:3:35:GLY:HA2	1.81	0.62
22:5:309:CLA:HHC	22:5:309:CLA:HBB1	1.82	0.62
22:A:826:CLA:HBB1	22:A:826:CLA:HMB1	1.82	0.62
22:4:811:CLA:HHC	22:4:811:CLA:HBB1	1.82	0.62
22:A:818:CLA:H8	22:A:836:CLA:CMA	2.30	0.62
22:B:807:CLA:HBB1	22:B:807:CLA:HMB1	1.82	0.62
22:Z:309:CLA:H102	22:Z:309:CLA:H142	1.80	0.62
19:9:124:THR:HG21	39:2:303:CHL:HED3	1.80	0.62
1:A:153:ILE:HA	1:A:158:GLN:OE1	2.00	0.61
1:A:541:PHE:HZ	22:B:806:CLA:HBB2	1.65	0.61
24:A:844:BCR:H17C	24:A:845:BCR:H382	1.80	0.61
2:B:6:PHE:HB3	2:B:7:PRO:HD3	1.82	0.61
23:B:843:PQN:H142	24:B:849:BCR:H281	1.81	0.61
39:1:312:CHL:HMB3	39:1:312:CHL:HBB1	1.81	0.61
13:3:82:LYS:HD2	13:3:210:TYR:HD2	1.64	0.61
22:3:313:CLA:H202	22:5:320:CLA:HHB	1.82	0.61
24:7:303:BCR:H332	25:8:317:LHG:H252	1.82	0.61
1:A:462:MET:HE2	1:A:462:MET:HA	1.82	0.61
39:Z:312:CHL:HBB1	39:Z:312:CHL:HMB3	1.80	0.61
13:3:163:TRP:HH2	24:3:305:BCR:H10C	1.65	0.61
22:7:322:CLA:ND	22:7:323:CLA:H122	2.16	0.61
15:8:170:PRO:HD2	38:8:302:LUT:H24	1.82	0.61
16:4:113:GLY:HA3	38:4:803:LUT:H182	1.83	0.61
16:4:219:ARG:HA	16:4:222:MET:HE3	1.80	0.61
19:9:56:LEU:HB2	22:9:306:CLA:H11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:166:LEU:HA	20:2:169:ILE:HG12	1.81	0.61
22:A:814:CLA:HBD	22:A:816:CLA:HMA1	1.81	0.61
2:B:597:TRP:CH2	2:B:613:SER:HB2	2.35	0.61
22:B:818:CLA:HBB1	22:B:818:CLA:HHC	1.82	0.61
12:1:140:ARG:HG2	22:1:313:CLA:HHC	1.81	0.61
22:1:306:CLA:HBC1	22:1:316:CLA:H101	1.81	0.61
24:6:306:BCR:H16C	39:6:315:CHL:C4C	2.29	0.61
38:9:302:LUT:H11	22:9:307:CLA:HAC2	1.82	0.61
1:A:508:ALA:HB3	1:A:523:MET:HG3	1.81	0.61
22:B:810:CLA:H11	8:I:79:PHE:HB3	1.81	0.61
22:F:301:CLA:H121	9:J:14:VAL:HG13	1.81	0.61
7:G:107:ALA:HA	24:G:203:BCR:H341	1.82	0.61
12:Z:157:PHE:HA	22:Z:313:CLA:H72	1.81	0.61
15:8:80:VAL:HG13	15:8:202:PHE:HE2	1.64	0.61
39:4:814:CHL:HMB3	39:4:814:CHL:HBB1	1.82	0.61
18:6:226:VAL:HG21	41:6:324:3PH:H221	1.80	0.61
22:A:829:CLA:H11	24:A:845:BCR:H311	1.82	0.61
2:B:54:GLN:HG2	22:B:808:CLA:CMA	2.30	0.61
8:I:67:TYR:CE2	8:I:69:PHE:HB2	2.36	0.61
22:5:307:CLA:H93	22:5:308:CLA:H62	1.81	0.61
18:6:188:PHE:CE1	18:6:199:PRO:HB3	2.36	0.61
22:A:829:CLA:H42	22:A:829:CLA:HBD	1.82	0.61
23:A:843:PQN:H212	22:F:301:CLA:C4B	2.31	0.61
12:1:98:ASN:HD21	12:1:101:ASP:HB2	1.63	0.61
38:Z:301:LUT:H28	22:Z:303:CLA:H52	1.83	0.61
13:3:120:ALA:HB2	22:3:319:CLA:H2	1.82	0.61
16:4:243:LEU:HB2	38:4:802:LUT:H22	1.81	0.61
22:6:312:CLA:H52	22:6:312:CLA:C3D	2.30	0.61
19:9:120:GLY:HA2	22:9:313:CLA:HAB	1.81	0.61
1:A:197:MET:HG3	22:A:813:CLA:HBC2	1.83	0.61
1:A:545:VAL:HG11	1:A:598:TRP:CE2	2.35	0.61
22:L:201:CLA:H162	22:L:201:CLA:H91	1.81	0.61
18:6:147:ASN:HB3	39:6:320:CHL:C4D	2.30	0.61
1:A:409:ALA:HB1	24:A:846:BCR:H271	1.83	0.61
1:A:694:GLN:HE21	5:E:80:TYR:HE1	1.49	0.61
22:A:821:CLA:H92	22:A:825:CLA:HMB3	1.83	0.61
22:A:832:CLA:HMB1	22:A:832:CLA:HBB1	1.83	0.61
22:A:833:CLA:HAB	22:A:834:CLA:CHB	2.30	0.61
22:B:817:CLA:HHB	24:B:846:BCR:HC8	1.83	0.61
13:3:190:LEU:HB2	24:3:307:BCR:H393	1.82	0.61
22:3:312:CLA:H112	22:3:318:CLA:H42	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:836:CLA:NB	22:K:203:CLA:H52	2.15	0.61
22:A:854:CLA:H142	24:I:4001:BCR:H271	1.83	0.61
2:B:413:LEU:HB3	6:F:227:ARG:HG3	1.82	0.61
22:B:812:CLA:H71	24:B:849:BCR:H343	1.82	0.61
13:3:38:PRO:HD2	38:3:303:LUT:H23	1.82	0.61
24:3:304:BCR:H382	24:3:305:BCR:H351	1.82	0.61
22:3:308:CLA:H51	22:3:309:CLA:HMA2	1.81	0.61
38:7:301:LUT:H383	22:7:314:CLA:H11	1.82	0.61
22:9:307:CLA:H2	22:9:307:CLA:HED2	1.81	0.61
2:B:694:TRP:CD1	2:B:698:PRO:HD3	2.36	0.61
25:B:803:LHG:HC5	22:B:807:CLA:HBA2	1.83	0.61
12:Z:188:PHE:HA	12:Z:191:GLN:NE2	2.15	0.61
22:4:815:CLA:H43	33:4:822:LMT:H91	1.83	0.61
17:5:131:TRP:CD1	24:5:304:BCR:H12C	2.36	0.61
38:5:303:LUT:C28	22:5:310:CLA:H72	2.31	0.61
24:5:304:BCR:H342	22:5:326:CLA:H61	1.83	0.61
2:B:38:MET:HE3	2:B:38:MET:HA	1.82	0.60
2:B:366:PHE:HB3	2:B:603:TRP:CZ3	2.36	0.60
22:B:806:CLA:H171	22:L:201:CLA:HMC3	1.83	0.60
16:4:159:PHE:CD2	24:4:804:BCR:H12C	2.36	0.60
18:6:95:VAL:HG13	18:6:103:LYS:HB2	1.82	0.60
19:9:84:ILE:HG23	19:9:96:TRP:CG	2.36	0.60
19:9:110:PRO:HG3	20:2:199:TYR:HB2	1.82	0.60
14:7:26:TYR:CE2	14:7:191:GLN:HB2	2.37	0.60
24:8:304:BCR:H282	22:8:310:CLA:NB	2.17	0.60
17:5:205:GLN:HG3	17:5:253:TRP:CZ3	2.35	0.60
22:9:311:CLA:HED3	22:9:311:CLA:H2A	1.83	0.60
1:A:211:LEU:HD23	24:A:844:BCR:H373	1.84	0.60
1:A:363:LEU:HD21	22:A:819:CLA:H72	1.83	0.60
22:B:828:CLA:H71	24:B:848:BCR:H16C	1.82	0.60
14:7:49:GLY:HA3	14:7:194:ILE:HG21	1.83	0.60
15:8:27:ARG:HD3	15:8:47:ASP:O	2.01	0.60
16:4:86:LEU:HD11	38:4:803:LUT:H221	1.83	0.60
38:4:803:LUT:H26	22:4:808:CLA:H52	1.83	0.60
38:9:301:LUT:H14	22:9:304:CLA:HBB1	1.83	0.60
1:A:157:LEU:HD23	22:A:816:CLA:HED1	1.82	0.60
22:Z:308:CLA:H61	22:Z:315:CLA:CAA	2.30	0.60
22:5:307:CLA:H72	22:5:308:CLA:CMA	2.31	0.60
39:5:317:CHL:HBB1	39:5:317:CHL:HMB1	1.84	0.60
2:B:57:ILE:HG21	22:B:809:CLA:HMD1	1.82	0.60
4:D:131:LYS:HE3	4:D:132:PHE:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:305:CLA:ND	22:1:310:CLA:H8	2.17	0.60
22:8:310:CLA:H121	43:8:319:LPX:H8A	1.83	0.60
38:5:303:LUT:H372	22:5:315:CLA:H72	1.82	0.60
24:5:304:BCR:H16C	39:5:317:CHL:HMB3	1.82	0.60
18:6:52:PHE:HB3	22:6:310:CLA:CAD	2.32	0.60
18:6:247:PRO:HB2	22:6:301:CLA:C1	2.30	0.60
22:A:828:CLA:H191	24:J:104:BCR:H19C	1.83	0.60
15:8:63:ARG:HG2	15:8:137:PHE:HE2	1.66	0.60
15:8:102:GLU:HA	39:8:312:CHL:HED3	1.84	0.60
22:5:307:CLA:H72	22:5:308:CLA:HMA2	1.82	0.60
39:9:312:CHL:H2	39:9:312:CHL:HMA3	1.82	0.60
22:A:823:CLA:HBA1	37:K:201:DAO:H51	1.82	0.60
22:B:828:CLA:HBA2	24:B:848:BCR:H10C	1.83	0.60
10:K:38:MET:HG2	22:K:202:CLA:C3D	2.31	0.60
10:K:97:HIS:ND1	24:K:206:BCR:H14C	2.15	0.60
22:1:306:CLA:C15	25:1:317:LHG:HC92	2.32	0.60
22:1:306:CLA:H172	25:1:317:LHG:H121	1.82	0.60
12:Z:144:GLU:HB3	12:Z:150:ARG:HG2	1.82	0.60
22:Z:304:CLA:HBC3	22:Z:309:CLA:H143	1.84	0.60
13:3:137:SER:HA	13:3:140:LYS:NZ	2.16	0.60
22:4:815:CLA:HMB2	33:4:822:LMT:H51	1.84	0.60
22:A:804:CLA:HBD	22:A:811:CLA:H2	1.83	0.60
22:A:811:CLA:HBB1	22:A:811:CLA:HHC	1.83	0.60
2:B:262:PHE:CE1	2:B:356:LEU:HA	2.37	0.60
22:B:821:CLA:HMB1	22:B:826:CLA:HED1	1.82	0.60
15:8:174:CYS:HB2	22:8:305:CLA:HAA2	1.83	0.60
16:4:159:PHE:CD1	24:4:804:BCR:H10C	2.37	0.60
18:6:176:LYS:HD3	22:6:313:CLA:O1D	2.01	0.60
1:A:680:ALA:CB	22:B:801:CLA:HBB2	2.32	0.60
2:B:155:TRP:CZ2	2:B:159:GLN:HG2	2.37	0.60
2:B:183:LEU:HD13	22:B:815:CLA:HHB	1.83	0.60
7:G:46:LEU:HD12	22:G:201:CLA:H11	1.82	0.60
7:G:49:GLY:HA3	7:G:105:TRP:CD2	2.37	0.60
10:K:97:HIS:CE1	24:K:206:BCR:H14C	2.37	0.60
22:Z:304:CLA:C1C	22:Z:309:CLA:H121	2.31	0.60
1:A:211:LEU:HD11	24:A:856:BCR:HC7	1.84	0.60
22:A:817:CLA:CAB	24:K:206:BCR:HC32	2.25	0.60
2:B:493:LEU:HD12	22:B:836:CLA:HED1	1.84	0.60
22:F:301:CLA:HHC	22:F:301:CLA:HBB1	1.84	0.60
16:4:228:PHE:HD1	16:4:239:PRO:HB3	1.67	0.60
17:5:98:VAL:HG11	22:5:312:CLA:HED2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:173:LYS:HD3	22:6:308:CLA:O1A	2.02	0.60
1:A:136:GLN:HE22	6:F:104:LEU:HD11	1.67	0.59
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.84	0.59
22:B:811:CLA:HBA1	22:B:811:CLA:CHA	2.31	0.59
22:G:201:CLA:HHC	22:G:201:CLA:CBB	2.31	0.59
17:5:181:GLU:OE2	17:5:185:LYS:HE2	2.02	0.59
22:Z:310:CLA:HBA2	22:Z:310:CLA:CHA	2.29	0.59
22:7:308:CLA:HBB1	22:7:308:CLA:HMB3	1.84	0.59
39:4:813:CHL:HAB	39:4:816:CHL:CBB	2.32	0.59
24:5:305:BCR:H333	18:6:227:VAL:HG21	1.83	0.59
19:9:115:GLU:HB2	39:9:312:CHL:HBB2	1.83	0.59
22:A:805:CLA:HBD	22:A:825:CLA:H52	1.83	0.59
2:B:155:TRP:CH2	2:B:159:GLN:HG2	2.37	0.59
24:B:853:BCR:HC42	22:L:202:CLA:NC	2.17	0.59
5:E:39:ARG:HH21	5:E:62:VAL:H	1.49	0.59
22:8:308:CLA:HBC3	41:8:320:3PH:H3C1	1.83	0.59
16:4:177:ASP:HB3	16:4:180:PHE:O	2.02	0.59
22:4:818:CLA:HBA1	22:4:818:CLA:CHA	2.32	0.59
22:6:309:CLA:HBC1	22:6:319:CLA:HAA1	1.83	0.59
39:9:312:CHL:HBD	39:9:312:CHL:HAA2	1.83	0.59
20:2:171:PHE:O	20:2:172:CYS:C	2.45	0.59
22:A:821:CLA:C4C	22:A:827:CLA:H161	2.32	0.59
2:B:195:LEU:HA	2:B:199:ALA:HB3	1.84	0.59
22:B:814:CLA:HHC	22:B:814:CLA:CBB	2.32	0.59
12:1:78:CYS:SG	12:1:182:MET:HE2	2.43	0.59
12:Z:157:PHE:CE2	22:Z:313:CLA:H161	2.37	0.59
22:Z:303:CLA:H62	22:Z:304:CLA:HMA2	1.83	0.59
13:3:190:LEU:HB2	24:3:307:BCR:C39	2.33	0.59
15:8:127:GLY:HA2	22:8:314:CLA:HMB1	1.83	0.59
22:5:310:CLA:H101	22:5:315:CLA:H121	1.85	0.59
22:5:326:CLA:HHC	22:5:326:CLA:HBB1	1.83	0.59
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.83	0.59
13:3:82:LYS:NZ	13:3:210:TYR:HB3	2.16	0.59
24:7:303:BCR:H11C	22:7:322:CLA:H41	1.84	0.59
16:4:138:GLY:HA2	39:4:816:CHL:HAC2	1.83	0.59
22:B:811:CLA:HBB2	22:B:812:CLA:HAA1	1.84	0.59
22:B:812:CLA:HMB1	22:B:812:CLA:HBB1	1.83	0.59
22:8:309:CLA:H43	22:8:309:CLA:HED3	1.84	0.59
1:A:598:TRP:HE1	22:A:854:CLA:C1D	2.15	0.59
22:A:814:CLA:H141	31:3:301:DGD:HA41	1.84	0.59
2:B:349:VAL:HA	22:B:820:CLA:H42	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:49:GLY:H	14:7:191:GLN:NE2	2.01	0.59
39:8:301:CHL:HAA2	39:8:301:CHL:HBD	1.84	0.59
24:5:305:BCR:H343	18:6:220:VAL:HG11	1.84	0.59
20:2:207:THR:HG23	22:2:301:CLA:H8	1.82	0.59
22:A:855:CLA:H102	22:B:840:CLA:H43	1.85	0.59
2:B:78:TRP:HA	2:B:85:VAL:HB	1.85	0.59
2:B:229:GLY:HA3	7:G:117:LEU:HD13	1.84	0.59
22:B:814:CLA:O1A	7:G:81:LEU:HD22	2.02	0.59
22:F:304:CLA:HMD2	33:F:307:LMT:H32	1.84	0.59
15:8:133:ARG:HH12	22:8:314:CLA:HED3	1.67	0.59
18:6:39:PRO:HB2	18:6:41:HIS:CE1	2.37	0.59
20:2:177:VAL:C	20:2:178:ARG:HG3	2.27	0.59
38:Z:302:LUT:H393	22:Z:306:CLA:H141	1.85	0.59
22:8:310:CLA:HMA2	39:8:315:CHL:C3C	2.33	0.59
24:5:305:BCR:C12	24:5:305:BCR:H341	2.32	0.59
18:6:41:HIS:CD2	18:6:42:LEU:HG	2.38	0.59
18:6:245:PHE:CZ	18:6:247:PRO:HB3	2.36	0.59
22:6:314:CLA:HHC	22:6:314:CLA:CBB	2.31	0.59
2:B:182:GLY:HA3	22:B:815:CLA:HBB1	1.84	0.59
22:B:818:CLA:H121	22:B:818:CLA:HMC3	1.85	0.59
22:B:822:CLA:HBA1	7:G:100:ILE:HG22	1.85	0.59
12:Z:135:ALA:HA	22:Z:314:CLA:HAB	1.84	0.59
22:Z:309:CLA:HHC	22:Z:309:CLA:HBB1	1.85	0.59
22:3:322:CLA:H52	25:7:318:LHG:H321	1.84	0.59
22:7:312:CLA:HHC	22:7:312:CLA:CBB	2.32	0.59
22:8:309:CLA:HMD2	26:8:318:NKP:HAZA	1.85	0.59
38:9:301:LUT:H181	22:9:305:CLA:HBB1	1.85	0.59
1:A:217:GLN:HA	1:A:221:SER:HB2	1.84	0.58
22:A:814:CLA:H11	22:A:816:CLA:CHB	2.33	0.58
22:B:811:CLA:HBA1	22:B:811:CLA:HBD	1.85	0.58
6:F:141:LEU:HD21	6:F:150:PHE:CE2	2.37	0.58
22:F:304:CLA:H12	22:F:304:CLA:NA	2.17	0.58
12:Z:153:PRO:HB3	22:Z:313:CLA:HBC2	1.85	0.58
15:8:40:LEU:HD11	15:8:51:ASP:HB2	1.84	0.58
22:A:808:CLA:H42	22:A:828:CLA:HMD2	1.85	0.58
22:B:811:CLA:HHC	22:B:811:CLA:CBB	2.28	0.58
4:D:184:VAL:HG11	4:D:194:ILE:HG21	1.85	0.58
15:8:39:HIS:HA	15:8:41:LYS:NZ	2.18	0.58
15:8:205:GLN:HB3	15:8:216:ASN:ND2	2.18	0.58
22:B:814:CLA:O1D	22:B:815:CLA:HMC1	2.03	0.58
22:B:819:CLA:HHC	22:B:819:CLA:HBB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:827:CLA:H121	22:B:842:CLA:H202	1.86	0.58
6:F:165:TYR:O	6:F:169:LEU:HG	2.03	0.58
10:K:62:ASP:HB2	10:K:68:VAL:CG2	2.33	0.58
10:K:66:LYS:HB2	10:K:66:LYS:NZ	2.18	0.58
11:L:73:PRO:HB3	11:L:87:GLU:OE1	2.02	0.58
16:4:116:VAL:HB	16:4:117:PRO:HD3	1.86	0.58
22:4:809:CLA:OBD	22:4:815:CLA:HAA1	2.04	0.58
17:5:160:PRO:HG2	17:5:179:ARG:NH1	2.18	0.58
17:5:176:LYS:HD2	17:5:177:GLY:N	2.19	0.58
24:A:856:BCR:C24	10:K:95:LEU:HD21	2.34	0.58
2:B:10:SER:HB3	31:B:852:DGD:HE2	1.84	0.58
22:B:814:CLA:H43	19:9:56:LEU:HD22	1.85	0.58
22:B:842:CLA:CHC	22:1:308:CLA:H12	2.34	0.58
38:1:302:LUT:H28	22:1:304:CLA:H2	1.83	0.58
13:3:129:TRP:CZ3	41:7:319:3PH:H322	2.39	0.58
39:7:313:CHL:CBB	22:7:316:CLA:HBB2	2.33	0.58
38:5:302:LUT:H30	22:5:307:CLA:C5	2.33	0.58
22:A:811:CLA:HBA1	22:A:811:CLA:CHA	2.33	0.58
22:B:819:CLA:H91	22:B:828:CLA:HMB3	1.84	0.58
6:F:116:ALA:HB1	6:F:120:LYS:HZ3	1.68	0.58
11:L:141:GLN:H	11:L:141:GLN:NE2	2.00	0.58
38:4:802:LUT:H28	22:4:805:CLA:C2	2.34	0.58
25:4:821:LHG:H142	22:6:321:CLA:C4C	2.33	0.58
17:5:49:LEU:HD13	17:5:71:ARG:HD3	1.84	0.58
1:A:375:PRO:HG2	1:A:381:ALA:HB2	1.85	0.58
22:A:855:CLA:HHC	22:A:855:CLA:HBB1	1.84	0.58
2:B:628:ASN:HB2	2:B:725:PHE:CE1	2.38	0.58
22:B:828:CLA:C7	24:B:848:BCR:H16C	2.34	0.58
22:B:841:CLA:CAC	24:B:849:BCR:H24C	2.34	0.58
12:Z:101:ASP:HA	12:Z:104:LEU:HD12	1.85	0.58
38:Z:301:LUT:H8	22:Z:305:CLA:HBB1	1.86	0.58
22:Z:307:CLA:H52	15:8:152:PHE:HB2	1.84	0.58
13:3:203:VAL:HG11	31:3:301:DGD:HA72	1.86	0.58
22:5:313:CLA:HBC1	25:5:324:LHG:H302	1.86	0.58
18:6:182:MET:HE3	22:6:310:CLA:HMC3	1.85	0.58
6:F:203:PRO:HB2	22:8:309:CLA:H101	1.86	0.58
11:L:96:LEU:HD11	11:L:124:LEU:HD23	1.84	0.58
12:Z:203:LEU:HA	22:Z:305:CLA:CMA	2.34	0.58
24:4:804:BCR:C19	39:4:816:CHL:HMA2	2.33	0.58
17:5:164:TYR:HB3	22:5:307:CLA:HED3	1.85	0.58
2:B:243:HIS:HA	2:B:249:ASP:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HG23	22:B:818:CLA:H192	1.86	0.58
4:D:178:ASN:HB3	4:D:191:THR:CG2	2.33	0.58
5:E:74:ARG:HD2	5:E:85:THR:HB	1.85	0.58
24:7:303:BCR:H292	42:7:321:SPH:H122	1.85	0.58
39:8:315:CHL:HAA2	39:8:315:CHL:HBD	1.86	0.58
39:4:813:CHL:HAA1	39:4:813:CHL:HBD	1.85	0.58
17:5:247:ILE:HG23	39:5:316:CHL:H42	1.86	0.58
22:5:313:CLA:HBC2	25:5:324:LHG:HC91	1.86	0.58
4:D:182:ILE:HG23	4:D:183:LYS:HD2	1.85	0.58
22:F:304:CLA:C8	22:F:304:CLA:H2	2.33	0.58
7:G:45:MET:HG3	7:G:109:GLY:HA2	1.85	0.58
10:K:25:ARG:HA	10:K:29:PHE:CE1	2.39	0.58
40:1:318:SQD:H132	15:8:134:TRP:CE2	2.39	0.58
20:2:177:VAL:HG21	22:2:304:CLA:HMD3	1.86	0.58
2:B:341:SER:HA	22:B:828:CLA:H51	1.84	0.58
12:1:37:PRO:O	39:8:301:CHL:HED1	2.03	0.58
17:5:84:GLY:HA2	38:5:303:LUT:H181	1.86	0.58
18:6:108:PHE:HB2	18:6:113:LEU:HG	1.85	0.58
22:2:301:CLA:HBA1	22:2:301:CLA:CHA	2.31	0.58
1:A:85:PHE:CE2	1:A:173:MET:HE3	2.39	0.57
22:3:313:CLA:HAA1	22:5:301:CLA:HMB3	1.86	0.57
14:7:77:ARG:HA	14:7:80:MET:HE3	1.86	0.57
22:A:816:CLA:HBA2	22:A:816:CLA:CHA	2.33	0.57
22:A:817:CLA:H121	22:A:817:CLA:HMC2	1.85	0.57
22:A:822:CLA:CMB	22:A:823:CLA:H2	2.34	0.57
2:B:296:PHE:CD2	22:B:822:CLA:HAA2	2.39	0.57
2:B:296:PHE:CE2	22:B:822:CLA:HBD	2.39	0.57
22:B:832:CLA:C4D	22:B:842:CLA:H52	2.33	0.57
22:B:832:CLA:H42	22:B:842:CLA:H62	1.86	0.57
8:I:88:PRO:CG	24:I:4001:BCR:H12C	2.34	0.57
12:1:76:ILE:HG13	22:1:314:CLA:O1D	2.04	0.57
22:4:810:CLA:CGA	22:4:818:CLA:HAB	2.34	0.57
39:6:320:CHL:HAA2	39:6:320:CHL:HBD	1.87	0.57
19:9:101:ALA:HB2	39:9:312:CHL:CBA	2.35	0.57
1:A:362:SER:O	1:A:366:ILE:HG13	2.04	0.57
1:A:670:LEU:HB3	22:A:802:CLA:H92	1.85	0.57
22:A:835:CLA:ND	24:A:847:BCR:H282	2.19	0.57
22:A:841:CLA:HBA1	22:A:841:CLA:CHA	2.34	0.57
2:B:54:GLN:HG2	22:B:808:CLA:HMA2	1.85	0.57
6:F:153:THR:O	6:F:157:LEU:HG	2.04	0.57
8:I:87:LEU:HB3	8:I:88:PRO:HD3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:157:PHE:HZ	22:Z:313:CLA:NB	2.01	0.57
14:7:153:PHE:HB3	14:7:160:PHE:HE2	1.69	0.57
15:8:129:VAL:HG11	24:8:304:BCR:H16C	1.86	0.57
15:8:193:ARG:HA	15:8:196:MET:HE3	1.87	0.57
39:9:312:CHL:HED1	39:9:312:CHL:C9	2.34	0.57
22:A:807:CLA:H102	36:J:105:C7Z:C11	2.34	0.57
22:A:810:CLA:HAB	22:A:813:CLA:H101	1.85	0.57
2:B:646:VAL:HA	22:B:812:CLA:HAC1	1.86	0.57
24:B:844:BCR:H343	7:G:104:ALA:HA	1.86	0.57
24:3:304:BCR:H392	22:3:319:CLA:HAA1	1.86	0.57
25:4:820:LHG:H151	22:6:302:CLA:H72	1.84	0.57
18:6:157:PRO:HG3	39:6:316:CHL:C1D	2.34	0.57
18:6:188:PHE:CD1	18:6:199:PRO:HB3	2.39	0.57
22:A:807:CLA:HAB	24:J:104:BCR:C6	2.34	0.57
22:A:832:CLA:H152	22:A:832:CLA:H8	1.87	0.57
22:B:824:CLA:O1A	22:B:824:CLA:HBD	2.05	0.57
22:F:304:CLA:H2	22:F:304:CLA:H92	1.86	0.57
22:1:310:CLA:HHC	22:1:310:CLA:CBB	2.32	0.57
24:3:304:BCR:H313	25:7:318:LHG:H111	1.86	0.57
15:8:169:ASP:OD2	15:8:174:CYS:HB2	2.04	0.57
18:6:120:ALA:HB1	24:6:305:BCR:H15C	1.85	0.57
38:9:302:LUT:H371	22:9:306:CLA:H112	1.86	0.57
22:A:816:CLA:HBB2	24:A:844:BCR:H12C	1.87	0.57
22:A:830:CLA:H151	22:A:841:CLA:HMA3	1.86	0.57
24:A:844:BCR:H20C	24:A:845:BCR:H23C	1.87	0.57
2:B:210:TRP:CD1	25:B:851:LHG:H02	2.22	0.57
2:B:681:TRP:O	2:B:685:LYS:HG2	2.05	0.57
4:D:174:ARG:HB2	4:D:177:GLU:HG3	1.85	0.57
8:I:75:ALA:HB3	8:I:76:PRO:HD3	1.87	0.57
8:I:98:TYR:HD2	8:I:99:ILE:HD12	1.68	0.57
22:3:314:CLA:HHC	22:3:314:CLA:HBB1	1.85	0.57
22:6:307:CLA:HMB2	22:6:308:CLA:HBA2	1.87	0.57
22:B:827:CLA:HAA2	22:B:828:CLA:OBD	2.05	0.57
11:L:87:GLU:HA	11:L:90:ARG:HH21	1.68	0.57
22:L:202:CLA:HBC1	24:L:204:BCR:H23C	1.87	0.57
22:1:304:CLA:HBB1	22:1:304:CLA:HMB1	1.87	0.57
22:1:308:CLA:C4B	22:1:314:CLA:H161	2.34	0.57
13:3:159:PRO:HD2	22:3:308:CLA:OBD	2.04	0.57
22:3:312:CLA:C4B	22:3:318:CLA:H122	2.35	0.57
22:7:309:CLA:CHD	42:7:321:SPH:H151	2.35	0.57
15:8:115:LEU:HD21	39:8:312:CHL:HHD	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TRP:CD1	22:A:828:CLA:HAB	2.39	0.57
1:A:604:SER:O	1:A:607:ILE:HG12	2.04	0.57
21:A:801:CL0:H21	2:B:626:TRP:HD1	1.69	0.57
22:A:819:CLA:H172	22:A:827:CLA:O2A	2.05	0.57
10:K:77:ILE:HD12	13:3:18:THR:HG23	1.86	0.57
38:1:303:LUT:H24	22:1:307:CLA:O1A	2.03	0.57
22:Z:316:CLA:NA	22:Z:316:CLA:H162	2.19	0.57
13:3:121:MET:HB2	22:3:318:CLA:HAB	1.86	0.57
13:3:149:VAL:CG2	13:3:163:TRP:HB2	2.35	0.57
14:7:234:PHE:CD1	22:7:306:CLA:H11	2.40	0.57
38:7:301:LUT:H403	22:7:304:CLA:H13	1.86	0.57
15:8:208:ALA:HA	15:8:234:ILE:HD13	1.87	0.57
16:4:71:LEU:HD21	22:4:808:CLA:HAA2	1.86	0.57
17:5:185:LYS:NZ	22:5:313:CLA:HBD	2.19	0.57
17:5:245:LEU:HD11	18:6:222:VAL:HB	1.86	0.57
1:A:160:TYR:O	1:A:164:ILE:HG12	2.03	0.57
12:1:102:ALA:H	12:1:103:PRO:HD2	1.69	0.57
15:8:173:MET:HB2	22:8:305:CLA:HBA1	1.86	0.57
22:5:301:CLA:H51	22:5:301:CLA:ND	2.20	0.57
19:9:126:ARG:HH22	22:9:313:CLA:CMA	2.17	0.57
1:A:204:GLY:HA2	1:A:208:LEU:HD12	1.87	0.57
22:A:808:CLA:HHC	22:A:808:CLA:CBB	2.32	0.57
22:A:819:CLA:ND	22:A:829:CLA:H72	2.19	0.57
22:A:823:CLA:C1C	37:K:201:DAO:H111	2.34	0.57
2:B:142:PHE:HZ	22:B:816:CLA:H122	1.68	0.57
22:F:302:CLA:HHC	22:F:302:CLA:CBB	2.31	0.57
11:L:171:THR:O	11:L:175:THR:HG23	2.04	0.57
39:1:312:CHL:HBD	39:1:312:CHL:HAA1	1.87	0.57
22:3:313:CLA:HMA3	22:3:319:CLA:C3C	2.35	0.57
22:3:313:CLA:H121	22:5:320:CLA:NC	2.20	0.57
14:7:25:ALA:HA	14:7:30:ARG:HB2	1.87	0.57
15:8:74:ARG:O	22:8:305:CLA:HMC1	2.04	0.57
16:4:116:VAL:HG11	22:4:810:CLA:HAC2	1.87	0.57
39:5:316:CHL:H141	39:5:316:CHL:H172	1.86	0.57
22:G:202:CLA:NC	24:G:203:BCR:H282	2.20	0.56
22:L:203:CLA:HBB1	22:L:203:CLA:HMB3	1.87	0.56
22:Z:306:CLA:H71	22:Z:307:CLA:CMA	2.35	0.56
39:4:814:CHL:HAA1	39:4:814:CHL:HBD	1.86	0.56
38:9:302:LUT:H162	22:9:308:CLA:HHB	1.87	0.56
20:2:178:ARG:NH1	20:2:203:VAL:HG22	2.19	0.56
1:A:355:ILE:HD13	24:A:846:BCR:H371	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ILE:HD13	1:A:576:ASP:HB2	1.87	0.56
22:A:821:CLA:H102	22:A:824:CLA:H93	1.87	0.56
7:G:56:LEU:HD11	33:G:204:LMT:H3'	1.87	0.56
22:8:307:CLA:H161	22:8:311:CLA:HMC3	1.87	0.56
16:4:159:PHE:CE1	24:4:804:BCR:HC8	2.40	0.56
25:4:820:LHG:H101	24:6:305:BCR:HC42	1.86	0.56
22:5:315:CLA:H2A	25:5:324:LHG:H151	1.85	0.56
18:6:128:ARG:HG3	39:6:316:CHL:C1D	2.35	0.56
22:A:803:CLA:HHC	22:A:803:CLA:CBB	2.35	0.56
22:A:824:CLA:C2	22:A:835:CLA:H171	2.30	0.56
22:A:841:CLA:NC	22:A:841:CLA:H52	2.19	0.56
22:B:815:CLA:H102	24:B:845:BCR:H381	1.88	0.56
22:B:834:CLA:NA	24:J:104:BCR:H282	2.21	0.56
10:K:95:LEU:HD13	22:K:204:CLA:HBB2	1.88	0.56
14:7:163:LYS:HD3	14:7:164:GLU:HG3	1.86	0.56
38:8:302:LUT:C28	22:8:305:CLA:H61	2.35	0.56
22:8:307:CLA:H101	25:8:317:LHG:H312	1.86	0.56
22:8:310:CLA:HBD	43:8:319:LPX:H3	1.86	0.56
16:4:210:LEU:HB3	22:4:805:CLA:HMA2	1.87	0.56
17:5:253:TRP:HD1	22:5:301:CLA:O1A	1.88	0.56
22:5:308:CLA:C4B	22:5:313:CLA:H121	2.35	0.56
38:6:304:LUT:C28	22:6:310:CLA:H61	2.26	0.56
19:9:62:ARG:HA	19:9:62:ARG:HE	1.69	0.56
19:9:112:THR:HG22	19:9:116:PHE:CZ	2.40	0.56
39:9:312:CHL:H141	39:9:312:CHL:CHD	2.35	0.56
1:A:26:PHE:HD2	34:J:101:LMG:HC1	1.69	0.56
1:A:622:VAL:HA	1:A:627:VAL:HG22	1.86	0.56
22:B:810:CLA:HAA2	8:I:80:VAL:HG22	1.87	0.56
39:Z:312:CHL:HAB	22:Z:315:CLA:HBB2	1.86	0.56
24:3:307:BCR:H352	22:3:315:CLA:C4D	2.34	0.56
15:8:118:LEU:HD21	39:8:315:CHL:CHD	2.35	0.56
16:4:81:PHE:HB3	22:4:808:CLA:C3D	2.35	0.56
18:6:245:PHE:CE2	22:6:301:CLA:H112	2.41	0.56
20:2:196:ASN:O	22:2:301:CLA:HAA1	2.06	0.56
1:A:303:VAL:HG12	22:A:817:CLA:H142	1.87	0.56
22:A:805:CLA:H171	24:A:844:BCR:H323	1.87	0.56
2:B:224:THR:HB	2:B:225:PRO:HD3	1.88	0.56
2:B:495:LEU:HB3	2:B:496:PRO:HD3	1.88	0.56
7:G:50:ARG:HG2	22:G:202:CLA:CAB	2.35	0.56
7:G:90:SER:HB2	19:9:34:ASN:O	2.05	0.56
15:8:170:PRO:CD	38:8:302:LUT:H24	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:8:317:LHG:H122	25:8:317:LHG:O7	2.05	0.56
18:6:184:ALA:HB1	38:6:303:LUT:H7	1.86	0.56
19:9:72:THR:HG21	22:9:313:CLA:O1D	2.05	0.56
38:9:301:LUT:C14	22:9:304:CLA:HBB1	2.35	0.56
22:2:301:CLA:C1C	22:2:301:CLA:H52	2.34	0.56
22:A:803:CLA:H8	9:J:16:LEU:HD23	1.87	0.56
22:A:831:CLA:HBA2	25:A:849:LHG:HC92	1.87	0.56
11:L:99:PRO:HA	22:L:203:CLA:HMB2	1.87	0.56
11:L:140:PHE:HD1	11:L:144:PRO:HD2	1.71	0.56
12:Z:176:LYS:HD3	22:Z:309:CLA:O1D	2.05	0.56
22:Z:309:CLA:H142	22:Z:309:CLA:H61	1.86	0.56
22:7:308:CLA:OBD	22:7:315:CLA:HBA2	2.04	0.56
22:6:309:CLA:H172	22:6:309:CLA:HMB3	1.88	0.56
39:6:318:CHL:HAA2	39:6:318:CHL:HBD	1.88	0.56
1:A:461:THR:HG21	22:B:812:CLA:HAB	1.87	0.56
22:A:812:CLA:HBA1	22:A:812:CLA:HBD	1.87	0.56
22:A:815:CLA:H121	24:3:306:BCR:H16C	1.88	0.56
22:A:818:CLA:HHD	22:A:835:CLA:H42	1.87	0.56
22:A:820:CLA:HHC	22:A:820:CLA:CBB	2.33	0.56
22:A:828:CLA:H43	22:A:828:CLA:HBA1	1.86	0.56
2:B:296:PHE:HB3	7:G:100:ILE:HG21	1.86	0.56
22:B:806:CLA:H13	24:B:849:BCR:H10C	1.88	0.56
39:Z:311:CHL:NC	25:Z:317:LHG:H102	2.21	0.56
38:3:303:LUT:H28	22:3:311:CLA:H2	1.87	0.56
15:8:78:THR:HG23	22:8:305:CLA:HMC2	1.87	0.56
15:8:110:GLN:HB3	43:8:319:LPX:H2	1.87	0.56
22:4:810:CLA:H12	39:4:816:CHL:C3D	2.35	0.56
19:9:51:PHE:HB3	22:9:306:CLA:CAD	2.36	0.56
1:A:201:HIS:O	1:A:205:LEU:HB3	2.05	0.56
21:A:801:CL0:H12	22:A:802:CLA:CAD	2.36	0.56
22:A:812:CLA:O1A	13:3:39:LEU:HB3	2.06	0.56
22:A:838:CLA:H91	22:A:838:CLA:H143	1.86	0.56
22:A:855:CLA:H111	22:B:840:CLA:H62	1.88	0.56
2:B:481:SER:O	2:B:484:SER:HB2	2.05	0.56
22:B:825:CLA:H141	22:B:832:CLA:HBC3	1.88	0.56
4:D:139:TYR:CE2	4:D:149:TYR:HD1	2.23	0.56
12:Z:159:PRO:HD2	38:Z:301:LUT:H23	1.88	0.56
31:3:301:DGD:HA21	31:3:301:DGD:HA61	1.86	0.56
39:8:312:CHL:HMC	26:8:318:NKP:HARA	1.86	0.56
18:6:123:PHE:CE1	22:6:302:CLA:HBD	2.41	0.56
18:6:245:PHE:CE2	22:6:301:CLA:H91	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:TRP:H	22:B:812:CLA:HED3	1.70	0.56
2:B:190:ALA:HB1	22:B:816:CLA:HAB	1.88	0.56
2:B:315:ARG:HB3	22:B:842:CLA:H43	1.88	0.56
2:B:349:VAL:HA	22:B:820:CLA:H11	1.88	0.56
2:B:470:LYS:HG2	2:B:473:TYR:CE2	2.41	0.56
22:B:814:CLA:HAB	22:B:822:CLA:H72	1.87	0.56
22:B:827:CLA:H172	22:B:833:CLA:HBC1	1.87	0.56
3:C:22:PRO:HB3	3:C:53:ARG:NH1	2.21	0.56
12:Z:100:TYR:O	12:Z:103:PRO:HD2	2.05	0.56
22:3:320:CLA:C4D	41:7:319:3PH:H392	2.35	0.56
14:7:164:GLU:HB2	14:7:167:TYR:HB2	1.87	0.56
14:7:186:TYR:O	14:7:190:LYS:HG3	2.06	0.56
22:7:322:CLA:HBA2	22:7:323:CLA:H102	1.88	0.56
1:A:677:PHE:HB2	22:A:802:CLA:HAA1	1.89	0.56
7:G:54:LEU:N	7:G:55:PRO:HD2	2.21	0.56
12:Z:206:HIS:CB	22:Z:305:CLA:HAA2	2.33	0.56
15:8:128:PHE:CZ	24:8:304:BCR:H10C	2.41	0.56
15:8:149:PHE:O	15:8:150:LEU:C	2.47	0.56
38:8:302:LUT:H392	22:8:313:CLA:H41	1.89	0.56
22:4:807:CLA:HBA1	22:4:807:CLA:CBD	2.33	0.56
22:4:809:CLA:HHC	22:4:809:CLA:CBB	2.31	0.56
19:9:51:PHE:HB3	22:9:306:CLA:C3D	2.36	0.56
2:B:569:CYS:HG	29:B:802:SF4:FE1	1.22	0.55
2:B:708:LEU:HD21	31:B:852:DGD:HA21	1.87	0.55
22:B:805:CLA:HHC	22:B:805:CLA:CBB	2.32	0.55
12:1:75:VAL:HG22	12:1:175:ILE:HD11	1.88	0.55
12:Z:57:PRO:HG2	38:Z:302:LUT:H23	1.87	0.55
22:Z:309:CLA:C2B	25:Z:317:LHG:HC2	2.35	0.55
22:3:313:CLA:H2	22:3:319:CLA:CAD	2.36	0.55
22:5:315:CLA:C1A	25:5:324:LHG:H142	2.36	0.55
18:6:79:MET:HE3	22:6:307:CLA:HMC3	1.88	0.55
18:6:238:ASP:HA	18:6:243:LYS:CA	2.19	0.55
39:2:303:CHL:HAA1	39:2:303:CHL:HBD	1.88	0.55
22:A:841:CLA:H111	22:B:801:CLA:H121	1.89	0.55
27:A:852:DGA:HBW1	31:3:301:DGD:HA31	1.87	0.55
2:B:427:SER:HB3	22:B:801:CLA:HBA1	1.89	0.55
22:F:304:CLA:H2	22:F:304:CLA:H8	1.88	0.55
38:8:303:LUT:H28	22:8:308:CLA:H72	1.87	0.55
24:8:304:BCR:H372	39:8:315:CHL:H162	1.87	0.55
38:4:803:LUT:H193	39:4:816:CHL:CBB	2.36	0.55
38:4:803:LUT:H30	22:4:808:CLA:H72	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:810:CLA:O1A	22:4:818:CLA:HHC	2.06	0.55
17:5:106:PRO:O	17:5:109:LEU:HB2	2.06	0.55
17:5:127:LEU:HD13	22:6:314:CLA:H8	1.87	0.55
17:5:182:LEU:HB3	22:5:307:CLA:HMA1	1.87	0.55
1:A:349:TRP:CD2	22:A:825:CLA:H192	2.42	0.55
1:A:535:VAL:HG22	1:A:539:HIS:NE2	2.22	0.55
22:A:814:CLA:H11	22:A:816:CLA:HHB	1.88	0.55
22:A:816:CLA:H43	22:A:816:CLA:HBA1	1.88	0.55
2:B:6:PHE:CE2	2:B:25:GLY:HA3	2.41	0.55
2:B:168:TRP:CE2	22:B:815:CLA:HAC2	2.41	0.55
2:B:291:MET:HB2	22:B:823:CLA:HAC2	1.88	0.55
11:L:131:ALA:HB1	24:L:204:BCR:C19	2.35	0.55
12:Z:102:ALA:HB3	12:Z:103:PRO:HD3	1.88	0.55
13:3:180:LEU:HB3	22:3:308:CLA:HMA2	1.87	0.55
15:8:190:LYS:HD3	22:8:311:CLA:O1D	2.06	0.55
17:5:202:VAL:HG22	17:5:252:LEU:HD12	1.89	0.55
22:5:307:CLA:HMD2	39:5:317:CHL:H11	1.89	0.55
18:6:89:GLU:HB3	18:6:200:LEU:HD12	1.88	0.55
38:6:304:LUT:H28	22:6:310:CLA:C6	2.26	0.55
6:F:126:GLY:H	6:F:132:HIS:CE1	2.24	0.55
22:1:304:CLA:H122	22:1:305:CLA:CMB	2.36	0.55
16:4:68:PRO:HG2	16:4:71:LEU:HD12	1.87	0.55
1:A:438:ILE:HG13	1:A:556:PHE:HE2	1.71	0.55
2:B:221:GLN:NE2	2:B:225:PRO:HG3	2.22	0.55
22:B:817:CLA:H111	24:B:844:BCR:H383	1.88	0.55
10:K:77:ILE:HG13	13:3:19:SER:HA	1.87	0.55
12:Z:206:HIS:CG	22:Z:305:CLA:HAA2	2.42	0.55
22:4:806:CLA:HMD3	22:4:811:CLA:C4D	2.37	0.55
17:5:151:ILE:HD12	39:5:321:CHL:HMB2	1.87	0.55
22:A:818:CLA:O1A	22:A:827:CLA:HBB2	2.05	0.55
2:B:54:GLN:HE22	22:B:809:CLA:C1D	2.19	0.55
2:B:87:PRO:HB3	2:B:122:TYR:CD1	2.42	0.55
2:B:183:LEU:HD11	22:B:815:CLA:H43	1.87	0.55
2:B:722:TYR:HB2	22:B:805:CLA:HED3	1.89	0.55
8:I:80:VAL:HB	8:I:81:PRO:HD3	1.89	0.55
13:3:68:MET:SD	22:3:308:CLA:HAB	2.46	0.55
22:3:312:CLA:NB	22:3:318:CLA:H122	2.22	0.55
22:6:308:CLA:OBD	22:6:313:CLA:HBD	2.06	0.55
1:A:426:LEU:O	1:A:430:VAL:HG23	2.07	0.55
2:B:408:VAL:O	2:B:412:MET:HG2	2.05	0.55
2:B:546:LYS:HG3	6:F:225:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:823:CLA:HHC	22:B:823:CLA:CBB	2.32	0.55
22:B:842:CLA:HBB2	22:1:307:CLA:H61	1.88	0.55
6:F:116:ALA:HB1	6:F:120:LYS:NZ	2.21	0.55
6:F:201:THR:HA	22:8:309:CLA:C15	2.36	0.55
8:I:63:ALA:HB2	20:2:206:GLU:OE2	2.07	0.55
13:3:186:LYS:HA	24:3:307:BCR:H282	1.87	0.55
22:3:320:CLA:C2D	41:7:319:3PH:H371	2.37	0.55
15:8:157:LYS:HB2	15:8:157:LYS:NZ	2.22	0.55
39:5:316:CHL:CBB	22:5:319:CLA:HBB2	2.37	0.55
19:9:123:GLU:HB3	19:9:126:ARG:HH21	1.71	0.55
20:2:211:VAL:HG13	39:2:303:CHL:H2	1.87	0.55
1:A:414:VAL:HG13	1:A:567:ALA:HA	1.88	0.55
1:A:575:CYS:HB3	1:A:584:CYS:HA	1.89	0.55
22:A:804:CLA:C4B	22:A:811:CLA:H122	2.37	0.55
22:A:806:CLA:HHC	22:A:806:CLA:CBB	2.37	0.55
22:B:816:CLA:H13	24:B:846:BCR:H19C	1.87	0.55
4:D:128:LEU:HA	4:D:132:PHE:HD2	1.72	0.55
13:3:97:ILE:HG22	13:3:99:PRO:HG2	1.89	0.55
14:7:186:TYR:CE2	14:7:190:LYS:HD2	2.42	0.55
22:A:824:CLA:CMD	22:A:825:CLA:HAB	2.34	0.55
22:A:833:CLA:H203	22:B:840:CLA:HMA2	1.89	0.55
2:B:493:LEU:O	2:B:496:PRO:HD2	2.07	0.55
22:F:304:CLA:H12	22:F:304:CLA:C4A	2.36	0.55
22:F:304:CLA:HBD	22:F:304:CLA:H151	1.88	0.55
7:G:99:LEU:HG	22:G:202:CLA:CGA	2.37	0.55
12:1:55:PHE:CD2	38:1:303:LUT:H383	2.41	0.55
18:6:162:PHE:CZ	18:6:164:PRO:HB3	2.42	0.55
2:B:40:GLU:O	2:B:44:TYR:HD1	1.90	0.55
22:Z:304:CLA:HED2	22:Z:304:CLA:H2A	1.88	0.55
22:8:305:CLA:HMB1	22:8:305:CLA:HBB1	1.88	0.55
16:4:85:SER:HB2	16:4:88:VAL:CG2	2.37	0.55
16:4:237:LYS:HB2	16:4:242:ASN:HD21	1.72	0.55
39:4:819:CHL:HAA2	39:4:819:CHL:HBD	1.89	0.55
17:5:88:VAL:HG22	17:5:100:TRP:CD1	2.42	0.55
18:6:237:THR:HG21	39:6:315:CHL:HED2	1.89	0.55
18:6:252:GLY:HA3	22:6:301:CLA:HED1	1.89	0.55
1:A:348:SER:O	22:A:825:CLA:H191	2.07	0.54
1:A:459:ASN:HB3	1:A:471:MET:HE3	1.89	0.54
22:A:822:CLA:C3D	24:A:856:BCR:H292	2.37	0.54
22:B:823:CLA:H62	22:B:824:CLA:H72	1.89	0.54
7:G:48:VAL:O	7:G:52:ALA:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:201:CLA:HHC	22:L:201:CLA:CBB	2.33	0.54
39:1:312:CHL:HBA1	31:1:319:DGD:HB31	1.89	0.54
40:1:318:SQD:H131	15:8:138:LEU:HG	1.89	0.54
13:3:121:MET:HE3	13:3:125:GLU:HG3	1.89	0.54
22:8:307:CLA:HBA1	22:8:307:CLA:CBD	2.33	0.54
22:5:301:CLA:H61	22:5:320:CLA:HED1	1.88	0.54
19:9:206:GLN:NE2	19:9:206:GLN:H	2.05	0.54
1:A:21:PRO:HD3	1:A:183:LYS:O	2.08	0.54
1:A:672:PHE:CE2	1:A:676:HIS:HE1	2.26	0.54
27:A:852:DGA:HA52	14:7:243:PHE:HB3	1.89	0.54
22:B:810:CLA:HMB3	22:B:811:CLA:HHB	1.89	0.54
22:B:833:CLA:HMB1	22:B:833:CLA:HBB1	1.90	0.54
6:F:196:THR:HB	22:F:305:CLA:HED2	1.89	0.54
13:3:114:PHE:CE2	22:3:316:CLA:H2	2.42	0.54
13:3:226:LEU:HA	13:3:229:PHE:CD2	2.42	0.54
25:7:318:LHG:H122	25:7:318:LHG:H322	1.89	0.54
22:5:307:CLA:H71	22:5:307:CLA:H41	1.87	0.54
1:A:13:VAL:HG12	22:A:812:CLA:H2A	1.88	0.54
22:A:805:CLA:HAA2	22:A:825:CLA:H41	1.90	0.54
22:A:825:CLA:HMA2	22:A:827:CLA:H92	1.90	0.54
2:B:23:TRP:HB3	31:B:852:DGD:HA41	1.89	0.54
12:Z:115:PHE:CD2	22:Z:308:CLA:HMD2	2.42	0.54
12:Z:195:THR:CG2	12:Z:197:LYS:HE2	2.37	0.54
17:5:103:ALA:HB1	22:5:312:CLA:HED3	1.89	0.54
1:A:75:SER:OG	1:A:181:TYR:HB2	2.07	0.54
1:A:247:ARG:NH1	31:3:301:DGD:HE4	2.22	0.54
22:B:807:CLA:HBA1	22:B:807:CLA:CHA	2.38	0.54
12:1:39:SER:HA	15:8:135:MET:HE2	1.89	0.54
12:Z:86:ALA:HB1	22:Z:303:CLA:H192	1.89	0.54
12:Z:185:CYS:HA	12:Z:188:PHE:CD2	2.42	0.54
22:Z:303:CLA:HBC2	22:Z:313:CLA:H12	1.88	0.54
14:7:66:ARG:HG2	14:7:142:PHE:CZ	2.43	0.54
15:8:220:HIS:HA	15:8:227:THR:OG1	2.08	0.54
17:5:58:LEU:HD22	22:5:315:CLA:H142	1.90	0.54
18:6:123:PHE:HB2	22:6:302:CLA:C1	2.37	0.54
18:6:139:ASP:O	18:6:148:LYS:HG3	2.06	0.54
22:A:816:CLA:H42	27:A:852:DGA:HAF1	1.89	0.54
22:A:822:CLA:HMA2	22:A:823:CLA:HBD	1.90	0.54
2:B:160:PRO:O	2:B:161:SER:HB3	2.07	0.54
2:B:298:ILE:HG22	7:G:57:HIS:CE1	2.43	0.54
2:B:549:PRO:HB2	3:C:62:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:138:MET:HE1	14:7:35:PRO:O	2.08	0.54
38:4:803:LUT:H28	22:4:808:CLA:C5	2.38	0.54
22:6:309:CLA:C4B	22:6:309:CLA:H62	2.37	0.54
2:B:92:ILE:HD11	2:B:115:ASN:ND2	2.23	0.54
2:B:617:LEU:HD21	22:B:805:CLA:H202	1.90	0.54
2:B:695:LYS:HD2	8:I:100:GLU:HB3	1.90	0.54
2:B:697:LYS:HD3	3:C:81:TYR:HD2	1.71	0.54
11:L:79:VAL:HB	11:L:84:ARG:HG3	1.90	0.54
11:L:102:LYS:HG2	22:L:203:CLA:HMA1	1.88	0.54
12:1:39:SER:HB2	40:1:318:SQD:H62	1.88	0.54
13:3:80:LEU:HD11	24:3:305:BCR:H401	1.89	0.54
13:3:216:HIS:CG	22:3:310:CLA:HAA1	2.42	0.54
22:3:316:CLA:HHC	22:3:316:CLA:CBB	2.34	0.54
17:5:192:ILE:HD11	22:5:313:CLA:HHD	1.89	0.54
22:5:326:CLA:CMD	22:6:309:CLA:H2	2.37	0.54
18:6:66:TRP:HE1	22:6:311:CLA:H11	1.72	0.54
18:6:87:VAL:C	18:6:89:GLU:H	2.16	0.54
18:6:254:TRP:CG	22:6:319:CLA:HED1	2.43	0.54
38:6:303:LUT:C30	22:6:307:CLA:H8	2.38	0.54
22:A:812:CLA:O1D	22:A:813:CLA:HMC1	2.07	0.54
24:A:848:BCR:H393	22:B:801:CLA:H102	1.90	0.54
2:B:263:HIS:HE1	2:B:265:GLN:HB3	1.73	0.54
2:B:680:VAL:HG13	2:B:694:TRP:CZ2	2.43	0.54
6:F:165:TYR:O	6:F:168:ARG:HG2	2.07	0.54
7:G:56:LEU:HG	7:G:59:ARG:HH22	1.72	0.54
14:7:198:ARG:HA	14:7:201:MET:HE2	1.90	0.54
22:7:322:CLA:HMC2	15:8:221:LEU:HD21	1.89	0.54
22:4:808:CLA:HBB2	22:4:809:CLA:CHB	2.37	0.54
17:5:182:LEU:HB3	22:5:307:CLA:HMA2	1.89	0.54
39:5:316:CHL:H122	39:5:316:CHL:C9	2.36	0.54
18:6:238:ASP:HB2	18:6:243:LYS:HG2	1.89	0.54
22:A:812:CLA:HBA1	22:A:812:CLA:CBD	2.37	0.54
22:A:815:CLA:H92	13:3:203:VAL:HG21	1.90	0.54
2:B:235:ALA:HA	2:B:257:THR:HG22	1.90	0.54
2:B:515:PRO:HG2	6:F:132:HIS:CD2	2.42	0.54
22:B:819:CLA:O1A	22:B:828:CLA:HBB2	2.07	0.54
22:1:305:CLA:HHC	22:1:305:CLA:CBB	2.32	0.54
12:Z:153:PRO:HD3	22:Z:313:CLA:CMD	2.35	0.54
38:7:302:LUT:C32	22:7:307:CLA:HAB	2.27	0.54
15:8:39:HIS:HA	15:8:41:LYS:HZ3	1.72	0.54
22:5:309:CLA:H11	22:5:314:CLA:HMD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:TYR:CD1	2:B:617:LEU:HG	2.43	0.54
39:7:313:CHL:HAA1	39:7:313:CHL:HBD	1.90	0.54
22:8:310:CLA:HBA2	43:8:319:LPX:H3	1.90	0.54
1:A:578:PRO:HG3	3:C:52:LYS:HD2	1.89	0.54
1:A:682:SER:HB2	1:A:727:GLY:O	2.08	0.54
22:A:804:CLA:C3B	22:A:811:CLA:H122	2.38	0.54
22:A:814:CLA:H43	22:A:816:CLA:H41	1.90	0.54
22:B:813:CLA:HMB3	22:B:813:CLA:CBB	2.35	0.54
22:B:823:CLA:C1B	22:B:824:CLA:H8	2.38	0.54
4:D:77:LYS:HG3	4:D:81:GLU:HB3	1.90	0.54
7:G:33:GLU:HB2	7:G:35:TYR:CD2	2.43	0.54
22:1:308:CLA:HHC	22:1:308:CLA:CBB	2.37	0.54
12:Z:157:PHE:HA	22:Z:313:CLA:C7	2.38	0.54
39:8:312:CHL:CMC	26:8:318:NKP:HARA	2.38	0.54
22:4:810:CLA:H43	39:4:816:CHL:HBD	1.90	0.54
38:5:302:LUT:H373	22:5:307:CLA:H42	1.89	0.54
22:5:308:CLA:HMB3	22:5:308:CLA:H151	1.89	0.54
25:5:324:LHG:H102	25:5:324:LHG:H281	1.89	0.54
18:6:251:GLN:HB2	22:6:301:CLA:HBA1	1.90	0.54
19:9:137:GLY:HA2	19:9:144:PHE:HB2	1.90	0.54
1:A:49:ILE:H	1:A:49:ILE:HD12	1.74	0.53
1:A:646:LEU:HD12	1:A:650:LEU:HD12	1.90	0.53
1:A:707:LEU:HD23	6:F:216:THR:HG22	1.90	0.53
22:A:805:CLA:H101	24:A:845:BCR:HC8	1.89	0.53
6:F:123:LEU:HD11	9:J:38:VAL:HG11	1.90	0.53
38:4:802:LUT:C14	22:4:806:CLA:HAB	2.37	0.53
17:5:128:LEU:HB3	24:5:304:BCR:H15C	1.89	0.53
18:6:219:ALA:HB2	18:6:229:PRO:HD3	1.90	0.53
19:9:29:PRO:HB3	22:9:311:CLA:HED2	1.90	0.53
1:A:80:GLN:O	1:A:83:VAL:HG22	2.08	0.53
22:A:805:CLA:H143	24:A:844:BCR:C5	2.38	0.53
22:A:812:CLA:H172	22:A:812:CLA:H143	1.89	0.53
2:B:200:ILE:HB	2:B:201:PRO:HD3	1.90	0.53
3:C:62:PHE:HE1	3:C:66:ARG:HH21	1.55	0.53
6:F:190:PRO:O	6:F:194:ARG:HG3	2.08	0.53
7:G:97:PHE:CD2	7:G:102:THR:HG22	2.43	0.53
8:I:67:TYR:CZ	8:I:69:PHE:HB2	2.43	0.53
11:L:140:PHE:HA	11:L:144:PRO:CD	2.38	0.53
12:Z:103:PRO:HB3	22:Z:315:CLA:HMC3	1.91	0.53
13:3:111:TYR:CE2	22:3:316:CLA:HMA2	2.42	0.53
38:7:301:LUT:H30	22:7:304:CLA:H72	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:202:PHE:CZ	38:8:302:LUT:H8	2.42	0.53
17:5:33:LYS:HB3	22:5:315:CLA:CBC	2.37	0.53
22:5:301:CLA:HHC	22:5:301:CLA:HBB1	1.89	0.53
22:A:812:CLA:HHC	22:A:812:CLA:CBB	2.36	0.53
22:A:821:CLA:C2C	22:A:827:CLA:H18	2.38	0.53
2:B:442:ASP:OD1	2:B:616:TYR:HB2	2.08	0.53
12:1:94:LEU:HD12	22:1:309:CLA:CMD	2.38	0.53
22:Z:308:CLA:HMA3	22:Z:315:CLA:C2C	2.38	0.53
13:3:78:GLU:HB3	13:3:82:LYS:HE3	1.91	0.53
24:3:305:BCR:H21C	22:3:313:CLA:CAC	2.36	0.53
22:3:312:CLA:HHC	22:3:312:CLA:CBB	2.38	0.53
22:7:307:CLA:H92	22:7:308:CLA:H72	1.90	0.53
17:5:124:TRP:NE1	22:5:326:CLA:HMA3	2.23	0.53
22:A:837:CLA:HHC	22:A:837:CLA:CBB	2.31	0.53
2:B:241:ALA:HA	2:B:264:PRO:HG3	1.90	0.53
2:B:590:TRP:CD1	22:B:805:CLA:H152	2.42	0.53
6:F:163:ILE:HG12	22:F:305:CLA:C4D	2.39	0.53
8:I:78:VAL:C	8:I:81:PRO:HD2	2.33	0.53
11:L:160:PRO:O	11:L:166:GLY:HA3	2.07	0.53
39:Z:312:CHL:CAB	22:Z:315:CLA:HBB2	2.38	0.53
15:8:136:ASP:O	15:8:140:PRO:HA	2.09	0.53
16:4:106:TRP:CH2	24:4:804:BCR:H372	2.44	0.53
22:4:806:CLA:C4D	22:4:811:CLA:H61	2.38	0.53
18:6:221:VAL:HB	22:6:322:CLA:C1C	2.39	0.53
22:A:806:CLA:CBB	24:A:845:BCR:HC31	2.39	0.53
2:B:48:PHE:HB2	2:B:169:PHE:HE1	1.74	0.53
2:B:355:SER:HB3	22:B:828:CLA:HAC2	1.89	0.53
22:B:827:CLA:C3B	24:B:848:BCR:H19C	2.38	0.53
22:B:828:CLA:C11	24:B:847:BCR:H373	2.38	0.53
22:3:312:CLA:C1D	22:3:318:CLA:H93	2.38	0.53
22:3:313:CLA:H202	22:5:320:CLA:CHB	2.37	0.53
24:7:303:BCR:H333	22:7:322:CLA:H8	1.90	0.53
22:4:807:CLA:H71	25:4:820:LHG:H171	1.90	0.53
22:4:807:CLA:HBB1	22:4:807:CLA:HMB1	1.90	0.53
17:5:140:TYR:OH	22:5:323:CLA:HBA2	2.09	0.53
24:6:305:BCR:H291	22:6:312:CLA:H2	1.91	0.53
22:6:307:CLA:HMD1	39:6:316:CHL:CGA	2.38	0.53
22:A:819:CLA:HHD	24:A:845:BCR:H352	1.90	0.53
2:B:244:VAL:HB	2:B:247:THR:OG1	2.09	0.53
2:B:320:HIS:O	2:B:323:LEU:HB2	2.08	0.53
2:B:379:ILE:O	2:B:383:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:61:THR:HA	10:K:67:LEU:HA	1.91	0.53
22:K:205:CLA:CMD	24:K:206:BCR:H21C	2.39	0.53
22:Z:304:CLA:HHC	22:Z:304:CLA:CBB	2.37	0.53
22:Z:316:CLA:HBD	22:Z:316:CLA:H72	1.91	0.53
15:8:110:GLN:HG2	43:8:319:LPX:H1	1.89	0.53
17:5:131:TRP:HH2	24:5:304:BCR:H323	1.74	0.53
38:5:302:LUT:H30	22:5:307:CLA:H51	1.91	0.53
1:A:44:ASN:HB3	5:E:78:GLN:NE2	2.23	0.53
1:A:95:GLY:HA2	1:A:99:SER:HB3	1.89	0.53
2:B:312:PRO:HB2	25:B:850:LHG:HC32	1.90	0.53
38:1:303:LUT:C28	22:1:307:CLA:H111	2.39	0.53
22:Z:304:CLA:ND	22:Z:309:CLA:H62	2.23	0.53
22:8:308:CLA:H12	22:8:308:CLA:CHB	2.39	0.53
22:6:311:CLA:HBB1	22:6:311:CLA:HMB3	1.89	0.53
22:2:302:CLA:HBA1	22:2:302:CLA:CHA	2.38	0.53
1:A:190:TRP:CD1	22:A:812:CLA:HED2	2.43	0.53
2:B:588:ILE:O	2:B:591:VAL:HG22	2.09	0.53
2:B:655:HIS:HB2	22:B:806:CLA:HBA1	1.89	0.53
22:B:825:CLA:H111	24:B:847:BCR:C15	2.38	0.53
22:B:830:CLA:HHC	22:B:830:CLA:CBB	2.35	0.53
6:F:107:THR:HA	6:F:110:ARG:HE	1.73	0.53
24:G:203:BCR:H341	24:G:203:BCR:C12	2.39	0.53
12:1:194:ALA:HB1	12:1:218:ASN:ND2	2.23	0.53
22:Z:313:CLA:H172	22:Z:313:CLA:CHC	2.39	0.53
22:3:311:CLA:HBB1	22:3:311:CLA:HMB1	1.90	0.53
38:7:302:LUT:H26	22:7:307:CLA:H61	1.89	0.53
22:6:302:CLA:C3D	24:6:305:BCR:HC41	2.38	0.53
19:9:111:LEU:HD22	39:9:312:CHL:HAB	1.89	0.53
1:A:248:GLN:CD	1:A:248:GLN:H	2.17	0.53
1:A:679:TRP:CE3	21:A:801:CL0:H6	2.43	0.53
22:A:809:CLA:O1A	22:A:809:CLA:HBD	2.08	0.53
22:A:812:CLA:H92	22:3:311:CLA:H112	1.91	0.53
22:A:812:CLA:H142	13:3:39:LEU:HD11	1.89	0.53
22:A:815:CLA:H2	13:3:203:VAL:CG1	2.38	0.53
24:A:856:BCR:C13	24:K:206:BCR:HC8	2.39	0.53
10:K:78:SER:HB2	10:K:85:THR:HG22	1.91	0.53
22:Z:316:CLA:HHC	22:Z:316:CLA:CBB	2.32	0.53
13:3:180:LEU:HB3	22:3:308:CLA:CMA	2.39	0.53
38:3:303:LUT:H183	22:3:313:CLA:C4B	2.38	0.53
14:7:76:ALA:HB1	14:7:197:GLY:HA3	1.91	0.53
22:7:323:CLA:CAB	25:8:317:LHG:H151	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:236:ILE:HD11	22:8:316:CLA:HBC3	1.89	0.53
22:8:307:CLA:CGA	22:8:307:CLA:C1A	2.86	0.53
24:5:304:BCR:H271	22:5:312:CLA:CHB	2.39	0.53
22:5:311:CLA:H52	22:5:323:CLA:HAB	1.91	0.53
18:6:66:TRP:CZ2	22:6:317:CLA:HAA2	2.44	0.53
18:6:157:PRO:HG2	22:6:307:CLA:HMD2	1.89	0.53
38:6:303:LUT:H26	22:6:307:CLA:O1A	2.08	0.53
1:A:204:GLY:HA3	22:A:813:CLA:HBB1	1.90	0.53
1:A:488:GLN:HA	1:A:510:TRP:HE3	1.74	0.53
22:A:821:CLA:H43	22:A:835:CLA:H143	1.91	0.53
12:Z:144:GLU:HB2	22:Z:313:CLA:HAC1	1.90	0.53
13:3:227:THR:O	13:3:231:LYS:HG2	2.09	0.53
16:4:133:PRO:HG2	16:4:136:GLU:CB	2.38	0.53
17:5:185:LYS:HZ3	22:5:313:CLA:HBD	1.73	0.53
17:5:227:TRP:NE1	22:5:314:CLA:HED2	2.23	0.53
18:6:141:ASP:HB3	18:6:144:PHE:O	2.08	0.53
19:9:81:VAL:CG1	38:9:301:LUT:H12	2.36	0.53
22:9:305:CLA:HBA1	22:9:305:CLA:HBD	1.90	0.53
1:A:264:PHE:HA	1:A:269:TRP:CD1	2.44	0.52
1:A:681:PHE:HZ	22:A:841:CLA:HBC2	1.74	0.52
22:A:802:CLA:H12	2:B:617:LEU:HD13	1.90	0.52
22:A:816:CLA:NC	27:A:852:DGA:HB52	2.24	0.52
22:B:810:CLA:H62	22:B:810:CLA:C1C	2.38	0.52
4:D:156:VAL:HG12	4:D:160:LYS:HB2	1.90	0.52
12:1:203:LEU:HB2	38:1:302:LUT:H22	1.91	0.52
22:Z:304:CLA:CAD	22:Z:309:CLA:HBD	2.39	0.52
22:Z:304:CLA:HMD3	22:Z:309:CLA:CHA	2.39	0.52
14:7:119:SER:HB3	15:8:226:LYS:HG3	1.91	0.52
16:4:185:LEU:HD11	16:4:197:PHE:CD2	2.44	0.52
18:6:147:ASN:HD21	39:6:320:CHL:HAA1	1.72	0.52
1:A:45:THR:HG23	5:E:78:GLN:NE2	2.21	0.52
1:A:247:ARG:HB2	31:3:301:DGD:O3D	2.09	0.52
22:A:855:CLA:H202	24:L:204:BCR:H391	1.91	0.52
2:B:394:PHE:HA	2:B:398:ASP:OD1	2.09	0.52
12:Z:88:CYS:HA	12:Z:99:TRP:HB3	1.90	0.52
12:Z:144:GLU:HG3	22:Z:313:CLA:HBC1	1.91	0.52
39:Z:312:CHL:HHC	22:Z:315:CLA:HAB	1.90	0.52
13:3:169:LEU:HB2	22:3:308:CLA:O1A	2.09	0.52
18:6:141:ASP:CB	18:6:147:ASN:HB2	2.40	0.52
20:2:180:LYS:HE2	22:2:301:CLA:HED3	1.91	0.52
22:1:307:CLA:H102	22:1:308:CLA:CMB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1:312:CHL:HAA2	31:1:319:DGD:O2G	2.09	0.52
22:3:322:CLA:HMB3	41:7:319:3PH:H2A1	1.89	0.52
17:5:33:LYS:HB3	22:5:315:CLA:HBC3	1.91	0.52
22:5:301:CLA:H62	22:5:301:CLA:NB	2.25	0.52
22:9:313:CLA:HHC	22:9:313:CLA:CBB	2.40	0.52
20:2:197:ASN:CA	22:2:301:CLA:HBA2	2.35	0.52
1:A:366:ILE:HG22	1:A:370:HIS:CE1	2.45	0.52
22:A:834:CLA:HMA1	11:L:103:LEU:HB3	1.91	0.52
2:B:561:ASP:CG	3:C:66:ARG:HH12	2.17	0.52
6:F:205:GLN:HG2	15:8:55:LEU:HD23	1.91	0.52
7:G:38:VAL:HG11	22:G:201:CLA:C3D	2.40	0.52
13:3:199:GLY:O	13:3:203:VAL:HG23	2.09	0.52
24:3:304:BCR:H402	22:3:313:CLA:C1B	2.39	0.52
22:4:810:CLA:HMA2	39:4:816:CHL:C4C	2.39	0.52
17:5:171:PRO:HD2	38:5:302:LUT:C23	2.38	0.52
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.74	0.52
22:A:818:CLA:HMD2	22:A:827:CLA:HMB1	1.92	0.52
22:A:826:CLA:HAA2	22:A:827:CLA:OBD	2.10	0.52
26:A:851:NKP:HAGA	26:A:851:NKP:OAE	2.09	0.52
2:B:628:ASN:HB2	2:B:725:PHE:CZ	2.44	0.52
2:B:708:LEU:HD21	31:B:852:DGD:HA51	1.91	0.52
22:B:818:CLA:NC	22:B:818:CLA:H51	2.24	0.52
3:C:12:ILE:HG12	29:C:102:SF4:S2	2.50	0.52
8:I:92:MET:HB3	24:L:204:BCR:H12C	1.91	0.52
38:1:303:LUT:H28	22:1:307:CLA:H8	1.90	0.52
14:7:189:TYR:HB3	22:7:304:CLA:CMA	2.40	0.52
39:9:312:CHL:H2A	39:9:312:CHL:O2A	2.09	0.52
1:A:278:PHE:HZ	22:A:818:CLA:H43	1.75	0.52
22:A:823:CLA:NB	37:K:201:DAO:H91	2.24	0.52
22:B:828:CLA:HHC	22:B:828:CLA:CBB	2.38	0.52
10:K:107:LEU:HD21	22:K:203:CLA:HBB1	1.91	0.52
24:3:307:BCR:H402	25:3:321:LHG:O6	2.09	0.52
22:8:311:CLA:HMA2	33:4:801:LMT:H5'	1.92	0.52
18:6:107:PRO:HD2	39:6:318:CHL:CMD	2.40	0.52
18:6:186:ILE:HD11	22:6:311:CLA:HAB	1.91	0.52
22:A:804:CLA:HED1	22:A:811:CLA:HBD	1.90	0.52
2:B:390:HIS:HA	2:B:393:ILE:HD12	1.91	0.52
22:Z:304:CLA:OBD	22:Z:309:CLA:HBD	2.08	0.52
13:3:38:PRO:HD2	38:3:303:LUT:C23	2.40	0.52
24:3:305:BCR:H24C	22:3:313:CLA:CAC	2.39	0.52
24:3:305:BCR:H342	39:3:317:CHL:HHB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:307:BCR:H311	22:3:315:CLA:HMA1	1.90	0.52
16:4:210:LEU:HB3	22:4:805:CLA:CMA	2.39	0.52
38:4:802:LUT:H382	22:4:805:CLA:C4D	2.39	0.52
17:5:95:ARG:NH1	17:5:110:PRO:HB3	2.25	0.52
17:5:138:GLN:NE2	18:6:35:GLY:HA3	2.25	0.52
22:5:311:CLA:OBD	22:5:318:CLA:HAA1	2.09	0.52
18:6:34:PRO:HD2	22:6:314:CLA:O1D	2.09	0.52
18:6:108:PHE:CD2	18:6:113:LEU:HD21	2.44	0.52
22:6:319:CLA:HHC	22:6:319:CLA:HBB1	1.91	0.52
1:A:197:MET:CG	22:A:813:CLA:HBC2	2.38	0.52
2:B:477:LEU:H	2:B:480:SER:HB2	1.75	0.52
2:B:688:LEU:HB2	24:B:853:BCR:HC31	1.92	0.52
22:B:827:CLA:HMB1	22:B:827:CLA:HBB1	1.92	0.52
12:Z:87:GLY:HA3	38:Z:302:LUT:H182	1.91	0.52
12:Z:203:LEU:HD22	38:Z:301:LUT:H172	1.92	0.52
14:7:55:PRO:HD2	38:7:302:LUT:H23	1.90	0.52
24:7:303:BCR:H292	22:7:309:CLA:H71	1.90	0.52
38:8:302:LUT:H373	22:8:305:CLA:H42	1.91	0.52
17:5:106:PRO:HG3	17:5:243:GLN:HG3	1.91	0.52
22:A:829:CLA:C1C	24:A:845:BCR:HC42	2.40	0.52
22:A:832:CLA:H121	22:A:834:CLA:H201	1.91	0.52
22:A:833:CLA:H202	24:L:204:BCR:C10	2.40	0.52
2:B:552:LYS:HD2	4:D:181:PRO:HD3	1.91	0.52
22:B:814:CLA:H3A	19:9:54:LEU:HD22	1.92	0.52
22:B:827:CLA:H2	22:B:839:CLA:HBA2	1.91	0.52
22:B:828:CLA:HBA2	24:B:848:BCR:C10	2.40	0.52
22:B:833:CLA:H112	22:F:302:CLA:H151	1.92	0.52
11:L:92:HIS:HA	11:L:95:PHE:HE2	1.75	0.52
12:1:60:LEU:CD1	22:1:307:CLA:H42	2.40	0.52
12:Z:105:TRP:CH2	12:Z:112:PRO:HG3	2.45	0.52
24:3:307:BCR:HC7	22:3:315:CLA:H3A	1.90	0.52
14:7:82:GLY:O	14:7:86:VAL:HG23	2.10	0.52
16:4:86:LEU:CD1	38:4:803:LUT:H221	2.40	0.52
16:4:139:LYS:HG3	39:4:813:CHL:O2D	2.10	0.52
17:5:131:TRP:CH2	24:5:304:BCR:H323	2.44	0.52
17:5:243:GLN:HB3	24:5:305:BCR:H312	1.91	0.52
18:6:76:ARG:HA	18:6:79:MET:HE3	1.92	0.52
18:6:88:GLN:NE2	38:6:304:LUT:H42	2.24	0.52
19:9:82:VAL:HG12	22:9:308:CLA:HBC2	1.91	0.52
19:9:101:ALA:N	39:9:312:CHL:HAA1	2.25	0.52
2:B:127:THR:HA	2:B:245:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:PHE:HZ	2:B:409:LEU:HD21	1.75	0.52
12:1:194:ALA:HB2	22:1:316:CLA:HED3	1.91	0.52
12:Z:53:TYR:CE1	39:Z:311:CHL:HAC2	2.45	0.52
14:7:175:PRO:HD2	38:7:301:LUT:C23	2.40	0.52
39:5:317:CHL:HAA1	39:5:317:CHL:HBD	1.90	0.52
22:6:312:CLA:H193	22:6:312:CLA:H152	1.92	0.52
22:A:824:CLA:HHC	22:A:824:CLA:CBB	2.41	0.51
2:B:394:PHE:CZ	2:B:409:LEU:HD21	2.45	0.51
22:B:824:CLA:C1C	33:1:301:LMT:H101	2.39	0.51
12:1:94:LEU:HD12	22:1:309:CLA:HMD1	1.92	0.51
22:1:313:CLA:CHC	22:1:313:CLA:H172	2.41	0.51
39:Z:311:CHL:CMA	25:Z:317:LHG:H192	2.40	0.51
14:7:149:GLY:HA3	14:7:161:LYS:HE3	1.93	0.51
22:4:806:CLA:HMD2	22:4:811:CLA:H2	1.91	0.51
1:A:360:PHE:HD1	22:A:829:CLA:H192	1.76	0.51
2:B:362:LEU:HD22	2:B:369:GLN:HE21	1.75	0.51
12:1:140:ARG:HG3	22:1:313:CLA:HMC2	1.92	0.51
12:Z:56:ASP:HA	38:Z:302:LUT:H24	1.91	0.51
13:3:42:LEU:HD13	22:3:311:CLA:HMA2	1.92	0.51
13:3:129:TRP:HZ3	41:7:319:3PH:H322	1.74	0.51
24:7:303:BCR:H383	22:7:316:CLA:NA	2.25	0.51
22:7:304:CLA:HMB2	22:7:305:CLA:HBA2	1.92	0.51
22:7:312:CLA:H72	22:7:312:CLA:C4B	2.40	0.51
22:7:323:CLA:H92	25:8:317:LHG:H321	1.93	0.51
15:8:143:GLN:HG3	22:8:313:CLA:HMC2	1.92	0.51
16:4:108:MET:SD	22:4:805:CLA:HAB	2.50	0.51
16:4:254:THR:HA	22:4:807:CLA:HBA2	1.91	0.51
22:6:319:CLA:C3D	25:6:323:LHG:H372	2.40	0.51
19:9:65:TRP:CZ2	22:9:313:CLA:HAA1	2.45	0.51
1:A:460:ASP:OD1	1:A:641:THR:HB	2.10	0.51
22:A:810:CLA:HBA2	22:A:810:CLA:H42	1.92	0.51
2:B:463:TRP:NE1	2:B:477:LEU:HG	2.24	0.51
22:B:810:CLA:H2	22:B:810:CLA:C4D	2.41	0.51
22:B:824:CLA:HBC2	22:B:825:CLA:HBA1	1.91	0.51
22:G:202:CLA:C4C	24:G:203:BCR:H282	2.41	0.51
22:1:310:CLA:C1C	25:1:317:LHG:HC41	2.41	0.51
13:3:139:SER:HB3	13:3:151:GLY:HA2	1.92	0.51
16:4:163:ARG:NH2	16:4:178:PRO:HG3	2.26	0.51
18:6:132:PHE:HD1	18:6:154:VAL:HG11	1.75	0.51
18:6:147:ASN:HB3	39:6:320:CHL:C3D	2.40	0.51
20:2:218:PRO:HD3	39:2:303:CHL:HMA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD12	10:K:34:THR:HG23	1.92	0.51
1:A:407:ALA:O	1:A:411:ILE:HG13	2.10	0.51
22:A:842:CLA:H42	22:A:842:CLA:HED2	1.92	0.51
2:B:530:THR:HG21	2:B:583:TRP:CE2	2.46	0.51
2:B:694:TRP:HA	22:B:840:CLA:O1D	2.10	0.51
22:B:811:CLA:HBA1	22:B:811:CLA:CBD	2.40	0.51
22:B:814:CLA:H112	22:B:814:CLA:C3B	2.41	0.51
22:B:840:CLA:H111	22:B:841:CLA:H142	1.92	0.51
10:K:59:ARG:N	10:K:69:ASP:HA	2.25	0.51
38:1:303:LUT:C28	22:1:307:CLA:H8	2.40	0.51
15:8:118:LEU:HD21	39:8:315:CHL:C1D	2.40	0.51
22:8:311:CLA:HHC	22:8:311:CLA:CBB	2.40	0.51
17:5:227:TRP:HH2	22:5:301:CLA:HBC2	1.75	0.51
22:5:326:CLA:H51	22:6:314:CLA:H61	1.93	0.51
18:6:79:MET:SD	22:6:307:CLA:HAB	2.50	0.51
1:A:413:MET:HG3	1:A:558:ARG:HG3	1.93	0.51
22:A:820:CLA:H143	10:K:90:LEU:HD21	1.91	0.51
2:B:687:PRO:C	2:B:689:ALA:H	2.19	0.51
10:K:32:SER:O	10:K:36:LEU:HG	2.10	0.51
17:5:82:MET:SD	22:5:307:CLA:HAB	2.51	0.51
18:6:235:GLN:HG2	18:6:245:PHE:HE1	1.76	0.51
1:A:75:SER:HA	1:A:78:PHE:HD2	1.76	0.51
1:A:104:TRP:CH2	1:A:149:ARG:HD2	2.45	0.51
22:A:816:CLA:CMB	24:A:844:BCR:H341	2.40	0.51
22:A:824:CLA:H11	24:A:846:BCR:H363	1.92	0.51
2:B:355:SER:CB	22:B:828:CLA:HAC2	2.41	0.51
22:B:842:CLA:HAB	12:1:70:PHE:CZ	2.45	0.51
3:C:29:VAL:HG12	4:D:165:ARG:HB3	1.92	0.51
6:F:162:TRP:CD1	22:F:305:CLA:HBD	2.46	0.51
11:L:123:GLY:HA2	22:L:201:CLA:H161	1.91	0.51
12:Z:100:TYR:O	39:Z:312:CHL:HED1	2.10	0.51
14:7:196:ASN:HD22	14:7:196:ASN:N	2.08	0.51
22:7:306:CLA:CMB	22:7:306:CLA:HBB1	2.41	0.51
22:7:310:CLA:HBA2	22:7:310:CLA:CHA	2.40	0.51
38:8:303:LUT:H163	39:8:315:CHL:HMC	1.92	0.51
39:8:312:CHL:HBD	39:8:312:CHL:HAA1	1.93	0.51
22:4:811:CLA:HHC	22:4:811:CLA:CBB	2.40	0.51
25:4:820:LHG:H312	22:6:321:CLA:HED1	1.92	0.51
18:6:120:ALA:HB1	24:6:305:BCR:C15	2.40	0.51
24:6:306:BCR:H352	39:6:315:CHL:HAC2	1.91	0.51
1:A:349:TRP:HZ3	22:A:825:CLA:H91	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:803:CLA:HMA1	22:A:808:CLA:H201	1.92	0.51
22:A:815:CLA:C4	24:3:306:BCR:HC8	2.40	0.51
2:B:93:TRP:CZ2	8:I:77:SER:HA	2.46	0.51
2:B:463:TRP:HD1	22:F:304:CLA:H193	1.75	0.51
22:B:842:CLA:HBB2	22:1:307:CLA:H41	1.93	0.51
6:F:78:LYS:HZ1	6:F:81:LYS:HD3	1.76	0.51
22:F:302:CLA:C1B	24:F:303:BCR:H10C	2.41	0.51
22:8:306:CLA:HHC	22:8:306:CLA:CBB	2.32	0.51
16:4:234:THR:HG22	22:4:817:CLA:O1D	2.10	0.51
17:5:165:PRO:HD2	22:5:307:CLA:OBD	2.10	0.51
18:6:106:LEU:CD1	18:6:110:ILE:HG23	2.41	0.51
1:A:396:TRP:HA	1:A:603:LEU:HD23	1.93	0.51
22:A:822:CLA:HBC3	22:A:823:CLA:H171	1.93	0.51
2:B:145:LEU:O	2:B:149:ILE:HG13	2.11	0.51
22:B:822:CLA:C1B	24:B:844:BCR:H351	2.40	0.51
22:B:823:CLA:HMD1	24:B:844:BCR:HC7	1.92	0.51
33:G:204:LMT:H62	22:1:308:CLA:HMD2	1.93	0.51
10:K:62:ASP:HB2	10:K:68:VAL:HG23	1.92	0.51
13:3:14:GLN:N	13:3:16:TYR:HH	2.09	0.51
16:4:157:PHE:CZ	22:4:815:CLA:HBC2	2.46	0.51
22:5:313:CLA:HHC	22:5:313:CLA:HBB1	1.93	0.51
22:5:326:CLA:HHC	22:5:326:CLA:CBB	2.41	0.51
22:A:810:CLA:C4C	22:A:813:CLA:H203	2.40	0.51
22:A:818:CLA:H41	22:A:836:CLA:HMA1	1.93	0.51
22:A:833:CLA:H43	22:A:855:CLA:H43	1.92	0.51
23:A:843:PQN:C19	24:F:303:BCR:H23C	2.41	0.51
22:F:304:CLA:H2	22:F:304:CLA:C9	2.41	0.51
9:J:1:MET:H2	34:J:101:LMG:C2	2.22	0.51
13:3:64:CYS:SG	13:3:192:MET:HE2	2.51	0.51
18:6:142:PRO:HD2	39:6:320:CHL:CHC	2.41	0.51
25:6:323:LHG:C12	25:6:323:LHG:H292	2.40	0.51
19:9:114:MET:SD	22:2:302:CLA:HAA1	2.51	0.51
19:9:204:HIS:HA	19:9:206:GLN:OE1	2.11	0.51
20:2:197:ASN:HA	22:2:301:CLA:CBA	2.34	0.51
1:A:453:PHE:HE1	22:B:806:CLA:HMA1	1.73	0.51
1:A:493:LEU:O	1:A:496:GLN:HG2	2.09	0.51
22:A:833:CLA:CAD	24:B:853:BCR:H10C	2.41	0.51
2:B:46:LYS:HG2	25:B:803:LHG:HC12	1.92	0.51
22:B:841:CLA:HBA2	23:B:843:PQN:H241	1.92	0.51
6:F:186:ILE:HG12	9:J:10:THR:HG22	1.92	0.51
11:L:94:PHE:O	11:L:97:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:58:LEU:HD12	38:1:303:LUT:H222	1.92	0.51
12:1:173:LYS:HD3	22:1:305:CLA:HAA2	1.92	0.51
15:8:164:PRO:HB3	22:8:313:CLA:HBC2	1.94	0.51
16:4:71:LEU:HB3	16:4:78:ASP:OD1	2.11	0.51
24:4:804:BCR:H282	22:4:818:CLA:HMC2	1.92	0.51
25:4:820:LHG:H131	22:6:302:CLA:H2	1.92	0.51
18:6:245:PHE:HE2	22:6:301:CLA:H91	1.76	0.51
22:2:304:CLA:HHC	22:2:304:CLA:CBB	2.41	0.51
1:A:526:ILE:HG23	1:A:613:LYS:HE3	1.93	0.50
22:A:829:CLA:HHC	22:A:829:CLA:HBB1	1.92	0.50
22:A:855:CLA:HHC	22:A:855:CLA:CBB	2.41	0.50
2:B:263:HIS:HB3	2:B:266:THR:OG1	2.11	0.50
2:B:276:HIS:ND1	22:B:819:CLA:HAB	2.26	0.50
22:B:825:CLA:HMB3	22:B:825:CLA:HBB1	1.91	0.50
22:F:304:CLA:C2D	22:F:304:CLA:H72	2.40	0.50
10:K:58:LYS:O	10:K:59:ARG:HB2	2.09	0.50
12:1:84:GLY:HA2	38:1:303:LUT:H181	1.93	0.50
24:3:305:BCR:H16C	39:3:317:CHL:H112	1.94	0.50
15:8:125:MET:HB3	24:8:304:BCR:C15	2.41	0.50
36:5:306:C7Z:C36	22:5:322:CLA:HAC1	2.42	0.50
22:A:809:CLA:H11	24:J:104:BCR:C12	2.41	0.50
22:A:840:CLA:H92	24:F:303:BCR:H17C	1.93	0.50
2:B:463:TRP:HE1	2:B:477:LEU:HG	1.75	0.50
2:B:597:TRP:HH2	2:B:613:SER:HB2	1.77	0.50
14:7:234:PHE:HD1	22:7:306:CLA:H11	1.75	0.50
22:7:310:CLA:H171	22:7:310:CLA:H122	1.94	0.50
38:5:303:LUT:H373	22:5:310:CLA:H8	1.94	0.50
22:6:309:CLA:HBA1	22:6:309:CLA:CBD	2.34	0.50
1:A:49:ILE:O	1:A:52:LEU:HD23	2.11	0.50
1:A:204:GLY:O	1:A:208:LEU:HB2	2.12	0.50
1:A:552:LYS:HD3	2:B:671:TYR:CE1	2.46	0.50
22:A:809:CLA:HHC	22:A:809:CLA:CBB	2.39	0.50
24:A:844:BCR:C40	24:A:856:BCR:H12C	2.42	0.50
2:B:488:SER:HA	2:B:491:GLN:CD	2.35	0.50
25:B:803:LHG:HC32	25:B:803:LHG:H242	1.91	0.50
12:Z:163:ALA:HB2	22:Z:303:CLA:HAA2	1.92	0.50
14:7:97:LEU:HD12	22:6:301:CLA:HMA1	1.94	0.50
22:7:311:CLA:HBA2	22:7:311:CLA:CHA	2.41	0.50
15:8:52:PRO:HD2	38:8:303:LUT:C23	2.31	0.50
15:8:152:PHE:HB3	15:8:156:PHE:CE2	2.47	0.50
15:8:169:ASP:HA	38:8:302:LUT:C24	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5:127:LEU:HD12	22:5:326:CLA:CBA	2.42	0.50
1:A:75:SER:O	1:A:78:PHE:HB2	2.11	0.50
1:A:190:TRP:CZ2	22:A:810:CLA:HMA1	2.45	0.50
22:A:833:CLA:CHA	24:B:853:BCR:H12C	2.41	0.50
2:B:340:ALA:HA	2:B:384:MET:HE3	1.93	0.50
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.94	0.50
6:F:155:GLY:O	6:F:159:VAL:HG12	2.11	0.50
22:F:302:CLA:H162	32:F:306:RRX:C40	2.42	0.50
11:L:92:HIS:HA	11:L:95:PHE:CE2	2.47	0.50
24:3:307:BCR:C31	22:3:315:CLA:HHB	2.38	0.50
18:6:214:THR:HA	22:6:309:CLA:CBA	2.40	0.50
25:6:323:LHG:HC92	25:6:323:LHG:H272	1.93	0.50
1:A:28:LYS:HE2	1:A:34:HIS:CG	2.47	0.50
22:A:806:CLA:C4	25:A:850:LHG:H262	2.42	0.50
2:B:444:MET:HB3	2:B:449:THR:O	2.11	0.50
24:B:847:BCR:H311	22:1:308:CLA:H72	1.93	0.50
6:F:114:ARG:C	6:F:116:ALA:H	2.20	0.50
15:8:169:ASP:N	15:8:170:PRO:HD3	2.27	0.50
38:5:302:LUT:C11	22:5:308:CLA:HMC1	2.41	0.50
22:A:839:CLA:H11	24:A:847:BCR:C15	2.41	0.50
24:A:844:BCR:H23C	24:3:306:BCR:C33	2.40	0.50
22:B:806:CLA:H171	22:L:201:CLA:CMC	2.41	0.50
22:B:811:CLA:CBB	22:B:812:CLA:HAA1	2.42	0.50
22:B:820:CLA:HMB3	22:B:820:CLA:CBB	2.37	0.50
22:B:825:CLA:NA	24:B:847:BCR:H362	2.27	0.50
11:L:99:PRO:HG3	22:L:203:CLA:CAB	2.41	0.50
12:1:160:LEU:H	12:1:160:LEU:HD12	1.77	0.50
38:Z:301:LUT:H30	22:Z:303:CLA:C5	2.39	0.50
14:7:129:LEU:HD21	25:8:317:LHG:H322	1.94	0.50
15:8:202:PHE:CD1	38:8:302:LUT:H41	2.47	0.50
16:4:183:ASN:HB3	39:4:819:CHL:C3D	2.41	0.50
38:4:803:LUT:H32	22:4:808:CLA:CAB	2.41	0.50
18:6:127:LYS:HB3	39:6:316:CHL:CMC	2.40	0.50
1:A:305:PHE:HE1	22:A:821:CLA:HAB	1.76	0.50
1:A:359:LEU:HD21	22:A:821:CLA:H93	1.94	0.50
22:A:814:CLA:H143	27:A:852:DGA:HBT1	1.94	0.50
2:B:16:ASP:OD2	2:B:20:ARG:HG3	2.12	0.50
22:B:811:CLA:CGA	22:B:811:CLA:C1A	2.89	0.50
22:B:817:CLA:H112	24:B:844:BCR:H21C	1.93	0.50
22:B:818:CLA:HHC	22:B:818:CLA:CBB	2.42	0.50
4:D:125:THR:HG22	4:D:129:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:35:ASP:N	9:J:36:PRO:HD3	2.27	0.50
22:1:305:CLA:C4D	22:1:310:CLA:H8	2.42	0.50
12:Z:221:SER:HA	22:Z:316:CLA:C4D	2.41	0.50
22:Z:306:CLA:H72	22:Z:307:CLA:HHB	1.92	0.50
38:9:301:LUT:H403	22:9:303:CLA:H13	1.93	0.50
38:9:302:LUT:H162	22:9:308:CLA:HMA1	1.94	0.50
38:9:302:LUT:C32	22:9:306:CLA:HAB	2.42	0.50
1:A:536:HIS:HA	1:A:539:HIS:HD2	1.76	0.50
1:A:572:ARG:HH21	25:A:850:LHG:C3	2.24	0.50
22:A:813:CLA:H201	22:3:312:CLA:H72	1.93	0.50
22:A:829:CLA:CHA	22:A:829:CLA:H12	2.42	0.50
2:B:5:LEU:HD12	8:I:101:LYS:HG3	1.94	0.50
2:B:222:GLY:O	2:B:225:PRO:HD2	2.12	0.50
22:B:830:CLA:H8	24:B:845:BCR:H19C	1.94	0.50
22:B:836:CLA:NC	31:1:319:DGD:HA82	2.26	0.50
11:L:86:VAL:HG22	11:L:90:ARG:HD3	1.93	0.50
11:L:120:SER:OG	22:L:201:CLA:H2	2.12	0.50
12:Z:58:LEU:HD21	15:8:170:PRO:HB3	1.93	0.50
22:Z:303:CLA:H102	22:Z:304:CLA:CMB	2.41	0.50
14:7:130:LEU:HB3	24:7:303:BCR:C15	2.42	0.50
25:4:820:LHG:H381	22:6:321:CLA:HBD	1.94	0.50
17:5:64:PRO:O	17:5:68:LYS:HG3	2.11	0.50
18:6:147:ASN:ND2	39:6:320:CHL:HAA1	2.27	0.50
18:6:157:PRO:HG3	39:6:316:CHL:C2D	2.42	0.50
22:6:309:CLA:HMB3	22:6:309:CLA:HBB1	1.94	0.50
22:9:307:CLA:HED2	22:9:307:CLA:H2A	1.94	0.50
20:2:166:LEU:HA	20:2:169:ILE:CG1	2.41	0.50
1:A:71:ARG:HH21	1:A:187:LYS:HA	1.77	0.50
1:A:245:LEU:HD23	31:3:301:DGD:HG12	1.93	0.50
1:A:697:ILE:O	1:A:701:ILE:HG13	2.12	0.50
22:A:815:CLA:H51	13:3:200:ALA:HA	1.93	0.50
2:B:13:LEU:HD21	2:B:20:ARG:HH11	1.76	0.50
12:1:211:TRP:CZ3	15:8:118:LEU:HA	2.47	0.50
12:Z:82:MET:HE3	22:Z:303:CLA:HMC3	1.93	0.50
12:Z:103:PRO:HG2	39:Z:312:CHL:CED	2.41	0.50
12:Z:140:ARG:HG2	22:Z:313:CLA:CAB	2.42	0.50
22:Z:309:CLA:CBB	24:4:804:BCR:H323	2.42	0.50
16:4:185:LEU:HD11	16:4:197:PHE:CE2	2.47	0.50
24:4:804:BCR:H402	22:4:810:CLA:C5	2.42	0.50
1:A:60:ASP:HA	1:A:69:ILE:HD13	1.93	0.49
22:A:854:CLA:HMA3	22:A:854:CLA:C2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:LEU:HD21	24:B:846:BCR:H24C	1.94	0.49
2:B:178:HIS:HB3	22:B:815:CLA:CAB	2.42	0.49
2:B:478:LEU:HD13	22:B:835:CLA:HHD	1.94	0.49
22:B:838:CLA:H152	32:F:306:RRX:C35	2.42	0.49
7:G:78:PHE:CG	7:G:78:PHE:O	2.65	0.49
7:G:114:PHE:CE2	22:G:201:CLA:HBC2	2.47	0.49
22:K:205:CLA:HMD3	24:K:206:BCR:H21C	1.94	0.49
22:1:307:CLA:HHD	39:8:301:CHL:HBB2	1.93	0.49
38:Z:302:LUT:H28	22:Z:306:CLA:H61	1.94	0.49
39:Z:311:CHL:HAA1	39:Z:311:CHL:HBD	1.93	0.49
22:7:315:CLA:HBB1	22:7:315:CLA:HMB3	1.93	0.49
38:8:302:LUT:C30	22:8:305:CLA:H61	2.41	0.49
17:5:188:LYS:HE3	25:5:324:LHG:HC61	1.94	0.49
19:9:115:GLU:CB	39:9:312:CHL:HBB2	2.41	0.49
1:A:197:MET:HE1	22:A:825:CLA:H71	1.93	0.49
22:A:823:CLA:HHC	22:A:823:CLA:CBB	2.33	0.49
24:A:856:BCR:H321	24:A:856:BCR:HC8	1.94	0.49
2:B:393:ILE:CG2	2:B:397:ARG:HD2	2.42	0.49
2:B:646:VAL:HG21	22:B:811:CLA:HAC1	1.93	0.49
22:B:815:CLA:H141	22:B:820:CLA:NB	2.27	0.49
6:F:138:GLY:HA3	22:F:304:CLA:C2D	2.41	0.49
12:1:160:LEU:HD12	12:1:160:LEU:N	2.28	0.49
12:Z:144:GLU:HG3	22:Z:313:CLA:HAC1	1.93	0.49
17:5:128:LEU:HB3	24:5:304:BCR:C15	2.42	0.49
38:9:301:LUT:H34	22:9:303:CLA:HBB2	1.94	0.49
38:9:301:LUT:H28	22:9:303:CLA:H2	1.92	0.49
22:A:816:CLA:HBB1	22:A:816:CLA:CMB	2.41	0.49
22:A:826:CLA:HHB	22:A:839:CLA:O2A	2.12	0.49
2:B:71:TRP:CD1	8:I:71:PRO:HD2	2.47	0.49
2:B:278:HIS:HA	2:B:281:ILE:HG12	1.94	0.49
2:B:349:VAL:O	2:B:353:MET:HB2	2.13	0.49
2:B:689:ALA:HB2	24:B:853:BCR:HC22	1.94	0.49
2:B:705:GLN:O	2:B:708:LEU:HG	2.11	0.49
3:C:18:VAL:C	3:C:20:ALA:H	2.19	0.49
22:F:301:CLA:HHC	22:F:301:CLA:CBB	2.42	0.49
12:Z:144:GLU:HG3	22:Z:313:CLA:CAC	2.43	0.49
22:3:311:CLA:H62	22:3:312:CLA:HHB	1.95	0.49
22:8:306:CLA:HMD3	22:8:311:CLA:C4D	2.43	0.49
22:4:812:CLA:C4D	22:6:302:CLA:H111	2.42	0.49
17:5:106:PRO:C	17:5:115:ASN:H	2.21	0.49
22:5:309:CLA:HHC	22:5:309:CLA:CBB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:140:ALA:HA	18:6:148:LYS:HA	1.93	0.49
19:9:84:ILE:HG22	19:9:183:PRO:HG2	1.94	0.49
19:9:126:ARG:HH22	22:9:313:CLA:HMA3	1.77	0.49
2:B:6:PHE:CE2	2:B:22:ILE:HA	2.47	0.49
2:B:478:LEU:CD1	22:B:835:CLA:HHD	2.42	0.49
4:D:184:VAL:CG1	4:D:194:ILE:HG21	2.42	0.49
22:1:304:CLA:H122	22:1:305:CLA:HMB2	1.95	0.49
22:1:305:CLA:HED2	22:1:305:CLA:H2A	1.93	0.49
22:1:316:CLA:HED1	22:1:316:CLA:H2	1.95	0.49
24:3:305:BCR:H312	39:3:317:CHL:HMB3	1.95	0.49
22:3:314:CLA:HHC	22:3:314:CLA:CBB	2.42	0.49
16:4:118:ASP:HA	16:4:121:ARG:HE	1.78	0.49
17:5:74:GLU:CD	17:5:187:ILE:HD11	2.38	0.49
17:5:106:PRO:HA	17:5:109:LEU:HD12	1.93	0.49
1:A:272:TYR:HB3	1:A:275:PHE:CZ	2.48	0.49
22:A:805:CLA:HAA2	22:A:825:CLA:C4	2.41	0.49
22:A:806:CLA:H8	22:A:830:CLA:HBC3	1.94	0.49
2:B:18:THR:HG22	3:C:79:LEU:HD11	1.94	0.49
2:B:107:ARG:HH22	2:B:115:ASN:HD22	1.60	0.49
25:Z:317:LHG:HC92	24:4:804:BCR:HC22	1.94	0.49
13:3:103:TYR:HE2	13:3:105:LYS:O	1.95	0.49
14:7:58:LEU:HD11	38:7:302:LUT:H221	1.94	0.49
17:5:127:LEU:HD12	22:5:326:CLA:HBA1	1.93	0.49
18:6:235:GLN:HE21	22:6:301:CLA:HHB	1.78	0.49
19:9:62:ARG:HB3	19:9:66:PHE:CE2	2.47	0.49
22:A:810:CLA:HMB3	22:A:810:CLA:HBB1	1.95	0.49
22:A:815:CLA:H122	13:3:196:PHE:CD2	2.47	0.49
22:A:841:CLA:H51	22:B:801:CLA:H203	1.94	0.49
22:A:855:CLA:H193	24:B:853:BCR:C35	2.43	0.49
2:B:548:MET:HE3	2:B:551:LYS:HA	1.93	0.49
2:B:651:PHE:CE2	2:B:655:HIS:HE1	2.31	0.49
2:B:715:SER:HB2	31:B:852:DGD:HBH2	1.95	0.49
39:1:312:CHL:HAB	22:1:315:CLA:HBB2	1.93	0.49
13:3:225:ILE:HG13	22:3:310:CLA:HMD3	1.95	0.49
14:7:202:VAL:HG21	25:7:318:LHG:H271	1.93	0.49
22:5:307:CLA:H101	22:5:308:CLA:H122	1.94	0.49
22:A:824:CLA:H141	25:A:849:LHG:H171	1.94	0.49
22:A:837:CLA:C3A	22:A:838:CLA:HAA2	2.42	0.49
22:A:841:CLA:HHC	22:A:841:CLA:HBB1	1.94	0.49
2:B:164:PRO:HB2	2:B:169:PHE:CE2	2.48	0.49
2:B:227:TRP:CZ2	22:B:817:CLA:H52	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:838:CLA:CGA	22:B:838:CLA:C1A	2.90	0.49
22:B:838:CLA:NC	22:B:838:CLA:H42	2.28	0.49
4:D:76:ARG:O	4:D:80:VAL:HG12	2.12	0.49
24:L:204:BCR:C12	24:L:204:BCR:H341	2.43	0.49
22:1:310:CLA:HBC3	25:1:317:LHG:O8	2.13	0.49
12:Z:191:GLN:HE22	12:Z:199:PRO:HG3	1.77	0.49
22:Z:307:CLA:H12	15:8:151:GLY:O	2.13	0.49
22:3:314:CLA:H41	22:3:314:CLA:H101	1.93	0.49
14:7:58:LEU:HB2	22:7:307:CLA:H11	1.94	0.49
14:7:83:ALA:HB1	38:7:301:LUT:H12	1.93	0.49
25:4:820:LHG:H122	24:6:305:BCR:H333	1.94	0.49
17:5:35:TRP:CZ3	22:5:315:CLA:HAA1	2.48	0.49
17:5:80:TRP:CE2	22:5:318:CLA:HBC3	2.47	0.49
18:6:73:VAL:HG21	18:6:128:ARG:CZ	2.41	0.49
22:6:310:CLA:H151	22:6:311:CLA:HBB1	1.94	0.49
22:A:807:CLA:HHC	22:A:807:CLA:HBB1	1.94	0.49
2:B:306:LEU:HD23	22:B:825:CLA:O1D	2.12	0.49
22:B:810:CLA:C1B	24:I:4001:BCR:HC22	2.42	0.49
13:3:121:MET:CB	22:3:318:CLA:HAB	2.42	0.49
38:8:303:LUT:H163	39:8:315:CHL:CMC	2.43	0.49
16:4:259:ASP:HB3	22:4:817:CLA:CHB	2.42	0.49
22:5:322:CLA:C14	22:6:310:CLA:H101	2.42	0.49
18:6:170:LEU:HB3	22:6:307:CLA:HMA1	1.95	0.49
1:A:21:PRO:HG2	1:A:185:ALA:HB3	1.95	0.49
1:A:53:HIS:HD2	22:A:804:CLA:HAC1	1.77	0.49
1:A:545:VAL:HG11	1:A:598:TRP:CZ2	2.48	0.49
22:A:815:CLA:HBC1	22:A:817:CLA:HMB2	1.95	0.49
2:B:71:TRP:CZ2	8:I:71:PRO:HB2	2.47	0.49
2:B:117:SER:HA	22:B:811:CLA:HMD1	1.94	0.49
22:B:809:CLA:H62	22:B:809:CLA:HMA3	1.95	0.49
6:F:138:GLY:O	6:F:142:LYS:HB2	2.13	0.49
7:G:71:LYS:HA	7:G:71:LYS:HE2	1.94	0.49
10:K:30:ILE:HA	10:K:35:ASN:ND2	2.28	0.49
22:1:306:CLA:H171	24:8:304:BCR:H321	1.93	0.49
22:Z:308:CLA:HBA2	22:Z:308:CLA:CHA	2.43	0.49
13:3:114:PHE:HB2	22:3:316:CLA:HAA1	1.95	0.49
38:9:301:LUT:H34	22:9:303:CLA:CBB	2.42	0.49
22:A:810:CLA:H142	22:A:813:CLA:H151	1.95	0.49
22:A:835:CLA:H201	22:A:842:CLA:HBB2	1.95	0.49
8:I:74:TRP:HZ2	22:2:304:CLA:HHB	1.78	0.49
10:K:38:MET:HE1	10:K:101:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:107:LEU:HD22	10:K:112:ASN:HD22	1.78	0.49
22:K:205:CLA:CHA	24:K:206:BCR:H393	2.43	0.49
22:Z:316:CLA:HMB2	22:8:310:CLA:H143	1.94	0.49
13:3:117:GLU:O	13:3:121:MET:HG2	2.13	0.49
13:3:203:VAL:O	31:3:301:DGD:HG31	2.12	0.49
39:7:313:CHL:C1C	39:7:313:CHL:H71	2.43	0.49
15:8:187:LYS:HD3	22:8:306:CLA:HBA1	1.94	0.49
16:4:180:PHE:HB3	16:4:182:ASN:OD1	2.12	0.49
39:4:816:CHL:HBA2	39:4:816:CHL:O2D	2.12	0.49
22:6:322:CLA:H112	22:6:322:CLA:H72	1.60	0.49
22:9:307:CLA:C3D	22:9:313:CLA:H43	2.43	0.49
20:2:178:ARG:HB3	22:2:304:CLA:HED2	1.94	0.49
1:A:202:LEU:O	1:A:305:PHE:HB3	2.12	0.48
1:A:203:ALA:HB2	1:A:309:GLY:HA3	1.93	0.48
1:A:668:TYR:CE1	22:A:808:CLA:HAC1	2.48	0.48
22:A:804:CLA:HBB1	22:A:804:CLA:HMB1	1.94	0.48
2:B:142:PHE:CZ	22:B:816:CLA:H122	2.48	0.48
3:C:5:VAL:HG11	3:C:26:LEU:HD21	1.95	0.48
6:F:107:THR:HA	6:F:110:ARG:NE	2.27	0.48
22:F:301:CLA:H122	22:F:301:CLA:H8	1.61	0.48
10:K:59:ARG:H	10:K:69:ASP:HA	1.78	0.48
12:Z:192:HIS:O	12:Z:196:GLY:HA2	2.12	0.48
15:8:77:MET:HE3	22:8:305:CLA:HMC3	1.94	0.48
15:8:153:GLU:HA	15:8:156:PHE:HD2	1.78	0.48
22:4:808:CLA:HBC1	25:4:820:LHG:H282	1.95	0.48
17:5:109:LEU:HD23	22:5:312:CLA:HAA2	1.95	0.48
18:6:110:ILE:CD1	24:6:306:BCR:HC8	2.38	0.48
18:6:141:ASP:HB2	18:6:147:ASN:HB2	1.95	0.48
22:6:309:CLA:NC	22:6:309:CLA:H51	2.28	0.48
19:9:127:TYR:HB2	22:9:313:CLA:HMA3	1.93	0.48
39:9:312:CHL:CHB	39:9:314:CHL:HBC2	2.43	0.48
1:A:396:TRP:CZ3	1:A:600:TYR:HA	2.48	0.48
2:B:223:LEU:HB3	2:B:227:TRP:NE1	2.28	0.48
2:B:412:MET:HA	2:B:415:HIS:CE1	2.48	0.48
12:Z:69:ARG:NH2	15:8:150:LEU:HD23	2.27	0.48
22:Z:309:CLA:HHC	22:Z:309:CLA:CBB	2.43	0.48
13:3:143:PHE:CE2	39:3:317:CHL:HBB2	2.48	0.48
13:3:159:PRO:HG3	39:3:317:CHL:HMD1	1.95	0.48
22:7:309:CLA:HMA2	22:7:316:CLA:C3C	2.43	0.48
16:4:258:ASN:O	16:4:262:ARG:HG3	2.13	0.48
17:5:105:GLU:HB3	17:5:107:GLN:NE2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5:305:BCR:H21C	24:5:305:BCR:H361	1.94	0.48
19:9:31:TRP:CD1	19:9:51:PHE:HA	2.48	0.48
1:A:501:THR:HG21	22:K:203:CLA:HED1	1.94	0.48
2:B:54:GLN:O	2:B:58:ILE:HG13	2.14	0.48
2:B:584:MET:O	2:B:588:ILE:HG12	2.13	0.48
22:B:814:CLA:HBB2	22:B:822:CLA:H93	1.95	0.48
13:3:149:VAL:HG22	13:3:163:TRP:HB2	1.93	0.48
14:7:82:GLY:HA2	38:7:302:LUT:H181	1.95	0.48
14:7:125:ALA:HB2	15:8:230:VAL:HG21	1.94	0.48
22:8:309:CLA:HAC1	39:8:312:CHL:HBB2	1.95	0.48
16:4:161:GLU:HG3	22:4:815:CLA:C4B	2.43	0.48
22:5:301:CLA:HHC	22:5:301:CLA:CBB	2.43	0.48
19:9:76:TRP:CD2	22:9:313:CLA:HAC2	2.47	0.48
1:A:678:VAL:HG21	24:A:848:BCR:H353	1.95	0.48
22:A:822:CLA:C4D	24:A:856:BCR:H292	2.44	0.48
23:A:843:PQN:H201	24:F:303:BCR:H382	1.95	0.48
24:A:848:BCR:H24C	22:B:801:CLA:H101	1.95	0.48
2:B:23:TRP:HB3	31:B:852:DGD:C4A	2.44	0.48
2:B:32:PHE:HB2	2:B:43:LEU:HD13	1.95	0.48
2:B:177:ASN:OD1	2:B:292:TYR:HD2	1.97	0.48
22:B:824:CLA:H11	33:G:204:LMT:C6'	2.43	0.48
22:B:841:CLA:H203	24:L:204:BCR:H15C	1.95	0.48
24:B:844:BCR:H272	24:B:846:BCR:H323	1.96	0.48
3:C:3:HIS:ND1	3:C:69:LEU:HA	2.28	0.48
6:F:121:ALA:HB3	6:F:123:LEU:HD13	1.95	0.48
22:F:304:CLA:C1D	22:F:304:CLA:H52	2.44	0.48
7:G:33:GLU:HB3	7:G:34:PRO:HD2	1.95	0.48
7:G:54:LEU:O	7:G:58:ARG:HG2	2.13	0.48
9:J:34:PRO:HD2	35:J:102:T7X:C5	2.43	0.48
12:1:79:ARG:HA	12:1:82:MET:HE3	1.95	0.48
12:1:191:GLN:HG3	12:1:192:HIS:N	2.27	0.48
22:7:310:CLA:H2	22:7:310:CLA:H61	1.64	0.48
22:8:306:CLA:HMD2	33:4:801:LMT:H61	1.95	0.48
39:8:312:CHL:CHD	39:8:315:CHL:HBC2	2.43	0.48
16:4:114:ILE:HG23	16:4:134:TRP:CD1	2.48	0.48
16:4:177:ASP:CB	16:4:183:ASN:HB2	2.42	0.48
18:6:159:PHE:O	38:6:303:LUT:H24	2.12	0.48
1:A:69:ILE:O	1:A:73:VAL:HG23	2.13	0.48
1:A:296:HIS:HB3	22:A:818:CLA:HMB1	1.95	0.48
1:A:382:THR:HG21	1:A:517:VAL:HB	1.94	0.48
1:A:487:ILE:HD11	22:A:837:CLA:H43	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ILE:HD11	1:A:583:THR:HB	1.95	0.48
22:A:810:CLA:O1A	22:A:813:CLA:H193	2.13	0.48
22:A:813:CLA:H191	22:3:312:CLA:H41	1.95	0.48
22:A:835:CLA:NB	24:A:847:BCR:H292	2.28	0.48
22:A:836:CLA:C4D	22:K:203:CLA:H12	2.44	0.48
22:A:841:CLA:H62	22:A:841:CLA:H102	1.48	0.48
22:B:819:CLA:HHC	22:B:819:CLA:CBB	2.43	0.48
22:B:821:CLA:H42	22:B:825:CLA:O1A	2.14	0.48
22:B:842:CLA:HBA1	25:B:850:LHG:HC42	1.95	0.48
33:1:301:LMT:H31	22:1:308:CLA:H42	1.95	0.48
13:3:163:TRP:O	13:3:166:LEU:HB3	2.14	0.48
38:3:302:LUT:H382	22:3:308:CLA:C4D	2.43	0.48
22:8:306:CLA:HMD3	22:8:311:CLA:CHA	2.43	0.48
25:4:820:LHG:HC91	25:4:820:LHG:H292	1.94	0.48
25:6:323:LHG:H292	25:6:323:LHG:H122	1.96	0.48
38:9:302:LUT:H161	39:9:314:CHL:HBB1	1.96	0.48
39:9:312:CHL:HBC2	39:9:312:CHL:CMC	2.39	0.48
1:A:25:SER:O	22:A:811:CLA:HHB	2.13	0.48
1:A:427:LEU:O	1:A:431:ILE:HG13	2.14	0.48
1:A:441:LEU:O	1:A:444:VAL:HG12	2.13	0.48
1:A:541:PHE:CZ	22:B:806:CLA:HBB2	2.46	0.48
22:A:811:CLA:HHC	22:A:811:CLA:CBB	2.42	0.48
22:A:823:CLA:NC	37:K:201:DAO:H111	2.29	0.48
2:B:490:SER:CB	2:B:495:LEU:HB2	2.44	0.48
22:B:832:CLA:H2	22:B:842:CLA:C3	2.43	0.48
22:Z:305:CLA:H43	22:Z:310:CLA:OBD	2.14	0.48
13:3:202:ALA:O	31:3:301:DGD:HB31	2.13	0.48
24:3:306:BCR:C12	24:3:306:BCR:H341	2.42	0.48
22:3:320:CLA:CMD	41:7:319:3PH:H342	2.36	0.48
15:8:208:ALA:HA	15:8:234:ILE:HG21	1.95	0.48
22:4:807:CLA:C1A	22:4:807:CLA:CGA	2.91	0.48
18:6:142:PRO:HB2	22:6:302:CLA:CMD	2.44	0.48
20:2:199:TYR:O	20:2:204:GLY:HA3	2.14	0.48
1:A:82:GLY:O	1:A:86:ILE:HG13	2.13	0.48
1:A:495:PRO:O	1:A:500:PRO:HA	2.13	0.48
1:A:673:LEU:HB3	22:A:802:CLA:O2A	2.13	0.48
1:A:684:MET:HE3	23:A:843:PQN:H2M1	1.94	0.48
22:A:814:CLA:HBA1	24:A:844:BCR:C34	2.44	0.48
22:A:814:CLA:HMC2	24:A:844:BCR:H352	1.94	0.48
22:A:821:CLA:H2	22:A:821:CLA:H61	1.56	0.48
22:A:821:CLA:C10	24:A:847:BCR:H10C	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:848:BCR:H292	22:F:302:CLA:HMA1	1.96	0.48
2:B:295:ASN:HB2	7:G:83:GLN:O	2.13	0.48
6:F:123:LEU:HB3	6:F:131:PRO:HB3	1.96	0.48
9:J:16:LEU:HD21	36:J:105:C7Z:C12	2.44	0.48
22:Z:303:CLA:H41	22:Z:304:CLA:HBA1	1.95	0.48
22:Z:304:CLA:HMD3	22:Z:309:CLA:HBA2	1.95	0.48
22:Z:305:CLA:HBC1	22:Z:316:CLA:C10	2.42	0.48
13:3:138:MET:HE2	13:3:138:MET:HA	1.96	0.48
14:7:243:PHE:HE2	22:7:317:CLA:CAB	2.26	0.48
16:4:183:ASN:OD1	39:4:819:CHL:HAA1	2.14	0.48
17:5:160:PRO:HG2	17:5:179:ARG:HH12	1.77	0.48
39:5:316:CHL:HAA1	39:5:316:CHL:HBD	1.95	0.48
18:6:237:THR:HG23	18:6:246:THR:OG1	2.13	0.48
22:6:311:CLA:CBB	22:6:319:CLA:H42	2.44	0.48
19:9:100:GLY:O	39:9:314:CHL:HBC1	2.14	0.48
39:9:312:CHL:HBC1	22:9:313:CLA:HBC3	1.94	0.48
22:A:822:CLA:H8	22:A:823:CLA:C9	2.44	0.48
2:B:613:SER:HA	2:B:616:TYR:CE1	2.49	0.48
22:B:834:CLA:O2A	9:J:36:PRO:HG2	2.14	0.48
22:B:836:CLA:HBB1	22:B:836:CLA:CMB	2.43	0.48
11:L:126:ILE:HD12	22:L:201:CLA:H152	1.96	0.48
14:7:137:LYS:HB3	22:7:314:CLA:HMC2	1.95	0.48
15:8:107:SER:OG	39:8:315:CHL:HAC1	2.14	0.48
22:5:312:CLA:HBA1	22:5:312:CLA:H3A	1.72	0.48
22:5:318:CLA:H92	22:6:322:CLA:H62	1.95	0.48
18:6:122:HIS:CE1	18:6:126:LEU:HD11	2.48	0.48
20:2:199:TYR:OH	20:2:211:VAL:HG21	2.13	0.48
1:A:26:PHE:CD2	34:J:101:LMG:HC1	2.49	0.48
22:A:805:CLA:C17	24:A:844:BCR:H323	2.44	0.48
22:A:822:CLA:O1A	22:K:204:CLA:HMB3	2.14	0.48
2:B:217:LEU:HD23	22:B:817:CLA:O1D	2.14	0.48
2:B:688:LEU:CB	24:B:853:BCR:HC31	2.43	0.48
22:B:815:CLA:H71	22:B:815:CLA:H111	1.56	0.48
22:B:815:CLA:H172	22:B:830:CLA:CAD	2.44	0.48
22:G:202:CLA:HED2	22:G:202:CLA:H2A	1.95	0.48
9:J:3:ASN:HB2	34:J:101:LMG:HC3	1.95	0.48
11:L:135:TYR:CZ	11:L:139:MET:HG3	2.49	0.48
39:Z:312:CHL:HAA1	39:Z:312:CHL:HBD	1.95	0.48
22:3:322:CLA:H141	22:7:317:CLA:HBC2	1.96	0.48
39:8:312:CHL:C1C	26:8:318:NKP:HAPA	2.44	0.48
16:4:100:GLU:CD	16:4:215:ILE:HD11	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:237:LYS:HB2	16:4:242:ASN:ND2	2.28	0.48
22:5:322:CLA:H2A	22:5:322:CLA:HED3	1.95	0.48
18:6:52:PHE:HB3	22:6:310:CLA:C3D	2.43	0.48
19:9:69:ALA:HA	19:9:72:THR:HG22	1.96	0.48
22:A:810:CLA:H51	22:3:312:CLA:H51	1.95	0.48
2:B:32:PHE:HB2	2:B:43:LEU:CD1	2.43	0.48
2:B:312:PRO:HD2	25:B:850:LHG:P	2.54	0.48
2:B:655:HIS:HB3	22:B:806:CLA:HBD	1.96	0.48
22:B:827:CLA:C3B	22:B:839:CLA:HMA3	2.44	0.48
5:E:47:ARG:HB3	5:E:50:SER:OG	2.13	0.48
11:L:96:LEU:HB3	11:L:97:PRO:HD3	1.95	0.48
12:Z:60:LEU:CD1	38:Z:302:LUT:H221	2.43	0.48
13:3:20:GLU:O	13:3:24:GLN:HG3	2.14	0.48
38:7:301:LUT:H26	22:7:304:CLA:O1A	2.14	0.48
22:4:812:CLA:H72	22:6:302:CLA:H121	1.96	0.48
22:6:309:CLA:HBD	22:6:309:CLA:CBA	2.38	0.48
1:A:307:VAL:CA	24:A:856:BCR:H17C	2.31	0.47
22:A:823:CLA:H12	37:K:201:DAO:H82	1.95	0.47
22:A:830:CLA:H112	25:A:850:LHG:H202	1.95	0.47
22:A:833:CLA:CBD	24:B:853:BCR:H12C	2.43	0.47
22:A:855:CLA:H141	24:B:853:BCR:C17	2.44	0.47
22:B:811:CLA:H111	22:B:811:CLA:H2	1.95	0.47
22:Z:303:CLA:HBB1	22:Z:303:CLA:CMB	2.44	0.47
14:7:58:LEU:CD1	38:7:302:LUT:H221	2.44	0.47
22:8:313:CLA:CHA	22:8:313:CLA:HBA2	2.44	0.47
22:8:313:CLA:CMA	39:8:315:CHL:H52	2.40	0.47
16:4:192:TYR:HB3	22:4:805:CLA:O1D	2.14	0.47
18:6:179:ARG:HA	18:6:182:MET:HE2	1.96	0.47
39:9:312:CHL:HHC	39:9:312:CHL:CBB	2.41	0.47
1:A:409:ALA:CB	24:A:846:BCR:H271	2.43	0.47
22:A:821:CLA:HMB1	22:A:821:CLA:HBB1	1.96	0.47
22:A:822:CLA:C1D	24:A:856:BCR:H402	2.43	0.47
22:A:833:CLA:H42	22:B:840:CLA:H41	1.96	0.47
22:A:835:CLA:O1A	22:A:836:CLA:HHB	2.13	0.47
22:A:842:CLA:CBB	24:A:846:BCR:H12C	2.44	0.47
22:B:810:CLA:C2B	24:I:4001:BCR:HC22	2.45	0.47
22:B:818:CLA:H143	22:B:818:CLA:H111	1.64	0.47
6:F:153:THR:HG21	32:F:306:RRX:H57	1.95	0.47
7:G:35:TYR:HA	22:G:201:CLA:OBD	2.15	0.47
33:1:301:LMT:H52	22:1:314:CLA:H42	1.95	0.47
12:Z:203:LEU:O	12:Z:207:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:306:CLA:H72	22:Z:307:CLA:HMB1	1.96	0.47
13:3:59:SER:OG	22:3:312:CLA:HAA1	2.14	0.47
13:3:70:GLY:HA2	38:3:303:LUT:C18	2.40	0.47
15:8:30:TRP:CH2	41:8:320:3PH:H332	2.49	0.47
16:4:183:ASN:HB3	39:4:819:CHL:C4D	2.43	0.47
17:5:134:VAL:HG12	22:6:314:CLA:HED1	1.95	0.47
22:5:307:CLA:H52	22:5:307:CLA:H8	1.66	0.47
19:9:195:GLY:O	19:9:196:TYR:C	2.57	0.47
22:A:805:CLA:OBD	22:A:825:CLA:H101	2.14	0.47
22:A:838:CLA:H72	22:A:839:CLA:HMD3	1.97	0.47
22:B:825:CLA:HHC	22:B:832:CLA:HMD1	1.95	0.47
3:C:66:ARG:HB3	3:C:68:TYR:CE1	2.48	0.47
5:E:50:SER:OG	5:E:88:PHE:HE1	1.97	0.47
7:G:112:LEU:O	7:G:116:PHE:HD1	1.97	0.47
12:Z:170:LEU:HA	12:Z:173:LYS:HD2	1.95	0.47
13:3:82:LYS:HD2	13:3:210:TYR:CD2	2.47	0.47
24:3:306:BCR:C21	22:3:318:CLA:H91	2.19	0.47
22:8:307:CLA:H62	22:8:307:CLA:CHC	2.44	0.47
17:5:107:GLN:H	17:5:107:GLN:CD	2.21	0.47
18:6:216:PHE:CD1	22:6:322:CLA:HBB1	2.48	0.47
19:9:123:GLU:HG3	22:9:313:CLA:C4B	2.43	0.47
22:A:805:CLA:H151	24:A:844:BCR:HC31	1.96	0.47
2:B:31:ASP:HB2	22:B:831:CLA:CAA	2.45	0.47
2:B:153:ALA:HB2	22:B:813:CLA:HBC2	1.95	0.47
2:B:680:VAL:HG13	2:B:694:TRP:HZ2	1.79	0.47
2:B:705:GLN:HG3	31:B:852:DGD:HA52	1.95	0.47
22:B:806:CLA:H72	22:B:806:CLA:H112	1.77	0.47
24:B:853:BCR:H272	22:L:201:CLA:H92	1.95	0.47
7:G:102:THR:HG21	22:G:202:CLA:HBA1	1.96	0.47
9:J:8:LEU:HA	9:J:13:VAL:HG11	1.96	0.47
12:Z:112:PRO:HB2	12:Z:119:VAL:HG23	1.97	0.47
22:Z:304:CLA:HMD2	22:Z:309:CLA:H12	1.96	0.47
13:3:127:ARG:HG3	22:3:322:CLA:O1D	2.14	0.47
16:4:176:GLN:NE2	16:4:181:THR:HA	2.29	0.47
17:5:55:PHE:CE1	22:5:315:CLA:HAA2	2.49	0.47
22:5:310:CLA:H172	22:5:311:CLA:HBB2	1.96	0.47
18:6:123:PHE:HZ	39:6:320:CHL:HBB2	1.76	0.47
22:A:821:CLA:H18	24:A:846:BCR:H272	1.96	0.47
2:B:330:SER:O	2:B:334:GLN:HG3	2.13	0.47
22:B:808:CLA:CBA	22:B:815:CLA:HBA1	2.38	0.47
22:B:840:CLA:HBB1	22:B:840:CLA:HMB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:MET:SD	4:D:192:MET:N	2.83	0.47
12:1:185:CYS:HA	12:1:188:PHE:CD2	2.49	0.47
38:Z:301:LUT:C28	22:Z:303:CLA:H52	2.45	0.47
13:3:131:ASP:O	13:3:135:PRO:HA	2.15	0.47
24:3:304:BCR:HC31	22:7:310:CLA:HAB	1.96	0.47
22:3:322:CLA:C4B	25:7:318:LHG:H101	2.44	0.47
22:7:306:CLA:H8	22:7:306:CLA:H51	1.48	0.47
25:4:820:LHG:H121	25:4:820:LHG:HC92	1.60	0.47
17:5:123:ALA:HB1	22:5:326:CLA:HAA1	1.95	0.47
22:5:315:CLA:H152	22:5:315:CLA:H18	1.76	0.47
18:6:73:VAL:HG21	18:6:128:ARG:NH1	2.30	0.47
18:6:123:PHE:HE1	24:6:305:BCR:H332	1.80	0.47
18:6:161:PRO:HD2	38:6:303:LUT:C23	2.44	0.47
18:6:251:GLN:HG2	18:6:254:TRP:CZ3	2.50	0.47
22:6:308:CLA:C1D	22:6:313:CLA:H72	2.44	0.47
19:9:111:LEU:HD11	39:9:314:CHL:C2D	2.45	0.47
22:2:302:CLA:HED2	22:2:302:CLA:H2A	1.95	0.47
1:A:87:TRP:O	1:A:91:MET:HG2	2.15	0.47
1:A:264:PHE:HA	1:A:269:TRP:HD1	1.80	0.47
1:A:437:ILE:HG23	22:A:839:CLA:HBB2	1.95	0.47
21:A:801:CL0:H34	21:A:801:CL0:H41	1.52	0.47
22:A:807:CLA:CHC	26:A:851:NKP:HAUA	2.44	0.47
22:A:831:CLA:CMA	11:L:57:THR:HG21	2.43	0.47
2:B:18:THR:HG21	3:C:77:MET:HG3	1.96	0.47
2:B:30:HIS:CD2	22:B:808:CLA:HBB2	2.50	0.47
2:B:269:LEU:HD21	2:B:356:LEU:HB3	1.95	0.47
22:B:823:CLA:HBD	7:G:57:HIS:HD2	1.79	0.47
22:B:842:CLA:HAB	12:1:70:PHE:HZ	1.79	0.47
6:F:157:LEU:HB3	22:F:302:CLA:H142	1.97	0.47
7:G:59:ARG:HG2	7:G:63:ARG:NE	2.24	0.47
9:J:11:ALA:N	9:J:12:PRO:HD2	2.29	0.47
22:L:202:CLA:H2	22:L:202:CLA:H92	1.97	0.47
12:Z:144:GLU:HG3	22:Z:313:CLA:CBC	2.45	0.47
13:3:203:VAL:CG1	31:3:301:DGD:HG32	2.42	0.47
15:8:37:PRO:HG2	15:8:40:LEU:HD12	1.96	0.47
15:8:51:ASP:HA	38:8:303:LUT:H24	1.96	0.47
15:8:62:LEU:HD12	22:8:308:CLA:HMA2	1.97	0.47
15:8:105:LYS:HB2	39:8:312:CHL:OBD	2.14	0.47
22:8:307:CLA:HBB1	22:8:307:CLA:HMB3	1.96	0.47
16:4:85:SER:HB2	16:4:88:VAL:HG23	1.95	0.47
16:4:192:TYR:HD1	22:4:805:CLA:O1D	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:5:311:CLA:O2D	22:5:311:CLA:HBA2	2.15	0.47
1:A:200:HIS:HB3	22:A:813:CLA:CAB	2.44	0.47
1:A:204:GLY:HA3	22:A:813:CLA:CBB	2.45	0.47
22:A:809:CLA:HAB	24:J:104:BCR:H383	1.97	0.47
22:A:829:CLA:HHC	22:A:829:CLA:CBB	2.45	0.47
2:B:27:ALA:C	2:B:29:ALA:H	2.22	0.47
2:B:31:ASP:HB2	22:B:831:CLA:HAA1	1.97	0.47
2:B:92:ILE:HG23	22:B:812:CLA:CAD	2.45	0.47
2:B:218:PRO:HD2	22:B:817:CLA:CAD	2.45	0.47
2:B:262:PHE:HZ	2:B:356:LEU:HD23	1.79	0.47
2:B:384:MET:HE1	24:B:848:BCR:H361	1.95	0.47
2:B:429:PHE:HA	22:F:302:CLA:O1D	2.15	0.47
22:B:808:CLA:HBB1	22:B:808:CLA:CMB	2.44	0.47
22:B:809:CLA:HMA2	22:B:831:CLA:C3B	2.44	0.47
22:B:811:CLA:H11	22:B:829:CLA:O1A	2.13	0.47
22:B:813:CLA:HBA1	22:B:814:CLA:H11	1.97	0.47
22:B:841:CLA:H91	22:B:841:CLA:H111	1.68	0.47
3:C:14:CYS:HB2	3:C:16:GLN:HG2	1.97	0.47
5:E:71:VAL:CG2	5:E:90:LEU:HD23	2.44	0.47
6:F:79:ARG:O	6:F:83:GLU:HB2	2.14	0.47
7:G:78:PHE:CD1	19:9:58:ALA:HB3	2.49	0.47
33:G:204:LMT:H91	22:1:308:CLA:HMD2	1.97	0.47
8:I:75:ALA:O	8:I:79:PHE:HD1	1.98	0.47
11:L:86:VAL:O	11:L:90:ARG:HG3	2.14	0.47
12:Z:83:LEU:HD11	22:Z:303:CLA:HAC1	1.94	0.47
12:Z:166:ASP:O	12:Z:170:LEU:HD13	2.14	0.47
39:7:313:CHL:HMC	22:7:316:CLA:HAB	1.95	0.47
22:7:323:CLA:H18	22:7:324:CLA:HMC2	1.95	0.47
15:8:72:HIS:HB3	15:8:196:MET:SD	2.55	0.47
16:4:210:LEU:C	22:4:805:CLA:HMA1	2.39	0.47
22:4:815:CLA:HBB1	22:4:815:CLA:CMB	2.44	0.47
22:5:311:CLA:C1B	22:5:318:CLA:H191	2.45	0.47
39:5:317:CHL:CHB	22:5:319:CLA:H71	2.44	0.47
18:6:125:GLU:HG2	22:6:317:CLA:CHB	2.45	0.47
22:9:311:CLA:NC	25:9:315:LHG:H271	2.30	0.47
22:A:809:CLA:CAB	24:J:104:BCR:H24C	2.45	0.47
22:A:827:CLA:C3B	22:A:835:CLA:HMA3	2.45	0.47
22:A:830:CLA:HMD1	25:A:850:LHG:H291	1.97	0.47
2:B:301:ARG:HG3	7:G:65:ALA:HA	1.97	0.47
2:B:395:TRP:NE1	24:B:848:BCR:H272	2.29	0.47
7:G:58:ARG:NH2	7:G:96:GLY:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:186:LYS:HD3	22:3:314:CLA:O1D	2.15	0.47
14:7:131:PHE:HB3	22:7:315:CLA:HAB	1.96	0.47
14:7:132:HIS:CD2	22:7:315:CLA:HMB3	2.50	0.47
15:8:80:VAL:HG13	15:8:202:PHE:CE2	2.46	0.47
38:8:303:LUT:C28	22:8:308:CLA:H72	2.45	0.47
22:8:305:CLA:H71	22:8:306:CLA:CMA	2.44	0.47
16:4:81:PHE:HB3	22:4:808:CLA:CAD	2.44	0.47
16:4:140:TYR:CD2	22:4:810:CLA:HED1	2.49	0.47
22:5:301:CLA:H61	22:5:301:CLA:H2	1.68	0.47
38:5:302:LUT:H183	22:5:309:CLA:C3B	2.45	0.47
24:5:304:BCR:H17C	22:5:319:CLA:H2	1.97	0.47
18:6:61:PRO:O	18:6:65:LYS:HG3	2.15	0.47
18:6:84:GLY:O	18:6:88:GLN:HG3	2.15	0.47
18:6:160:ALA:HA	22:6:307:CLA:HBA2	1.97	0.47
1:A:262:ALA:HB3	1:A:263:PRO:HD3	1.97	0.47
22:A:804:CLA:HAA1	22:A:811:CLA:H2	1.97	0.47
22:A:821:CLA:H72	24:A:846:BCR:C36	2.44	0.47
22:A:833:CLA:C1D	22:A:834:CLA:H121	2.45	0.47
2:B:54:GLN:HG2	22:B:808:CLA:HMA1	1.97	0.47
2:B:219:HIS:CG	2:B:220:PRO:HD2	2.50	0.47
2:B:705:GLN:HG3	31:B:852:DGD:C5A	2.45	0.47
22:B:813:CLA:H42	22:9:307:CLA:H72	1.96	0.47
22:B:823:CLA:HED2	22:B:823:CLA:H2A	1.97	0.47
22:B:828:CLA:H143	22:B:828:CLA:H111	1.75	0.47
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.96	0.47
22:F:302:CLA:H162	32:F:306:RRX:H6	1.95	0.47
22:G:201:CLA:HHB	24:G:203:BCR:H363	1.96	0.47
15:8:97:VAL:HG13	22:8:310:CLA:O1D	2.14	0.47
38:4:803:LUT:H24	22:4:808:CLA:O1A	2.15	0.47
22:5:318:CLA:HBB1	22:5:318:CLA:HMB1	1.96	0.47
18:6:69:GLU:HG3	18:6:132:PHE:CD1	2.50	0.47
18:6:248:CYS:O	18:6:249:LEU:C	2.57	0.47
22:6:301:CLA:C1	22:6:301:CLA:H92	2.45	0.47
22:6:309:CLA:H121	25:6:323:LHG:H122	1.97	0.47
19:9:49:PHE:HZ	19:9:160:LYS:HE2	1.80	0.47
19:9:87:GLN:HG2	22:9:308:CLA:C1D	2.45	0.47
22:9:306:CLA:HBB1	22:9:306:CLA:CMB	2.44	0.47
1:A:410:ALA:O	1:A:414:VAL:HG23	2.15	0.47
22:A:817:CLA:H62	22:A:817:CLA:H41	1.51	0.47
2:B:208:VAL:HG22	2:B:216:GLN:HG2	1.97	0.47
22:B:830:CLA:H72	24:B:846:BCR:H372	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:157:PHE:HZ	22:1:313:CLA:NB	2.13	0.47
12:Z:195:THR:HG22	12:Z:197:LYS:H	1.80	0.47
38:Z:301:LUT:H26	22:Z:303:CLA:C2	2.44	0.47
22:3:311:CLA:C6	22:3:312:CLA:HMA3	2.45	0.47
14:7:55:PRO:HG2	38:7:302:LUT:H23	1.97	0.47
42:7:321:SPH:H4	42:7:321:SPH:H71	1.72	0.47
15:8:50:PHE:HB3	22:8:308:CLA:CAD	2.45	0.47
15:8:124:PHE:CD1	39:8:301:CHL:H51	2.50	0.47
22:8:309:CLA:HBD	22:8:314:CLA:HBD	1.97	0.47
17:5:188:LYS:HD3	22:5:313:CLA:O1D	2.15	0.47
39:6:315:CHL:HAB	39:6:318:CHL:HBB2	1.96	0.47
19:9:62:ARG:HB3	19:9:66:PHE:CZ	2.50	0.47
19:9:117:LEU:HD23	20:2:215:CYS:SG	2.55	0.47
20:2:214:LEU:HB3	39:2:303:CHL:HBA1	1.97	0.47
22:2:302:CLA:HHC	22:2:302:CLA:HBB1	1.96	0.47
1:A:301:ILE:HD12	1:A:305:PHE:CE2	2.50	0.46
22:A:814:CLA:HBA1	24:A:844:BCR:H341	1.97	0.46
2:B:187:SER:O	22:B:816:CLA:HBB2	2.15	0.46
2:B:495:LEU:O	2:B:495:LEU:HD22	2.15	0.46
22:B:812:CLA:HBB1	22:B:812:CLA:CMB	2.45	0.46
22:B:823:CLA:CMB	33:1:301:LMT:H71	2.45	0.46
7:G:86:SER:HB3	19:9:36:ASN:HB2	1.97	0.46
10:K:35:ASN:HA	22:K:202:CLA:OBD	2.15	0.46
22:Z:307:CLA:CBC	22:Z:314:CLA:HAC1	2.45	0.46
13:3:146:LEU:HD11	22:5:315:CLA:C17	2.42	0.46
13:3:149:VAL:HG21	17:5:57:PRO:O	2.15	0.46
13:3:149:VAL:HG23	13:3:162:PRO:HD2	1.96	0.46
24:3:304:BCR:H312	22:3:322:CLA:C1D	2.44	0.46
22:3:316:CLA:CHA	22:3:316:CLA:HBA1	2.45	0.46
42:7:321:SPH:H5	42:7:321:SPH:H2	1.58	0.46
15:8:184:LEU:C	22:8:305:CLA:HMA1	2.40	0.46
16:4:198:ASP:HA	38:4:802:LUT:C24	2.31	0.46
38:4:802:LUT:H181	38:4:802:LUT:H8	1.97	0.46
24:4:804:BCR:H271	22:4:810:CLA:C4A	2.45	0.46
24:4:804:BCR:H271	22:4:810:CLA:NA	2.30	0.46
22:4:818:CLA:C2D	22:4:818:CLA:H42	2.45	0.46
18:6:164:PRO:O	18:6:170:LEU:HD21	2.15	0.46
22:6:307:CLA:H71	22:6:308:CLA:HMA2	1.97	0.46
22:6:314:CLA:NC	25:6:323:LHG:HC91	2.29	0.46
1:A:114:SER:CB	1:A:131:VAL:HG21	2.46	0.46
1:A:310:HIS:HB2	24:A:856:BCR:H19C	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TRP:HH2	22:A:812:CLA:HHB	1.80	0.46
1:A:528:LEU:HD11	22:A:837:CLA:CAD	2.46	0.46
22:A:807:CLA:HHC	22:A:807:CLA:CBB	2.46	0.46
3:C:7:ILE:HG13	3:C:40:ALA:O	2.15	0.46
3:C:25:VAL:HG13	3:C:45:THR:HA	1.97	0.46
11:L:129:ALA:CB	11:L:175:THR:HG22	2.45	0.46
12:Z:85:ALA:HB1	38:Z:301:LUT:H12	1.96	0.46
12:Z:195:THR:HG22	12:Z:197:LYS:HE2	1.96	0.46
13:3:228:ASN:HA	13:3:231:LYS:HG2	1.96	0.46
14:7:117:ASP:HB3	15:8:226:LYS:HD2	1.97	0.46
24:7:303:BCR:H271	22:7:309:CLA:C4A	2.44	0.46
22:8:307:CLA:H111	22:8:307:CLA:H152	1.66	0.46
22:5:313:CLA:HHC	22:5:313:CLA:CBB	2.46	0.46
18:6:167:MET:SD	18:6:171:LYS:HE3	2.55	0.46
1:A:366:ILE:HA	22:A:826:CLA:HED2	1.96	0.46
1:A:498:THR:HG21	22:A:835:CLA:HMD2	1.97	0.46
22:A:808:CLA:HAB	24:J:104:BCR:H352	1.98	0.46
2:B:196:VAL:HA	2:B:200:ILE:HD12	1.98	0.46
2:B:632:LEU:HD11	2:B:651:PHE:HB2	1.97	0.46
3:C:58:CYS:HA	29:C:102:SF4:S4	2.56	0.46
4:D:150:LEU:O	4:D:153:LYS:HE3	2.15	0.46
22:F:302:CLA:H61	32:F:306:RRX:H7	1.96	0.46
22:F:304:CLA:H72	22:F:304:CLA:C3D	2.44	0.46
10:K:38:MET:HB3	22:K:202:CLA:CAD	2.46	0.46
12:1:98:ASN:ND2	12:1:101:ASP:HB2	2.29	0.46
22:1:304:CLA:HMB2	22:1:305:CLA:HBA2	1.97	0.46
22:1:315:CLA:HBB1	22:1:315:CLA:HMB1	1.96	0.46
13:3:137:SER:HA	13:3:140:LYS:HZ1	1.78	0.46
13:3:177:MET:HE1	22:3:308:CLA:HAA2	1.96	0.46
38:7:301:LUT:H382	22:7:304:CLA:C4D	2.44	0.46
25:7:318:LHG:H111	25:7:318:LHG:HC81	1.41	0.46
22:7:322:CLA:C2	22:7:323:CLA:H101	2.45	0.46
15:8:157:LYS:HB2	15:8:157:LYS:HZ3	1.80	0.46
15:8:196:MET:HE3	22:8:308:CLA:HMC3	1.97	0.46
38:8:303:LUT:H162	22:8:310:CLA:HHB	1.96	0.46
16:4:237:LYS:HB3	16:4:241:GLN:OE1	2.15	0.46
17:5:131:TRP:HZ2	17:5:150:PRO:HG3	1.80	0.46
17:5:171:PRO:HD2	38:5:302:LUT:C24	2.45	0.46
17:5:248:PRO:O	39:5:316:CHL:H2	2.14	0.46
22:5:310:CLA:H92	22:5:310:CLA:H61	1.64	0.46
18:6:149:LEU:HD13	18:6:150:ALA:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:215:ILE:HG13	22:6:322:CLA:HBB2	1.97	0.46
39:9:312:CHL:HAA2	39:9:312:CHL:CBD	2.46	0.46
22:2:301:CLA:HHC	22:2:301:CLA:HBB1	1.97	0.46
1:A:80:GLN:O	1:A:84:ILE:HG13	2.16	0.46
1:A:91:MET:HE1	22:A:808:CLA:HMA2	1.97	0.46
1:A:175:PHE:CD2	22:A:810:CLA:HAC2	2.50	0.46
1:A:289:LEU:HD21	1:A:374:MET:HB3	1.97	0.46
22:A:827:CLA:C4B	22:A:835:CLA:HMA3	2.45	0.46
2:B:450:PRO:O	2:B:453:GLN:HG2	2.16	0.46
2:B:543:ARG:CB	2:B:552:LYS:HB3	2.39	0.46
2:B:601:THR:HG21	2:B:610:PHE:HB2	1.97	0.46
22:B:824:CLA:HHC	24:B:847:BCR:C10	2.45	0.46
22:B:842:CLA:HED2	24:B:847:BCR:H11C	1.97	0.46
7:G:98:THR:OG1	7:G:100:ILE:HG12	2.15	0.46
12:1:79:ARG:O	12:1:83:LEU:HG	2.15	0.46
12:Z:220:VAL:HG12	22:Z:316:CLA:H2A	1.97	0.46
13:3:65:ARG:HA	13:3:68:MET:HE3	1.96	0.46
22:3:313:CLA:H121	22:5:320:CLA:C1C	2.45	0.46
24:7:303:BCR:H291	42:7:321:SPH:H142	1.98	0.46
39:8:312:CHL:HHD	39:8:315:CHL:HBC2	1.96	0.46
18:6:141:ASP:HA	39:6:320:CHL:C1C	2.46	0.46
19:9:106:VAL:HG13	19:9:111:LEU:HD12	1.98	0.46
22:9:307:CLA:HMD3	22:9:313:CLA:C1D	2.46	0.46
1:A:150:ALA:HB2	1:A:378:PRO:CD	2.46	0.46
1:A:450:PHE:CD2	22:A:854:CLA:H12	2.51	0.46
1:A:493:LEU:HB3	1:A:496:GLN:NE2	2.30	0.46
22:A:803:CLA:H193	24:J:104:BCR:H17C	1.98	0.46
22:A:826:CLA:HBB1	22:A:826:CLA:CMB	2.44	0.46
22:A:830:CLA:HBB1	22:A:830:CLA:CMB	2.42	0.46
22:A:832:CLA:HBB1	22:A:832:CLA:CMB	2.45	0.46
2:B:256:LEU:HD11	22:B:817:CLA:HBC1	1.98	0.46
2:B:337:LEU:HD13	22:B:826:CLA:C3B	2.46	0.46
24:B:844:BCR:C36	24:G:203:BCR:H312	2.36	0.46
4:D:125:THR:HA	4:D:136:PRO:HG2	1.97	0.46
7:G:49:GLY:HA3	7:G:105:TRP:CE2	2.50	0.46
7:G:98:THR:O	7:G:102:THR:HG23	2.15	0.46
22:Z:307:CLA:OBD	22:Z:314:CLA:HAA1	2.15	0.46
39:Z:312:CHL:HMC	22:Z:315:CLA:HAB	1.97	0.46
22:3:308:CLA:CMD	39:3:317:CHL:HBA2	2.45	0.46
22:8:307:CLA:H18	22:8:311:CLA:HAC2	1.98	0.46
39:8:312:CHL:ND	26:8:318:NKP:HAL	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:230:ALA:CB	22:4:807:CLA:HAC2	2.46	0.46
22:5:307:CLA:CHB	22:5:307:CLA:H2	2.46	0.46
22:6:301:CLA:H41	22:6:301:CLA:H61	1.75	0.46
38:6:303:LUT:H35	38:6:303:LUT:H401	1.73	0.46
38:6:303:LUT:H30	22:6:307:CLA:H52	1.96	0.46
39:6:315:CHL:HBC3	39:6:318:CHL:CBC	2.45	0.46
22:6:322:CLA:HBC2	41:6:324:3PH:H281	1.98	0.46
22:2:301:CLA:HHC	22:2:301:CLA:CBB	2.46	0.46
1:A:119:TRP:HE3	22:A:809:CLA:H2A	1.81	0.46
1:A:526:ILE:CG2	1:A:613:LYS:HE3	2.46	0.46
1:A:694:GLN:O	1:A:698:GLU:HG3	2.14	0.46
22:A:812:CLA:H142	22:A:812:CLA:HMB2	1.97	0.46
22:A:826:CLA:HMA1	24:A:847:BCR:H15C	1.98	0.46
2:B:263:HIS:CE1	2:B:265:GLN:HB3	2.48	0.46
2:B:692:VAL:HG13	11:L:135:TYR:CE1	2.50	0.46
22:B:841:CLA:H161	24:L:204:BCR:H15C	1.97	0.46
4:D:125:THR:O	4:D:129:ARG:HG3	2.16	0.46
10:K:66:LYS:O	10:K:68:VAL:HG23	2.16	0.46
12:1:153:PRO:HD2	22:1:304:CLA:OBD	2.16	0.46
12:Z:182:MET:HE3	22:Z:306:CLA:CMC	2.45	0.46
38:3:303:LUT:H42	44:3:402:HOH:O	2.16	0.46
15:8:151:GLY:O	15:8:152:PHE:HB2	2.16	0.46
16:4:231:GLN:HB3	16:4:242:ASN:OD1	2.16	0.46
22:4:806:CLA:H12	22:4:806:CLA:H52	1.66	0.46
17:5:61:GLY:HA3	22:5:310:CLA:HBA1	1.96	0.46
17:5:164:TYR:CE1	17:5:183:GLN:HG2	2.50	0.46
22:5:315:CLA:H2	22:5:315:CLA:H61	1.55	0.46
18:6:66:TRP:NE1	22:6:311:CLA:H11	2.30	0.46
18:6:164:PRO:CG	22:6:308:CLA:H12	2.45	0.46
22:6:308:CLA:ND	22:6:313:CLA:H72	2.30	0.46
22:A:806:CLA:HBB2	24:A:845:BCR:HC31	1.96	0.46
22:A:821:CLA:H43	22:A:824:CLA:H12	1.98	0.46
22:A:825:CLA:H122	22:A:825:CLA:H8	1.65	0.46
22:A:828:CLA:H191	24:J:104:BCR:C19	2.45	0.46
2:B:190:ALA:CB	22:B:816:CLA:HAB	2.44	0.46
22:B:822:CLA:HBA2	22:B:822:CLA:H12	1.73	0.46
9:J:4:PHE:O	9:J:8:LEU:HG	2.16	0.46
14:7:53:PHE:HB3	22:7:307:CLA:C3D	2.45	0.46
14:7:218:PRO:C	14:7:220:GLN:H	2.24	0.46
39:7:313:CHL:HMC	22:7:316:CLA:CAB	2.46	0.46
39:4:813:CHL:HHC	39:4:816:CHL:HAB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:815:CLA:H2A	22:4:815:CLA:CED	2.43	0.46
18:6:173:LYS:HG3	22:6:313:CLA:HED2	1.97	0.46
22:6:314:CLA:H11	22:6:314:CLA:H51	1.75	0.46
22:2:302:CLA:HHC	22:2:302:CLA:CBB	2.46	0.46
1:A:87:TRP:HA	22:A:807:CLA:HBB2	1.97	0.46
1:A:178:TRP:HB2	22:A:811:CLA:HMC2	1.97	0.46
1:A:687:PHE:HB2	22:B:801:CLA:HBC2	1.97	0.46
22:A:805:CLA:H202	22:A:805:CLA:H161	1.71	0.46
22:A:839:CLA:H11	24:A:847:BCR:H15C	1.98	0.46
27:A:852:DGA:HAW1	27:A:852:DGA:HAN2	1.57	0.46
2:B:87:PRO:HB3	2:B:122:TYR:CG	2.51	0.46
2:B:296:PHE:HE2	22:B:822:CLA:HBD	1.79	0.46
2:B:358:PRO:HG3	22:B:820:CLA:HBA1	1.98	0.46
2:B:401:PRO:HD2	4:D:180:ASN:ND2	2.30	0.46
2:B:540:LEU:HD21	24:B:847:BCR:H282	1.97	0.46
22:B:812:CLA:H8	22:B:812:CLA:H51	1.27	0.46
4:D:131:LYS:HE3	4:D:132:PHE:CZ	2.51	0.46
22:F:304:CLA:HMC1	33:F:307:LMT:H121	1.98	0.46
7:G:33:GLU:CD	7:G:33:GLU:H	2.23	0.46
7:G:99:LEU:HD21	19:9:32:LEU:HD21	1.98	0.46
10:K:107:LEU:CD2	22:K:203:CLA:HBB1	2.45	0.46
22:Z:304:CLA:C4D	22:Z:309:CLA:H62	2.45	0.46
31:3:301:DGD:O2G	31:3:301:DGD:HD1	2.16	0.46
17:5:73:SER:OG	22:5:311:CLA:HAA2	2.15	0.46
17:5:105:GLU:OE1	17:5:240:VAL:HG21	2.16	0.46
17:5:153:LYS:HA	17:5:153:LYS:HD3	1.69	0.46
18:6:250:PHE:H	22:6:301:CLA:C4	2.27	0.46
18:6:250:PHE:N	22:6:301:CLA:H43	2.28	0.46
1:A:200:HIS:CD2	22:A:813:CLA:HAB	2.50	0.46
1:A:263:PRO:HB2	1:A:272:TYR:CZ	2.50	0.46
1:A:695:GLU:HA	1:A:698:GLU:CD	2.41	0.46
24:A:844:BCR:H15C	24:A:844:BCR:H351	1.39	0.46
22:B:808:CLA:H43	24:B:845:BCR:H24C	1.97	0.46
22:B:810:CLA:CAA	8:I:80:VAL:HG22	2.46	0.46
22:B:816:CLA:C6	24:B:846:BCR:H362	2.46	0.46
22:B:817:CLA:C4B	24:B:844:BCR:H271	2.46	0.46
24:B:847:BCR:H15C	24:B:847:BCR:H351	1.75	0.46
6:F:218:LYS:HE2	6:F:218:LYS:HB2	1.63	0.46
7:G:92:ASN:HB3	22:G:202:CLA:OBD	2.16	0.46
12:1:61:CYS:SG	12:1:67:LEU:HA	2.56	0.46
12:1:82:MET:HE3	22:1:304:CLA:HMC3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:308:CLA:CMD	22:1:314:CLA:ND	2.79	0.46
25:Z:317:LHG:H121	25:Z:317:LHG:HC91	1.78	0.46
22:3:313:CLA:HBB1	22:3:313:CLA:CMB	2.44	0.46
22:7:308:CLA:HBB1	22:7:308:CLA:CMB	2.45	0.46
42:7:320:SPH:H11	42:7:320:SPH:H4	1.55	0.46
16:4:128:PRO:HD2	22:4:818:CLA:HMA1	1.98	0.46
16:4:163:ARG:NE	39:4:819:CHL:OMC	2.49	0.46
17:5:57:PRO:HB2	17:5:58:LEU:HD12	1.97	0.46
22:5:326:CLA:HBA1	22:5:326:CLA:CBD	2.45	0.46
24:6:306:BCR:H19C	39:6:315:CHL:H2	1.98	0.46
22:6:311:CLA:HED3	22:6:317:CLA:CGA	2.46	0.46
19:9:51:PHE:HE1	22:9:311:CLA:HBC3	1.80	0.46
38:9:302:LUT:C16	22:9:308:CLA:HMA1	2.46	0.46
20:2:163:LEU:C	20:2:165:MET:H	2.24	0.46
1:A:12:LYS:HE3	1:A:12:LYS:HB3	1.70	0.46
22:A:814:CLA:H121	22:A:816:CLA:CBB	2.44	0.46
22:A:823:CLA:H172	24:A:856:BCR:H403	1.98	0.46
2:B:172:ALA:O	2:B:173:GLU:C	2.59	0.46
2:B:653:PHE:HD1	22:B:806:CLA:H71	1.81	0.46
22:B:809:CLA:H71	22:B:809:CLA:H111	1.52	0.46
24:B:853:BCR:H372	24:I:4001:BCR:H403	1.98	0.46
10:K:98:ILE:HG12	24:K:206:BCR:H311	1.98	0.46
22:K:202:CLA:HBB1	22:K:202:CLA:CMB	2.45	0.46
22:1:306:CLA:C4B	22:1:306:CLA:H72	2.46	0.46
22:Z:307:CLA:HBC1	22:Z:314:CLA:HAC1	1.98	0.46
22:Z:308:CLA:HMA3	22:Z:315:CLA:C1C	2.45	0.46
39:Z:311:CHL:C1C	25:Z:317:LHG:H102	2.46	0.46
13:3:182:LEU:HA	13:3:185:ILE:HG22	1.98	0.46
24:3:307:BCR:C19	22:3:310:CLA:H91	2.46	0.46
16:4:119:LEU:O	16:4:123:VAL:HG23	2.16	0.46
24:5:305:BCR:H343	18:6:220:VAL:HG21	1.97	0.46
22:5:315:CLA:HHC	22:5:315:CLA:HBB1	1.97	0.46
39:5:316:CHL:H152	22:6:322:CLA:HAA1	1.97	0.46
18:6:96:PHE:HZ	18:6:192:ALA:HB1	1.81	0.46
18:6:249:LEU:O	18:6:250:PHE:C	2.58	0.46
22:6:309:CLA:HBC2	22:6:319:CLA:HBD	1.98	0.46
22:6:311:CLA:HBB1	22:6:311:CLA:CMB	2.46	0.46
39:6:315:CHL:HBC3	39:6:318:CHL:HBC3	1.97	0.46
19:9:142:PHE:HB3	19:9:143:PRO:CD	2.40	0.46
1:A:572:ARG:HH21	25:A:850:LHG:HC31	1.82	0.45
1:A:676:HIS:HB3	22:A:802:CLA:HBD	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:802:CLA:H202	22:A:830:CLA:H192	1.97	0.45
22:A:817:CLA:H122	22:A:817:CLA:H8	1.64	0.45
2:B:470:LYS:HG2	2:B:473:TYR:HE2	1.80	0.45
25:B:803:LHG:HC32	25:B:803:LHG:H262	1.98	0.45
22:B:821:CLA:H93	22:B:821:CLA:H111	1.63	0.45
5:E:53:TYR:C	5:E:55:GLN:H	2.25	0.45
6:F:199:GLY:O	6:F:202:TRP:HD1	1.99	0.45
22:F:304:CLA:H172	22:F:304:CLA:HAA1	1.98	0.45
8:I:95:LEU:CD1	24:L:204:BCR:HC8	2.46	0.45
12:Z:190:ALA:CB	22:Z:316:CLA:H61	2.41	0.45
22:3:308:CLA:HMD3	39:3:317:CHL:HBA2	1.98	0.45
22:7:324:CLA:H102	22:4:817:CLA:C4B	2.45	0.45
15:8:202:PHE:HD1	38:8:302:LUT:H41	1.81	0.45
16:4:66:LYS:CD	25:4:821:LHG:HC31	2.44	0.45
17:5:151:ILE:HD12	39:5:321:CHL:CMB	2.46	0.45
24:5:305:BCR:H351	39:5:316:CHL:HAC1	1.97	0.45
22:6:319:CLA:HHC	22:6:319:CLA:CBB	2.45	0.45
19:9:59:ASP:OD1	19:9:62:ARG:HB2	2.16	0.45
19:9:119:MET:HE3	39:9:314:CHL:HHB	1.98	0.45
20:2:163:LEU:HB3	20:2:165:MET:HG2	1.99	0.45
1:A:578:PRO:HD3	2:B:562:GLY:HA2	1.97	0.45
22:A:842:CLA:HMB1	24:A:846:BCR:C12	2.44	0.45
27:A:852:DGA:HA61	14:7:242:PRO:HB2	1.97	0.45
2:B:423:LEU:HD11	22:B:839:CLA:HMB1	1.98	0.45
22:B:808:CLA:H18	22:B:815:CLA:HMD3	1.97	0.45
22:B:824:CLA:HMB2	22:B:842:CLA:ND	2.31	0.45
22:B:829:CLA:ND	22:B:829:CLA:H8	2.31	0.45
22:B:836:CLA:O2A	31:1:319:DGD:HA72	2.16	0.45
22:B:842:CLA:HHC	12:1:70:PHE:HZ	1.81	0.45
9:J:2:LYS:HE3	9:J:2:LYS:HB3	1.59	0.45
12:1:37:PRO:HG2	39:8:301:CHL:CMD	2.46	0.45
24:3:307:BCR:H11C	24:3:307:BCR:H341	1.67	0.45
22:3:322:CLA:H92	22:7:306:CLA:H72	1.99	0.45
15:8:201:GLY:O	15:8:205:GLN:HG2	2.16	0.45
18:6:126:LEU:CD1	22:6:302:CLA:HBA1	2.42	0.45
18:6:219:ALA:CB	18:6:229:PRO:HD3	2.47	0.45
20:2:223:ALA:HB3	20:2:226:SER:OG	2.16	0.45
1:A:516:ALA:HB2	1:A:622:VAL:HG21	1.98	0.45
22:A:812:CLA:C1C	22:A:812:CLA:H51	2.46	0.45
22:A:815:CLA:HBB1	22:A:815:CLA:CMB	2.45	0.45
2:B:226:PHE:HA	2:B:231:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:LEU:HG	2:B:352:HIS:CE1	2.52	0.45
4:D:127:GLN:HG3	4:D:131:LYS:HE2	1.98	0.45
4:D:129:ARG:O	4:D:133:LYS:HA	2.16	0.45
4:D:141:VAL:HG22	4:D:147:VAL:HG22	1.98	0.45
22:G:202:CLA:HBB1	22:G:202:CLA:HMB3	1.98	0.45
13:3:192:MET:SD	22:3:311:CLA:HAB	2.57	0.45
24:3:307:BCR:H401	22:3:314:CLA:CHD	2.47	0.45
22:7:322:CLA:HBB1	22:7:322:CLA:CMB	2.44	0.45
22:8:310:CLA:H62	22:8:310:CLA:H2	1.72	0.45
17:5:118:MET:HB3	24:5:305:BCR:H12C	1.98	0.45
17:5:131:TRP:HZ3	24:5:304:BCR:HC41	1.81	0.45
39:5:316:CHL:H13	22:6:322:CLA:HBD	1.98	0.45
39:6:315:CHL:HBD	39:6:315:CHL:HAA1	1.97	0.45
22:9:311:CLA:CGA	25:9:315:LHG:HC62	2.47	0.45
1:A:265:PHE:HA	22:K:202:CLA:HAC2	1.99	0.45
1:A:700:ILE:HG23	22:A:840:CLA:O1D	2.16	0.45
22:A:802:CLA:H51	2:B:439:VAL:HG13	1.98	0.45
22:A:833:CLA:H13	22:B:840:CLA:HBA1	1.98	0.45
22:A:834:CLA:HBC3	22:A:854:CLA:H13	1.97	0.45
2:B:293:ARG:HD2	2:B:301:ARG:HD3	1.98	0.45
2:B:321:LYS:HD2	2:B:322:GLY:N	2.31	0.45
25:B:803:LHG:H111	22:B:807:CLA:C1D	2.46	0.45
22:B:816:CLA:H61	22:B:816:CLA:H2	1.52	0.45
22:B:825:CLA:H13	24:B:847:BCR:H17C	1.99	0.45
22:B:827:CLA:CHB	22:B:839:CLA:HAA2	2.47	0.45
22:B:834:CLA:HBA2	22:B:834:CLA:CHA	2.43	0.45
3:C:10:THR:O	3:C:60:THR:HG21	2.17	0.45
6:F:125:CYS:HB3	6:F:131:PRO:HA	1.99	0.45
10:K:60:GLY:O	10:K:67:LEU:HG	2.16	0.45
22:Z:306:CLA:HBC1	25:Z:317:LHG:H292	1.98	0.45
22:7:322:CLA:H72	22:7:323:CLA:H171	1.99	0.45
22:8:305:CLA:HBB1	22:8:306:CLA:HAA1	1.98	0.45
22:8:311:CLA:C2B	25:8:317:LHG:HC2	2.46	0.45
1:A:101:TYR:O	1:A:105:LEU:HG	2.16	0.45
1:A:113:PRO:O	1:A:139:GLN:HA	2.17	0.45
1:A:248:GLN:H	1:A:248:GLN:NE2	2.14	0.45
1:A:442:ASN:HD22	2:B:675:LEU:HD11	1.82	0.45
22:A:810:CLA:H121	22:A:812:CLA:HBC1	1.98	0.45
22:A:814:CLA:H92	27:A:852:DGA:HB81	1.99	0.45
22:A:815:CLA:C1B	24:A:856:BCR:HC42	2.47	0.45
22:A:829:CLA:H11	24:A:845:BCR:H321	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:THR:O	7:G:34:PRO:HG3	2.17	0.45
2:B:616:TYR:HD2	2:B:618:MET:HB3	1.81	0.45
22:B:806:CLA:C19	22:B:812:CLA:H52	2.46	0.45
6:F:151:ILE:HB	6:F:152:PRO:HD3	1.97	0.45
7:G:46:LEU:HB3	22:G:202:CLA:HMB3	1.98	0.45
11:L:134:ILE:HG13	24:L:204:BCR:H363	1.97	0.45
12:1:72:GLU:O	12:1:76:ILE:HG12	2.17	0.45
12:1:112:PRO:HB3	22:1:315:CLA:HMD1	1.97	0.45
12:1:138:GLU:HG3	22:1:314:CLA:C4B	2.47	0.45
38:Z:302:LUT:C28	22:Z:306:CLA:H61	2.47	0.45
13:3:191:ALA:O	13:3:195:VAL:HG23	2.17	0.45
24:4:804:BCR:H393	22:4:810:CLA:CHC	2.47	0.45
25:4:820:LHG:HC61	22:6:302:CLA:HAC2	1.99	0.45
18:6:66:TRP:HZ2	22:6:317:CLA:HAA2	1.80	0.45
18:6:101:PRO:HG3	39:6:318:CHL:OMC	2.16	0.45
19:9:57:GLY:HA3	19:9:63:LEU:HD13	1.98	0.45
38:9:302:LUT:C37	22:9:306:CLA:H112	2.47	0.45
20:2:197:ASN:CB	22:2:301:CLA:HBA2	2.47	0.45
20:2:216:VAL:O	20:2:220:ILE:HG13	2.16	0.45
1:A:49:ILE:HD12	1:A:49:ILE:N	2.32	0.45
1:A:403:VAL:HG11	1:A:596:LEU:CD2	2.46	0.45
22:A:822:CLA:H71	22:K:204:CLA:CAB	2.45	0.45
23:A:843:PQN:H262	23:A:843:PQN:H302	1.63	0.45
2:B:647:TRP:CZ2	2:B:727:ILE:HG21	2.52	0.45
22:B:818:CLA:H112	22:B:818:CLA:H93	1.69	0.45
4:D:117:ARG:HB3	4:D:120:GLN:HG3	1.99	0.45
6:F:163:ILE:HG23	22:F:305:CLA:C1D	2.47	0.45
7:G:78:PHE:CE1	19:9:58:ALA:HB3	2.52	0.45
11:L:129:ALA:HB2	11:L:175:THR:HG22	1.97	0.45
12:Z:147:ALA:HA	12:Z:150:ARG:CD	2.47	0.45
22:3:313:CLA:H111	22:3:313:CLA:H152	1.68	0.45
14:7:118:TRP:CZ3	14:7:123:LEU:HA	2.52	0.45
15:8:78:THR:HG23	22:8:305:CLA:HMC1	1.97	0.45
22:8:307:CLA:NC	22:8:307:CLA:H51	2.32	0.45
17:5:60:LEU:HD12	38:5:303:LUT:H221	1.99	0.45
17:5:104:GLY:HA2	22:5:319:CLA:HAC2	1.98	0.45
18:6:127:LYS:O	18:6:138:VAL:HG21	2.16	0.45
22:6:302:CLA:C4D	24:6:305:BCR:HC41	2.47	0.45
19:9:94:PRO:HB2	19:9:99:ALA:HA	1.98	0.45
1:A:175:PHE:CE2	22:A:810:CLA:HAC2	2.52	0.45
21:A:801:CL0:H72	21:A:801:CL0:H10	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ARG:NH2	2:B:115:ASN:HA	2.32	0.45
2:B:227:TRP:CH2	22:B:817:CLA:H52	2.50	0.45
2:B:243:HIS:CD2	2:B:251:ALA:HA	2.52	0.45
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.97	0.45
22:B:810:CLA:C1D	22:B:810:CLA:H51	2.46	0.45
22:B:824:CLA:NC	33:1:301:LMT:H101	2.32	0.45
22:B:825:CLA:H2	22:B:825:CLA:H61	1.76	0.45
22:B:825:CLA:O1A	24:B:847:BCR:H16C	2.16	0.45
22:B:835:CLA:CMB	24:B:848:BCR:H332	2.47	0.45
22:F:301:CLA:H152	9:J:18:TRP:CE3	2.46	0.45
13:3:164:PHE:HB3	22:3:308:CLA:OBD	2.16	0.45
41:7:319:3PH:H362	41:7:319:3PH:H231	1.98	0.45
15:8:101:TYR:CD1	15:8:102:GLU:HG3	2.52	0.45
16:4:156:LEU:O	24:4:804:BCR:H14C	2.17	0.45
22:4:805:CLA:H61	22:4:805:CLA:H92	1.74	0.45
17:5:60:LEU:HD11	22:5:315:CLA:C14	2.47	0.45
22:5:301:CLA:HBA1	22:5:320:CLA:HED3	1.97	0.45
38:5:303:LUT:H183	22:5:312:CLA:C3B	2.47	0.45
22:5:310:CLA:HMB2	22:5:310:CLA:H51	1.99	0.45
18:6:97:TRP:HH2	18:6:189:THR:HG22	1.80	0.45
24:6:305:BCR:C27	22:6:312:CLA:H101	2.46	0.45
24:6:306:BCR:H11C	24:6:306:BCR:H341	1.80	0.45
19:9:65:TRP:HZ2	22:9:313:CLA:HAA1	1.81	0.45
19:9:106:VAL:HG22	19:9:111:LEU:HB2	1.98	0.45
19:9:120:GLY:CA	22:9:313:CLA:HAB	2.44	0.45
1:A:114:SER:HB3	1:A:131:VAL:HG21	1.99	0.45
1:A:222:LEU:N	1:A:223:PRO:HD2	2.32	0.45
1:A:571:PHE:HD2	22:A:830:CLA:HED1	1.82	0.45
22:A:829:CLA:H61	24:A:845:BCR:H342	1.97	0.45
22:A:841:CLA:HHC	22:A:841:CLA:CBB	2.47	0.45
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.99	0.45
2:B:262:PHE:HE1	2:B:356:LEU:HA	1.82	0.45
22:B:821:CLA:H172	22:B:826:CLA:H203	1.99	0.45
22:B:825:CLA:H141	22:B:832:CLA:CBC	2.47	0.45
22:B:829:CLA:O1D	22:B:830:CLA:HHB	2.16	0.45
3:C:74:THR:HG23	3:C:79:LEU:HB2	1.98	0.45
5:E:39:ARG:HE	5:E:62:VAL:N	2.15	0.45
6:F:158:TYR:HA	6:F:202:TRP:HZ2	1.82	0.45
9:J:24:ALA:O	9:J:28:GLU:HG2	2.17	0.45
12:1:134:MET:HE2	22:1:314:CLA:HMC2	1.98	0.45
22:Z:306:CLA:H3A	22:Z:306:CLA:HBA2	1.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:157:ALA:O	13:3:159:PRO:HD3	2.17	0.45
14:7:122:THR:O	14:7:126:THR:HG23	2.17	0.45
15:8:50:PHE:CZ	41:8:320:3PH:H391	2.52	0.45
15:8:83:ILE:HG23	15:8:100:TRP:HB3	1.99	0.45
16:4:204:LYS:H	16:4:204:LYS:HG2	1.66	0.45
17:5:46:ASN:HB2	17:5:48:GLU:OE1	2.17	0.45
17:5:83:LEU:HG	22:5:307:CLA:HMC3	1.97	0.45
22:5:307:CLA:H3A	22:5:307:CLA:HBA2	1.35	0.45
22:5:311:CLA:OBD	22:5:318:CLA:H12	2.17	0.45
22:9:313:CLA:CHA	22:9:313:CLA:HBA2	2.45	0.45
22:2:301:CLA:HBC1	22:2:304:CLA:HMD1	1.99	0.45
1:A:80:GLN:HE21	1:A:84:ILE:HG13	1.82	0.45
22:A:821:CLA:H101	24:A:847:BCR:C10	2.40	0.45
2:B:475:PHE:HB3	22:F:304:CLA:C19	2.44	0.45
2:B:548:MET:HG2	2:B:565:ARG:NH2	2.32	0.45
2:B:561:ASP:HB3	2:B:568:THR:HG21	1.99	0.45
2:B:681:TRP:CZ2	4:D:71:THR:HB	2.52	0.45
5:E:42:GLN:HA	5:E:57:GLY:O	2.16	0.45
14:7:53:PHE:HZ	41:7:319:3PH:H282	1.82	0.45
15:8:115:LEU:HD21	39:8:312:CHL:CHD	2.47	0.45
15:8:139:LYS:HB3	15:8:139:LYS:HE2	1.71	0.45
17:5:169:PHE:HD1	39:5:317:CHL:O1A	1.98	0.45
22:5:308:CLA:C1C	22:5:313:CLA:H143	2.47	0.45
22:6:322:CLA:H2	22:6:322:CLA:H121	1.99	0.45
1:A:85:PHE:HE1	24:A:844:BCR:HC21	1.82	0.45
2:B:293:ARG:HH22	7:G:61:LEU:HB3	1.81	0.45
22:B:838:CLA:H152	32:F:306:RRX:H37	1.98	0.45
6:F:162:TRP:CD1	6:F:162:TRP:C	2.94	0.45
7:G:80:SER:O	7:G:83:GLN:HB3	2.17	0.45
22:G:201:CLA:HAB	24:G:203:BCR:H352	1.98	0.45
8:I:87:LEU:C	8:I:87:LEU:HD13	2.42	0.45
10:K:68:VAL:O	10:K:68:VAL:HG12	2.16	0.45
12:Z:147:ALA:HA	12:Z:150:ARG:HD2	1.99	0.45
38:Z:301:LUT:H15	38:Z:301:LUT:H201	1.79	0.45
24:3:304:BCR:H341	24:3:304:BCR:H11C	1.34	0.45
14:7:58:LEU:HD11	22:7:308:CLA:H92	1.99	0.45
15:8:113:ILE:HG22	15:8:118:LEU:HB2	1.99	0.45
16:4:140:TYR:HD2	16:4:142:TYR:CE1	2.35	0.45
24:4:804:BCR:C37	39:4:816:CHL:HHB	2.44	0.45
17:5:69:TRP:CG	22:5:323:CLA:HAA1	2.52	0.45
22:5:311:CLA:CMD	22:6:322:CLA:H92	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:5:326:CLA:C1	22:6:314:CLA:H152	2.46	0.45
19:9:133:THR:C	19:9:135:SER:H	2.25	0.45
39:9:312:CHL:H2A	39:9:312:CHL:C2	2.47	0.45
1:A:172:ALA:HA	22:3:312:CLA:H18	1.99	0.44
1:A:442:ASN:ND2	2:B:675:LEU:HD11	2.33	0.44
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.99	0.44
1:A:536:HIS:HA	1:A:539:HIS:CD2	2.52	0.44
22:A:807:CLA:HAB	24:J:104:BCR:C7	2.47	0.44
22:A:820:CLA:H62	22:A:820:CLA:H2	1.41	0.44
22:A:840:CLA:HBB2	6:F:167:GLY:HA3	1.99	0.44
27:A:852:DGA:HA22	27:A:852:DGA:HA51	1.65	0.44
2:B:181:SER:HB3	2:B:289:GLY:HA3	2.00	0.44
22:B:801:CLA:H122	22:B:801:CLA:H161	1.67	0.44
22:B:811:CLA:C3D	22:B:829:CLA:HBA1	2.47	0.44
22:B:842:CLA:C4B	22:1:308:CLA:H51	2.47	0.44
22:B:842:CLA:HBC1	33:1:301:LMT:O6'	2.16	0.44
6:F:224:ILE:HB	6:F:227:ARG:NH2	2.30	0.44
7:G:94:PRO:O	7:G:95:ALA:HB3	2.17	0.44
11:L:128:LEU:HB3	24:L:204:BCR:H401	1.99	0.44
12:1:144:GLU:CB	22:1:313:CLA:HAC1	2.47	0.44
12:Z:145:THR:CA	12:Z:150:ARG:HH21	2.22	0.44
38:3:303:LUT:H32	22:3:311:CLA:CAB	2.47	0.44
22:7:308:CLA:HMD3	22:7:315:CLA:ND	2.32	0.44
38:4:803:LUT:H32	22:4:808:CLA:HAB	1.99	0.44
22:4:805:CLA:HMD1	39:4:814:CHL:O1A	2.16	0.44
17:5:131:TRP:CZ3	22:6:314:CLA:HBA2	2.52	0.44
41:5:325:3PH:H221	41:5:325:3PH:H2	1.51	0.44
19:9:64:LYS:HD2	19:9:64:LYS:C	2.42	0.44
19:9:145:ASP:N	19:9:146:PRO:HD2	2.27	0.44
19:9:187:LEU:HD13	38:9:301:LUT:H163	1.99	0.44
1:A:53:HIS:CD2	22:A:804:CLA:HAC1	2.52	0.44
1:A:658:ILE:HD12	2:B:622:ARG:HG3	2.00	0.44
22:A:804:CLA:C4A	22:A:811:CLA:H71	2.48	0.44
22:A:816:CLA:O1A	27:A:852:DGA:HG12	2.16	0.44
22:A:817:CLA:C4D	22:A:817:CLA:H12	2.47	0.44
22:A:830:CLA:H151	22:A:841:CLA:CMA	2.48	0.44
22:A:832:CLA:H101	22:L:202:CLA:H11	2.00	0.44
22:A:836:CLA:H61	22:K:203:CLA:CBA	2.39	0.44
2:B:32:PHE:HA	2:B:35:HIS:CG	2.52	0.44
2:B:548:MET:HE1	2:B:554:PHE:CD1	2.52	0.44
2:B:622:ARG:HA	2:B:626:TRP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:811:CLA:H202	22:B:811:CLA:H162	1.64	0.44
22:B:819:CLA:H111	22:B:819:CLA:H71	1.25	0.44
22:B:824:CLA:H91	22:B:824:CLA:H111	1.75	0.44
22:B:826:CLA:HMA1	22:B:826:CLA:H92	1.99	0.44
22:B:827:CLA:HBB1	22:B:827:CLA:CMB	2.47	0.44
6:F:186:ILE:HA	9:J:10:THR:HA	1.97	0.44
12:1:57:PRO:CD	38:1:303:LUT:H23	2.45	0.44
12:1:211:TRP:HZ3	15:8:118:LEU:HA	1.81	0.44
12:Z:68:LYS:HD2	12:Z:147:ALA:CB	2.44	0.44
13:3:36:PHE:HB3	22:3:311:CLA:HMD3	1.98	0.44
22:3:309:CLA:HMC2	22:3:314:CLA:H143	1.98	0.44
22:3:312:CLA:HBD	22:3:318:CLA:HBD	1.99	0.44
14:7:157:THR:O	14:7:161:LYS:HD3	2.17	0.44
14:7:198:ARG:HA	14:7:201:MET:CE	2.47	0.44
22:7:306:CLA:HBB1	22:7:306:CLA:HMB3	1.98	0.44
22:7:310:CLA:H122	22:7:310:CLA:C17	2.46	0.44
15:8:50:PHE:HB3	22:8:308:CLA:C3D	2.48	0.44
15:8:205:GLN:HG3	38:8:302:LUT:H42	1.99	0.44
22:4:809:CLA:HBA1	22:4:809:CLA:H11	1.62	0.44
25:4:821:LHG:H142	22:6:321:CLA:CHD	2.47	0.44
25:5:324:LHG:H111	25:5:324:LHG:HC82	1.50	0.44
22:A:809:CLA:HBA1	24:J:104:BCR:H363	1.99	0.44
22:A:833:CLA:H41	22:A:855:CLA:HBC2	1.99	0.44
24:A:844:BCR:C20	24:A:845:BCR:H23C	2.47	0.44
24:A:844:BCR:H21C	24:A:845:BCR:H271	1.99	0.44
27:A:852:DGA:HG11	14:7:243:PHE:HB3	1.99	0.44
2:B:135:ASP:HB3	22:B:816:CLA:HED1	1.99	0.44
2:B:292:TYR:CD1	2:B:302:MET:HG2	2.52	0.44
2:B:649:TRP:CZ2	22:B:806:CLA:H72	2.52	0.44
22:B:823:CLA:NA	22:B:824:CLA:H92	2.32	0.44
22:B:839:CLA:H61	22:B:839:CLA:H2	1.67	0.44
33:G:204:LMT:H62	33:G:204:LMT:H91	1.79	0.44
12:Z:193:ALA:HB3	22:Z:316:CLA:HED1	1.99	0.44
22:Z:303:CLA:H62	22:Z:304:CLA:CMA	2.47	0.44
22:Z:309:CLA:HBB2	24:4:804:BCR:H323	1.99	0.44
13:3:71:ALA:CB	38:3:302:LUT:H12	2.47	0.44
13:3:146:LEU:O	13:3:149:VAL:N	2.46	0.44
24:3:307:BCR:H342	22:3:315:CLA:HAA1	1.98	0.44
39:3:317:CHL:H61	39:3:317:CHL:H101	1.65	0.44
14:7:141:ASP:HB2	14:7:148:GLN:HG2	1.98	0.44
22:7:310:CLA:HBC1	25:7:318:LHG:H281	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:51:ASP:OD2	22:8:308:CLA:HBA1	2.18	0.44
22:8:310:CLA:H72	22:8:310:CLA:H112	1.31	0.44
16:4:83:PRO:HD2	38:4:803:LUT:C23	2.42	0.44
16:4:193:PRO:HB2	16:4:197:PHE:HB2	2.00	0.44
22:4:805:CLA:HBA2	22:4:805:CLA:H3A	1.29	0.44
39:4:813:CHL:CAB	39:4:816:CHL:HBB2	2.41	0.44
17:5:230:ASN:HA	17:5:233:HIS:HE2	1.82	0.44
38:5:303:LUT:H15	38:5:303:LUT:H201	1.85	0.44
19:9:31:TRP:NE1	19:9:51:PHE:HA	2.32	0.44
1:A:212:SER:HA	22:A:815:CLA:HBB2	1.98	0.44
1:A:269:TRP:HB3	22:A:817:CLA:HHB	1.98	0.44
1:A:369:HIS:HA	1:A:372:TYR:CD2	2.53	0.44
1:A:412:PHE:CD1	1:A:416:ASP:HB2	2.53	0.44
22:A:821:CLA:NC	22:A:827:CLA:H161	2.32	0.44
2:B:52:PHE:HD1	2:B:150:PHE:HD1	1.64	0.44
2:B:287:VAL:HB	22:B:818:CLA:H202	1.98	0.44
25:B:803:LHG:H262	22:B:807:CLA:HAA2	2.00	0.44
22:B:831:CLA:HBB1	22:B:831:CLA:CMB	2.45	0.44
22:B:835:CLA:HBA2	22:B:835:CLA:H3A	1.25	0.44
24:B:848:BCR:C8	24:B:848:BCR:H321	2.47	0.44
5:E:70:PRO:HD2	5:E:89:ALA:HA	1.97	0.44
10:K:62:ASP:HB2	10:K:68:VAL:HG21	1.99	0.44
12:Z:160:LEU:HB2	38:Z:301:LUT:H222	1.99	0.44
13:3:127:ARG:HD3	39:3:317:CHL:CBB	2.47	0.44
15:8:105:LYS:NZ	15:8:105:LYS:HB3	2.32	0.44
15:8:152:PHE:O	15:8:153:GLU:C	2.60	0.44
22:4:818:CLA:HBA1	22:4:818:CLA:C2	2.45	0.44
17:5:100:TRP:HD1	38:5:303:LUT:H41	1.82	0.44
17:5:245:LEU:HD22	18:6:220:VAL:HG11	1.99	0.44
22:5:307:CLA:H43	22:5:308:CLA:H2	1.99	0.44
18:6:57:LEU:CD1	38:6:304:LUT:H221	2.47	0.44
1:A:367:VAL:HG12	1:A:371:MET:HE2	1.98	0.44
1:A:454:GLY:C	1:A:456:TYR:H	2.25	0.44
22:A:815:CLA:H143	13:3:196:PHE:HA	1.98	0.44
27:A:852:DGA:HA22	27:A:852:DGA:HG12	1.72	0.44
2:B:373:TYR:CE2	2:B:377:GLN:HG3	2.52	0.44
2:B:667:SER:C	2:B:668:TRP:HD1	2.26	0.44
22:L:203:CLA:HBB1	22:L:203:CLA:CMB	2.47	0.44
22:1:308:CLA:C1C	22:1:314:CLA:H18	2.48	0.44
39:1:312:CHL:CAA	31:1:319:DGD:HG31	2.42	0.44
25:1:317:LHG:C10	24:8:304:BCR:H313	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:79:ARG:O	12:Z:83:LEU:HG	2.17	0.44
12:Z:190:ALA:CB	22:Z:305:CLA:HAC2	2.47	0.44
15:8:114:ALA:HB3	15:8:117:PRO:HD2	2.00	0.44
15:8:126:CYS:HB2	22:8:314:CLA:HAB	1.99	0.44
22:8:306:CLA:CMD	22:8:311:CLA:C4D	2.96	0.44
38:5:302:LUT:H401	38:5:302:LUT:H35	1.77	0.44
18:6:253:LEU:HA	41:6:324:3PH:H292	1.98	0.44
38:9:302:LUT:H28	22:9:306:CLA:C5	2.40	0.44
22:9:306:CLA:H111	22:9:306:CLA:H72	1.27	0.44
20:2:182:PRO:HG2	20:2:183:ILE:H	1.81	0.44
1:A:71:ARG:HD3	1:A:185:ALA:HB1	1.99	0.44
22:A:812:CLA:H91	22:A:812:CLA:H111	1.71	0.44
22:A:814:CLA:H41	22:A:814:CLA:H61	1.65	0.44
22:A:832:CLA:H13	22:A:832:CLA:H91	2.00	0.44
24:A:844:BCR:C21	24:A:845:BCR:H291	2.47	0.44
2:B:423:LEU:HB3	2:B:533:LEU:HD13	1.98	0.44
2:B:429:PHE:CE2	22:B:838:CLA:HAB	2.52	0.44
2:B:473:TYR:HB3	2:B:475:PHE:CE2	2.53	0.44
22:B:818:CLA:H72	22:B:818:CLA:H122	1.99	0.44
22:B:818:CLA:HBA2	22:B:818:CLA:H3A	1.53	0.44
3:C:49:VAL:HG11	4:D:117:ARG:HH21	1.82	0.44
4:D:115:PHE:HB3	4:D:120:GLN:NE2	2.29	0.44
22:F:304:CLA:H92	22:F:304:CLA:H61	1.57	0.44
22:G:201:CLA:C1C	24:G:203:BCR:H10C	2.48	0.44
10:K:107:LEU:HD22	10:K:112:ASN:CB	2.47	0.44
22:Z:307:CLA:H12	22:Z:307:CLA:H51	1.70	0.44
24:3:307:BCR:C39	22:3:314:CLA:HAC2	2.46	0.44
22:7:309:CLA:C2	22:7:309:CLA:H72	2.44	0.44
22:7:310:CLA:CBC	25:7:318:LHG:H281	2.48	0.44
22:8:311:CLA:C4A	33:4:801:LMT:H62	2.47	0.44
16:4:113:GLY:O	38:4:803:LUT:H42	2.17	0.44
16:4:121:ARG:NH2	16:4:133:PRO:HA	2.28	0.44
16:4:164:ARG:HH12	22:4:815:CLA:CED	2.31	0.44
22:5:307:CLA:HMB2	22:5:308:CLA:HBA2	2.00	0.44
22:5:310:CLA:H51	22:5:310:CLA:C2B	2.48	0.44
22:6:309:CLA:HBC1	22:6:319:CLA:CAA	2.46	0.44
22:6:312:CLA:H52	22:6:312:CLA:C2D	2.48	0.44
19:9:102:LYS:HD2	22:9:308:CLA:HED1	2.00	0.44
1:A:511:GLY:HA2	1:A:525:PRO:HB3	1.99	0.44
1:A:606:ALA:HB2	22:A:837:CLA:HBB2	1.99	0.44
21:A:801:CL0:CAC	2:B:626:TRP:HD1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:812:CLA:C4	13:3:41:LEU:HD21	2.48	0.44
22:B:840:CLA:C2	22:B:841:CLA:H143	2.47	0.44
24:B:844:BCR:H341	24:B:844:BCR:H11C	1.52	0.44
3:C:28:MET:CE	3:C:38:GLN:HB3	2.48	0.44
22:F:302:CLA:H62	22:F:302:CLA:H2	1.48	0.44
22:F:304:CLA:H111	22:F:304:CLA:H152	1.71	0.44
13:3:203:VAL:HG11	31:3:301:DGD:C7A	2.48	0.44
14:7:187:LYS:HD3	14:7:190:LYS:HD3	1.98	0.44
22:7:309:CLA:C3C	42:7:321:SPH:H162	2.48	0.44
41:7:319:3PH:H372	41:7:319:3PH:H3A1	1.41	0.44
22:8:309:CLA:H93	22:8:309:CLA:H111	1.71	0.44
18:6:235:GLN:NE2	22:6:301:CLA:HHB	2.32	0.44
41:6:324:3PH:H221	41:6:324:3PH:H251	1.52	0.44
1:A:399:GLY:HA3	1:A:603:LEU:HD21	2.00	0.44
22:A:807:CLA:H2	22:A:807:CLA:H61	1.62	0.44
2:B:178:HIS:CE1	22:B:822:CLA:HMD3	2.53	0.44
2:B:183:LEU:CD1	22:B:815:CLA:H43	2.47	0.44
2:B:695:LYS:HE2	11:L:141:GLN:NE2	2.32	0.44
22:B:821:CLA:O1A	22:B:826:CLA:H142	2.17	0.44
22:B:830:CLA:H193	24:B:846:BCR:H17C	1.99	0.44
22:L:201:CLA:HBA2	22:L:201:CLA:HBD	1.99	0.44
22:L:202:CLA:CBC	24:L:204:BCR:H23C	2.48	0.44
12:1:209:ASN:ND2	12:1:212:GLY:HA3	2.33	0.44
38:1:303:LUT:H11	38:1:303:LUT:H191	1.88	0.44
38:1:303:LUT:H382	22:1:307:CLA:O2A	2.17	0.44
12:Z:149:LYS:CB	22:Z:313:CLA:HBC1	2.40	0.44
12:Z:177:ASN:HD22	12:Z:177:ASN:H	1.65	0.44
13:3:149:VAL:HG21	13:3:163:TRP:HB2	2.00	0.44
14:7:135:GLU:HG3	22:7:315:CLA:C4B	2.48	0.44
38:7:301:LUT:C14	22:7:305:CLA:HAB	2.48	0.44
15:8:115:LEU:HD22	15:8:115:LEU:HA	1.74	0.44
15:8:141:GLY:HA2	15:8:157:LYS:O	2.18	0.44
39:8:315:CHL:H61	39:8:315:CHL:H111	1.98	0.44
38:4:803:LUT:H28	22:4:808:CLA:H72	2.00	0.44
22:4:807:CLA:H152	22:4:807:CLA:H111	1.67	0.44
17:5:155:ASN:HB3	39:5:321:CHL:C2D	2.47	0.44
17:5:179:ARG:O	17:5:183:GLN:HG3	2.17	0.44
39:6:320:CHL:HHC	39:6:320:CHL:CBB	2.46	0.44
1:A:453:PHE:CE1	22:B:806:CLA:HMA1	2.52	0.44
2:B:258:PHE:CD1	2:B:494:TRP:HB3	2.53	0.44
22:B:808:CLA:H122	22:B:808:CLA:HBD	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:817:CLA:H3A	22:B:817:CLA:HBA2	1.21	0.44
6:F:222:ILE:O	6:F:222:ILE:HD12	2.18	0.44
38:1:302:LUT:C30	22:1:304:CLA:H8	2.47	0.44
12:Z:114:TRP:HB2	22:Z:308:CLA:CGA	2.47	0.44
38:Z:302:LUT:H8	22:Z:308:CLA:HBB1	2.00	0.44
13:3:42:LEU:HD12	13:3:53:PRO:HA	2.00	0.44
13:3:81:GLY:HA3	13:3:88:ASP:HA	2.00	0.44
13:3:146:LEU:O	13:3:147:GLU:C	2.61	0.44
22:3:313:CLA:H112	22:5:320:CLA:ND	2.33	0.44
22:7:305:CLA:HAC2	22:7:306:CLA:H191	2.00	0.44
39:4:816:CHL:HAC2	39:4:816:CHL:OMC	2.18	0.44
17:5:179:ARG:HG2	17:5:183:GLN:HG3	2.00	0.44
24:5:304:BCR:HC32	22:6:314:CLA:C1D	2.48	0.44
19:9:57:GLY:N	22:9:306:CLA:O1A	2.51	0.44
20:2:173:SER:HB2	20:2:176:ALA:C	2.43	0.44
1:A:316:TRP:CZ3	22:A:820:CLA:HBD	2.52	0.43
1:A:693:TRP:HZ3	22:B:801:CLA:O1D	2.01	0.43
22:A:818:CLA:H62	22:A:818:CLA:NC	2.32	0.43
22:A:823:CLA:HBA2	37:K:201:DAO:H81	2.00	0.43
2:B:231:TRP:HB2	22:B:818:CLA:O1A	2.18	0.43
2:B:320:HIS:HA	2:B:323:LEU:HD12	2.00	0.43
2:B:351:GLN:HG3	22:B:827:CLA:CED	2.44	0.43
2:B:388:PHE:CZ	24:B:848:BCR:H20C	2.53	0.43
2:B:449:THR:HB	2:B:452:LYS:HG3	1.99	0.43
2:B:471:ALA:O	2:B:472:PHE:C	2.60	0.43
2:B:616:TYR:CD2	2:B:618:MET:HB3	2.52	0.43
22:B:817:CLA:NC	24:B:844:BCR:H291	2.33	0.43
22:B:825:CLA:HBB1	22:B:825:CLA:CMB	2.48	0.43
22:B:827:CLA:C2B	22:B:839:CLA:HMA3	2.48	0.43
22:B:829:CLA:H92	22:B:829:CLA:H62	1.55	0.43
22:B:833:CLA:HBB1	22:B:833:CLA:CMB	2.48	0.43
22:B:834:CLA:C2	24:F:303:BCR:HC42	2.47	0.43
7:G:50:ARG:HG2	22:G:202:CLA:C3B	2.48	0.43
11:L:96:LEU:O	11:L:99:PRO:HD2	2.18	0.43
12:Z:179:ARG:HA	12:Z:182:MET:CE	2.48	0.43
39:Z:311:CHL:HBC3	39:Z:311:CHL:CHD	2.44	0.43
13:3:21:SER:HA	13:3:24:GLN:CD	2.43	0.43
13:3:115:PHE:O	13:3:119:ILE:HG12	2.18	0.43
22:3:311:CLA:HBB1	22:3:311:CLA:CMB	2.47	0.43
16:4:259:ASP:HA	16:4:262:ARG:HD3	1.99	0.43
22:5:315:CLA:HHC	22:5:315:CLA:CBB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:302:CLA:HHC	22:6:302:CLA:CBB	2.48	0.43
1:A:32:PRO:HB2	1:A:48:TRP:CH2	2.53	0.43
1:A:127:LEU:HD22	1:A:667:ALA:HB2	2.00	0.43
1:A:227:LEU:HD12	1:A:237:ILE:HG23	2.00	0.43
1:A:338:HIS:CE1	25:A:849:LHG:HC12	2.36	0.43
1:A:392:THR:HG23	1:A:607:ILE:HG21	2.00	0.43
22:A:817:CLA:H61	22:A:817:CLA:C4C	2.48	0.43
22:A:821:CLA:H11	22:A:827:CLA:H122	2.00	0.43
23:A:843:PQN:H142	24:F:303:BCR:H291	2.00	0.43
2:B:5:LEU:HB3	2:B:8:LYS:HE3	2.00	0.43
2:B:520:VAL:O	2:B:524:ILE:HG13	2.18	0.43
22:B:821:CLA:HMB2	22:B:826:CLA:HMA3	1.99	0.43
22:B:831:CLA:HMD2	31:B:852:DGD:HB62	2.00	0.43
22:B:833:CLA:H18	22:B:833:CLA:H152	1.74	0.43
9:J:1:MET:N	34:J:101:LMG:HC71	2.32	0.43
12:1:57:PRO:HD2	38:1:303:LUT:C23	2.46	0.43
22:Z:316:CLA:C2	22:Z:316:CLA:H71	2.42	0.43
13:3:103:TYR:CE2	13:3:105:LYS:HB2	2.53	0.43
14:7:70:HIS:CE1	14:7:138:ARG:HH11	2.35	0.43
22:7:308:CLA:HMA3	22:7:308:CLA:H43	2.00	0.43
38:4:803:LUT:H28	22:4:808:CLA:H52	2.00	0.43
24:5:304:BCR:HC42	25:6:323:LHG:HC81	2.00	0.43
22:5:318:CLA:H12	22:5:318:CLA:H51	1.80	0.43
22:5:322:CLA:HED1	25:6:323:LHG:H301	2.00	0.43
22:6:312:CLA:HMA3	39:6:318:CHL:HAC2	1.99	0.43
39:6:316:CHL:HBD	39:6:316:CHL:HAA1	2.00	0.43
19:9:35:LEU:HG	19:9:36:ASN:N	2.32	0.43
19:9:129:GLY:HA3	19:9:142:PHE:CE1	2.53	0.43
20:2:186:LEU:HD23	20:2:186:LEU:C	2.42	0.43
1:A:521:VAL:HG21	1:A:627:VAL:HG11	1.99	0.43
1:A:550:LEU:CB	24:A:847:BCR:H322	2.48	0.43
22:A:835:CLA:H51	22:A:835:CLA:H12	1.76	0.43
2:B:16:ASP:HB3	2:B:21:ARG:HB3	1.98	0.43
22:B:812:CLA:NB	24:B:849:BCR:H322	2.34	0.43
22:B:817:CLA:H51	22:B:817:CLA:H11	1.76	0.43
22:B:821:CLA:HAA2	22:B:825:CLA:OBD	2.17	0.43
22:B:825:CLA:H111	24:B:847:BCR:C16	2.49	0.43
22:B:838:CLA:HHC	22:B:838:CLA:H102	2.01	0.43
3:C:66:ARG:HD3	3:C:66:ARG:HA	1.84	0.43
12:1:55:PHE:HZ	40:1:318:SQD:H271	1.83	0.43
12:1:69:ARG:NH2	22:1:308:CLA:O1D	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:82:MET:SD	22:Z:303:CLA:HAB	2.58	0.43
38:Z:301:LUT:H362	22:Z:313:CLA:H42	1.99	0.43
22:7:324:CLA:H143	22:4:817:CLA:ND	2.32	0.43
15:8:74:ARG:HA	15:8:77:MET:HE3	1.99	0.43
15:8:121:VAL:O	15:8:125:MET:HG3	2.18	0.43
24:8:304:BCR:H19C	39:8:315:CHL:CGA	2.49	0.43
22:8:316:CLA:CBB	22:8:316:CLA:HHC	2.48	0.43
22:8:316:CLA:HHC	22:8:316:CLA:HBB1	2.00	0.43
17:5:230:ASN:HA	17:5:233:HIS:CE1	2.53	0.43
22:5:308:CLA:H151	22:5:308:CLA:CMB	2.48	0.43
22:5:318:CLA:HBC2	22:5:319:CLA:HMB1	2.00	0.43
18:6:215:ILE:O	18:6:218:LYS:HG2	2.18	0.43
18:6:240:GLN:HB2	24:6:306:BCR:H313	1.99	0.43
24:6:305:BCR:H20C	22:6:312:CLA:H203	1.99	0.43
19:9:30:THR:HB	19:9:35:LEU:HB3	2.00	0.43
1:A:412:PHE:HD1	1:A:416:ASP:HB2	1.83	0.43
1:A:675:ALA:HB1	1:A:734:GLY:O	2.18	0.43
22:A:823:CLA:H191	10:K:98:ILE:CD1	2.46	0.43
22:A:828:CLA:C9	24:J:104:BCR:H341	2.48	0.43
22:B:820:CLA:CMB	22:B:820:CLA:CBB	2.96	0.43
22:B:823:CLA:NB	22:B:824:CLA:H8	2.33	0.43
3:C:14:CYS:SG	29:C:102:SF4:S4	3.17	0.43
4:D:160:LYS:HB3	4:D:160:LYS:HE2	1.78	0.43
5:E:78:GLN:CB	5:E:84:THR:HG22	2.38	0.43
6:F:137:PRO:HG2	22:F:304:CLA:C2C	2.49	0.43
33:G:204:LMT:H111	22:1:314:CLA:HMC3	2.00	0.43
12:1:143:ASP:O	12:1:145:THR:HG23	2.18	0.43
38:1:302:LUT:H35	38:1:302:LUT:H401	1.84	0.43
13:3:142:TYR:HA	13:3:147:GLU:CD	2.44	0.43
39:3:317:CHL:HAA1	39:3:317:CHL:HBD	1.99	0.43
38:7:301:LUT:H35	38:7:301:LUT:H401	1.83	0.43
15:8:228:THR:HA	22:8:307:CLA:CBA	2.48	0.43
22:8:308:CLA:C17	22:8:308:CLA:H122	2.48	0.43
16:4:101:LEU:HD12	16:4:101:LEU:HA	1.82	0.43
17:5:135:ARG:HB3	39:5:317:CHL:CMC	2.48	0.43
17:5:178:ASN:ND2	17:5:181:GLU:HB2	2.32	0.43
38:5:303:LUT:H31	38:5:303:LUT:H391	1.91	0.43
22:5:318:CLA:H2	22:5:323:CLA:HAC1	1.99	0.43
18:6:235:GLN:HG2	18:6:245:PHE:CE1	2.53	0.43
24:6:305:BCR:H16C	39:6:316:CHL:CMB	2.42	0.43
22:6:309:CLA:H203	22:6:309:CLA:H152	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:9:305:CLA:H92	22:9:305:CLA:H61	1.68	0.43
1:A:26:PHE:H	34:J:101:LMG:HC5	1.83	0.43
22:A:804:CLA:HED1	22:A:811:CLA:HED2	2.00	0.43
22:A:807:CLA:ND	26:A:851:NKP:HARA	2.33	0.43
22:A:810:CLA:HAA1	13:3:51:VAL:HG21	2.01	0.43
22:A:814:CLA:HBB1	22:A:814:CLA:CMB	2.46	0.43
22:A:814:CLA:H61	27:A:852:DGA:HB62	1.99	0.43
22:A:841:CLA:CAB	22:B:801:CLA:H162	2.48	0.43
22:A:842:CLA:H62	22:A:842:CLA:H2	1.65	0.43
2:B:32:PHE:C	2:B:34:SER:N	2.76	0.43
2:B:258:PHE:HE1	22:B:819:CLA:H52	1.83	0.43
25:B:803:LHG:H122	22:B:807:CLA:ND	2.32	0.43
22:B:807:CLA:HAB	22:B:809:CLA:CAD	2.48	0.43
22:B:817:CLA:H111	24:B:844:BCR:H23C	2.01	0.43
22:B:835:CLA:HMB3	24:B:848:BCR:H332	1.99	0.43
4:D:191:THR:O	4:D:194:ILE:HG22	2.19	0.43
12:Z:164:LYS:HB2	12:Z:164:LYS:NZ	2.34	0.43
14:7:80:MET:SD	22:7:304:CLA:HAB	2.58	0.43
15:8:82:GLY:O	15:8:86:PRO:HG2	2.19	0.43
16:4:193:PRO:HD2	22:4:805:CLA:OBD	2.18	0.43
17:5:131:TRP:HB2	22:6:314:CLA:H2	2.00	0.43
22:5:309:CLA:H12	22:5:309:CLA:C1A	2.49	0.43
22:6:312:CLA:C4D	22:6:312:CLA:H52	2.48	0.43
39:6:315:CHL:HBB2	39:6:318:CHL:HBB2	2.00	0.43
39:6:315:CHL:HBB2	22:6:317:CLA:HBC1	2.00	0.43
19:9:194:PRO:HB3	22:9:310:CLA:HMB2	2.00	0.43
1:A:161:THR:HG21	22:A:816:CLA:HAA2	2.00	0.43
1:A:343:GLU:H	1:A:343:GLU:CD	2.26	0.43
1:A:487:ILE:HG21	22:A:837:CLA:HED1	2.01	0.43
1:A:674:GLY:HA2	24:A:848:BCR:H17C	2.00	0.43
22:A:833:CLA:H102	22:B:840:CLA:C5	2.48	0.43
2:B:48:PHE:HB2	2:B:169:PHE:CE1	2.54	0.43
2:B:262:PHE:CZ	2:B:356:LEU:HA	2.54	0.43
2:B:687:PRO:HG2	22:L:202:CLA:C5	2.45	0.43
22:B:831:CLA:CHA	22:B:831:CLA:HBA1	2.42	0.43
22:B:832:CLA:HAA1	22:B:842:CLA:H41	2.00	0.43
22:B:838:CLA:H122	32:F:306:RRX:H38	2.00	0.43
4:D:56:PRO:HD2	4:D:149:TYR:CZ	2.54	0.43
5:E:39:ARG:HG3	5:E:61:SER:HA	1.98	0.43
5:E:86:ASN:HB3	5:E:88:PHE:CE2	2.53	0.43
22:F:304:CLA:OBD	22:F:304:CLA:H122	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:J:101:LMG:HC8	14:7:57:GLY:HA3	2.00	0.43
12:1:100:TYR:O	12:1:103:PRO:HD2	2.17	0.43
22:1:307:CLA:C1B	22:1:307:CLA:H2	2.49	0.43
14:7:205:LEU:HD21	22:7:307:CLA:H171	2.00	0.43
22:7:323:CLA:HED2	15:8:31:MET:HG2	2.00	0.43
41:8:320:3PH:H3A1	41:8:320:3PH:H3D1	1.45	0.43
16:4:196:ILE:HD12	16:4:196:ILE:HA	1.80	0.43
24:4:804:BCR:H281	22:4:810:CLA:NB	2.33	0.43
17:5:242:VAL:HG21	39:5:316:CHL:HMD3	1.99	0.43
22:5:308:CLA:H72	22:5:308:CLA:H112	1.68	0.43
22:5:323:CLA:O1A	22:5:323:CLA:H2A	2.19	0.43
18:6:88:GLN:HG2	22:6:312:CLA:C3D	2.48	0.43
1:A:119:TRP:CE3	22:A:809:CLA:H2A	2.53	0.43
1:A:651:TRP:HD1	22:B:805:CLA:CAC	2.31	0.43
1:A:673:LEU:HD12	22:A:802:CLA:H42	1.99	0.43
22:A:834:CLA:H92	22:A:834:CLA:H61	1.71	0.43
2:B:38:MET:O	4:D:186:PHE:HD1	2.02	0.43
2:B:590:TRP:CG	22:B:805:CLA:H152	2.53	0.43
22:B:833:CLA:C1B	32:F:306:RRX:H26	2.48	0.43
22:B:838:CLA:HMA2	22:B:839:CLA:HED2	2.01	0.43
33:G:204:LMT:H111	22:1:314:CLA:CMC	2.47	0.43
9:J:1:MET:N	34:J:101:LMG:HC2	2.29	0.43
12:1:173:LYS:HG3	22:1:310:CLA:HED2	2.00	0.43
22:1:304:CLA:HBB1	22:1:304:CLA:CMB	2.47	0.43
22:1:308:CLA:HMD3	22:1:314:CLA:ND	2.34	0.43
12:Z:144:GLU:CG	22:Z:313:CLA:HAC1	2.49	0.43
12:Z:144:GLU:CD	12:Z:146:ASP:H	2.27	0.43
12:Z:195:THR:HG23	12:Z:197:LYS:HE2	2.01	0.43
38:Z:301:LUT:H35	38:Z:301:LUT:H401	1.81	0.43
22:Z:306:CLA:C1B	22:Z:306:CLA:H2	2.49	0.43
13:3:52:THR:HG23	13:3:55:TRP:H	1.84	0.43
14:7:204:ASN:CG	38:7:302:LUT:H12	2.44	0.43
38:7:302:LUT:C28	22:7:307:CLA:H61	2.44	0.43
24:4:804:BCR:H343	39:4:819:CHL:HAB	2.01	0.43
22:4:805:CLA:H71	22:4:806:CLA:CMA	2.49	0.43
24:5:304:BCR:HC7	39:5:321:CHL:HBB2	2.01	0.43
22:5:318:CLA:H2	22:5:323:CLA:CAC	2.49	0.43
38:9:302:LUT:H35	38:9:302:LUT:H401	1.81	0.43
21:A:801:CL0:H22	2:B:626:TRP:CD1	2.54	0.43
22:A:816:CLA:H92	27:A:852:DGA:HB61	2.01	0.43
22:A:821:CLA:H111	22:A:821:CLA:H152	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:826:CLA:O1A	22:A:839:CLA:HAA2	2.19	0.43
22:A:832:CLA:C11	22:L:202:CLA:H171	2.47	0.43
2:B:126:TYR:O	2:B:131:ARG:NH1	2.51	0.43
2:B:431:GLY:HA3	22:B:801:CLA:H11	2.00	0.43
22:B:815:CLA:H142	22:B:815:CLA:H112	1.80	0.43
22:B:815:CLA:H151	22:B:820:CLA:C4D	2.48	0.43
22:B:824:CLA:HBC2	22:B:825:CLA:CBA	2.48	0.43
22:F:304:CLA:CBB	32:F:306:RRX:H51	2.45	0.43
7:G:45:MET:HG3	7:G:109:GLY:CA	2.47	0.43
12:Z:35:TRP:HD1	39:Z:311:CHL:C1B	2.32	0.43
12:Z:160:LEU:HB3	12:Z:162:PHE:CZ	2.54	0.43
12:Z:166:ASP:OD1	12:Z:169:THR:OG1	2.28	0.43
31:3:301:DGD:HE5	31:3:301:DGD:O4D	2.18	0.43
24:3:304:BCR:H23C	24:3:305:BCR:H353	2.01	0.43
24:3:305:BCR:C16	39:3:317:CHL:H112	2.48	0.43
14:7:59:SER:HB2	14:7:65:MET:HG2	2.01	0.43
14:7:135:GLU:HG3	22:7:315:CLA:C1B	2.48	0.43
22:7:308:CLA:H92	22:7:308:CLA:H62	1.71	0.43
15:8:37:PRO:O	15:8:38:ALA:HB2	2.19	0.43
22:8:307:CLA:O1D	22:8:307:CLA:H2A	2.19	0.43
16:4:70:HIS:CD2	16:4:71:LEU:HG	2.54	0.43
16:4:105:ARG:HB3	39:4:814:CHL:HED2	2.00	0.43
17:5:78:ALA:HB1	17:5:190:GLY:HA3	2.01	0.43
24:5:304:BCR:H381	22:5:319:CLA:NC	2.34	0.43
22:5:310:CLA:H152	22:5:311:CLA:HBB1	2.00	0.43
18:6:167:MET:O	18:6:171:LYS:HG3	2.19	0.43
18:6:173:LYS:NZ	22:6:308:CLA:H43	2.34	0.43
19:9:32:LEU:O	19:9:35:LEU:HB2	2.18	0.43
20:2:177:VAL:O	20:2:178:ARG:HG3	2.19	0.43
1:A:521:VAL:HG11	1:A:524:MET:HB2	2.00	0.43
22:A:819:CLA:H151	22:A:819:CLA:H18	1.74	0.43
22:A:821:CLA:O2A	22:A:824:CLA:HBA2	2.19	0.43
2:B:669:ARG:NE	2:B:700:ALA:HB3	2.34	0.43
22:B:805:CLA:H51	22:B:805:CLA:H8	1.64	0.43
22:B:814:CLA:H2	22:B:814:CLA:ND	2.33	0.43
22:B:827:CLA:HBA1	22:B:827:CLA:H12	1.73	0.43
5:E:53:TYR:C	5:E:55:GLN:N	2.77	0.43
6:F:201:THR:O	6:F:205:GLN:HG3	2.19	0.43
12:1:56:ASP:HA	38:1:303:LUT:H24	2.00	0.43
22:1:316:CLA:H141	39:8:301:CHL:H111	2.00	0.43
38:3:303:LUT:H15	38:3:303:LUT:H201	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:4:808:CLA:H62	22:4:808:CLA:H41	1.58	0.43
17:5:58:LEU:HD12	17:5:58:LEU:N	2.34	0.43
22:5:309:CLA:C1	22:5:314:CLA:HMD2	2.49	0.43
38:6:303:LUT:C28	22:6:307:CLA:H52	2.49	0.43
19:9:119:MET:HE3	39:9:314:CHL:HMB3	2.01	0.43
22:2:301:CLA:HBA1	22:2:301:CLA:H11	1.61	0.43
1:A:494:ALA:HB1	1:A:498:THR:OG1	2.18	0.43
1:A:726:VAL:HG22	22:A:841:CLA:O1D	2.19	0.43
22:A:822:CLA:HAA2	10:K:61:THR:CG2	2.47	0.43
22:A:832:CLA:H112	22:L:202:CLA:H152	2.00	0.43
2:B:482:SER:C	2:B:484:SER:H	2.27	0.43
2:B:652:LEU:O	22:B:806:CLA:HBA1	2.19	0.43
22:B:809:CLA:CBC	22:B:811:CLA:H193	2.49	0.43
22:B:819:CLA:H93	22:B:835:CLA:HBA1	2.00	0.43
24:B:848:BCR:H321	24:B:848:BCR:HC8	2.00	0.43
3:C:79:LEU:HD22	3:C:81:TYR:CE2	2.54	0.43
6:F:70:CYS:HA	6:F:73:SER:HB3	2.01	0.43
22:G:202:CLA:CHC	24:G:203:BCR:H402	2.49	0.43
8:I:74:TRP:CZ2	22:2:304:CLA:HHB	2.54	0.43
38:Z:301:LUT:H371	22:Z:303:CLA:H92	2.01	0.43
13:3:109:ASP:OD1	13:3:109:ASP:N	2.52	0.43
38:3:302:LUT:H30	22:3:308:CLA:H72	1.98	0.43
22:3:308:CLA:H3A	22:3:308:CLA:HBA2	1.17	0.43
22:3:312:CLA:H61	22:3:312:CLA:H2	1.73	0.43
22:3:312:CLA:H61	22:3:312:CLA:H92	1.76	0.43
22:3:322:CLA:HHC	22:3:322:CLA:HBB1	2.01	0.43
42:7:320:SPH:H91	42:7:320:SPH:H61	1.63	0.43
15:8:105:LYS:O	15:8:109:GLU:HG2	2.19	0.43
16:4:225:PHE:HA	16:4:228:PHE:HD2	1.83	0.43
22:4:805:CLA:H71	22:4:806:CLA:HMA2	2.00	0.43
22:4:806:CLA:HBA1	22:4:806:CLA:H61	2.01	0.43
17:5:94:LEU:O	17:5:96:PRO:HD3	2.18	0.43
17:5:227:TRP:N	22:5:309:CLA:O1A	2.52	0.43
18:6:121:MET:HE2	22:6:317:CLA:C2C	2.49	0.43
18:6:222:VAL:CG1	18:6:224:GLY:H	2.32	0.43
24:6:306:BCR:H19C	39:6:315:CHL:C2	2.49	0.43
24:6:306:BCR:C8	24:6:306:BCR:H311	2.48	0.43
1:A:694:GLN:NE2	5:E:80:TYR:HE1	2.16	0.42
22:A:819:CLA:H203	22:A:827:CLA:HAA1	2.00	0.42
22:A:840:CLA:H11	22:A:840:CLA:C1A	2.49	0.42
2:B:600:LEU:HD23	2:B:600:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:809:CLA:HBA1	22:B:809:CLA:H3A	1.55	0.42
24:B:844:BCR:C22	24:G:203:BCR:HC42	2.49	0.42
3:C:74:THR:HG21	4:D:81:GLU:OE1	2.18	0.42
5:E:47:ARG:HD2	5:E:50:SER:OG	2.18	0.42
12:Z:149:LYS:HB3	22:Z:313:CLA:CBC	2.40	0.42
14:7:113:THR:HG22	14:7:115:HIS:H	1.84	0.42
24:8:304:BCR:H19C	39:8:315:CHL:CMA	2.49	0.42
16:4:106:TRP:CZ3	24:4:804:BCR:H372	2.54	0.42
16:4:216:LYS:HD2	22:4:811:CLA:O1D	2.19	0.42
17:5:69:TRP:CZ2	22:5:318:CLA:HAA2	2.54	0.42
22:5:309:CLA:H11	22:5:314:CLA:CMD	2.49	0.42
18:6:87:VAL:C	18:6:89:GLU:N	2.76	0.42
18:6:242:THR:HG23	24:6:306:BCR:H312	2.01	0.42
38:6:304:LUT:H15	38:6:304:LUT:H201	1.84	0.42
20:2:198:ILE:HD12	22:2:301:CLA:CHD	2.48	0.42
1:A:365:ILE:CD1	1:A:398:GLY:HA3	2.49	0.42
22:A:806:CLA:H12	22:A:806:CLA:HBA2	1.53	0.42
22:A:821:CLA:H93	22:A:821:CLA:H62	1.85	0.42
22:A:831:CLA:HAB	22:A:839:CLA:CBB	2.49	0.42
2:B:107:ARG:HE	2:B:116:ILE:HG12	1.84	0.42
2:B:371:SER:HA	2:B:726:LEU:HD21	2.00	0.42
2:B:513:ILE:HG22	2:B:517:ASP:OD2	2.19	0.42
22:B:833:CLA:HMC2	22:B:839:CLA:HAC1	2.00	0.42
24:B:847:BCR:HC31	22:1:314:CLA:H41	2.00	0.42
5:E:38:LYS:HB3	5:E:38:LYS:HE3	1.65	0.42
11:L:165:GLU:H	11:L:165:GLU:CD	2.26	0.42
12:1:134:MET:HE2	22:1:314:CLA:C2C	2.48	0.42
22:1:308:CLA:C1D	22:1:314:CLA:H93	2.49	0.42
12:Z:115:PHE:H	22:Z:308:CLA:CAD	2.32	0.42
22:Z:309:CLA:HMC2	24:4:804:BCR:HC21	2.01	0.42
39:Z:312:CHL:HAB	22:Z:315:CLA:CBB	2.49	0.42
14:7:65:MET:O	14:7:69:VAL:HG23	2.20	0.42
24:7:303:BCR:H373	22:7:316:CLA:HHB	2.00	0.42
22:7:310:CLA:H93	22:7:310:CLA:H62	1.80	0.42
15:8:135:MET:HE3	15:8:139:LYS:HB2	2.01	0.42
15:8:164:PRO:HD3	22:8:313:CLA:HMD1	2.01	0.42
16:4:85:SER:HB2	16:4:88:VAL:HG21	2.00	0.42
17:5:227:TRP:HE1	22:5:314:CLA:HED2	1.83	0.42
22:5:314:CLA:CBB	22:5:314:CLA:HHC	2.49	0.42
19:9:59:ASP:OD2	19:9:62:ARG:HG3	2.19	0.42
38:9:301:LUT:H162	22:9:305:CLA:HHB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HG13	1:A:395:ASN:HA	2.01	0.42
1:A:366:ILE:HD12	22:A:827:CLA:H42	2.01	0.42
22:A:810:CLA:CAB	22:A:813:CLA:H121	2.48	0.42
22:A:814:CLA:C2C	24:A:844:BCR:H352	2.49	0.42
2:B:5:LEU:HG	8:I:103:ASN:HB2	2.01	0.42
2:B:176:LEU:HD12	2:B:176:LEU:HA	1.87	0.42
2:B:211:ASP:HB3	25:B:851:LHG:HC42	2.01	0.42
2:B:527:GLY:HA2	2:B:583:TRP:CZ3	2.53	0.42
22:B:835:CLA:HBB1	22:B:835:CLA:CMB	2.44	0.42
24:B:853:BCR:HC32	22:L:202:CLA:C4C	2.49	0.42
22:F:304:CLA:C2	22:F:304:CLA:HBA1	2.49	0.42
22:G:202:CLA:HBB1	22:G:202:CLA:CMB	2.50	0.42
8:I:98:TYR:CD2	8:I:99:ILE:HD12	2.51	0.42
10:K:33:THR:O	10:K:37:ILE:HG13	2.19	0.42
38:Z:301:LUT:C30	22:Z:303:CLA:H8	2.49	0.42
22:3:309:CLA:O1D	22:3:314:CLA:H51	2.19	0.42
22:7:307:CLA:H18	22:7:307:CLA:H151	1.80	0.42
38:8:302:LUT:H30	22:8:305:CLA:H61	2.00	0.42
22:4:807:CLA:HBB1	22:4:807:CLA:CMB	2.49	0.42
18:6:46:LEU:H	18:6:46:LEU:CD1	2.27	0.42
18:6:170:LEU:HB3	22:6:307:CLA:CMA	2.49	0.42
18:6:216:PHE:HA	22:6:322:CLA:HMB1	2.01	0.42
24:6:305:BCR:H402	22:6:312:CLA:C1B	2.50	0.42
1:A:483:PHE:HB3	22:A:837:CLA:C3	2.48	0.42
22:A:812:CLA:C9	38:3:303:LUT:H372	2.49	0.42
22:A:824:CLA:H52	24:A:847:BCR:H363	2.01	0.42
22:A:832:CLA:H18	22:A:832:CLA:H151	1.69	0.42
22:A:835:CLA:H11	22:A:835:CLA:HBA1	1.72	0.42
2:B:43:LEU:O	2:B:47:ILE:HG13	2.20	0.42
2:B:159:GLN:O	2:B:160:PRO:C	2.62	0.42
2:B:243:HIS:HD2	2:B:251:ALA:HA	1.84	0.42
22:B:815:CLA:H192	22:B:830:CLA:H93	2.01	0.42
22:B:817:CLA:HBA1	19:9:177:LEU:HD22	2.00	0.42
22:B:834:CLA:HMA3	35:J:102:T7X:C15	2.48	0.42
3:C:15:THR:HG22	3:C:28:MET:HE2	2.00	0.42
4:D:138:PHE:CZ	4:D:151:HIS:HB2	2.54	0.42
6:F:162:TRP:CZ3	6:F:200:ALA:HA	2.54	0.42
7:G:77:TYR:CG	7:G:78:PHE:N	2.87	0.42
12:1:158:ASP:O	12:1:161:ASN:ND2	2.50	0.42
38:Z:302:LUT:H35	38:Z:302:LUT:H401	1.83	0.42
13:3:182:LEU:HD23	22:3:314:CLA:HED2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:231:LYS:C	31:3:301:DGD:HE2	2.44	0.42
22:3:318:CLA:H62	22:3:318:CLA:H2	1.64	0.42
38:7:302:LUT:H35	38:7:302:LUT:H401	1.87	0.42
42:7:320:SPH:H121	42:7:320:SPH:H152	1.45	0.42
15:8:155:SER:HB3	15:8:167:PRO:HD3	2.02	0.42
22:8:310:CLA:H62	43:8:319:LPX:H5A	2.01	0.42
39:8:312:CHL:C1D	26:8:318:NKP:HAL	2.50	0.42
16:4:62:PHE:HD2	16:4:65:SER:HB3	1.85	0.42
18:6:72:ARG:O	18:6:76:ARG:HG3	2.20	0.42
18:6:91:VAL:O	18:6:93:PRO:HD3	2.20	0.42
18:6:95:VAL:HA	18:6:103:LYS:HE2	2.02	0.42
18:6:123:PHE:CD2	24:6:305:BCR:H12C	2.54	0.42
22:6:302:CLA:HHC	22:6:302:CLA:HBB1	2.01	0.42
22:6:310:CLA:H13	22:6:310:CLA:H102	1.82	0.42
19:9:110:PRO:HB2	20:2:194:TRP:CZ3	2.54	0.42
19:9:125:LYS:NZ	19:9:125:LYS:HB3	2.35	0.42
20:2:189:HIS:ND1	22:2:301:CLA:HAA2	2.34	0.42
1:A:101:TYR:CZ	1:A:105:LEU:HD21	2.54	0.42
1:A:150:ALA:HB2	1:A:378:PRO:HD2	2.02	0.42
1:A:650:LEU:HD13	22:B:805:CLA:CBB	2.50	0.42
1:A:686:LEU:HG	1:A:727:GLY:HA3	2.00	0.42
22:A:808:CLA:H93	22:A:808:CLA:H62	1.87	0.42
22:A:810:CLA:HBD	13:3:51:VAL:HG23	2.00	0.42
22:A:829:CLA:H2	22:A:829:CLA:H62	1.73	0.42
22:A:838:CLA:HHB	22:A:839:CLA:O1D	2.19	0.42
24:A:846:BCR:H15C	24:A:846:BCR:H351	1.66	0.42
2:B:231:TRP:CH2	22:B:818:CLA:H92	2.54	0.42
22:B:840:CLA:HBB1	22:B:840:CLA:CMB	2.49	0.42
22:B:841:CLA:NB	24:B:849:BCR:H15C	2.35	0.42
24:B:844:BCR:H20C	24:B:844:BCR:H361	1.42	0.42
25:B:850:LHG:HC81	25:B:850:LHG:HC5	1.83	0.42
4:D:86:ILE:HG21	4:D:124:LEU:HD23	2.01	0.42
8:I:95:LEU:HD13	24:L:204:BCR:HC8	2.00	0.42
12:Z:160:LEU:N	12:Z:160:LEU:HD22	2.34	0.42
12:Z:188:PHE:HA	12:Z:191:GLN:HE22	1.82	0.42
38:Z:302:LUT:H15	38:Z:302:LUT:H201	1.83	0.42
39:Z:312:CHL:HED2	39:Z:312:CHL:H2A	2.00	0.42
13:3:41:LEU:HD12	13:3:41:LEU:N	2.34	0.42
24:3:307:BCR:H351	24:3:307:BCR:H15C	1.46	0.42
14:7:149:GLY:HA3	14:7:161:LYS:HD2	2.02	0.42
14:7:167:TYR:CZ	14:7:190:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:7:302:LUT:H15	38:7:302:LUT:H201	1.83	0.42
22:8:307:CLA:HBB1	22:8:307:CLA:CMB	2.50	0.42
16:4:118:ASP:HB2	16:4:240:LEU:HD23	2.01	0.42
22:4:812:CLA:H61	22:4:812:CLA:H2	1.60	0.42
22:5:318:CLA:H11	22:6:322:CLA:H91	2.00	0.42
18:6:80:LEU:HD11	22:6:307:CLA:CBC	2.49	0.42
22:6:311:CLA:OBD	22:6:317:CLA:HAA1	2.19	0.42
1:A:278:PHE:HB2	22:A:817:CLA:O1D	2.20	0.42
1:A:490:THR:O	1:A:494:ALA:HB2	2.20	0.42
22:A:805:CLA:H93	22:A:805:CLA:H111	1.71	0.42
22:A:812:CLA:H2	22:A:812:CLA:ND	2.35	0.42
22:A:812:CLA:H71	22:A:812:CLA:CHC	2.48	0.42
22:A:841:CLA:HBC1	24:F:303:BCR:H392	2.00	0.42
2:B:166:LEU:HD11	2:B:170:LYS:HE3	2.01	0.42
2:B:517:ASP:HA	2:B:520:VAL:HG12	2.01	0.42
2:B:712:THR:O	2:B:716:VAL:HG23	2.19	0.42
22:B:821:CLA:O1A	22:B:826:CLA:H112	2.20	0.42
6:F:192:ALA:O	6:F:196:THR:HG23	2.18	0.42
7:G:122:LEU:HD22	7:G:122:LEU:HA	1.83	0.42
12:1:192:HIS:O	12:1:196:GLY:HA2	2.19	0.42
12:Z:218:ASN:ND2	22:Z:305:CLA:HMD2	2.35	0.42
13:3:15:LEU:HA	13:3:34:PHE:O	2.19	0.42
22:7:324:CLA:H11	22:7:324:CLA:H51	1.83	0.42
15:8:186:LEU:HD23	22:8:311:CLA:HED3	2.00	0.42
16:4:225:PHE:CD2	38:4:803:LUT:H14	2.54	0.42
38:4:802:LUT:H31	38:4:802:LUT:H391	1.90	0.42
22:4:812:CLA:H93	24:6:305:BCR:H311	2.01	0.42
17:5:55:PHE:HB3	22:5:310:CLA:C3D	2.50	0.42
22:6:322:CLA:HBB1	22:6:322:CLA:HMB1	2.02	0.42
19:9:76:TRP:CE3	22:9:313:CLA:HAC2	2.55	0.42
1:A:161:THR:HA	27:A:852:DGA:HAW1	2.01	0.42
22:A:810:CLA:HBB1	22:A:810:CLA:CMB	2.49	0.42
22:A:817:CLA:H61	22:A:817:CLA:C3C	2.50	0.42
22:A:829:CLA:C2	24:A:845:BCR:HC7	2.41	0.42
23:A:843:PQN:H18	23:A:843:PQN:H222	1.42	0.42
2:B:33:GLU:H	2:B:33:GLU:HG3	1.48	0.42
2:B:61:TRP:CG	22:B:809:CLA:HBC1	2.54	0.42
2:B:443:VAL:HG21	22:B:834:CLA:HAC2	2.01	0.42
2:B:453:GLN:NE2	2:B:455:LEU:HD11	2.32	0.42
22:B:822:CLA:NB	24:B:844:BCR:H351	2.35	0.42
22:B:823:CLA:CMD	24:B:844:BCR:HC7	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:829:CLA:H111	22:B:829:CLA:C2D	2.50	0.42
6:F:202:TRP:N	6:F:203:PRO:CD	2.83	0.42
22:L:201:CLA:H62	22:L:201:CLA:H102	1.30	0.42
12:1:122:ASP:O	12:1:123:LEU:C	2.62	0.42
38:Z:302:LUT:H8	22:Z:308:CLA:HMB2	2.01	0.42
13:3:72:ALA:HB1	24:3:305:BCR:H383	2.01	0.42
22:3:320:CLA:NA	41:7:319:3PH:H3D2	2.34	0.42
22:3:322:CLA:CMB	41:7:319:3PH:H2A1	2.49	0.42
14:7:34:TYR:O	14:7:35:PRO:C	2.62	0.42
22:7:307:CLA:HBB1	22:7:307:CLA:HMB3	2.01	0.42
16:4:111:ALA:HB1	38:4:802:LUT:H12	2.00	0.42
16:4:185:LEU:HD23	39:4:819:CHL:HMD2	2.02	0.42
17:5:252:LEU:HD23	41:5:325:3PH:H342	2.00	0.42
22:6:301:CLA:H11	22:6:301:CLA:H52	1.71	0.42
22:6:314:CLA:H93	22:6:314:CLA:H112	1.63	0.42
19:9:113:ALA:HA	19:9:116:PHE:HD2	1.84	0.42
20:2:165:MET:O	20:2:169:ILE:HG12	2.20	0.42
1:A:478:GLN:HB3	1:A:480:GLN:HE21	1.83	0.42
22:A:804:CLA:HBB1	22:A:804:CLA:CMB	2.49	0.42
22:A:805:CLA:H62	22:A:805:CLA:H2	1.55	0.42
22:A:822:CLA:CBB	37:K:201:DAO:H112	2.46	0.42
22:A:833:CLA:HBB1	22:L:203:CLA:HBB2	2.02	0.42
2:B:67:PHE:HZ	8:I:71:PRO:HG2	1.85	0.42
2:B:89:ALA:HB1	22:B:811:CLA:O2D	2.19	0.42
25:B:803:LHG:HC91	22:B:807:CLA:C3D	2.50	0.42
22:B:829:CLA:H62	22:B:829:CLA:H2	1.63	0.42
5:E:79:ASN:OD1	5:E:83:VAL:N	2.53	0.42
6:F:220:GLU:H	6:F:220:GLU:HG3	1.50	0.42
7:G:36:LEU:HD13	7:G:36:LEU:C	2.43	0.42
22:Z:316:CLA:H111	22:Z:316:CLA:H152	1.49	0.42
22:3:311:CLA:H62	22:3:311:CLA:H93	1.80	0.42
22:3:322:CLA:HHC	22:3:322:CLA:CBB	2.48	0.42
14:7:67:TRP:CH2	22:7:315:CLA:HAA1	2.54	0.42
14:7:135:GLU:HG3	22:7:315:CLA:NB	2.35	0.42
22:7:323:CLA:H93	22:7:323:CLA:H111	1.68	0.42
15:8:205:GLN:NE2	38:8:302:LUT:H42	2.35	0.42
22:8:305:CLA:HBB1	22:8:305:CLA:CMB	2.48	0.42
22:8:307:CLA:H51	22:8:307:CLA:C4C	2.50	0.42
39:8:315:CHL:HAA2	39:8:315:CHL:CBD	2.50	0.42
24:4:804:BCR:H24C	39:4:816:CHL:HAA1	2.01	0.42
17:5:100:TRP:CH2	17:5:201:VAL:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5:123:ALA:CB	22:5:326:CLA:HAA1	2.50	0.42
39:5:316:CHL:HMC	22:5:319:CLA:CAB	2.45	0.42
18:6:214:THR:HA	22:6:309:CLA:HBA2	2.01	0.42
18:6:248:CYS:HB3	18:6:254:TRP:CH2	2.55	0.42
39:9:312:CHL:H162	39:9:312:CHL:H121	1.85	0.42
20:2:214:LEU:C	39:2:303:CHL:HAA2	2.44	0.42
1:A:341:LEU:HD11	1:A:426:LEU:CD1	2.50	0.42
1:A:426:LEU:HB2	22:A:824:CLA:HMC2	2.01	0.42
1:A:461:THR:CG2	22:B:812:CLA:HAB	2.48	0.42
22:A:815:CLA:C1C	24:A:856:BCR:H312	2.49	0.42
2:B:13:LEU:HD11	31:B:852:DGD:HE1	2.02	0.42
2:B:297:GLY:O	2:B:298:ILE:C	2.63	0.42
2:B:653:PHE:CD1	22:B:806:CLA:H71	2.54	0.42
22:B:801:CLA:H152	22:B:801:CLA:H18	1.83	0.42
22:B:819:CLA:H43	22:B:835:CLA:HED1	2.02	0.42
6:F:114:ARG:HB2	9:J:35:ASP:OD2	2.20	0.42
13:3:216:HIS:CD2	22:3:310:CLA:HAA1	2.54	0.42
14:7:127:MET:HE3	14:7:127:MET:HB3	1.94	0.42
14:7:209:ALA:CB	22:7:317:CLA:H8	2.48	0.42
22:7:305:CLA:C4B	22:7:310:CLA:H121	2.50	0.42
15:8:187:LYS:HG2	22:8:306:CLA:HBD	2.01	0.42
17:5:158:PRO:HB2	17:5:160:PRO:HD3	2.02	0.42
24:5:304:BCR:H19C	22:5:319:CLA:CBA	2.28	0.42
19:9:52:ASP:CG	19:9:55:GLY:HA2	2.44	0.42
39:9:312:CHL:H18	39:9:312:CHL:C1C	2.50	0.42
39:9:314:CHL:HED2	20:2:194:TRP:CH2	2.54	0.42
1:A:129:GLY:O	1:A:136:GLN:HA	2.20	0.42
1:A:205:LEU:HD12	24:A:845:BCR:H363	2.02	0.42
1:A:278:PHE:CZ	22:A:818:CLA:H43	2.54	0.42
1:A:369:HIS:HA	1:A:372:TYR:CE2	2.55	0.42
1:A:651:TRP:CD1	22:B:805:CLA:HBC1	2.55	0.42
22:A:806:CLA:H62	22:A:806:CLA:H2	1.64	0.42
22:A:815:CLA:O1A	13:3:203:VAL:HG12	2.20	0.42
22:A:840:CLA:HHD	24:F:303:BCR:H383	2.01	0.42
2:B:229:GLY:O	2:B:231:TRP:N	2.50	0.42
2:B:419:ILE:HG23	22:B:839:CLA:HBB2	2.02	0.42
2:B:490:SER:HB3	2:B:495:LEU:HB2	2.01	0.42
2:B:712:THR:HG22	31:B:852:DGD:HBW1	2.02	0.42
3:C:23:LEU:O	3:C:24:ASP:C	2.62	0.42
8:I:93:ALA:HB1	11:L:134:ILE:HG21	2.00	0.42
11:L:140:PHE:CD1	11:L:144:PRO:HD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:206:HIS:HA	12:1:213:SER:OG	2.20	0.42
22:1:315:CLA:HBB1	22:1:315:CLA:CMB	2.50	0.42
12:Z:186:LEU:HG	22:Z:305:CLA:HAC1	2.02	0.42
22:Z:309:CLA:HHD	25:Z:317:LHG:H242	2.02	0.42
39:Z:311:CHL:HMA1	25:Z:317:LHG:H192	2.01	0.42
22:3:320:CLA:C4A	41:7:319:3PH:H3D2	2.50	0.42
22:7:307:CLA:H93	22:7:307:CLA:H111	1.77	0.42
22:8:309:CLA:HMD1	22:8:314:CLA:C4C	2.50	0.42
16:4:193:PRO:HD2	22:4:805:CLA:CAD	2.50	0.42
25:4:820:LHG:H352	22:6:321:CLA:C1	2.50	0.42
18:6:85:ILE:HG12	38:6:304:LUT:H41	2.01	0.42
18:6:100:ALA:HB3	18:6:101:PRO:HD3	2.02	0.42
39:6:315:CHL:H61	39:6:315:CHL:H41	1.88	0.42
39:6:318:CHL:H62	39:6:318:CHL:H41	1.74	0.42
19:9:102:LYS:CD	22:9:308:CLA:HED1	2.50	0.42
19:9:175:GLN:OE1	38:9:301:LUT:H42	2.19	0.42
22:9:305:CLA:H142	22:9:305:CLA:H112	1.89	0.42
20:2:171:PHE:C	20:2:174:GLN:H	2.27	0.42
1:A:634:ASN:O	1:A:638:SER:HB2	2.19	0.41
22:A:820:CLA:H71	22:A:820:CLA:H111	1.20	0.41
22:A:832:CLA:H112	22:A:832:CLA:H152	1.66	0.41
22:A:855:CLA:H161	24:B:853:BCR:H351	2.01	0.41
2:B:198:VAL:C	2:B:201:PRO:HD2	2.45	0.41
2:B:687:PRO:O	2:B:688:LEU:HB2	2.20	0.41
22:B:821:CLA:HMB1	22:B:826:CLA:H2	2.02	0.41
22:B:824:CLA:HMB3	22:B:824:CLA:HBB1	2.02	0.41
22:B:826:CLA:H92	22:B:826:CLA:H61	1.65	0.41
3:C:15:THR:HG22	3:C:28:MET:HG3	2.02	0.41
11:L:61:SER:O	11:L:62:THR:C	2.63	0.41
38:Z:301:LUT:H403	22:Z:303:CLA:C14	2.47	0.41
22:3:314:CLA:H41	22:3:314:CLA:H62	1.32	0.41
14:7:241:VAL:CG1	14:7:244:TYR:HB3	2.50	0.41
22:7:312:CLA:HED2	22:7:312:CLA:HBD	1.85	0.41
39:7:313:CHL:CMC	22:7:316:CLA:HAB	2.50	0.41
38:8:302:LUT:H35	38:8:302:LUT:H401	1.79	0.41
38:5:302:LUT:C33	22:5:308:CLA:HMB2	2.50	0.41
38:5:303:LUT:H35	38:5:303:LUT:H401	1.85	0.41
22:6:307:CLA:H41	22:6:308:CLA:HBA1	2.02	0.41
22:6:308:CLA:H51	22:6:308:CLA:H11	1.63	0.41
39:6:320:CHL:OMC	39:6:320:CHL:HAC2	2.20	0.41
22:6:322:CLA:HMC3	41:6:324:3PH:H2A1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:111:LEU:HD23	19:9:111:LEU:C	2.44	0.41
1:A:179:PHE:O	1:A:183:LYS:HB2	2.20	0.41
1:A:483:PHE:HB3	22:A:837:CLA:H42	2.01	0.41
22:A:823:CLA:H111	22:A:823:CLA:H152	1.46	0.41
24:A:844:BCR:H393	24:3:306:BCR:HC42	2.02	0.41
2:B:105:PHE:HD2	2:B:107:ARG:HH12	1.67	0.41
2:B:388:PHE:HZ	22:B:827:CLA:HAB	1.85	0.41
2:B:495:LEU:HD22	2:B:495:LEU:C	2.46	0.41
2:B:587:THR:O	2:B:591:VAL:HG13	2.21	0.41
2:B:656:LEU:HA	22:B:806:CLA:HAA1	2.01	0.41
2:B:727:ILE:CD1	22:B:829:CLA:H12	2.50	0.41
22:B:806:CLA:H92	22:B:806:CLA:H62	1.71	0.41
22:B:810:CLA:C1	8:I:79:PHE:HB3	2.50	0.41
22:B:822:CLA:HMA2	7:G:103:MET:HE3	2.00	0.41
22:B:825:CLA:HAB	22:B:832:CLA:HMD1	2.01	0.41
22:B:830:CLA:H52	24:B:845:BCR:C23	2.50	0.41
6:F:222:ILE:H	6:F:222:ILE:HG13	1.79	0.41
33:G:204:LMT:H41	33:G:204:LMT:H12	1.79	0.41
12:Z:167:ILE:O	12:Z:171:LYS:HG3	2.20	0.41
13:3:183:ASN:HB3	22:3:309:CLA:CAA	2.51	0.41
14:7:155:GLY:N	42:7:320:SPH:H62	2.35	0.41
38:7:302:LUT:H24	22:7:307:CLA:O1A	2.20	0.41
15:8:111:THR:HG21	39:8:315:CHL:CMD	2.50	0.41
38:8:303:LUT:H15	38:8:303:LUT:H201	1.95	0.41
16:4:156:LEU:HD22	24:4:804:BCR:H15C	2.02	0.41
22:4:810:CLA:HMA2	39:4:816:CHL:C2C	2.49	0.41
17:5:172:LEU:HD12	38:5:302:LUT:H222	2.01	0.41
22:5:311:CLA:CHB	22:5:318:CLA:H191	2.51	0.41
22:5:318:CLA:C9	22:6:322:CLA:H62	2.49	0.41
19:9:31:TRP:CZ3	19:9:32:LEU:HD23	2.55	0.41
1:A:46:THR:CG2	1:A:715:PRO:HA	2.51	0.41
1:A:376:PRO:HG3	22:A:819:CLA:HBA1	2.03	0.41
22:A:828:CLA:H72	22:A:828:CLA:H111	1.19	0.41
22:A:828:CLA:H93	24:J:104:BCR:H353	2.01	0.41
22:A:841:CLA:H141	22:A:841:CLA:H162	1.94	0.41
2:B:495:LEU:HD22	2:B:499:LEU:HG	2.02	0.41
22:B:811:CLA:H51	22:B:811:CLA:H8	1.22	0.41
22:B:816:CLA:HMB3	22:B:830:CLA:H13	2.02	0.41
22:B:821:CLA:H41	22:B:825:CLA:H91	2.02	0.41
22:B:823:CLA:HAA2	7:G:60:ASP:OD2	2.21	0.41
22:B:830:CLA:C1D	24:B:845:BCR:H272	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:204:VAL:CG2	22:8:309:CLA:H72	2.42	0.41
22:1:308:CLA:HBC1	22:1:314:CLA:HAC1	2.02	0.41
22:1:313:CLA:H102	22:1:313:CLA:H13	1.88	0.41
12:Z:83:LEU:HB2	22:Z:308:CLA:HBB2	2.02	0.41
13:3:114:PHE:CD1	22:3:316:CLA:HBD	2.55	0.41
13:3:122:GLN:HE21	13:3:122:GLN:HB3	1.73	0.41
13:3:158:TYR:CE1	13:3:181:LYS:HG2	2.55	0.41
22:3:311:CLA:H61	22:3:312:CLA:HMA3	2.01	0.41
14:7:150:ASP:OD1	14:7:150:ASP:N	2.53	0.41
39:4:813:CHL:HAB	39:4:816:CHL:CAB	2.50	0.41
38:5:303:LUT:H162	22:5:312:CLA:HMB3	2.00	0.41
24:5:305:BCR:H363	39:5:316:CHL:ND	2.34	0.41
22:5:308:CLA:CMA	22:5:308:CLA:HBA1	2.49	0.41
22:5:314:CLA:HHC	22:5:314:CLA:HBB1	2.02	0.41
18:6:194:VAL:HG21	22:6:309:CLA:HMD1	2.02	0.41
22:6:309:CLA:H62	22:6:309:CLA:CHC	2.51	0.41
1:A:346:THR:HG23	22:A:825:CLA:HBC1	2.00	0.41
1:A:690:ARG:HG3	1:A:717:ALA:CB	2.48	0.41
1:A:740:TRP:CG	24:A:848:BCR:HC41	2.55	0.41
22:A:808:CLA:CAD	22:A:828:CLA:HAA2	2.51	0.41
22:A:823:CLA:C11	24:A:856:BCR:H401	2.41	0.41
22:A:840:CLA:CBB	6:F:167:GLY:HA3	2.51	0.41
27:A:852:DGA:HB91	22:3:316:CLA:HMC1	2.03	0.41
2:B:356:LEU:HD13	22:B:819:CLA:HAA2	2.03	0.41
2:B:439:VAL:HG12	22:B:834:CLA:HAC1	2.03	0.41
2:B:513:ILE:HG23	22:B:837:CLA:HMD3	2.02	0.41
22:B:824:CLA:HBB1	22:B:824:CLA:CMB	2.50	0.41
22:B:827:CLA:C2	22:B:839:CLA:HBD	2.46	0.41
3:C:5:VAL:HA	3:C:66:ARG:O	2.21	0.41
22:F:304:CLA:NB	22:F:304:CLA:H43	2.36	0.41
32:F:306:RRX:H40	32:F:306:RRX:H36	1.34	0.41
22:L:202:CLA:H2	22:L:202:CLA:H61	1.61	0.41
12:1:140:ARG:HG2	22:1:313:CLA:CHC	2.50	0.41
38:1:302:LUT:H15	38:1:302:LUT:H201	1.86	0.41
22:1:313:CLA:O1A	22:1:313:CLA:H93	2.21	0.41
12:Z:85:ALA:CB	38:Z:301:LUT:H12	2.51	0.41
39:Z:311:CHL:HAA2	16:4:162:PHE:HB2	2.01	0.41
13:3:38:PRO:HD2	38:3:303:LUT:C24	2.50	0.41
13:3:111:TYR:CE2	14:7:244:TYR:HB2	2.55	0.41
38:3:303:LUT:H31	38:3:303:LUT:H391	1.92	0.41
24:3:306:BCR:H393	22:3:318:CLA:H92	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:322:CLA:C2C	25:7:318:LHG:HC82	2.51	0.41
22:7:305:CLA:O1D	22:7:310:CLA:H92	2.19	0.41
16:4:85:SER:OG	33:4:801:LMT:H1B	2.20	0.41
17:5:240:VAL:HG13	17:5:247:ILE:HB	2.03	0.41
38:5:302:LUT:H11	22:5:308:CLA:CMC	2.47	0.41
24:5:304:BCR:H382	22:5:319:CLA:NB	2.36	0.41
22:5:315:CLA:H93	22:5:315:CLA:H62	1.75	0.41
22:5:318:CLA:H42	22:5:323:CLA:HAC2	2.02	0.41
18:6:95:VAL:HA	18:6:103:LYS:HZ3	1.85	0.41
18:6:245:PHE:HE2	22:6:301:CLA:H112	1.85	0.41
22:6:308:CLA:HBB1	22:6:308:CLA:CMB	2.45	0.41
22:6:309:CLA:HBB1	22:6:309:CLA:CMB	2.49	0.41
39:6:316:CHL:H12	39:6:316:CHL:HBA1	1.52	0.41
38:9:302:LUT:H31	38:9:302:LUT:H391	1.90	0.41
1:A:495:PRO:HA	1:A:499:ALA:O	2.20	0.41
22:A:814:CLA:C9	27:A:852:DGA:HB81	2.50	0.41
22:A:817:CLA:C1A	22:A:817:CLA:CGA	2.98	0.41
22:A:822:CLA:CBC	22:A:823:CLA:H171	2.50	0.41
22:A:834:CLA:CHC	24:I:4001:BCR:H291	2.51	0.41
2:B:298:ILE:HG22	7:G:57:HIS:NE2	2.35	0.41
2:B:398:ASP:OD2	4:D:185:LYS:HE3	2.21	0.41
2:B:559:PRO:HB3	2:B:703:ILE:HB	2.02	0.41
22:B:815:CLA:H102	24:B:845:BCR:C38	2.50	0.41
22:B:829:CLA:HBC3	31:B:852:DGD:HBG3	2.02	0.41
22:B:838:CLA:HAC2	32:F:306:RRX:H2	2.02	0.41
22:B:838:CLA:C19	22:F:302:CLA:H101	2.51	0.41
22:B:842:CLA:CED	24:B:847:BCR:H11C	2.51	0.41
3:C:22:PRO:O	4:D:122:LEU:HD23	2.20	0.41
12:1:162:PHE:HB2	22:1:304:CLA:O2A	2.20	0.41
22:1:310:CLA:H91	22:1:310:CLA:H111	1.77	0.41
12:Z:140:ARG:HG3	22:Z:313:CLA:CMC	2.50	0.41
12:Z:174:GLU:HG3	22:Z:303:CLA:C4B	2.50	0.41
14:7:136:GLN:HG3	22:7:323:CLA:HBA1	2.02	0.41
14:7:241:VAL:HG12	14:7:244:TYR:H	1.85	0.41
22:7:309:CLA:C4C	42:7:321:SPH:H151	2.49	0.41
15:8:61:ALA:HB1	15:8:65:TYR:CE2	2.56	0.41
15:8:106:VAL:O	15:8:110:GLN:HB2	2.21	0.41
39:8:315:CHL:H111	39:8:315:CHL:C6	2.46	0.41
39:4:816:CHL:HBB1	39:4:816:CHL:CMB	2.45	0.41
17:5:112:PRO:C	17:5:114:GLN:N	2.78	0.41
22:5:307:CLA:HBB1	22:5:307:CLA:HMB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:5:322:CLA:H152	22:6:319:CLA:H52	2.03	0.41
18:6:77:TRP:HZ2	18:6:121:MET:HE1	1.85	0.41
38:6:304:LUT:H35	38:6:304:LUT:H401	1.86	0.41
24:6:305:BCR:H271	22:6:312:CLA:H101	2.03	0.41
24:6:306:BCR:H363	39:6:315:CHL:C4D	2.50	0.41
22:6:322:CLA:H2A	22:6:322:CLA:CED	2.49	0.41
19:9:110:PRO:HG2	20:2:200:THR:HG23	2.02	0.41
20:2:177:VAL:O	20:2:178:ARG:C	2.63	0.41
1:A:14:LYS:HA	22:A:812:CLA:HAA1	2.03	0.41
1:A:15:ILE:HG12	22:A:812:CLA:OBD	2.21	0.41
1:A:211:LEU:CD2	24:A:844:BCR:H373	2.50	0.41
1:A:584:CYS:HB3	2:B:668:TRP:HE3	1.86	0.41
22:A:809:CLA:NC	22:A:828:CLA:H172	2.35	0.41
22:A:813:CLA:H42	22:A:813:CLA:HMA2	2.02	0.41
22:A:814:CLA:H43	22:A:816:CLA:C4	2.50	0.41
2:B:78:TRP:HH2	2:B:123:GLN:HA	1.85	0.41
22:B:808:CLA:H2	22:B:808:CLA:H61	1.61	0.41
22:B:808:CLA:H143	22:B:815:CLA:C3D	2.50	0.41
22:B:830:CLA:H52	24:B:845:BCR:H23C	2.02	0.41
12:1:206:HIS:CG	22:1:306:CLA:HAA2	2.56	0.41
22:Z:316:CLA:H141	22:Z:316:CLA:H172	2.01	0.41
22:Z:316:CLA:ND	22:Z:316:CLA:H13	2.35	0.41
22:3:313:CLA:H13	22:5:320:CLA:NB	2.35	0.41
22:3:313:CLA:H3A	22:3:313:CLA:HBA2	1.46	0.41
22:3:322:CLA:HBC1	14:7:31:PRO:HB2	2.03	0.41
22:7:322:CLA:H61	22:7:322:CLA:H2	1.66	0.41
22:7:322:CLA:C3	22:7:323:CLA:H193	2.50	0.41
22:7:323:CLA:H161	22:7:323:CLA:H121	1.79	0.41
22:5:308:CLA:HMA2	22:5:308:CLA:HBA1	2.02	0.41
19:9:56:LEU:CD1	38:9:302:LUT:H221	2.45	0.41
19:9:113:ALA:HA	19:9:116:PHE:CD2	2.56	0.41
1:A:368:ALA:HB2	1:A:394:HIS:HB2	2.03	0.41
1:A:377:TYR:CE2	22:A:829:CLA:HED2	2.56	0.41
1:A:396:TRP:HZ3	1:A:600:TYR:HA	1.85	0.41
1:A:406:GLY:CA	24:A:847:BCR:H323	2.51	0.41
1:A:499:ALA:HB1	22:A:836:CLA:HED3	2.02	0.41
22:A:803:CLA:HBA2	22:A:803:CLA:H12	1.72	0.41
22:A:807:CLA:O2D	22:A:809:CLA:HED1	2.19	0.41
22:A:822:CLA:CHD	24:A:856:BCR:H402	2.50	0.41
22:A:823:CLA:C9	22:K:204:CLA:HMB2	2.50	0.41
22:A:832:CLA:HMA2	2:B:685:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:836:CLA:HBA2	22:A:836:CLA:CHA	2.49	0.41
22:A:840:CLA:HMC2	23:A:843:PQN:H272	2.01	0.41
2:B:24:PHE:O	2:B:28:VAL:HG23	2.21	0.41
2:B:413:LEU:HA	2:B:416:LYS:HB3	2.03	0.41
22:B:819:CLA:C9	22:B:828:CLA:HAB	2.41	0.41
22:B:832:CLA:CHA	22:B:842:CLA:H52	2.51	0.41
3:C:9:ASP:C	3:C:11:CYS:H	2.29	0.41
4:D:106:MET:SD	4:D:134:PHE:HE2	2.43	0.41
6:F:142:LYS:HA	33:F:307:LMT:H2'	2.03	0.41
12:1:157:PHE:CE2	22:1:313:CLA:H161	2.55	0.41
22:1:308:CLA:HMD1	22:1:314:CLA:C4C	2.50	0.41
12:Z:215:PHE:CG	22:Z:305:CLA:H42	2.55	0.41
22:3:312:CLA:ND	22:3:318:CLA:H101	2.35	0.41
15:8:124:PHE:HD1	39:8:301:CHL:H51	1.85	0.41
22:8:305:CLA:HBB1	22:8:306:CLA:CAA	2.51	0.41
16:4:78:ASP:HA	22:4:808:CLA:O1D	2.21	0.41
16:4:83:PRO:CD	38:4:803:LUT:H23	2.42	0.41
16:4:150:PHE:HB2	39:4:813:CHL:HAC2	2.01	0.41
16:4:238:THR:HB	16:4:239:PRO:HD2	2.03	0.41
17:5:161:GLU:HG3	17:5:179:ARG:HH22	1.86	0.41
22:5:322:CLA:H121	22:6:311:CLA:HMB2	2.03	0.41
18:6:95:VAL:CG1	18:6:100:ALA:HA	2.50	0.41
39:9:312:CHL:C3C	39:9:314:CHL:CBB	2.98	0.41
1:A:575:CYS:SG	29:B:802:SF4:S1	3.19	0.41
1:A:661:TYR:OH	1:A:670:LEU:HD23	2.21	0.41
22:A:817:CLA:H12	22:A:817:CLA:ND	2.35	0.41
2:B:32:PHE:HD1	2:B:35:HIS:CE1	2.38	0.41
2:B:143:LEU:HD21	24:B:846:BCR:C24	2.50	0.41
2:B:243:HIS:HB2	2:B:250:GLY:O	2.21	0.41
2:B:315:ARG:HB2	22:B:842:CLA:O1A	2.21	0.41
2:B:331:LEU:HD23	2:B:331:LEU:HA	1.90	0.41
22:B:830:CLA:ND	24:B:845:BCR:H282	2.35	0.41
22:B:838:CLA:H2	22:B:839:CLA:CMD	2.51	0.41
6:F:153:THR:HG21	32:F:306:RRX:C4	2.51	0.41
22:F:305:CLA:HMB3	22:F:305:CLA:CBB	2.46	0.41
38:1:303:LUT:H161	22:1:309:CLA:HMB2	2.02	0.41
12:Z:176:LYS:HE2	22:Z:309:CLA:C2D	2.50	0.41
38:Z:302:LUT:H371	22:Z:306:CLA:H142	2.02	0.41
22:3:312:CLA:H162	22:3:312:CLA:H141	1.85	0.41
14:7:73:LEU:HD13	14:7:166:GLY:HA3	2.03	0.41
14:7:129:LEU:O	22:7:323:CLA:H11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:173:PHE:HZ	22:7:314:CLA:CHC	2.34	0.41
22:7:322:CLA:C3D	22:7:323:CLA:H91	2.51	0.41
15:8:184:LEU:HB3	22:8:305:CLA:CMA	2.50	0.41
16:4:109:LEU:HB3	22:4:810:CLA:HAB	2.03	0.41
18:6:164:PRO:HG2	22:6:308:CLA:H12	2.03	0.41
19:9:82:VAL:HG21	38:9:301:LUT:H401	2.03	0.41
19:9:111:LEU:HD21	39:9:314:CHL:ND	2.35	0.41
1:A:59:PHE:HB2	1:A:69:ILE:HG23	2.03	0.41
1:A:205:LEU:HD13	22:A:813:CLA:HHB	2.03	0.41
22:A:807:CLA:H91	22:A:807:CLA:H111	1.69	0.41
22:A:808:CLA:CHC	22:A:809:CLA:HMD2	2.51	0.41
22:A:816:CLA:HBC2	22:3:316:CLA:CBB	2.51	0.41
22:A:821:CLA:O1A	22:A:824:CLA:HBD	2.21	0.41
22:A:828:CLA:H91	24:J:104:BCR:H11C	2.02	0.41
22:A:829:CLA:NC	24:A:845:BCR:HC42	2.35	0.41
22:A:838:CLA:H52	22:A:838:CLA:NC	2.36	0.41
24:A:847:BCR:H311	24:A:847:BCR:HC7	1.81	0.41
2:B:74:ASN:ND2	2:B:88:ILE:HG13	2.35	0.41
2:B:94:ASP:C	2:B:96:HIS:H	2.28	0.41
2:B:127:THR:HA	2:B:245:PHE:HZ	1.84	0.41
2:B:168:TRP:NE1	22:B:815:CLA:HAC2	2.36	0.41
2:B:302:MET:HB2	2:B:324:PHE:CE2	2.55	0.41
2:B:362:LEU:HD22	2:B:369:GLN:NE2	2.35	0.41
2:B:478:LEU:HD13	22:B:835:CLA:CMD	2.51	0.41
2:B:575:ASP:HA	2:B:578:TYR:HB3	2.02	0.41
22:B:812:CLA:H41	22:B:812:CLA:H62	1.88	0.41
22:B:821:CLA:H51	22:B:828:CLA:H101	2.03	0.41
22:B:826:CLA:H161	22:B:826:CLA:H122	1.67	0.41
22:B:827:CLA:HBA1	22:B:828:CLA:HED2	2.03	0.41
24:B:853:BCR:H312	22:L:202:CLA:C2C	2.50	0.41
34:F:308:LMG:H161	34:F:308:LMG:H132	1.83	0.41
22:J:103:CLA:HED1	15:8:240:LEU:HB2	2.03	0.41
22:K:202:CLA:HMB3	24:K:206:BCR:H352	2.03	0.41
22:K:205:CLA:NA	24:K:206:BCR:H281	2.36	0.41
38:1:303:LUT:H35	38:1:303:LUT:H401	1.84	0.41
39:1:312:CHL:H11	31:1:319:DGD:HD3	2.02	0.41
12:Z:92:GLU:OE1	12:Z:199:PRO:HD2	2.20	0.41
12:Z:92:GLU:OE1	12:Z:200:LEU:HD23	2.20	0.41
12:Z:103:PRO:HB2	39:Z:312:CHL:C1D	2.51	0.41
13:3:54:GLN:H	13:3:54:GLN:CD	2.29	0.41
13:3:98:PRO:N	13:3:99:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:111:TYR:CZ	22:3:316:CLA:HMA2	2.55	0.41
13:3:158:TYR:HB3	22:3:308:CLA:HED3	2.03	0.41
24:3:304:BCR:H383	22:3:313:CLA:CAB	2.51	0.41
22:3:313:CLA:H13	22:5:320:CLA:C4B	2.51	0.41
14:7:58:LEU:CD1	22:7:308:CLA:H92	2.51	0.41
24:7:303:BCR:C29	42:7:321:SPH:H122	2.50	0.41
22:7:308:CLA:CMD	22:7:315:CLA:C1D	2.99	0.41
15:8:77:MET:SD	22:8:305:CLA:HAB	2.61	0.41
15:8:113:ILE:CG2	15:8:118:LEU:HB2	2.51	0.41
15:8:144:SER:OG	15:8:157:LYS:HD3	2.21	0.41
15:8:189:ILE:HD12	15:8:189:ILE:HA	1.62	0.41
22:8:305:CLA:H111	43:8:319:LPX:H19A	2.03	0.41
16:4:132:VAL:HG21	16:4:140:TYR:CD1	2.56	0.41
16:4:231:GLN:NE2	38:4:802:LUT:H42	2.35	0.41
16:4:251:TRP:HB3	18:6:108:PHE:HB3	2.02	0.41
38:4:803:LUT:H31	38:4:803:LUT:H391	1.91	0.41
22:4:807:CLA:HBB1	22:4:807:CLA:H171	2.02	0.41
22:5:318:CLA:HBB1	22:5:318:CLA:CMB	2.50	0.41
18:6:61:PRO:HG2	18:6:62:GLU:OE1	2.21	0.41
18:6:215:ILE:HA	18:6:218:LYS:HG2	2.01	0.41
22:6:310:CLA:HBC1	25:6:323:LHG:H282	2.03	0.41
39:6:315:CHL:CBB	39:6:318:CHL:HBB2	2.51	0.41
19:9:36:ASN:O	19:9:37:PRO:C	2.64	0.41
38:9:302:LUT:H32	22:9:306:CLA:CAB	2.50	0.41
22:9:308:CLA:HMB3	22:9:308:CLA:HBB1	2.03	0.41
20:2:178:ARG:O	20:2:178:ARG:NE	2.52	0.41
20:2:194:TRP:O	20:2:200:THR:HG21	2.21	0.41
1:A:562:LEU:HB2	2:B:677:GLU:OE2	2.21	0.41
22:A:803:CLA:HMA2	22:A:808:CLA:H191	2.03	0.41
22:A:836:CLA:H42	22:K:203:CLA:C2D	2.51	0.41
22:A:840:CLA:H61	22:A:840:CLA:H2	1.75	0.41
2:B:53:GLY:O	2:B:57:ILE:HG13	2.21	0.41
22:B:809:CLA:HMA2	22:B:831:CLA:C4B	2.51	0.41
24:B:847:BCR:C8	22:1:308:CLA:H92	2.51	0.41
3:C:21:CYS:HA	29:C:101:SF4:S4	2.61	0.41
6:F:79:ARG:HB2	6:F:79:ARG:NH1	2.36	0.41
10:K:59:ARG:NH2	10:K:67:LEU:HD22	2.36	0.41
24:K:206:BCR:H15C	24:K:206:BCR:H351	1.96	0.41
12:1:36:LEU:HD21	40:1:318:SQD:H161	2.03	0.41
12:1:167:ILE:O	12:1:171:LYS:HG3	2.20	0.41
22:1:306:CLA:H112	25:1:317:LHG:H312	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:307:CLA:H61	22:1:307:CLA:H92	1.76	0.41
12:Z:60:LEU:CD1	22:Z:306:CLA:H42	2.51	0.41
12:Z:77:HIS:HB3	12:Z:182:MET:SD	2.61	0.41
38:3:302:LUT:H31	38:3:302:LUT:H391	1.88	0.41
24:3:307:BCR:H10C	22:3:315:CLA:C1B	2.50	0.41
22:3:309:CLA:HBB1	22:3:309:CLA:CMB	2.46	0.41
39:7:313:CHL:OMC	39:7:313:CHL:HAC1	2.20	0.41
22:8:306:CLA:CMD	33:4:801:LMT:H61	2.51	0.41
39:8:315:CHL:HAC2	39:8:315:CHL:OMC	2.20	0.41
16:4:225:PHE:CE1	38:4:803:LUT:H10	2.56	0.41
18:6:99:ASP:CB	39:6:315:CHL:HED3	2.48	0.41
18:6:123:PHE:CG	24:6:305:BCR:H10C	2.55	0.41
18:6:157:PRO:HG2	22:6:307:CLA:CMD	2.51	0.41
18:6:199:PRO:HB2	38:6:303:LUT:H183	2.03	0.41
22:6:317:CLA:HBA2	22:6:317:CLA:H12	1.69	0.41
39:9:314:CHL:HHC	39:9:314:CHL:CBB	2.48	0.41
20:2:177:VAL:HG22	22:2:301:CLA:HHD	2.03	0.41
1:A:578:PRO:HB3	2:B:560:CYS:SG	2.60	0.40
22:A:807:CLA:HAA2	22:A:809:CLA:O2D	2.22	0.40
22:A:821:CLA:HBB1	22:A:821:CLA:CMB	2.50	0.40
22:A:834:CLA:HED2	22:A:834:CLA:H2A	2.02	0.40
31:B:852:DGD:HE5	31:B:852:DGD:HD4	2.03	0.40
4:D:117:ARG:HD2	4:D:119:GLU:HB3	2.03	0.40
4:D:192:MET:HG2	4:D:193:ASP:N	2.36	0.40
5:E:52:TRP:O	5:E:55:GLN:HB2	2.21	0.40
10:K:106:GLY:HA3	22:K:203:CLA:C1B	2.52	0.40
13:3:126:LEU:HD13	22:3:318:CLA:HMB3	2.02	0.40
22:7:310:CLA:HBC3	25:7:318:LHG:O8	2.21	0.40
22:8:311:CLA:CMA	33:4:801:LMT:H5'	2.51	0.40
16:4:150:PHE:O	16:4:153:MET:HG2	2.22	0.40
16:4:258:ASN:HD22	16:4:258:ASN:H	1.69	0.40
17:5:101:TYR:HD1	39:5:316:CHL:HED3	1.86	0.40
22:5:308:CLA:HBB1	22:5:308:CLA:HMB1	2.03	0.40
18:6:57:LEU:HD11	38:6:304:LUT:H221	2.01	0.40
18:6:60:ASN:OD1	18:6:61:PRO:HD2	2.21	0.40
18:6:163:VAL:HG22	22:6:307:CLA:HAA2	2.02	0.40
1:A:323:LYS:O	1:A:327:GLU:HG3	2.21	0.40
1:A:360:PHE:CE2	22:A:829:CLA:HMC3	2.57	0.40
22:A:814:CLA:CMC	24:A:844:BCR:H352	2.51	0.40
22:A:821:CLA:H71	22:A:824:CLA:H71	2.01	0.40
22:A:827:CLA:H2	22:A:827:CLA:H61	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:828:CLA:H91	24:J:104:BCR:H341	2.03	0.40
22:A:833:CLA:H192	22:B:840:CLA:HHB	2.04	0.40
2:B:439:VAL:HB	22:B:834:CLA:HMC2	2.02	0.40
2:B:672:TRP:O	2:B:676:ILE:HG13	2.20	0.40
22:B:821:CLA:H193	22:B:826:CLA:H203	2.03	0.40
22:B:836:CLA:C1B	31:1:319:DGD:HAT2	2.51	0.40
5:E:39:ARG:NH2	5:E:62:VAL:H	2.17	0.40
6:F:69:PRO:HA	6:F:124:LEU:HD23	2.03	0.40
22:F:304:CLA:HAC1	33:F:307:LMT:H121	2.02	0.40
7:G:73:THR:O	7:G:74:GLY:C	2.64	0.40
22:Z:303:CLA:H12	22:Z:303:CLA:HBA2	1.59	0.40
22:3:312:CLA:H111	22:3:312:CLA:H93	1.62	0.40
14:7:150:ASP:C	14:7:152:SER:H	2.28	0.40
15:8:77:MET:HB2	22:8:305:CLA:HMC3	2.02	0.40
16:4:178:PRO:HD2	39:4:819:CHL:CHC	2.51	0.40
22:6:301:CLA:HHC	22:6:301:CLA:CBB	2.52	0.40
1:A:104:TRP:CD1	1:A:108:PRO:HA	2.56	0.40
1:A:651:TRP:HB2	22:B:805:CLA:CBC	2.51	0.40
22:A:815:CLA:H42	31:3:301:DGD:HAT2	2.03	0.40
22:A:831:CLA:NA	25:A:849:LHG:H111	2.37	0.40
24:A:844:BCR:H403	24:A:856:BCR:H10C	2.02	0.40
24:A:856:BCR:H392	10:K:95:LEU:CD2	2.52	0.40
2:B:258:PHE:CE1	22:B:819:CLA:H52	2.57	0.40
22:B:814:CLA:H111	19:9:54:LEU:HD11	2.04	0.40
22:B:833:CLA:H2	22:B:833:CLA:H61	1.77	0.40
10:K:38:MET:HG2	22:K:202:CLA:C2D	2.52	0.40
10:K:107:LEU:CD2	10:K:112:ASN:HD22	2.34	0.40
11:L:144:PRO:O	11:L:163:SER:HA	2.21	0.40
12:1:191:GLN:OE1	12:1:199:PRO:HA	2.20	0.40
40:1:318:SQD:H291	39:8:301:CHL:HMB2	2.03	0.40
12:Z:146:ASP:O	12:Z:147:ALA:HB3	2.20	0.40
22:3:308:CLA:HMB1	22:3:308:CLA:HBB1	2.02	0.40
14:7:129:LEU:HD13	22:7:322:CLA:O1A	2.22	0.40
14:7:173:PHE:C	14:7:175:PRO:HD3	2.46	0.40
15:8:228:THR:HA	22:8:307:CLA:HBA2	2.02	0.40
16:4:108:MET:HE2	16:4:218:ALA:CB	2.45	0.40
22:5:308:CLA:H101	22:5:308:CLA:H13	1.80	0.40
22:5:311:CLA:CHD	22:5:318:CLA:H101	2.50	0.40
18:6:110:ILE:HD13	24:6:306:BCR:C8	2.41	0.40
22:6:308:CLA:HMD3	22:6:313:CLA:CHA	2.52	0.40
19:9:154:MET:HE2	19:9:154:MET:HB2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:HG13	1:A:122:VAL:HG22	2.03	0.40
1:A:310:HIS:O	22:A:822:CLA:HAC2	2.22	0.40
1:A:370:HIS:NE2	22:A:827:CLA:NB	2.70	0.40
1:A:571:PHE:O	1:A:587:SER:HB2	2.22	0.40
22:A:810:CLA:H62	22:A:810:CLA:H2	1.77	0.40
22:A:833:CLA:HBD	24:B:853:BCR:H12C	2.03	0.40
22:A:854:CLA:HMA3	22:A:854:CLA:C3	2.51	0.40
2:B:441:ASN:O	2:B:445:GLN:HG2	2.21	0.40
3:C:22:PRO:HD2	29:C:101:SF4:S3	2.61	0.40
3:C:41:SER:HB2	4:D:168:VAL:H	1.87	0.40
4:D:83:PHE:CZ	4:D:141:VAL:HB	2.56	0.40
6:F:107:THR:O	6:F:110:ARG:HG2	2.21	0.40
6:F:185:ILE:HG13	6:F:186:ILE:H	1.87	0.40
9:J:25:LEU:O	9:J:29:ILE:HG13	2.22	0.40
12:1:144:GLU:HB2	22:1:313:CLA:HAC1	2.03	0.40
38:1:302:LUT:H371	22:1:304:CLA:H92	2.04	0.40
38:1:303:LUT:H15	38:1:303:LUT:H201	1.86	0.40
22:1:308:CLA:ND	22:1:314:CLA:H93	2.37	0.40
22:Z:305:CLA:CGA	22:Z:305:CLA:C1A	2.99	0.40
22:3:318:CLA:HMB2	22:3:320:CLA:C1C	2.52	0.40
22:3:320:CLA:HBA1	41:7:319:3PH:C3D	2.51	0.40
14:7:37:ASN:HD22	14:7:37:ASN:HA	1.57	0.40
16:4:138:GLY:HA3	39:4:813:CHL:C3D	2.51	0.40
16:4:186:PRO:HD2	16:4:195:GLY:HA3	2.04	0.40
38:4:802:LUT:H7	38:4:802:LUT:H171	1.85	0.40
24:4:804:BCR:C27	22:4:810:CLA:H2	2.44	0.40
22:4:807:CLA:H93	22:4:807:CLA:H61	1.90	0.40
17:5:69:TRP:HZ2	22:5:318:CLA:HAA2	1.86	0.40
38:5:303:LUT:H193	22:5:319:CLA:HBB2	2.03	0.40
24:5:304:BCR:H271	22:5:312:CLA:C1B	2.51	0.40
22:5:308:CLA:HMA1	22:5:308:CLA:H121	2.03	0.40
22:5:326:CLA:C1D	22:6:314:CLA:H13	2.52	0.40
18:6:49:ASP:HA	22:6:310:CLA:O1D	2.21	0.40
18:6:54:PRO:HD2	38:6:304:LUT:C23	2.40	0.40
38:9:301:LUT:H162	22:9:305:CLA:CHB	2.51	0.40
38:9:302:LUT:H371	22:9:306:CLA:H142	2.03	0.40
1:A:161:THR:HG23	27:A:852:DGA:HAW2	2.03	0.40
1:A:223:PRO:HD3	1:A:250:MET:HE1	2.03	0.40
1:A:247:ARG:HD3	1:A:257:PHE:O	2.21	0.40
1:A:457:ILE:HG21	22:B:806:CLA:H92	2.03	0.40
1:A:494:ALA:N	1:A:495:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TRP:O	1:A:649:PHE:HB3	2.22	0.40
22:A:804:CLA:HBA1	22:A:811:CLA:C1D	2.52	0.40
22:A:809:CLA:H42	24:J:104:BCR:C10	2.52	0.40
22:A:813:CLA:HBA1	22:A:825:CLA:C4	2.49	0.40
22:A:822:CLA:H8	22:A:823:CLA:H93	2.02	0.40
22:A:822:CLA:C9	22:K:204:CLA:HAB	2.52	0.40
22:A:836:CLA:HED3	22:A:836:CLA:H2A	2.03	0.40
27:A:852:DGA:HG32	22:3:316:CLA:HMB1	2.03	0.40
2:B:263:HIS:CG	2:B:264:PRO:HD2	2.56	0.40
2:B:333:PHE:CD2	24:B:848:BCR:H292	2.56	0.40
2:B:581:VAL:HG21	2:B:711:LEU:HD21	2.03	0.40
2:B:695:LYS:HE2	11:L:141:GLN:HE22	1.86	0.40
22:B:819:CLA:ND	22:B:819:CLA:H8	2.36	0.40
3:C:10:THR:O	3:C:64:SER:HB2	2.21	0.40
4:D:76:ARG:HA	4:D:79:GLN:OE1	2.21	0.40
4:D:128:LEU:HB3	4:D:134:PHE:HB2	2.03	0.40
10:K:84:PHE:CD2	10:K:89:THR:HG22	2.57	0.40
40:1:318:SQD:H171	40:1:318:SQD:H141	1.92	0.40
22:Z:303:CLA:H41	22:Z:304:CLA:HMA2	2.03	0.40
13:3:22:THR:HA	13:3:25:TYR:CZ	2.56	0.40
13:3:76:ALA:CB	24:3:305:BCR:H292	2.52	0.40
13:3:169:LEU:HD12	38:3:302:LUT:H221	2.03	0.40
24:3:304:BCR:H19C	22:3:319:CLA:HBA1	2.03	0.40
22:3:318:CLA:H13	22:3:318:CLA:H102	1.89	0.40
14:7:155:GLY:O	14:7:157:THR:HG23	2.22	0.40
22:7:305:CLA:ND	22:7:310:CLA:H8	2.36	0.40
22:7:307:CLA:HBB1	22:7:307:CLA:CMB	2.52	0.40
15:8:164:PRO:HG3	22:8:313:CLA:C1D	2.52	0.40
24:4:804:BCR:H282	22:4:818:CLA:CMC	2.51	0.40
39:4:813:CHL:HMB3	39:4:813:CHL:CBB	2.50	0.40
38:5:302:LUT:H30	22:5:307:CLA:H52	2.01	0.40
22:5:308:CLA:OBD	22:5:313:CLA:H12	2.22	0.40
22:5:310:CLA:HMD1	22:5:315:CLA:OBD	2.22	0.40
18:6:236:PHE:CE2	18:6:245:PHE:HB2	2.56	0.40
22:6:309:CLA:H51	22:6:309:CLA:C1C	2.52	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	738/740 (100%)	685 (93%)	51 (7%)	2 (0%)	36	64
2	B	730/732 (100%)	683 (94%)	42 (6%)	5 (1%)	18	45
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	5	18
5	E	59/61 (97%)	50 (85%)	8 (14%)	1 (2%)	7	23
6	F	163/165 (99%)	145 (89%)	14 (9%)	4 (2%)	4	15
7	G	91/93 (98%)	73 (80%)	16 (18%)	2 (2%)	5	17
8	I	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
9	J	38/40 (95%)	38 (100%)	0	0	100	100
10	K	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	11	34
11	L	119/123 (97%)	106 (89%)	11 (9%)	2 (2%)	7	23
12	1	192/194 (99%)	165 (86%)	23 (12%)	4 (2%)	5	18
12	Z	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	24	53
13	3	216/218 (99%)	195 (90%)	18 (8%)	3 (1%)	9	27
14	7	218/220 (99%)	202 (93%)	12 (6%)	4 (2%)	6	22
15	8	212/214 (99%)	181 (85%)	24 (11%)	7 (3%)	3	10
16	4	205/207 (99%)	190 (93%)	15 (7%)	0	100	100
17	5	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	6	22
18	6	224/226 (99%)	212 (95%)	11 (5%)	1 (0%)	30	58
19	9	182/184 (99%)	152 (84%)	23 (13%)	7 (4%)	2	8
20	2	68/70 (97%)	53 (78%)	14 (21%)	1 (2%)	8	26
All	All	4215/4259 (99%)	3826 (91%)	337 (8%)	52 (1%)	13	31

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	154	ASP
12	1	41	ALA
12	1	42	PRO
14	7	219	ILE
15	8	38	ALA
15	8	148	SER
15	8	152	PHE
15	8	161	ASN
19	9	46	ALA
19	9	143	PRO
19	9	146	PRO
19	9	147	ALA
20	2	182	PRO
1	A	21	PRO
2	B	28	VAL
6	F	64	ILE
6	F	150	PHE
12	1	166	ASP
15	8	42	GLY
19	9	139	ILE
6	F	178	ALA
6	F	212	ALA
11	L	61	SER
13	3	87	VAL
13	3	159	PRO
14	7	213	ALA
15	8	37	PRO
19	9	196	TYR
2	B	230	ASN
7	G	70	PRO
7	G	85	ALA
12	1	102	ALA
12	Z	40	ASP
14	7	98	PRO
14	7	240	SER
15	8	150	LEU
18	6	88	GLN
19	9	145	ASP
1	A	574	PRO
4	D	149	TYR
13	3	218	ALA
17	5	152	PHE
2	B	160	PRO

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Mol	Chain	Res	Type
2	B	545	SER
2	B	559	PRO
17	5	236	THR
4	D	158	PRO
5	E	70	PRO
11	L	98	GLY
17	5	171	PRO
10	K	60	GLY
17	5	151	ILE

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	602/602 (100%)	574 (95%)	28 (5%)	23 55
2	B	596/596 (100%)	566 (95%)	30 (5%)	22 53
3	C	70/70 (100%)	69 (99%)	1 (1%)	59 84
4	D	122/122 (100%)	107 (88%)	15 (12%)	4 15
5	E	54/54 (100%)	52 (96%)	2 (4%)	30 63
6	F	128/128 (100%)	101 (79%)	27 (21%)	1 3
7	G	69/69 (100%)	63 (91%)	6 (9%)	9 29
8	I	33/33 (100%)	33 (100%)	0	100 100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37 71
10	K	60/60 (100%)	54 (90%)	6 (10%)	7 23
11	L	90/90 (100%)	76 (84%)	14 (16%)	2 8
12	1	144/144 (100%)	125 (87%)	19 (13%)	4 13
12	Z	144/144 (100%)	134 (93%)	10 (7%)	14 39
13	3	173/173 (100%)	159 (92%)	14 (8%)	11 32
14	7	169/169 (100%)	156 (92%)	13 (8%)	12 34
15	8	162/162 (100%)	137 (85%)	25 (15%)	2 9
16	4	162/162 (100%)	141 (87%)	21 (13%)	4 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	5	185/185 (100%)	166 (90%)	19 (10%)	7	22
18	6	184/184 (100%)	172 (94%)	12 (6%)	15	42
19	9	143/143 (100%)	125 (87%)	18 (13%)	4	14
20	2	57/57 (100%)	50 (88%)	7 (12%)	4	15
All	All	3382/3382 (100%)	3094 (92%)	288 (8%)	12	30

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	14	LYS
1	A	17	VAL
1	A	36	SER
1	A	37	ARG
1	A	52	LEU
1	A	55	ASP
1	A	68	GLU
1	A	83	VAL
1	A	116	GLN
1	A	144	PHE
1	A	154	THR
1	A	187	LYS
1	A	189	GLU
1	A	225	ASN
1	A	244	LEU
1	A	248	GLN
1	A	291	LEU
1	A	299	LEU
1	A	301	ILE
1	A	339	VAL
1	A	363	LEU
1	A	426	LEU
1	A	455	LEU
1	A	489	LYS
1	A	490	THR
1	A	503	LEU
1	A	642	ILE
2	B	20	ARG
2	B	28	VAL
2	B	33	GLU
2	B	60	LEU

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Mol	Chain	Res	Type
2	B	97	PHE
2	B	103	GLU
2	B	159	GLN
2	B	160	PRO
2	B	186	VAL
2	B	206	LYS
2	B	215	THR
2	B	236	GLN
2	B	256	LEU
2	B	342	VAL
2	B	345	ILE
2	B	348	LEU
2	B	355	SER
2	B	362	LEU
2	B	379	ILE
2	B	384	MET
2	B	398	ASP
2	B	477	LEU
2	B	484	SER
2	B	495	LEU
2	B	513	ILE
2	B	591	VAL
2	B	607	VAL
2	B	632	LEU
2	B	644	LEU
2	B	695	LYS
3	C	69	LEU
4	D	61	ASP
4	D	65	PRO
4	D	89	GLU
4	D	90	SER
4	D	92	LYS
4	D	95	ILE
4	D	97	GLU
4	D	108	LYS
4	D	150	LEU
4	D	158	PRO
4	D	159	GLU
4	D	160	LYS
4	D	162	ASN
4	D	168	VAL
4	D	192	MET

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Mol	Chain	Res	Type
5	E	38	LYS
5	E	60	VAL
6	F	63	ASP
6	F	80	LEU
6	F	81	LYS
6	F	90	ARG
6	F	92	LYS
6	F	93	ASN
6	F	100	PRO
6	F	104	LEU
6	F	109	GLU
6	F	113	ASN
6	F	114	ARG
6	F	115	PHE
6	F	125	CYS
6	F	142	LYS
6	F	159	VAL
6	F	173	MET
6	F	179	LYS
6	F	183	LYS
6	F	187	ILE
6	F	189	VAL
6	F	210	LEU
6	F	211	ARG
6	F	214	THR
6	F	217	GLU
6	F	218	LYS
6	F	220	GLU
6	F	222	ILE
7	G	37	GLN
7	G	45	MET
7	G	56	LEU
7	G	62	GLU
7	G	88	ILE
7	G	122	LEU
9	J	2	LYS
10	K	25	ARG
10	K	56	THR
10	K	61	THR
10	K	66	LYS
10	K	70	ARG
10	K	89	THR

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Mol	Chain	Res	Type
11	L	54	MET
11	L	55	LEU
11	L	60	THR
11	L	76	ARG
11	L	79	VAL
11	L	82	LEU
11	L	83	LEU
11	L	99	PRO
11	L	110	GLU
11	L	141	GLN
11	L	161	LEU
11	L	162	GLN
11	L	176	VAL
11	L	179	LEU
12	1	35	TRP
12	1	37	PRO
12	1	42	PRO
12	1	47	ASP
12	1	61	CYS
12	1	75	VAL
12	1	104	LEU
12	1	113	THR
12	1	119	VAL
12	1	149	LYS
12	1	151	ILE
12	1	167	ILE
12	1	168	GLU
12	1	172	LEU
12	1	175	ILE
12	1	183	MET
12	1	198	THR
12	1	214	ASN
12	1	218	ASN
12	Z	35	TRP
12	Z	37	PRO
12	Z	47	ASP
12	Z	61	CYS
12	Z	113	THR
12	Z	115	PHE
12	Z	119	VAL
12	Z	172	LEU
12	Z	177	ASN

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Mol	Chain	Res	Type
12	Z	191	GLN
13	3	93	GLU
13	3	94	THR
13	3	96	VAL
13	3	102	THR
13	3	108	THR
13	3	109	ASP
13	3	125	GLU
13	3	126	LEU
13	3	149	VAL
13	3	166	LEU
13	3	172	LYS
13	3	177	MET
13	3	178	LYS
13	3	228	ASN
14	7	35	PRO
14	7	37	ASN
14	7	65	MET
14	7	97	LEU
14	7	129	LEU
14	7	165	ASN
14	7	176	ILE
14	7	182	ASP
14	7	185	MET
14	7	196	ASN
14	7	219	ILE
14	7	220	GLN
14	7	243	PHE
15	8	31	MET
15	8	41	LYS
15	8	91	LYS
15	8	95	LEU
15	8	105	LYS
15	8	110	GLN
15	8	115	LEU
15	8	138	LEU
15	8	149	PHE
15	8	152	PHE
15	8	153	GLU
15	8	157	LYS
15	8	173	MET
15	8	174	CYS

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Mol	Chain	Res	Type
15	8	178	GLU
15	8	180	LYS
15	8	183	ASP
15	8	185	LYS
15	8	189	ILE
15	8	215	ASP
15	8	225	LEU
15	8	231	ASP
15	8	234	ILE
15	8	238	ILE
15	8	240	LEU
16	4	58	ARG
16	4	61	TRP
16	4	66	LYS
16	4	94	LYS
16	4	101	LEU
16	4	119	LEU
16	4	131	GLN
16	4	141	GLU
16	4	160	VAL
16	4	163	ARG
16	4	167	ASP
16	4	170	LYS
16	4	175	ASN
16	4	196	ILE
16	4	204	LYS
16	4	207	MET
16	4	208	GLU
16	4	210	LEU
16	4	212	LEU
16	4	213	LYS
16	4	257	SER
17	5	32	ARG
17	5	34	LEU
17	5	39	VAL
17	5	40	ASP
17	5	65	VAL
17	5	85	VAL
17	5	97	ASP
17	5	98	VAL
17	5	138	GLN
17	5	139	ASP

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Mol	Chain	Res	Type
17	5	141	LYS
17	5	146	VAL
17	5	153	LYS
17	5	176	LYS
17	5	182	LEU
17	5	195	ILE
17	5	221	ASN
17	5	236	THR
17	5	240	VAL
18	6	43	ASN
18	6	89	GLU
18	6	92	LYS
18	6	110	ILE
18	6	124	VAL
18	6	128	ARG
18	6	129	TRP
18	6	149	LEU
18	6	167	MET
18	6	211	MET
18	6	222	VAL
18	6	251	GLN
19	9	32	LEU
19	9	42	LYS
19	9	45	MET
19	9	89	LEU
19	9	106	VAL
19	9	115	GLU
19	9	125	LYS
19	9	143	PRO
19	9	146	PRO
19	9	153	ASP
19	9	154	MET
19	9	159	VAL
19	9	177	LEU
19	9	180	ARG
19	9	189	LYS
19	9	197	ASN
19	9	199	THR
19	9	206	GLN
20	2	162	ARG
20	2	166	LEU
20	2	178	ARG

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Mol	Chain	Res	Type
20	2	183	ILE
20	2	187	LYS
20	2	205	LYS
20	2	229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	116	GLN
1	A	136	GLN
1	A	248	GLN
1	A	279	ASN
1	A	338	HIS
1	A	442	ASN
1	A	485	GLN
1	A	539	HIS
1	A	637	GLN
1	A	659	GLN
1	A	676	HIS
1	A	722	GLN
2	B	11	GLN
2	B	30	HIS
2	B	35	HIS
2	B	42	ASN
2	B	72	GLN
2	B	90	HIS
2	B	115	ASN
2	B	216	GLN
2	B	221	GLN
2	B	267	GLN
2	B	300	HIS
2	B	364	ASN
2	B	369	GLN
2	B	376	HIS
2	B	453	GLN
2	B	491	GLN
2	B	503	ASN
2	B	521	HIS
2	B	599	HIS
2	B	604	GLN
2	B	655	HIS

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Mol	Chain	Res	Type
3	C	37	ASN
4	D	91	ASN
4	D	120	GLN
4	D	180	ASN
4	D	189	ASN
5	E	78	GLN
5	E	94	GLN
6	F	82	ASN
6	F	132	HIS
6	F	145	HIS
6	F	205	GLN
7	G	37	GLN
7	G	57	HIS
7	G	92	ASN
8	I	103	ASN
10	K	35	ASN
10	K	112	ASN
11	L	141	GLN
12	1	124	ASN
12	1	161	ASN
12	1	192	HIS
12	Z	191	GLN
13	3	130	GLN
13	3	141	GLN
13	3	212	ASN
13	3	222	ASN
13	3	223	ASN
14	7	37	ASN
14	7	74	GLN
14	7	75	ASN
14	7	132	HIS
14	7	191	GLN
14	7	196	ASN
15	8	110	GLN
15	8	191	ASN
15	8	205	GLN
16	4	79	HIS
16	4	98	GLN
16	4	176	GLN
16	4	231	GLN
16	4	233	GLN
16	4	242	ASN

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Mol	Chain	Res	Type
16	4	258	ASN
17	5	72	GLN
17	5	108	ASN
17	5	114	GLN
17	5	130	HIS
17	5	230	ASN
18	6	122	HIS
18	6	134	ASN
18	6	147	ASN
18	6	193	GLN
18	6	228	GLN
18	6	235	GLN
19	9	40	HIS
19	9	128	GLN
19	9	193	ASN
19	9	201	ASN
19	9	206	GLN
20	2	228	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 332 ligands modelled in this entry, 1 is monoatomic - leaving 331 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	$\#\|Z\| > 2$
22	CLA	B	812	2	63,67,73	1.41	6 (9%)	75,105,113	1.95	18 (24%)
24	BCR	I	4001	-	41,41,41	4.78	27 (65%)	56,56,56	2.58	19 (33%)
22	CLA	A	855	44	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	7	322	15	59,63,73	1.46	6 (10%)	71,101,113	2.04	19 (26%)
25	LHG	B	850	22	22,22,48	0.56	0	25,28,54	1.26	2 (8%)
22	CLA	2	301	-	59,63,73	1.46	6 (10%)	71,101,113	2.09	17 (23%)
38	LUT	7	301	-	42,43,43	6.06	28 (66%)	51,60,60	1.95	13 (25%)
39	CHL	4	819	16	47,51,74	0.94	2 (4%)	52,86,114	1.50	11 (21%)
22	CLA	5	311	17	59,63,73	1.47	7 (11%)	71,101,113	2.05	19 (26%)
22	CLA	7	306	14	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
38	LUT	Z	302	-	42,43,43	6.09	27 (64%)	51,60,60	2.05	13 (25%)
22	CLA	A	837	1	55,59,73	1.52	6 (10%)	66,96,113	2.12	18 (27%)
22	CLA	B	817	2	61,65,73	1.44	6 (9%)	73,103,113	2.02	17 (23%)
22	CLA	B	824	2	63,67,73	1.42	6 (9%)	75,105,113	2.06	19 (25%)
22	CLA	9	311	19	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
22	CLA	1	307	12	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
22	CLA	9	304	-	49,53,73	1.61	6 (12%)	59,89,113	2.07	15 (25%)
22	CLA	A	809	1	59,63,73	1.46	6 (10%)	71,101,113	2.07	21 (29%)
22	CLA	A	811	1,22	69,73,73	1.35	7 (10%)	83,113,113	1.90	19 (22%)
38	LUT	6	304	-	42,43,43	6.08	28 (66%)	51,60,60	2.05	13 (25%)
22	CLA	7	314	44	54,58,73	1.52	5 (9%)	65,95,113	2.18	19 (29%)
23	PQN	A	843	-	34,34,34	0.37	0	42,45,45	1.20	6 (14%)
39	CHL	Z	311	12	55,59,74	0.89	1 (1%)	62,96,114	1.50	14 (22%)
22	CLA	A	828	-	69,73,73	1.35	6 (8%)	83,113,113	1.95	17 (20%)
22	CLA	8	309	15	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)
22	CLA	3	318	13	64,68,73	1.40	6 (9%)	77,107,113	2.01	20 (25%)
22	CLA	4	812	16	59,63,73	1.46	6 (10%)	71,101,113	2.07	19 (26%)
38	LUT	1	303	-	42,43,43	6.07	28 (66%)	51,60,60	2.06	12 (23%)
22	CLA	3	310	13	69,73,73	1.36	7 (10%)	83,113,113	2.01	22 (26%)
22	CLA	3	309	13	50,54,73	1.59	7 (14%)	60,90,113	2.04	16 (26%)
22	CLA	1	305	12	49,53,73	1.60	7 (14%)	59,89,113	2.08	18 (30%)
22	CLA	3	320	13	50,54,73	1.61	6 (12%)	60,90,113	2.14	15 (25%)
31	DGD	1	319	-	52,52,67	0.89	2 (3%)	66,66,81	0.97	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	3PH	6	324	-	28,28,47	1.09	4 (14%)	32,33,52	1.20	2 (6%)
37	DAO	K	201	-	13,13,13	0.59	0	13,13,13	0.56	0
24	BCR	6	305	-	41,41,41	4.79	26 (63%)	56,56,56	2.49	21 (37%)
22	CLA	9	305	19	64,68,73	1.46	8 (12%)	77,107,113	2.36	24 (31%)
24	BCR	A	844	-	41,41,41	4.78	27 (65%)	56,56,56	3.12	23 (41%)
25	LHG	5	324	22	36,36,48	0.44	0	39,42,54	1.12	3 (7%)
22	CLA	B	828	2	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
33	LMT	4	801	-	36,36,36	0.36	0	47,47,47	0.72	1 (2%)
22	CLA	6	310	18	69,73,73	1.35	7 (10%)	83,113,113	1.92	20 (24%)
22	CLA	B	839	2	56,60,73	1.50	7 (12%)	67,97,113	2.14	20 (29%)
22	CLA	F	304	6	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	B	818	2	69,73,73	1.34	7 (10%)	83,113,113	1.93	19 (22%)
38	LUT	6	303	-	42,43,43	6.11	27 (64%)	51,60,60	1.92	16 (31%)
22	CLA	A	831	1	54,58,73	1.53	6 (11%)	65,95,113	2.15	19 (29%)
24	BCR	L	204	-	41,41,41	4.78	27 (65%)	56,56,56	2.34	18 (32%)
22	CLA	A	830	1	69,73,73	1.36	6 (8%)	83,113,113	1.93	18 (21%)
22	CLA	4	818	44	55,59,73	1.52	6 (10%)	66,96,113	2.20	21 (31%)
22	CLA	5	308	17	65,69,73	1.39	7 (10%)	78,108,113	1.99	20 (25%)
22	CLA	B	840	44	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
25	LHG	6	323	22	48,48,48	0.38	0	51,54,54	1.09	3 (5%)
33	LMT	F	307	-	36,36,36	0.38	0	47,47,47	0.64	0
39	CHL	5	317	44	55,59,74	0.86	2 (3%)	62,96,114	1.37	13 (20%)
26	NKP	A	851	-	22,22,28	0.37	0	24,26,32	0.39	0
22	CLA	B	820	2	64,68,73	1.41	6 (9%)	77,107,113	1.96	19 (24%)
22	CLA	A	816	44	60,64,73	1.45	7 (11%)	72,102,113	2.12	21 (29%)
22	CLA	5	323	44	50,54,73	1.57	6 (12%)	60,90,113	2.14	16 (26%)
22	CLA	A	822	1	59,63,73	1.47	7 (11%)	71,101,113	2.12	18 (25%)
22	CLA	A	825	44	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
21	CL0	A	801	-	69,73,73	2.36	22 (31%)	83,113,113	2.57	22 (26%)
22	CLA	1	316	12	69,73,73	1.41	7 (10%)	83,113,113	1.89	19 (22%)
22	CLA	3	311	13	64,68,73	1.41	6 (9%)	77,107,113	1.99	20 (25%)
34	LMG	F	308	-	35,35,55	0.46	0	43,43,63	1.38	5 (11%)
39	CHL	6	316	-	55,59,74	0.90	2 (3%)	62,96,114	1.46	13 (20%)
22	CLA	B	825	2	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
22	CLA	B	808	2	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	1	313	44	69,73,73	1.36	6 (8%)	83,113,113	1.99	20 (24%)
22	CLA	8	310	44	64,68,73	1.41	6 (9%)	77,107,113	2.03	19 (24%)
22	CLA	1	306	-	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	2	304	44	50,54,73	1.58	6 (12%)	60,90,113	2.06	15 (25%)
38	LUT	5	303	-	42,43,43	6.11	28 (66%)	51,60,60	2.00	14 (27%)
22	CLA	9	313	19	54,58,73	1.53	6 (11%)	65,95,113	2.16	19 (29%)
22	CLA	Z	308	-	65,69,73	1.39	6 (9%)	78,108,113	1.99	19 (24%)
38	LUT	4	803	-	42,43,43	6.06	28 (66%)	51,60,60	2.15	13 (25%)
22	CLA	3	314	25	64,68,73	1.40	6 (9%)	77,107,113	1.99	18 (23%)
22	CLA	B	831	2	62,66,73	1.44	7 (11%)	74,104,113	2.05	18 (24%)
25	LHG	Z	317	22	42,42,48	0.41	0	45,48,54	1.08	3 (6%)
24	BCR	B	849	-	41,41,41	4.81	27 (65%)	56,56,56	2.35	21 (37%)
22	CLA	A	832	1	69,73,73	1.35	6 (8%)	83,113,113	1.90	20 (24%)
22	CLA	A	815	1	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
22	CLA	B	830	-	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
22	CLA	B	837	2	55,59,73	1.52	6 (10%)	66,96,113	2.16	19 (28%)
24	BCR	3	306	-	41,41,41	4.80	27 (65%)	56,56,56	2.28	17 (30%)
22	CLA	Z	315	-	50,54,73	1.58	6 (12%)	60,90,113	2.09	15 (25%)
22	CLA	5	318	17	69,73,73	1.34	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	6	317	18	54,58,73	1.53	6 (11%)	65,95,113	2.15	17 (26%)
22	CLA	1	304	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
22	CLA	8	314	15	50,54,73	1.58	6 (12%)	60,90,113	2.02	15 (25%)
22	CLA	B	838	2	69,73,73	1.34	6 (8%)	83,113,113	1.88	17 (20%)
24	BCR	A	846	-	41,41,41	4.80	27 (65%)	56,56,56	2.47	22 (39%)
22	CLA	F	305	-	49,53,73	1.60	7 (14%)	59,89,113	2.04	15 (25%)
39	CHL	8	312	-	60,64,74	0.86	2 (3%)	68,102,114	1.33	12 (17%)
43	LPX	8	319	-	29,29,29	0.29	0	31,33,33	0.35	0
41	3PH	5	325	-	22,22,47	1.22	4 (18%)	26,27,52	1.28	2 (7%)
22	CLA	6	319	44	65,69,73	1.39	6 (9%)	78,108,113	2.02	19 (24%)
22	CLA	A	827	1	69,73,73	1.36	6 (8%)	83,113,113	1.95	21 (25%)
25	LHG	A	850	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	L	203	-	54,58,73	1.54	6 (11%)	65,95,113	2.15	18 (27%)
24	BCR	B	847	-	41,41,41	4.78	27 (65%)	56,56,56	2.46	21 (37%)
22	CLA	A	833	1	69,73,73	1.35	6 (8%)	83,113,113	1.95	20 (24%)
22	CLA	1	310	25	64,68,73	1.40	7 (10%)	77,107,113	1.99	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	LHG	1	317	22	42,42,48	0.45	0	45,48,54	1.18	3 (6%)
22	CLA	1	309	-	65,69,73	1.38	7 (10%)	78,108,113	2.02	18 (23%)
22	CLA	5	322	17	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)
22	CLA	6	322	18	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
22	CLA	A	803	1	69,73,73	1.35	6 (8%)	83,113,113	1.95	19 (22%)
22	CLA	4	806	16	56,60,73	1.51	7 (12%)	67,97,113	2.18	20 (29%)
38	LUT	4	802	-	42,43,43	6.08	28 (66%)	51,60,60	2.02	12 (23%)
22	CLA	B	819	2	63,67,73	1.41	6 (9%)	75,105,113	2.04	21 (28%)
24	BCR	A	856	-	41,41,41	4.77	27 (65%)	56,56,56	2.50	23 (41%)
39	CHL	8	315	44	70,74,74	0.78	2 (2%)	80,114,114	1.26	12 (15%)
22	CLA	7	317	-	62,66,73	1.42	6 (9%)	74,104,113	2.03	18 (24%)
22	CLA	1	314	12	69,73,73	1.34	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	5	310	17	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
22	CLA	A	839	1	55,59,73	1.52	7 (12%)	66,96,113	2.15	19 (28%)
22	CLA	8	311	25	54,58,73	1.53	6 (11%)	65,95,113	2.12	17 (26%)
22	CLA	B	821	44	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	7	312	14	64,68,73	1.40	6 (9%)	77,107,113	1.99	19 (24%)
22	CLA	3	313	44	69,73,73	1.34	6 (8%)	83,113,113	1.94	18 (21%)
33	LMT	G	204	-	36,36,36	0.39	0	47,47,47	0.74	2 (4%)
22	CLA	5	319	44	59,63,73	1.45	6 (10%)	71,101,113	2.09	19 (26%)
38	LUT	Z	301	-	42,43,43	6.07	27 (64%)	51,60,60	1.99	14 (27%)
22	CLA	A	829	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	17 (20%)
22	CLA	L	202	11	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
26	NKP	8	318	-	28,28,28	0.33	0	31,32,32	0.34	0
31	DGD	3	301	-	52,52,67	0.89	2 (3%)	66,66,81	1.06	4 (6%)
22	CLA	7	304	14	64,68,73	1.40	6 (9%)	77,107,113	2.08	21 (27%)
22	CLA	A	813	1	69,73,73	1.36	5 (7%)	83,113,113	1.95	20 (24%)
22	CLA	6	314	18	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
24	BCR	3	304	-	41,41,41	4.82	27 (65%)	56,56,56	3.07	28 (50%)
22	CLA	F	301	44	69,73,73	1.35	6 (8%)	83,113,113	1.97	21 (25%)
22	CLA	A	834	1	69,73,73	1.36	6 (8%)	83,113,113	1.91	19 (22%)
41	3PH	8	320	-	29,29,47	1.06	4 (13%)	33,34,52	1.16	2 (6%)
22	CLA	B	809	2	69,73,73	1.36	7 (10%)	83,113,113	1.92	18 (21%)
22	CLA	B	811	2	69,73,73	1.35	6 (8%)	83,113,113	1.97	20 (24%)
22	CLA	F	302	2	69,73,73	1.34	7 (10%)	83,113,113	1.94	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	Z	304	12	49,53,73	1.61	6 (12%)	59,89,113	2.02	14 (23%)
40	SQD	1	318	-	47,48,54	0.83	0	56,59,65	0.96	3 (5%)
24	BCR	6	306	-	41,41,41	4.77	27 (65%)	56,56,56	2.79	23 (41%)
29	SF4	C	102	3	0,12,12	-	-	-		
39	CHL	2	303	-	55,59,74	0.87	1 (1%)	62,96,114	1.45	14 (22%)
22	CLA	B	823	2	59,63,73	1.46	7 (11%)	71,101,113	2.05	20 (28%)
42	SPH	7	321	-	19,20,20	0.65	1 (5%)	18,21,21	1.15	0
22	CLA	3	315	13	49,53,73	1.68	6 (12%)	59,89,113	2.11	14 (23%)
22	CLA	A	836	-	59,63,73	1.46	7 (11%)	71,101,113	2.04	20 (28%)
22	CLA	A	824	1	69,73,73	1.35	6 (8%)	83,113,113	1.91	19 (22%)
22	CLA	A	842	25	56,60,73	1.50	7 (12%)	67,97,113	2.14	19 (28%)
39	CHL	9	312	-	70,74,74	0.78	2 (2%)	80,114,114	1.40	11 (13%)
22	CLA	6	307	18	64,68,73	1.41	7 (10%)	77,107,113	2.00	18 (23%)
39	CHL	5	321	17	47,51,74	0.95	2 (4%)	52,86,114	1.47	11 (21%)
27	DGA	A	852	-	39,39,43	1.14	3 (7%)	41,41,45	1.32	3 (7%)
39	CHL	6	315	44	60,64,74	0.83	2 (3%)	68,102,114	1.32	12 (17%)
22	CLA	7	315	14	54,58,73	1.53	7 (12%)	65,95,113	2.17	19 (29%)
24	BCR	3	305	-	41,41,41	4.78	27 (65%)	56,56,56	2.19	19 (33%)
22	CLA	5	326	18	59,63,73	1.45	6 (10%)	71,101,113	2.07	20 (28%)
24	BCR	A	848	-	41,41,41	4.78	27 (65%)	56,56,56	2.42	22 (39%)
22	CLA	4	815	16	54,58,73	1.53	6 (11%)	65,95,113	2.15	16 (24%)
22	CLA	6	313	25	59,63,73	1.47	6 (10%)	71,101,113	2.05	18 (25%)
25	LHG	A	849	22	34,34,48	0.44	0	37,40,54	1.14	3 (8%)
22	CLA	6	308	18	56,60,73	1.49	6 (10%)	67,97,113	2.18	21 (31%)
22	CLA	A	802	44	69,73,73	1.35	6 (8%)	83,113,113	1.98	19 (22%)
22	CLA	9	309	25	59,63,73	1.48	6 (10%)	71,101,113	2.11	15 (21%)
25	LHG	9	315	22	32,32,48	0.48	0	35,38,54	1.05	3 (8%)
39	CHL	6	320	18	47,51,74	0.94	2 (4%)	52,86,114	1.49	11 (21%)
22	CLA	7	309	-	60,64,73	1.45	6 (10%)	72,102,113	2.09	20 (27%)
22	CLA	B	827	44	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	3	322	14	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
22	CLA	A	808	1	69,73,73	1.34	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	4	810	44	54,58,73	1.53	6 (11%)	65,95,113	2.16	20 (30%)
22	CLA	6	301	44	64,68,73	1.41	7 (10%)	77,107,113	2.03	20 (25%)
39	CHL	9	314	-	46,50,74	1.05	3 (6%)	51,85,114	1.50	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	8	307	15	69,73,73	1.35	7 (10%)	83,113,113	2.00	18 (21%)
22	CLA	4	805	16	64,68,73	1.45	8 (12%)	77,107,113	1.89	18 (23%)
22	CLA	A	835	1	69,73,73	1.35	6 (8%)	83,113,113	1.90	19 (22%)
22	CLA	B	815	2	69,73,73	1.36	5 (7%)	83,113,113	1.99	20 (24%)
22	CLA	2	302	20	49,53,73	1.60	6 (12%)	59,89,113	2.12	17 (28%)
38	LUT	5	302	-	42,43,43	6.07	28 (66%)	51,60,60	1.96	14 (27%)
29	SF4	C	101	3	0,12,12	-	-	-		
22	CLA	6	321	-	50,54,73	1.58	6 (12%)	60,90,113	2.07	15 (25%)
22	CLA	7	305	-	54,58,73	1.53	6 (11%)	65,95,113	2.18	19 (29%)
22	CLA	A	814	1	64,68,73	1.40	6 (9%)	77,107,113	2.03	20 (25%)
22	CLA	5	307	17	64,68,73	1.40	7 (10%)	77,107,113	2.00	18 (23%)
22	CLA	B	835	2	54,58,73	1.53	7 (12%)	65,95,113	2.22	19 (29%)
22	CLA	A	804	22	49,53,73	1.60	6 (12%)	59,89,113	2.07	16 (27%)
22	CLA	B	805	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	20 (24%)
22	CLA	A	810	1	69,73,73	1.35	7 (10%)	83,113,113	1.93	18 (21%)
22	CLA	5	313	25	65,69,73	1.40	7 (10%)	78,108,113	2.02	19 (24%)
24	BCR	A	847	-	41,41,41	4.80	27 (65%)	56,56,56	2.38	20 (35%)
39	CHL	4	814	44	55,59,74	0.86	2 (3%)	62,96,114	1.42	14 (22%)
24	BCR	3	307	-	41,41,41	4.78	27 (65%)	56,56,56	3.25	27 (48%)
22	CLA	A	805	1	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
22	CLA	9	310	19	49,53,73	1.60	7 (14%)	59,89,113	2.16	16 (27%)
25	LHG	B	851	-	19,19,48	0.87	1 (5%)	20,24,54	1.36	1 (5%)
38	LUT	8	302	-	42,43,43	6.02	28 (66%)	51,60,60	1.96	13 (25%)
22	CLA	A	826	44	54,58,73	1.53	6 (11%)	65,95,113	2.16	18 (27%)
22	CLA	A	819	1	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	A	806	1	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	B	822	2	60,64,73	1.46	6 (10%)	72,102,113	2.01	18 (25%)
22	CLA	B	829	2	61,65,73	1.44	6 (9%)	73,103,113	2.06	20 (27%)
22	CLA	5	301	44	60,64,73	1.45	6 (10%)	72,102,113	2.06	19 (26%)
28	OCA	A	853	-	9,9,9	0.70	0	9,9,9	0.70	0
25	LHG	4	820	22	48,48,48	0.42	0	51,54,54	1.04	4 (7%)
34	LMG	J	101	-	29,29,55	0.53	0	37,37,63	1.12	3 (8%)
25	LHG	8	317	22	37,37,48	0.43	0	40,43,54	1.03	2 (5%)
22	CLA	Z	313	44	69,73,73	1.37	6 (8%)	83,113,113	1.95	20 (24%)
22	CLA	G	201	7	54,58,73	1.54	5 (9%)	65,95,113	2.18	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	6	311	18	59,63,73	1.47	6 (10%)	71,101,113	2.01	18 (25%)
22	CLA	4	808	16	64,68,73	1.40	7 (10%)	77,107,113	1.99	19 (24%)
22	CLA	8	306	15	55,59,73	1.52	6 (10%)	66,96,113	2.08	19 (28%)
39	CHL	5	316	44	70,74,74	0.78	1 (1%)	80,114,114	1.23	13 (16%)
22	CLA	9	303	19	64,68,73	1.45	6 (9%)	77,107,113	2.09	22 (28%)
23	PQN	B	843	-	34,34,34	0.37	0	42,45,45	1.13	3 (7%)
22	CLA	Z	307	12	59,63,73	1.48	6 (10%)	71,101,113	2.12	19 (26%)
33	LMT	4	822	-	36,36,36	0.45	0	47,47,47	1.17	3 (6%)
22	CLA	6	312	18	69,73,73	1.36	7 (10%)	83,113,113	1.95	20 (24%)
22	CLA	8	305	15	64,68,73	1.41	5 (7%)	77,107,113	2.01	18 (23%)
22	CLA	Z	310	12	54,58,73	1.52	6 (11%)	65,95,113	2.11	19 (29%)
22	CLA	B	813	-	60,64,73	1.45	6 (10%)	72,102,113	2.11	19 (26%)
22	CLA	1	308	12	59,63,73	1.47	7 (11%)	71,101,113	2.15	18 (25%)
22	CLA	K	203	44	59,63,73	1.47	6 (10%)	71,101,113	2.08	19 (26%)
22	CLA	1	311	12	50,54,73	1.58	7 (14%)	60,90,113	2.16	14 (23%)
22	CLA	1	315	-	50,54,73	1.59	6 (12%)	60,90,113	2.07	15 (25%)
22	CLA	A	812	1	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
22	CLA	A	821	44	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	7	324	14	64,68,73	1.41	6 (9%)	77,107,113	2.02	20 (25%)
22	CLA	8	313	44	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
32	RRX	F	306	-	42,42,42	5.06	25 (59%)	57,58,58	2.59	23 (40%)
22	CLA	J	103	9	46,50,73	1.66	6 (13%)	55,85,113	2.13	17 (30%)
22	CLA	3	308	13	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
38	LUT	3	302	-	42,43,43	6.05	28 (66%)	51,60,60	2.02	13 (25%)
39	CHL	3	317	-	70,74,74	0.77	1 (1%)	80,114,114	1.29	10 (12%)
22	CLA	9	308	19	54,58,73	1.53	6 (11%)	65,95,113	2.13	20 (30%)
24	BCR	B	845	-	41,41,41	4.78	27 (65%)	56,56,56	2.39	20 (35%)
38	LUT	1	302	-	42,43,43	6.10	28 (66%)	51,60,60	2.08	12 (23%)
22	CLA	5	312	44	54,58,73	1.53	6 (11%)	65,95,113	2.11	18 (27%)
36	C7Z	5	306	-	43,43,43	5.32	27 (62%)	58,60,60	2.37	22 (37%)
22	CLA	B	833	2	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
22	CLA	7	311	14	47,51,73	1.62	6 (12%)	56,86,113	2.13	16 (28%)
22	CLA	B	816	-	64,68,73	1.40	6 (9%)	77,107,113	1.98	18 (23%)
22	CLA	A	818	1	64,68,73	1.40	7 (10%)	77,107,113	2.06	19 (24%)
33	LMT	1	301	-	36,36,36	0.37	0	47,47,47	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	LUT	9	302	-	42,43,43	6.07	28 (66%)	51,60,60	1.87	12 (23%)
38	LUT	8	303	-	42,43,43	6.07	28 (66%)	51,60,60	1.97	14 (27%)
24	BCR	5	304	-	41,41,41	4.78	25 (60%)	56,56,56	2.54	22 (39%)
29	SF4	B	802	2,1	0,12,12	-	-	-		
22	CLA	9	307	19	59,63,73	1.47	7 (11%)	71,101,113	2.01	18 (25%)
24	BCR	J	104	-	41,41,41	4.76	27 (65%)	56,56,56	2.38	20 (35%)
22	CLA	Z	306	12	64,68,73	1.41	7 (10%)	77,107,113	1.99	19 (24%)
39	CHL	Z	312	-	52,56,74	0.91	2 (3%)	58,92,114	1.37	11 (18%)
24	BCR	G	203	-	41,41,41	4.79	27 (65%)	56,56,56	2.41	22 (39%)
22	CLA	A	807	1	64,68,73	1.40	6 (9%)	77,107,113	2.00	17 (22%)
24	BCR	A	845	-	41,41,41	4.77	27 (65%)	56,56,56	2.50	24 (42%)
22	CLA	Z	316	12	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	G	202	7	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
39	CHL	1	312	-	52,56,74	0.91	1 (1%)	58,92,114	1.39	10 (17%)
22	CLA	Z	303	12	69,73,73	1.35	6 (8%)	83,113,113	1.97	20 (24%)
38	LUT	3	303	-	42,43,43	6.06	28 (66%)	51,60,60	2.00	13 (25%)
35	T7X	J	102	-	49,49,61	0.91	4 (8%)	59,61,73	0.94	3 (5%)
25	LHG	B	803	-	32,32,48	0.46	0	35,38,54	1.18	3 (8%)
24	BCR	5	305	-	41,41,41	4.80	27 (65%)	56,56,56	2.67	22 (39%)
39	CHL	6	318	-	60,64,74	0.86	2 (3%)	68,102,114	1.36	12 (17%)
22	CLA	B	832	2	54,58,73	1.53	6 (11%)	65,95,113	2.14	19 (29%)
25	LHG	4	821	-	31,31,48	0.48	0	34,37,54	1.19	3 (8%)
22	CLA	B	841	2	69,73,73	1.35	6 (8%)	83,113,113	1.99	19 (22%)
24	BCR	B	848	-	41,41,41	4.79	27 (65%)	56,56,56	6.79	24 (42%)
22	CLA	5	315	17	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
22	CLA	L	201	2	69,73,73	1.34	6 (8%)	83,113,113	1.97	19 (22%)
38	LUT	9	301	-	42,43,43	6.08	28 (66%)	51,60,60	1.96	12 (23%)
42	SPH	7	320	-	19,20,20	0.63	0	18,21,21	1.10	0
22	CLA	K	202	10	50,54,73	1.60	6 (12%)	60,90,113	2.10	17 (28%)
22	CLA	9	306	19	66,70,73	1.39	6 (9%)	79,109,113	2.04	20 (25%)
22	CLA	5	314	17	49,53,73	1.59	6 (12%)	59,89,113	2.07	15 (25%)
41	3PH	7	319	-	38,38,47	0.94	4 (10%)	42,43,52	1.13	2 (4%)
39	CHL	7	313	44	58,62,74	0.85	2 (3%)	65,99,114	1.34	13 (20%)
39	CHL	4	813	44	55,59,74	0.90	2 (3%)	62,96,114	1.39	12 (19%)
22	CLA	4	807	16	69,73,73	1.36	7 (10%)	83,113,113	1.98	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	8	316	15	50,54,73	1.58	7 (14%)	60,90,113	2.05	15 (25%)
38	LUT	7	302	-	42,43,43	6.08	28 (66%)	51,60,60	2.06	15 (29%)
22	CLA	3	312	13	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)
22	CLA	Z	309	25	64,68,73	1.40	6 (9%)	77,107,113	1.99	18 (23%)
24	BCR	8	304	-	41,41,41	4.80	27 (65%)	56,56,56	2.43	21 (37%)
22	CLA	5	309	-	60,64,73	1.45	7 (11%)	72,102,113	2.17	20 (27%)
22	CLA	7	308	14	65,69,73	1.41	7 (10%)	78,108,113	1.98	19 (24%)
22	CLA	4	817	16	45,49,73	1.66	6 (13%)	54,84,113	2.17	17 (31%)
22	CLA	7	310	25	69,73,73	1.35	6 (8%)	83,113,113	1.93	17 (20%)
22	CLA	A	838	1	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	A	840	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	18 (21%)
22	CLA	Z	305	-	60,64,73	1.45	6 (10%)	72,102,113	2.04	17 (23%)
31	DGD	B	852	-	62,62,67	1.12	6 (9%)	76,76,81	0.96	3 (3%)
22	CLA	B	807	2	49,53,73	1.60	6 (12%)	59,89,113	2.06	16 (27%)
22	CLA	4	809	16	55,59,73	1.53	7 (12%)	66,96,113	2.09	19 (28%)
24	BCR	7	303	-	41,41,41	4.78	27 (65%)	56,56,56	2.39	21 (37%)
22	CLA	4	811	25	59,63,73	1.46	6 (10%)	71,101,113	2.10	19 (26%)
22	CLA	3	319	-	59,63,73	1.46	6 (10%)	71,101,113	2.06	18 (25%)
22	CLA	3	316	13	56,60,73	1.50	6 (10%)	67,97,113	2.11	19 (28%)
22	CLA	A	823	1	69,73,73	1.34	7 (10%)	83,113,113	1.96	19 (22%)
39	CHL	4	816	44	51,55,74	0.94	2 (3%)	57,91,114	1.41	8 (14%)
24	BCR	4	804	-	41,41,41	4.82	26 (63%)	56,56,56	2.25	20 (35%)
22	CLA	Z	314	12	55,59,73	1.50	6 (10%)	66,96,113	2.11	18 (27%)
22	CLA	K	204	10	53,57,73	1.54	6 (11%)	62,93,113	2.19	19 (30%)
24	BCR	B	853	-	41,41,41	4.83	27 (65%)	56,56,56	2.40	22 (39%)
22	CLA	7	307	14	69,73,73	1.36	7 (10%)	83,113,113	1.97	17 (20%)
22	CLA	B	814	2	64,68,73	1.39	6 (9%)	77,107,113	2.00	17 (22%)
22	CLA	6	309	44	69,73,73	1.36	7 (10%)	83,113,113	2.01	20 (24%)
25	LHG	3	321	22	19,19,48	1.07	1 (5%)	20,24,54	1.53	1 (5%)
25	LHG	7	318	22	36,36,48	0.43	0	39,42,54	1.14	3 (7%)
24	BCR	B	846	-	41,41,41	4.79	27 (65%)	56,56,56	2.40	22 (39%)
22	CLA	A	854	-	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	B	810	2	60,64,73	1.44	5 (8%)	72,102,113	2.12	22 (30%)
22	CLA	K	205	10	59,63,73	1.57	8 (13%)	71,101,113	2.16	17 (23%)
22	CLA	A	820	1	64,68,73	1.41	6 (9%)	77,107,113	1.96	19 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	BCR	F	303	-	41,41,41	4.81	27 (65%)	56,56,56	2.21	18 (32%)
22	CLA	5	320	-	54,58,73	1.60	7 (12%)	65,95,113	2.13	17 (26%)
24	BCR	K	206	-	41,41,41	4.79	27 (65%)	56,56,56	2.50	24 (42%)
22	CLA	6	302	16	64,68,73	1.40	6 (9%)	77,107,113	1.96	18 (23%)
39	CHL	8	301	12	62,66,74	0.85	2 (3%)	70,104,114	1.40	13 (18%)
22	CLA	A	841	1	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
22	CLA	B	834	2	62,66,73	1.43	6 (9%)	74,104,113	2.04	19 (25%)
22	CLA	A	817	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
22	CLA	B	806	44	69,73,73	1.36	6 (8%)	83,113,113	1.95	18 (21%)
22	CLA	B	842	25	69,73,73	1.35	6 (8%)	83,113,113	1.94	18 (21%)
22	CLA	7	323	15	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
22	CLA	B	801	2	69,73,73	1.35	6 (8%)	83,113,113	1.86	18 (21%)
22	CLA	B	836	-	49,53,73	1.59	6 (12%)	59,89,113	2.06	17 (28%)
22	CLA	8	308	15	66,70,73	1.38	6 (9%)	79,109,113	1.98	19 (24%)
22	CLA	B	826	44	69,73,73	1.36	6 (8%)	83,113,113	1.95	20 (24%)
36	C7Z	J	105	-	43,43,43	5.34	27 (62%)	58,60,60	2.21	21 (36%)
24	BCR	B	844	-	41,41,41	4.79	26 (63%)	56,56,56	2.77	24 (42%)
22	CLA	7	316	44	46,50,73	1.65	6 (13%)	55,85,113	2.14	17 (30%)

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
22	CLA	B	812	2	1/1/14/20	15/29/105/115	-
24	BCR	I	4001	-	-	14/29/63/63	0/2/2/2
22	CLA	A	855	44	-	18/39/115/115	-
22	CLA	7	322	15	-	9/27/103/115	-
25	LHG	B	850	22	-	16/26/26/53	-
22	CLA	2	301	-	-	11/27/103/115	-
38	LUT	7	301	-	-	9/29/67/67	0/2/2/2
39	CHL	4	819	16	-	0/14/90/117	-
22	CLA	5	311	17	-	11/27/103/115	-
22	CLA	7	306	14	-	16/39/115/115	-
38	LUT	Z	302	-	-	7/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	837	1	-	10/23/99/115	-
22	CLA	B	817	2	-	18/30/106/115	-
22	CLA	B	824	2	-	19/32/108/115	-
22	CLA	9	311	19	-	5/17/93/115	-
22	CLA	1	307	12	-	18/33/109/115	-
22	CLA	9	304	-	-	5/15/91/115	-
22	CLA	A	809	1	-	7/27/103/115	-
22	CLA	A	811	1,22	-	20/39/115/115	-
38	LUT	6	304	-	-	6/29/67/67	0/2/2/2
22	CLA	7	314	44	-	7/21/97/115	-
23	PQN	A	843	-	-	8/23/43/43	0/2/2/2
39	CHL	Z	311	12	-	10/23/99/117	-
22	CLA	A	828	-	-	21/39/115/115	-
22	CLA	8	309	15	-	17/39/115/115	-
22	CLA	3	318	13	-	11/33/109/115	-
22	CLA	4	812	16	-	10/27/103/115	-
38	LUT	1	303	-	-	8/29/67/67	0/2/2/2
22	CLA	3	310	13	-	14/39/115/115	-
22	CLA	3	309	13	-	6/17/93/115	-
22	CLA	1	305	12	-	6/15/91/115	-
22	CLA	3	320	13	-	7/17/93/115	-
31	DGD	1	319	-	-	14/40/80/95	0/2/2/2
41	3PH	6	324	-	-	11/30/30/49	-
37	DAO	K	201	-	-	1/11/11/11	-
24	BCR	6	305	-	-	13/29/63/63	0/2/2/2
22	CLA	9	305	19	-	20/33/109/115	-
24	BCR	A	844	-	-	13/29/63/63	0/2/2/2
25	LHG	5	324	22	-	24/41/41/53	-
22	CLA	B	828	2	-	18/39/115/115	-
33	LMT	4	801	-	-	1/21/61/61	0/2/2/2
22	CLA	6	310	18	-	18/39/115/115	-
22	CLA	B	839	2	-	11/24/100/115	-
22	CLA	F	304	6	-	24/39/115/115	-
22	CLA	B	818	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	6	303	-	-	9/29/67/67	0/2/2/2
22	CLA	A	831	1	-	10/21/97/115	-
24	BCR	L	204	-	-	13/29/63/63	0/2/2/2
22	CLA	A	830	1	-	14/39/115/115	-
22	CLA	4	818	44	-	12/23/99/115	-
22	CLA	5	308	17	-	17/35/111/115	-
22	CLA	B	840	44	-	9/39/115/115	-
25	LHG	6	323	22	-	38/53/53/53	-
33	LMT	F	307	-	-	8/21/61/61	0/2/2/2
39	CHL	5	317	44	-	7/23/99/117	-
26	NKP	A	851	-	-	9/22/22/28	-
22	CLA	B	820	2	-	18/33/109/115	-
22	CLA	A	816	44	-	14/29/105/115	-
22	CLA	5	323	44	-	9/17/93/115	-
22	CLA	A	822	1	-	12/27/103/115	-
22	CLA	A	825	44	-	16/39/115/115	-
21	CL0	A	801	-	-	13/39/115/115	-
22	CLA	1	316	12	-	22/39/115/115	-
22	CLA	3	311	13	-	13/33/109/115	-
34	LMG	F	308	-	-	16/30/50/70	0/1/1/1
39	CHL	6	316	-	-	10/23/99/117	-
22	CLA	B	825	2	-	19/39/115/115	-
22	CLA	B	808	2	-	15/39/115/115	-
22	CLA	1	313	44	-	12/39/115/115	-
22	CLA	8	310	44	-	15/33/109/115	-
22	CLA	1	306	-	-	18/39/115/115	-
22	CLA	2	304	44	-	9/17/93/115	-
38	LUT	5	303	-	-	6/29/67/67	0/2/2/2
22	CLA	9	313	19	-	6/21/97/115	-
22	CLA	Z	308	-	-	14/35/111/115	-
38	LUT	4	803	-	-	8/29/67/67	0/2/2/2
22	CLA	3	314	25	-	19/33/109/115	-
22	CLA	B	831	2	-	17/31/107/115	-
25	LHG	Z	317	22	-	27/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	849	-	-	13/29/63/63	0/2/2/2
22	CLA	A	832	1	-	17/39/115/115	-
22	CLA	A	815	1	-	16/39/115/115	-
22	CLA	B	830	-	-	13/39/115/115	-
22	CLA	B	837	2	-	9/23/99/115	-
24	BCR	3	306	-	-	13/29/63/63	0/2/2/2
22	CLA	Z	315	-	-	10/17/93/115	-
22	CLA	5	318	17	-	14/39/115/115	-
22	CLA	6	317	18	-	10/21/97/115	-
22	CLA	1	304	-	-	13/39/115/115	-
22	CLA	8	314	15	-	10/17/93/115	-
22	CLA	B	838	2	-	15/39/115/115	-
24	BCR	A	846	-	-	13/29/63/63	0/2/2/2
22	CLA	F	305	-	-	6/15/91/115	-
39	CHL	8	312	-	-	10/29/105/117	-
43	LPX	8	319	-	-	6/31/31/31	-
41	3PH	5	325	-	-	5/24/24/49	-
22	CLA	6	319	44	-	17/35/111/115	-
22	CLA	A	827	1	-	17/39/115/115	-
25	LHG	A	850	-	-	29/53/53/53	-
22	CLA	L	203	-	-	7/21/97/115	-
24	BCR	B	847	-	-	11/29/63/63	0/2/2/2
22	CLA	A	833	1	-	14/39/115/115	-
22	CLA	1	310	25	-	17/33/109/115	-
25	LHG	1	317	22	-	22/47/47/53	-
22	CLA	1	309	-	-	13/35/111/115	-
22	CLA	5	322	17	-	11/39/115/115	-
22	CLA	6	322	18	-	15/39/115/115	-
22	CLA	A	803	1	-	12/39/115/115	-
22	CLA	4	806	16	-	12/24/100/115	-
38	LUT	4	802	-	-	10/29/67/67	0/2/2/2
22	CLA	B	819	2	-	15/32/108/115	-
24	BCR	A	856	-	-	16/29/63/63	0/2/2/2
39	CHL	8	315	44	-	13/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	317	-	-	15/31/107/115	-
22	CLA	1	314	12	-	13/39/115/115	-
22	CLA	5	310	17	-	13/39/115/115	-
22	CLA	A	839	1	-	10/23/99/115	-
22	CLA	8	311	25	-	10/21/97/115	-
22	CLA	B	821	44	-	18/39/115/115	-
22	CLA	7	312	14	-	18/33/109/115	-
22	CLA	3	313	44	-	17/39/115/115	-
33	LMT	G	204	-	-	6/21/61/61	0/2/2/2
22	CLA	5	319	44	-	13/27/103/115	-
38	LUT	Z	301	-	-	7/29/67/67	0/2/2/2
22	CLA	A	829	-	-	11/39/115/115	-
22	CLA	L	202	11	-	21/39/115/115	-
26	NKP	8	318	-	-	7/28/28/28	-
31	DGD	3	301	-	-	12/40/80/95	0/2/2/2
22	CLA	7	304	14	-	13/33/109/115	-
22	CLA	A	813	1	-	14/39/115/115	-
22	CLA	6	314	18	-	15/39/115/115	-
24	BCR	3	304	-	-	10/29/63/63	0/2/2/2
22	CLA	F	301	44	-	13/39/115/115	-
22	CLA	A	834	1	-	15/39/115/115	-
41	3PH	8	320	-	-	13/31/31/49	-
22	CLA	B	809	2	-	19/39/115/115	-
22	CLA	B	811	2	-	15/39/115/115	-
22	CLA	F	302	2	-	17/39/115/115	-
22	CLA	Z	304	12	-	6/15/91/115	-
40	SQD	1	318	-	-	12/43/63/69	0/1/1/1
24	BCR	6	306	-	-	16/29/63/63	0/2/2/2
39	CHL	2	303	-	-	8/23/99/117	-
29	SF4	C	102	3	-	-	0/6/5/5
22	CLA	B	823	2	-	13/27/103/115	-
42	SPH	7	321	-	-	11/21/21/21	-
22	CLA	3	315	13	-	8/15/91/115	-
22	CLA	A	836	-	-	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	824	1	-	17/39/115/115	-
22	CLA	A	842	25	-	12/24/100/115	-
39	CHL	9	312	-	-	16/41/117/117	-
22	CLA	6	307	18	-	12/33/109/115	-
39	CHL	5	321	17	-	4/14/90/117	-
27	DGA	A	852	-	-	23/41/41/45	-
39	CHL	6	315	44	-	12/29/105/117	-
22	CLA	7	315	14	-	8/21/97/115	-
24	BCR	3	305	-	-	14/29/63/63	0/2/2/2
22	CLA	5	326	18	-	8/27/103/115	-
24	BCR	A	848	-	-	15/29/63/63	0/2/2/2
22	CLA	4	815	16	-	8/21/97/115	-
22	CLA	6	313	25	-	9/27/103/115	-
25	LHG	A	849	22	-	27/39/39/53	-
22	CLA	6	308	18	-	8/24/100/115	-
22	CLA	A	802	44	-	17/39/115/115	-
22	CLA	9	309	25	-	9/27/103/115	-
25	LHG	9	315	22	-	20/37/37/53	-
39	CHL	6	320	18	-	1/14/90/117	-
22	CLA	7	309	-	-	14/29/105/115	-
22	CLA	B	827	44	-	14/39/115/115	-
22	CLA	3	322	14	-	14/39/115/115	-
22	CLA	A	808	1	-	19/39/115/115	-
22	CLA	4	810	44	-	8/21/97/115	-
22	CLA	6	301	44	-	18/33/109/115	-
39	CHL	9	314	-	-	0/12/88/117	-
22	CLA	8	307	15	-	12/39/115/115	-
22	CLA	4	805	16	-	15/33/109/115	-
22	CLA	A	835	1	-	13/39/115/115	-
22	CLA	B	815	2	-	13/39/115/115	-
22	CLA	2	302	20	-	8/15/91/115	-
38	LUT	5	302	-	-	9/29/67/67	0/2/2/2
29	SF4	C	101	3	-	-	0/6/5/5
22	CLA	6	321	-	-	6/17/93/115	-
22	CLA	7	305	-	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	814	1	-	19/33/109/115	-
22	CLA	5	307	17	-	14/33/109/115	-
22	CLA	B	835	2	-	8/21/97/115	-
22	CLA	A	804	22	-	6/15/91/115	-
22	CLA	B	805	-	-	16/39/115/115	-
22	CLA	A	810	1	-	17/39/115/115	-
22	CLA	5	313	25	-	12/35/111/115	-
24	BCR	A	847	-	-	16/29/63/63	0/2/2/2
39	CHL	4	814	44	-	11/23/99/117	-
24	BCR	3	307	-	-	13/29/63/63	0/2/2/2
22	CLA	A	805	1	-	19/39/115/115	-
22	CLA	9	310	19	-	6/15/91/115	-
25	LHG	B	851	-	-	15/22/22/53	-
38	LUT	8	302	-	-	8/29/67/67	0/2/2/2
22	CLA	A	826	44	-	6/21/97/115	-
22	CLA	A	819	1	-	12/39/115/115	-
22	CLA	A	806	1	-	16/39/115/115	-
22	CLA	B	822	2	-	17/29/105/115	-
22	CLA	B	829	2	-	15/30/106/115	-
22	CLA	5	301	44	-	13/29/105/115	-
28	OCA	A	853	-	-	3/7/7/7	-
25	LHG	4	820	22	-	30/53/53/53	-
34	LMG	J	101	-	-	7/24/44/70	0/1/1/1
25	LHG	8	317	22	-	27/42/42/53	-
22	CLA	Z	313	44	-	13/39/115/115	-
22	CLA	G	201	7	-	10/21/97/115	-
22	CLA	6	311	18	-	12/27/103/115	-
22	CLA	4	808	16	-	16/33/109/115	-
22	CLA	8	306	15	-	9/23/99/115	-
39	CHL	5	316	44	-	12/41/117/117	-
22	CLA	9	303	19	-	13/33/109/115	-
23	PQN	B	843	-	-	9/23/43/43	0/2/2/2
22	CLA	Z	307	12	-	10/27/103/115	-
33	LMT	4	822	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	312	18	-	15/39/115/115	-
22	CLA	8	305	15	-	14/33/109/115	-
22	CLA	Z	310	12	-	10/21/97/115	-
22	CLA	B	813	-	-	14/29/105/115	-
22	CLA	1	308	12	-	13/27/103/115	-
22	CLA	K	203	44	-	9/27/103/115	-
22	CLA	1	311	12	-	8/17/93/115	-
22	CLA	1	315	-	-	7/17/93/115	-
22	CLA	A	812	1	-	16/39/115/115	-
22	CLA	A	821	44	-	12/39/115/115	-
22	CLA	7	324	14	-	23/33/109/115	-
22	CLA	8	313	44	-	7/21/97/115	-
32	RRX	F	306	-	-	15/29/65/65	0/2/2/2
22	CLA	J	103	9	-	5/12/88/115	-
22	CLA	3	308	13	-	18/39/115/115	-
38	LUT	3	302	-	-	4/29/67/67	0/2/2/2
39	CHL	3	317	-	-	13/41/117/117	-
22	CLA	9	308	19	-	8/21/97/115	-
24	BCR	B	845	-	-	16/29/63/63	0/2/2/2
38	LUT	1	302	-	-	9/29/67/67	0/2/2/2
22	CLA	5	312	44	-	6/21/97/115	-
36	C7Z	5	306	-	-	13/29/67/67	0/2/2/2
22	CLA	B	833	2	-	19/39/115/115	-
22	CLA	7	311	14	-	6/13/89/115	-
22	CLA	B	816	-	-	13/33/109/115	-
22	CLA	A	818	1	-	15/33/109/115	-
33	LMT	1	301	-	-	4/21/61/61	0/2/2/2
38	LUT	9	302	-	-	4/29/67/67	0/2/2/2
38	LUT	8	303	-	-	3/29/67/67	0/2/2/2
24	BCR	5	304	-	-	14/29/63/63	0/2/2/2
29	SF4	B	802	2,1	-	-	0/6/5/5
22	CLA	9	307	19	-	10/27/103/115	-
24	BCR	J	104	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	306	12	-	20/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Z	312	-	-	10/20/96/117	-
24	BCR	G	203	-	-	15/29/63/63	0/2/2/2
22	CLA	A	807	1	-	17/33/109/115	-
24	BCR	A	845	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	316	12	-	21/39/115/115	-
22	CLA	G	202	7	-	8/17/93/115	-
39	CHL	1	312	-	-	4/20/96/117	-
22	CLA	Z	303	12	-	16/39/115/115	-
38	LUT	3	303	-	-	7/29/67/67	0/2/2/2
35	T7X	J	102	-	-	17/44/68/80	0/1/1/1
25	LHG	B	803	-	-	22/37/37/53	-
24	BCR	5	305	-	-	13/29/63/63	0/2/2/2
39	CHL	6	318	-	-	9/29/105/117	-
22	CLA	B	832	2	-	6/21/97/115	-
25	LHG	4	821	-	-	16/36/36/53	-
22	CLA	B	841	2	-	13/39/115/115	-
24	BCR	B	848	-	-	16/29/63/63	0/2/2/2
22	CLA	5	315	17	-	14/39/115/115	-
22	CLA	L	201	2	-	17/39/115/115	-
38	LUT	9	301	-	-	5/29/67/67	0/2/2/2
42	SPH	7	320	-	-	11/21/21/21	-
22	CLA	K	202	10	-	10/17/93/115	-
22	CLA	9	306	19	-	14/36/112/115	-
22	CLA	5	314	17	-	6/15/91/115	-
41	3PH	7	319	-	-	17/40/40/49	-
39	CHL	7	313	44	-	7/27/103/117	-
39	CHL	4	813	44	-	7/23/99/117	-
22	CLA	4	807	16	-	12/39/115/115	-
22	CLA	8	316	15	-	11/17/93/115	-
38	LUT	7	302	-	-	5/29/67/67	0/2/2/2
22	CLA	3	312	13	-	12/39/115/115	-
22	CLA	Z	309	25	-	16/33/109/115	-
24	BCR	8	304	-	-	12/29/63/63	0/2/2/2
22	CLA	5	309	-	-	17/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	308	14	-	16/35/111/115	-
22	CLA	4	817	16	-	2/10/86/115	-
22	CLA	7	310	25	-	17/39/115/115	-
22	CLA	A	838	1	-	15/39/115/115	-
22	CLA	A	840	-	-	18/39/115/115	-
22	CLA	Z	305	-	-	12/29/105/115	-
31	DGD	B	852	-	-	11/50/90/95	0/2/2/2
22	CLA	B	807	2	-	8/15/91/115	-
22	CLA	4	809	16	-	5/23/99/115	-
24	BCR	7	303	-	-	16/29/63/63	0/2/2/2
22	CLA	4	811	25	-	9/27/103/115	-
22	CLA	3	319	-	-	9/27/103/115	-
22	CLA	3	316	13	-	8/24/100/115	-
22	CLA	A	823	1	-	15/39/115/115	-
39	CHL	4	816	44	-	7/19/95/117	-
24	BCR	4	804	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	314	12	-	9/23/99/115	-
22	CLA	K	204	10	-	12/20/96/115	-
24	BCR	B	853	-	-	17/29/63/63	0/2/2/2
22	CLA	7	307	14	-	14/39/115/115	-
22	CLA	B	814	2	-	19/33/109/115	-
22	CLA	6	309	44	-	17/39/115/115	-
25	LHG	3	321	22	-	11/22/22/53	-
25	LHG	7	318	22	-	25/41/41/53	-
24	BCR	B	846	-	-	17/29/63/63	0/2/2/2
22	CLA	A	854	-	-	13/39/115/115	-
22	CLA	B	810	2	-	11/29/105/115	-
22	CLA	K	205	10	-	17/27/103/115	-
22	CLA	A	820	1	-	21/33/109/115	-
24	BCR	F	303	-	-	15/29/63/63	0/2/2/2
22	CLA	5	320	-	-	11/21/97/115	-
24	BCR	K	206	-	-	13/29/63/63	0/2/2/2
22	CLA	6	302	16	-	17/33/109/115	-
39	CHL	8	301	12	-	5/32/108/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	841	1	-	10/39/115/115	-
22	CLA	B	834	2	-	15/31/107/115	-
22	CLA	A	817	-	-	13/33/109/115	-
22	CLA	B	806	44	-	12/39/115/115	-
22	CLA	B	842	25	-	17/39/115/115	-
22	CLA	7	323	15	-	19/39/115/115	-
22	CLA	B	801	2	-	15/39/115/115	-
22	CLA	B	836	-	-	6/15/91/115	-
22	CLA	8	308	15	-	15/36/112/115	-
22	CLA	B	826	44	-	17/39/115/115	-
36	C7Z	J	105	-	-	13/29/67/67	0/2/2/2
24	BCR	B	844	-	-	12/29/63/63	0/2/2/2
22	CLA	7	316	44	-	6/12/88/115	-

All (2818) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	303	LUT	C24-C25	23.39	1.62	1.33
38	5	303	LUT	C24-C25	23.37	1.62	1.33
38	1	302	LUT	C24-C25	23.34	1.62	1.33
38	7	302	LUT	C24-C25	23.27	1.62	1.33
38	Z	302	LUT	C24-C25	23.26	1.62	1.33
38	6	304	LUT	C24-C25	23.22	1.62	1.33
38	5	302	LUT	C24-C25	23.21	1.62	1.33
38	4	803	LUT	C24-C25	23.19	1.62	1.33
38	1	303	LUT	C24-C25	23.18	1.62	1.33
38	9	302	LUT	C24-C25	23.17	1.62	1.33
38	9	301	LUT	C24-C25	23.16	1.62	1.33
38	8	303	LUT	C24-C25	23.12	1.62	1.33
38	3	303	LUT	C24-C25	23.10	1.61	1.33
38	4	802	LUT	C24-C25	23.09	1.61	1.33
38	3	302	LUT	C24-C25	23.07	1.61	1.33
38	Z	301	LUT	C24-C25	23.04	1.61	1.33
38	7	301	LUT	C24-C25	22.90	1.61	1.33
38	8	302	LUT	C24-C25	22.74	1.61	1.33
36	J	105	C7Z	C25-C26	15.85	1.61	1.34
32	F	306	RRX	C26-C25	15.80	1.61	1.34
36	5	306	C7Z	C25-C26	15.76	1.61	1.34
24	5	305	BCR	C26-C25	15.60	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	848	BCR	C26-C25	15.57	1.61	1.34
24	6	306	BCR	C26-C25	15.55	1.61	1.34
24	F	303	BCR	C26-C25	15.52	1.61	1.34
24	7	303	BCR	C26-C25	15.49	1.61	1.34
24	A	846	BCR	C26-C25	15.46	1.61	1.34
24	3	304	BCR	C26-C25	15.45	1.61	1.34
24	4	804	BCR	C26-C25	15.45	1.61	1.34
24	6	305	BCR	C26-C25	15.42	1.61	1.34
24	8	304	BCR	C26-C25	15.42	1.61	1.34
24	B	844	BCR	C26-C25	15.41	1.61	1.34
24	B	846	BCR	C26-C25	15.40	1.61	1.34
24	A	847	BCR	C26-C25	15.39	1.61	1.34
24	G	203	BCR	C26-C25	15.36	1.61	1.34
24	B	853	BCR	C26-C25	15.36	1.61	1.34
24	A	848	BCR	C26-C25	15.31	1.61	1.34
24	3	307	BCR	C26-C25	15.31	1.61	1.34
24	A	845	BCR	C26-C25	15.30	1.60	1.34
38	4	802	LUT	C5-C6	15.30	1.60	1.34
24	L	204	BCR	C26-C25	15.29	1.60	1.34
38	6	303	LUT	C5-C6	15.28	1.60	1.34
24	B	849	BCR	C26-C25	15.27	1.60	1.34
38	5	303	LUT	C5-C6	15.26	1.60	1.34
24	3	306	BCR	C26-C25	15.26	1.60	1.34
38	1	302	LUT	C5-C6	15.22	1.60	1.34
38	9	302	LUT	C5-C6	15.21	1.60	1.34
38	7	301	LUT	C5-C6	15.19	1.60	1.34
38	Z	301	LUT	C5-C6	15.19	1.60	1.34
38	9	301	LUT	C5-C6	15.17	1.60	1.34
24	K	206	BCR	C26-C25	15.17	1.60	1.34
24	3	305	BCR	C26-C25	15.16	1.60	1.34
38	7	302	LUT	C5-C6	15.15	1.60	1.34
38	8	302	LUT	C5-C6	15.14	1.60	1.34
24	B	847	BCR	C26-C25	15.13	1.60	1.34
38	6	304	LUT	C5-C6	15.11	1.60	1.34
38	Z	302	LUT	C5-C6	15.10	1.60	1.34
24	I	4001	BCR	C26-C25	15.10	1.60	1.34
24	B	845	BCR	C26-C25	15.10	1.60	1.34
38	8	303	LUT	C5-C6	15.09	1.60	1.34
24	A	844	BCR	C26-C25	15.09	1.60	1.34
36	J	105	C7Z	C5-C6	15.09	1.60	1.34
24	5	304	BCR	C26-C25	15.08	1.60	1.34
38	5	302	LUT	C5-C6	15.07	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	3	302	LUT	C5-C6	15.07	1.60	1.34
38	3	303	LUT	C5-C6	15.06	1.60	1.34
38	1	303	LUT	C5-C6	15.05	1.60	1.34
38	4	803	LUT	C5-C6	15.01	1.60	1.34
24	A	856	BCR	C26-C25	15.01	1.60	1.34
24	J	104	BCR	C26-C25	15.00	1.60	1.34
36	5	306	C7Z	C5-C6	14.91	1.60	1.34
32	F	306	RRX	C5-C6	14.38	1.59	1.34
24	3	304	BCR	C5-C6	14.21	1.59	1.34
24	B	849	BCR	C5-C6	14.20	1.59	1.34
24	4	804	BCR	C5-C6	14.20	1.59	1.34
24	F	303	BCR	C5-C6	14.11	1.58	1.34
24	A	844	BCR	C5-C6	14.08	1.58	1.34
24	B	853	BCR	C5-C6	14.08	1.58	1.34
24	A	847	BCR	C5-C6	14.08	1.58	1.34
24	B	847	BCR	C5-C6	14.06	1.58	1.34
24	3	305	BCR	C5-C6	14.04	1.58	1.34
24	A	846	BCR	C5-C6	14.02	1.58	1.34
24	B	844	BCR	C5-C6	14.01	1.58	1.34
24	G	203	BCR	C5-C6	14.00	1.58	1.34
24	K	206	BCR	C5-C6	13.99	1.58	1.34
24	B	846	BCR	C5-C6	13.99	1.58	1.34
24	5	304	BCR	C5-C6	13.97	1.58	1.34
24	6	305	BCR	C5-C6	13.96	1.58	1.34
24	5	305	BCR	C5-C6	13.94	1.58	1.34
24	A	856	BCR	C5-C6	13.93	1.58	1.34
24	6	306	BCR	C5-C6	13.91	1.58	1.34
24	B	845	BCR	C5-C6	13.88	1.58	1.34
24	B	848	BCR	C5-C6	13.87	1.58	1.34
24	J	104	BCR	C5-C6	13.82	1.58	1.34
24	I	4001	BCR	C5-C6	13.81	1.58	1.34
24	3	306	BCR	C5-C6	13.81	1.58	1.34
24	A	845	BCR	C5-C6	13.79	1.58	1.34
24	8	304	BCR	C5-C6	13.73	1.58	1.34
24	L	204	BCR	C5-C6	13.72	1.58	1.34
24	A	848	BCR	C5-C6	13.68	1.58	1.34
24	3	307	BCR	C5-C6	13.67	1.58	1.34
24	7	303	BCR	C5-C6	13.64	1.58	1.34
38	4	802	LUT	C22-C21	-13.09	1.38	1.54
38	5	302	LUT	C22-C21	-13.07	1.38	1.54
38	5	303	LUT	C22-C21	-13.06	1.38	1.54
38	6	303	LUT	C22-C21	-13.04	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	803	LUT	C22-C21	-12.98	1.38	1.54
38	8	303	LUT	C22-C21	-12.98	1.38	1.54
38	6	304	LUT	C22-C21	-12.93	1.38	1.54
38	Z	302	LUT	C22-C21	-12.93	1.38	1.54
38	7	301	LUT	C22-C21	-12.88	1.38	1.54
38	9	302	LUT	C22-C21	-12.85	1.38	1.54
38	7	302	LUT	C22-C21	-12.84	1.38	1.54
38	1	303	LUT	C22-C21	-12.84	1.38	1.54
38	9	301	LUT	C22-C21	-12.83	1.38	1.54
38	3	303	LUT	C22-C21	-12.82	1.38	1.54
38	1	302	LUT	C22-C21	-12.80	1.38	1.54
38	3	302	LUT	C22-C21	-12.72	1.38	1.54
38	Z	301	LUT	C22-C21	-12.65	1.38	1.54
38	8	302	LUT	C22-C21	-12.53	1.39	1.54
36	J	105	C7Z	C24-C23	11.66	1.72	1.52
36	5	306	C7Z	C24-C23	11.62	1.72	1.52
38	4	802	LUT	C2-C3	-11.26	1.36	1.52
38	7	301	LUT	C2-C3	-11.09	1.36	1.52
38	9	301	LUT	C2-C3	-11.06	1.36	1.52
38	5	302	LUT	C2-C3	-11.04	1.36	1.52
38	9	302	LUT	C2-C3	-11.03	1.36	1.52
38	3	302	LUT	C2-C3	-11.03	1.36	1.52
38	8	302	LUT	C2-C3	-11.02	1.36	1.52
36	J	105	C7Z	C22-C23	-11.02	1.36	1.52
38	5	303	LUT	C2-C3	-11.01	1.36	1.52
38	3	303	LUT	C2-C3	-10.97	1.36	1.52
36	5	306	C7Z	C22-C23	-10.95	1.36	1.52
38	1	302	LUT	C2-C3	-10.95	1.36	1.52
38	7	302	LUT	C2-C3	-10.92	1.36	1.52
38	4	803	LUT	C2-C3	-10.88	1.36	1.52
38	6	304	LUT	C2-C3	-10.87	1.36	1.52
38	1	303	LUT	C2-C3	-10.85	1.36	1.52
38	Z	302	LUT	C2-C3	-10.85	1.36	1.52
38	8	303	LUT	C2-C3	-10.84	1.36	1.52
38	Z	301	LUT	C2-C3	-10.81	1.36	1.52
38	6	303	LUT	C2-C3	-10.79	1.36	1.52
32	F	306	RRX	C29-C28	-10.64	1.37	1.52
36	J	105	C7Z	C2-C3	-9.85	1.38	1.52
36	5	306	C7Z	C2-C3	-9.83	1.38	1.52
21	A	801	CL0	MG-NA	9.22	2.28	2.06
36	5	306	C7Z	C4-C3	8.54	1.67	1.52
36	J	105	C7Z	C4-C3	8.47	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	303	LUT	C22-C23	8.33	1.66	1.53
38	3	302	LUT	C22-C23	8.26	1.66	1.53
38	6	303	LUT	C22-C23	8.18	1.66	1.53
38	8	302	LUT	C22-C23	8.17	1.66	1.53
38	Z	301	LUT	C22-C23	8.15	1.66	1.53
38	7	301	LUT	C22-C23	8.13	1.66	1.53
38	9	302	LUT	C22-C23	8.12	1.66	1.53
38	5	303	LUT	C22-C23	8.10	1.66	1.53
38	8	303	LUT	C22-C23	8.08	1.66	1.53
38	7	302	LUT	C22-C23	8.08	1.66	1.53
38	4	803	LUT	C22-C23	8.08	1.66	1.53
32	F	306	RRX	C27-C28	8.05	1.66	1.52
38	Z	302	LUT	C22-C23	8.05	1.66	1.53
38	6	304	LUT	C22-C23	8.04	1.66	1.53
38	3	302	LUT	C4-C3	8.02	1.66	1.52
38	1	302	LUT	C4-C3	8.02	1.66	1.52
38	1	302	LUT	C22-C23	7.99	1.66	1.53
38	5	302	LUT	C22-C23	7.99	1.66	1.53
38	9	301	LUT	C22-C23	7.98	1.66	1.53
38	3	303	LUT	C22-C23	7.97	1.66	1.53
38	Z	301	LUT	C4-C3	7.96	1.66	1.52
38	4	802	LUT	C22-C23	7.96	1.66	1.53
38	1	303	LUT	C4-C3	7.95	1.66	1.52
38	6	303	LUT	C4-C3	7.92	1.66	1.52
38	Z	302	LUT	C4-C3	7.90	1.66	1.52
38	8	302	LUT	C4-C3	7.88	1.65	1.52
38	5	303	LUT	C4-C3	7.87	1.65	1.52
38	5	302	LUT	C4-C3	7.87	1.65	1.52
38	9	301	LUT	C4-C3	7.86	1.65	1.52
38	6	304	LUT	C4-C3	7.85	1.65	1.52
38	3	303	LUT	C4-C3	7.83	1.65	1.52
38	8	303	LUT	C4-C3	7.81	1.65	1.52
38	7	301	LUT	C4-C3	7.80	1.65	1.52
38	7	302	LUT	C4-C3	7.79	1.65	1.52
38	4	803	LUT	C4-C3	7.78	1.65	1.52
38	4	802	LUT	C4-C3	7.73	1.65	1.52
38	9	302	LUT	C4-C3	7.62	1.65	1.52
38	Z	301	LUT	C32-C33	7.61	1.62	1.45
38	7	302	LUT	C32-C33	7.50	1.62	1.45
38	1	303	LUT	C32-C33	7.49	1.62	1.45
38	1	302	LUT	C32-C33	7.49	1.62	1.45
38	5	303	LUT	C32-C33	7.47	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Z	302	LUT	C32-C33	7.46	1.62	1.45
38	7	301	LUT	C32-C33	7.43	1.61	1.45
38	6	304	LUT	C32-C33	7.42	1.61	1.45
38	3	303	LUT	C32-C33	7.42	1.61	1.45
38	6	303	LUT	C32-C33	7.40	1.61	1.45
38	3	302	LUT	C32-C33	7.40	1.61	1.45
38	9	301	LUT	C32-C33	7.39	1.61	1.45
38	4	802	LUT	C32-C33	7.36	1.61	1.45
38	8	303	LUT	C32-C33	7.36	1.61	1.45
38	9	302	LUT	C32-C33	7.35	1.61	1.45
38	4	803	LUT	C32-C33	7.35	1.61	1.45
38	5	302	LUT	C32-C33	7.32	1.61	1.45
38	8	302	LUT	C32-C33	7.28	1.61	1.45
24	3	306	BCR	C30-C25	-7.11	1.44	1.53
24	5	304	BCR	C30-C25	-7.10	1.44	1.53
24	B	845	BCR	C30-C25	-7.03	1.44	1.53
24	L	204	BCR	C30-C25	-7.03	1.44	1.53
24	B	847	BCR	C30-C25	-7.02	1.44	1.53
24	A	844	BCR	C30-C25	-7.02	1.44	1.53
24	I	4001	BCR	C30-C25	-7.02	1.44	1.53
24	A	847	BCR	C30-C25	-6.99	1.44	1.53
24	K	206	BCR	C30-C25	-6.95	1.44	1.53
24	8	304	BCR	C1-C6	-6.89	1.44	1.53
24	3	305	BCR	C30-C25	-6.89	1.44	1.53
24	I	4001	BCR	C1-C6	-6.88	1.44	1.53
24	B	853	BCR	C30-C25	-6.86	1.44	1.53
24	B	849	BCR	C30-C25	-6.86	1.44	1.53
24	A	856	BCR	C30-C25	-6.85	1.44	1.53
24	J	104	BCR	C30-C25	-6.84	1.44	1.53
24	B	848	BCR	C30-C25	-6.80	1.44	1.53
24	A	848	BCR	C30-C25	-6.80	1.44	1.53
24	3	307	BCR	C30-C25	-6.79	1.44	1.53
24	4	804	BCR	C30-C25	-6.79	1.44	1.53
24	B	844	BCR	C30-C25	-6.78	1.44	1.53
24	3	304	BCR	C2-C3	-6.78	1.35	1.52
24	A	845	BCR	C30-C25	-6.77	1.44	1.53
24	A	846	BCR	C30-C25	-6.77	1.44	1.53
24	5	305	BCR	C30-C25	-6.77	1.44	1.53
24	6	305	BCR	C30-C25	-6.74	1.44	1.53
24	6	306	BCR	C30-C25	-6.73	1.44	1.53
24	7	303	BCR	C30-C25	-6.72	1.44	1.53
24	3	304	BCR	C30-C25	-6.71	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	847	BCR	C1-C6	-6.70	1.44	1.53
24	L	204	BCR	C1-C6	-6.70	1.44	1.53
24	F	303	BCR	C30-C25	-6.69	1.44	1.53
24	8	304	BCR	C30-C25	-6.69	1.44	1.53
24	G	203	BCR	C2-C3	-6.69	1.36	1.52
24	B	845	BCR	C1-C6	-6.68	1.44	1.53
24	6	305	BCR	C2-C3	-6.68	1.36	1.52
24	A	844	BCR	C2-C3	-6.67	1.36	1.52
24	5	304	BCR	C2-C3	-6.67	1.36	1.52
24	B	844	BCR	C2-C3	-6.67	1.36	1.52
24	K	206	BCR	C2-C3	-6.66	1.36	1.52
24	3	305	BCR	C2-C3	-6.66	1.36	1.52
24	3	307	BCR	C1-C6	-6.66	1.44	1.53
24	B	849	BCR	C2-C3	-6.66	1.36	1.52
24	B	848	BCR	C2-C3	-6.65	1.36	1.52
24	4	804	BCR	C2-C3	-6.65	1.36	1.52
24	F	303	BCR	C2-C3	-6.65	1.36	1.52
24	B	846	BCR	C2-C3	-6.64	1.36	1.52
24	5	304	BCR	C1-C6	-6.63	1.44	1.53
24	A	846	BCR	C2-C3	-6.63	1.36	1.52
24	B	846	BCR	C30-C25	-6.62	1.44	1.53
24	K	206	BCR	C1-C6	-6.62	1.44	1.53
24	5	305	BCR	C2-C3	-6.61	1.36	1.52
24	A	847	BCR	C2-C3	-6.61	1.36	1.52
24	B	847	BCR	C2-C3	-6.61	1.36	1.52
24	A	848	BCR	C1-C6	-6.59	1.44	1.53
24	A	856	BCR	C2-C3	-6.57	1.36	1.52
24	B	853	BCR	C2-C3	-6.57	1.36	1.52
24	G	203	BCR	C30-C25	-6.56	1.44	1.53
24	A	847	BCR	C1-C6	-6.54	1.44	1.53
24	3	306	BCR	C2-C3	-6.54	1.36	1.52
24	6	306	BCR	C2-C3	-6.53	1.36	1.52
24	I	4001	BCR	C2-C3	-6.53	1.36	1.52
32	F	306	RRX	C2-C3	-6.51	1.36	1.52
24	6	306	BCR	C1-C6	-6.51	1.44	1.53
24	A	845	BCR	C2-C3	-6.50	1.36	1.52
24	B	846	BCR	C1-C6	-6.50	1.44	1.53
22	4	805	CLA	MG-NA	6.49	2.21	2.06
24	G	203	BCR	C1-C6	-6.48	1.44	1.53
32	F	306	RRX	C30-C25	-6.48	1.44	1.53
24	3	305	BCR	C1-C6	-6.48	1.44	1.53
24	J	104	BCR	C1-C6	-6.47	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	845	BCR	C2-C3	-6.46	1.36	1.52
24	J	104	BCR	C2-C3	-6.45	1.36	1.52
24	A	846	BCR	C1-C6	-6.45	1.44	1.53
24	A	856	BCR	C1-C6	-6.45	1.44	1.53
24	L	204	BCR	C2-C3	-6.45	1.36	1.52
24	8	304	BCR	C2-C3	-6.44	1.36	1.52
24	A	848	BCR	C2-C3	-6.43	1.36	1.52
22	8	307	CLA	MG-NA	6.42	2.21	2.06
24	5	305	BCR	C29-C28	-6.42	1.36	1.52
24	3	307	BCR	C2-C3	-6.41	1.36	1.52
24	6	305	BCR	C29-C28	-6.41	1.36	1.52
24	A	847	BCR	C29-C28	-6.41	1.36	1.52
24	B	844	BCR	C1-C6	-6.40	1.45	1.53
24	B	849	BCR	C1-C6	-6.40	1.45	1.53
24	7	303	BCR	C29-C28	-6.40	1.36	1.52
24	A	845	BCR	C1-C6	-6.40	1.45	1.53
22	4	807	CLA	MG-NA	6.40	2.21	2.06
24	B	848	BCR	C29-C28	-6.39	1.36	1.52
22	4	806	CLA	MG-NA	6.38	2.21	2.06
22	7	308	CLA	MG-NA	6.38	2.21	2.06
22	4	809	CLA	MG-NA	6.38	2.21	2.06
24	4	804	BCR	C29-C28	-6.38	1.36	1.52
38	6	303	LUT	C1-C6	-6.38	1.45	1.53
24	F	303	BCR	C29-C28	-6.38	1.36	1.52
22	6	309	CLA	MG-NA	6.38	2.21	2.06
22	A	816	CLA	MG-NA	6.37	2.21	2.06
22	5	311	CLA	MG-NA	6.37	2.21	2.06
24	8	304	BCR	C29-C28	-6.37	1.36	1.52
22	B	820	CLA	MG-NA	6.37	2.21	2.06
22	7	306	CLA	MG-NA	6.36	2.21	2.06
22	3	310	CLA	MG-NA	6.36	2.21	2.06
22	A	817	CLA	MG-NA	6.36	2.21	2.06
22	3	312	CLA	MG-NA	6.36	2.21	2.06
24	7	303	BCR	C2-C3	-6.36	1.36	1.52
24	6	306	BCR	C29-C28	-6.36	1.36	1.52
22	A	825	CLA	MG-NA	6.36	2.21	2.06
22	5	315	CLA	MG-NA	6.35	2.21	2.06
22	B	828	CLA	MG-NA	6.35	2.21	2.06
22	Z	313	CLA	MG-NA	6.34	2.21	2.06
22	7	324	CLA	MG-NA	6.34	2.21	2.06
24	B	853	BCR	C1-C6	-6.34	1.45	1.53
22	6	301	CLA	MG-NA	6.34	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	MG-NA	6.34	2.21	2.06
24	7	303	BCR	C1-C6	-6.33	1.45	1.53
22	1	315	CLA	MG-NA	6.33	2.21	2.06
22	5	313	CLA	MG-NA	6.33	2.21	2.06
22	G	201	CLA	MG-NA	6.33	2.21	2.06
22	B	826	CLA	MG-NA	6.33	2.21	2.06
24	3	304	BCR	C29-C28	-6.33	1.36	1.52
22	A	820	CLA	MG-NA	6.32	2.21	2.06
24	B	844	BCR	C29-C28	-6.32	1.37	1.52
22	A	822	CLA	MG-NA	6.32	2.21	2.06
24	B	846	BCR	C29-C28	-6.32	1.37	1.52
22	5	322	CLA	MG-NA	6.32	2.21	2.06
24	A	846	BCR	C29-C28	-6.32	1.37	1.52
24	4	804	BCR	C1-C6	-6.32	1.45	1.53
22	A	813	CLA	MG-NA	6.32	2.21	2.06
22	A	829	CLA	MG-NA	6.32	2.21	2.06
22	F	301	CLA	MG-NA	6.31	2.21	2.06
22	K	203	CLA	MG-NA	6.31	2.21	2.06
22	9	308	CLA	MG-NA	6.31	2.21	2.06
22	1	310	CLA	MG-NA	6.31	2.21	2.06
22	8	306	CLA	MG-NA	6.31	2.21	2.06
24	G	203	BCR	C29-C28	-6.31	1.37	1.52
22	5	326	CLA	MG-NA	6.31	2.21	2.06
22	3	322	CLA	MG-NA	6.31	2.21	2.06
22	5	309	CLA	MG-NA	6.31	2.21	2.06
22	B	810	CLA	MG-NA	6.31	2.21	2.06
22	L	203	CLA	MG-NA	6.31	2.21	2.06
22	B	824	CLA	MG-NA	6.30	2.21	2.06
22	B	840	CLA	MG-NA	6.30	2.21	2.06
22	7	323	CLA	MG-NA	6.30	2.21	2.06
22	A	840	CLA	MG-NA	6.30	2.21	2.06
22	L	202	CLA	MG-NA	6.30	2.21	2.06
22	4	811	CLA	MG-NA	6.30	2.21	2.06
22	1	305	CLA	MG-NA	6.30	2.21	2.06
22	A	834	CLA	MG-NA	6.30	2.21	2.06
22	J	103	CLA	MG-NA	6.30	2.21	2.06
22	B	829	CLA	MG-NA	6.30	2.21	2.06
22	Z	315	CLA	MG-NA	6.30	2.21	2.06
22	8	309	CLA	MG-NA	6.30	2.21	2.06
22	9	307	CLA	MG-NA	6.30	2.21	2.06
22	6	319	CLA	MG-NA	6.30	2.21	2.06
22	B	834	CLA	MG-NA	6.30	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	806	CLA	MG-NA	6.30	2.21	2.06
22	1	304	CLA	MG-NA	6.30	2.21	2.06
22	A	807	CLA	MG-NA	6.30	2.21	2.06
22	7	310	CLA	MG-NA	6.30	2.21	2.06
22	A	839	CLA	MG-NA	6.29	2.21	2.06
22	A	855	CLA	MG-NA	6.29	2.21	2.06
22	Z	304	CLA	MG-NA	6.29	2.21	2.06
22	K	202	CLA	MG-NA	6.29	2.21	2.06
22	2	302	CLA	MG-NA	6.29	2.21	2.06
22	F	302	CLA	MG-NA	6.29	2.21	2.06
22	Z	310	CLA	MG-NA	6.29	2.21	2.06
22	7	305	CLA	MG-NA	6.29	2.21	2.06
22	2	304	CLA	MG-NA	6.29	2.21	2.06
22	A	814	CLA	MG-NA	6.29	2.21	2.06
22	7	312	CLA	MG-NA	6.29	2.21	2.06
22	A	824	CLA	MG-NA	6.29	2.21	2.06
22	B	823	CLA	MG-NA	6.29	2.21	2.06
22	B	822	CLA	MG-NA	6.29	2.21	2.06
22	7	317	CLA	MG-NA	6.29	2.21	2.06
22	6	311	CLA	MG-NA	6.29	2.21	2.06
22	B	842	CLA	MG-NA	6.29	2.21	2.06
22	A	812	CLA	MG-NA	6.29	2.21	2.06
22	F	305	CLA	MG-NA	6.29	2.21	2.06
22	A	841	CLA	MG-NA	6.29	2.21	2.06
22	A	808	CLA	MG-NA	6.28	2.21	2.06
22	A	809	CLA	MG-NA	6.28	2.21	2.06
22	B	833	CLA	MG-NA	6.28	2.21	2.06
22	B	815	CLA	MG-NA	6.28	2.21	2.06
24	F	303	BCR	C1-C6	-6.28	1.45	1.53
22	6	322	CLA	MG-NA	6.28	2.21	2.06
22	4	812	CLA	MG-NA	6.28	2.21	2.06
22	B	837	CLA	MG-NA	6.28	2.21	2.06
22	9	313	CLA	MG-NA	6.28	2.21	2.06
22	K	204	CLA	MG-NA	6.28	2.21	2.06
22	A	826	CLA	MG-NA	6.28	2.21	2.06
22	4	808	CLA	MG-NA	6.28	2.21	2.06
22	A	827	CLA	MG-NA	6.28	2.21	2.06
22	Z	307	CLA	MG-NA	6.28	2.21	2.06
24	3	306	BCR	C29-C28	-6.28	1.37	1.52
22	7	315	CLA	MG-NA	6.27	2.21	2.06
22	B	805	CLA	MG-NA	6.27	2.21	2.06
22	6	314	CLA	MG-NA	6.27	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	314	CLA	MG-NA	6.27	2.21	2.06
22	A	810	CLA	MG-NA	6.27	2.21	2.06
22	A	842	CLA	MG-NA	6.27	2.21	2.06
22	L	201	CLA	MG-NA	6.27	2.21	2.06
22	3	319	CLA	MG-NA	6.27	2.21	2.06
22	B	827	CLA	MG-NA	6.27	2.21	2.06
22	3	309	CLA	MG-NA	6.26	2.21	2.06
22	3	316	CLA	MG-NA	6.26	2.21	2.06
22	6	313	CLA	MG-NA	6.26	2.21	2.06
22	B	839	CLA	MG-NA	6.26	2.21	2.06
22	7	311	CLA	MG-NA	6.26	2.21	2.06
22	6	321	CLA	MG-NA	6.26	2.21	2.06
22	B	821	CLA	MG-NA	6.26	2.21	2.06
22	9	311	CLA	MG-NA	6.26	2.21	2.06
38	8	303	LUT	C1-C6	-6.26	1.45	1.53
22	B	819	CLA	MG-NA	6.26	2.21	2.06
24	3	307	BCR	C29-C28	-6.26	1.37	1.52
22	1	307	CLA	MG-NA	6.26	2.21	2.06
22	1	306	CLA	MG-NA	6.26	2.21	2.06
22	B	811	CLA	MG-NA	6.25	2.21	2.06
22	6	312	CLA	MG-NA	6.25	2.21	2.06
22	Z	314	CLA	MG-NA	6.25	2.21	2.06
22	Z	316	CLA	MG-NA	6.25	2.21	2.06
22	A	830	CLA	MG-NA	6.25	2.21	2.06
22	A	802	CLA	MG-NA	6.25	2.21	2.06
22	7	316	CLA	MG-NA	6.25	2.21	2.06
22	4	818	CLA	MG-NA	6.25	2.21	2.06
22	6	302	CLA	MG-NA	6.25	2.21	2.06
38	Z	301	LUT	C1-C6	-6.25	1.45	1.53
24	K	206	BCR	C29-C28	-6.25	1.37	1.52
22	A	803	CLA	MG-NA	6.25	2.21	2.06
22	A	806	CLA	MG-NA	6.25	2.21	2.06
22	7	309	CLA	MG-NA	6.25	2.21	2.06
22	A	833	CLA	MG-NA	6.25	2.21	2.06
22	B	831	CLA	MG-NA	6.25	2.21	2.06
22	1	314	CLA	MG-NA	6.25	2.21	2.06
38	4	803	LUT	C1-C6	-6.25	1.45	1.53
22	8	314	CLA	MG-NA	6.25	2.21	2.06
22	A	815	CLA	MG-NA	6.25	2.21	2.06
24	A	845	BCR	C29-C28	-6.25	1.37	1.52
22	5	310	CLA	MG-NA	6.25	2.21	2.06
22	6	310	CLA	MG-NA	6.25	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	832	CLA	MG-NA	6.25	2.21	2.06
22	B	816	CLA	MG-NA	6.24	2.21	2.06
22	B	825	CLA	MG-NA	6.24	2.21	2.06
22	F	304	CLA	MG-NA	6.24	2.21	2.06
22	B	841	CLA	MG-NA	6.24	2.21	2.06
22	8	316	CLA	MG-NA	6.24	2.21	2.06
22	B	809	CLA	MG-NA	6.24	2.21	2.06
22	B	813	CLA	MG-NA	6.24	2.21	2.06
22	1	313	CLA	MG-NA	6.24	2.21	2.06
22	A	854	CLA	MG-NA	6.24	2.21	2.06
22	4	817	CLA	MG-NA	6.24	2.21	2.06
22	6	317	CLA	MG-NA	6.24	2.21	2.06
22	3	314	CLA	MG-NA	6.24	2.21	2.06
22	5	308	CLA	MG-NA	6.24	2.21	2.06
22	5	319	CLA	MG-NA	6.24	2.21	2.06
38	1	303	LUT	C1-C6	-6.23	1.45	1.53
22	5	314	CLA	MG-NA	6.23	2.21	2.06
22	A	811	CLA	MG-NA	6.23	2.21	2.06
22	Z	309	CLA	MG-NA	6.23	2.21	2.06
22	A	818	CLA	MG-NA	6.23	2.21	2.06
22	B	807	CLA	MG-NA	6.23	2.21	2.06
22	B	808	CLA	MG-NA	6.23	2.21	2.06
22	Z	308	CLA	MG-NA	6.23	2.21	2.06
22	8	311	CLA	MG-NA	6.23	2.21	2.06
22	5	307	CLA	MG-NA	6.23	2.21	2.06
24	A	848	BCR	C29-C28	-6.23	1.37	1.52
22	8	310	CLA	MG-NA	6.23	2.21	2.06
38	3	302	LUT	C1-C6	-6.23	1.45	1.53
22	A	831	CLA	MG-NA	6.23	2.21	2.06
22	B	812	CLA	MG-NA	6.23	2.21	2.06
22	B	830	CLA	MG-NA	6.22	2.21	2.06
22	4	815	CLA	MG-NA	6.22	2.21	2.06
22	G	202	CLA	MG-NA	6.22	2.21	2.06
22	5	312	CLA	MG-NA	6.22	2.21	2.06
22	B	836	CLA	MG-NA	6.22	2.21	2.06
22	A	804	CLA	MG-NA	6.22	2.21	2.06
22	A	819	CLA	MG-NA	6.22	2.21	2.06
22	4	810	CLA	MG-NA	6.22	2.21	2.06
24	A	844	BCR	C1-C6	-6.22	1.45	1.53
22	A	821	CLA	MG-NA	6.22	2.21	2.06
22	5	301	CLA	MG-NA	6.22	2.21	2.06
22	B	801	CLA	MG-NA	6.22	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	838	CLA	MG-NA	6.21	2.21	2.06
22	6	308	CLA	MG-NA	6.21	2.21	2.06
22	9	306	CLA	MG-NA	6.21	2.21	2.06
22	B	835	CLA	MG-NA	6.21	2.21	2.06
24	B	848	BCR	C1-C6	-6.21	1.45	1.53
22	3	308	CLA	MG-NA	6.21	2.21	2.06
24	5	305	BCR	C1-C6	-6.21	1.45	1.53
22	8	313	CLA	MG-NA	6.20	2.21	2.06
22	3	311	CLA	MG-NA	6.20	2.21	2.06
22	8	308	CLA	MG-NA	6.20	2.21	2.06
22	A	805	CLA	MG-NA	6.20	2.21	2.06
22	B	832	CLA	MG-NA	6.20	2.21	2.06
22	6	307	CLA	MG-NA	6.20	2.21	2.06
22	5	318	CLA	MG-NA	6.20	2.21	2.06
24	B	849	BCR	C29-C28	-6.20	1.37	1.52
22	7	322	CLA	MG-NA	6.20	2.21	2.06
22	B	817	CLA	MG-NA	6.19	2.21	2.06
24	3	306	BCR	C1-C6	-6.19	1.45	1.53
22	B	838	CLA	MG-NA	6.19	2.21	2.06
22	2	301	CLA	MG-NA	6.19	2.21	2.06
22	A	823	CLA	MG-NA	6.19	2.21	2.06
22	7	307	CLA	MG-NA	6.19	2.21	2.06
38	8	302	LUT	C1-C6	-6.18	1.45	1.53
22	A	828	CLA	MG-NA	6.18	2.21	2.06
22	Z	306	CLA	MG-NA	6.18	2.21	2.06
22	1	308	CLA	MG-NA	6.18	2.21	2.06
38	1	302	LUT	C1-C6	-6.18	1.45	1.53
22	3	318	CLA	MG-NA	6.18	2.20	2.06
38	Z	302	LUT	C1-C6	-6.18	1.45	1.53
24	3	305	BCR	C29-C28	-6.17	1.37	1.52
24	5	304	BCR	C29-C28	-6.17	1.37	1.52
24	B	847	BCR	C29-C28	-6.17	1.37	1.52
38	3	303	LUT	C1-C6	-6.16	1.45	1.53
24	6	305	BCR	C1-C6	-6.16	1.45	1.53
24	B	845	BCR	C29-C28	-6.15	1.37	1.52
38	5	302	LUT	C1-C6	-6.15	1.45	1.53
22	5	323	CLA	MG-NA	6.15	2.20	2.06
22	Z	303	CLA	MG-NA	6.15	2.20	2.06
38	6	304	LUT	C1-C6	-6.15	1.45	1.53
22	B	818	CLA	MG-NA	6.15	2.20	2.06
22	Z	305	CLA	MG-NA	6.15	2.20	2.06
22	A	835	CLA	MG-NA	6.15	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	844	BCR	C29-C28	-6.15	1.37	1.52
22	1	309	CLA	MG-NA	6.14	2.20	2.06
22	A	836	CLA	MG-NA	6.14	2.20	2.06
22	B	814	CLA	MG-NA	6.14	2.20	2.06
24	L	204	BCR	C29-C28	-6.13	1.37	1.52
32	F	306	RRX	C19-C18	6.12	1.59	1.45
22	3	313	CLA	MG-NA	6.12	2.20	2.06
24	3	304	BCR	C1-C6	-6.11	1.45	1.53
24	I	4001	BCR	C29-C28	-6.11	1.37	1.52
24	B	853	BCR	C29-C28	-6.10	1.37	1.52
22	7	304	CLA	MG-NA	6.10	2.20	2.06
22	8	305	CLA	MG-NA	6.10	2.20	2.06
22	1	316	CLA	MG-NA	6.09	2.20	2.06
24	J	104	BCR	C29-C28	-6.09	1.37	1.52
22	9	304	CLA	MG-NA	6.09	2.20	2.06
38	7	302	LUT	C1-C6	-6.09	1.45	1.53
38	9	301	LUT	C1-C6	-6.05	1.45	1.53
22	9	310	CLA	MG-NA	6.05	2.20	2.06
38	5	303	LUT	C1-C6	-6.04	1.45	1.53
24	A	856	BCR	C29-C28	-6.02	1.37	1.52
38	9	302	LUT	C1-C6	-6.02	1.45	1.53
36	J	105	C7Z	C12-C13	6.02	1.58	1.45
38	7	301	LUT	C1-C6	-6.01	1.45	1.53
24	B	853	BCR	C12-C13	6.00	1.58	1.45
22	K	205	CLA	MG-NA	5.99	2.20	2.06
22	9	309	CLA	MG-NA	5.96	2.20	2.06
22	3	315	CLA	MG-NA	5.95	2.20	2.06
22	5	320	CLA	MG-NA	5.93	2.20	2.06
36	5	306	C7Z	C12-C13	5.92	1.58	1.45
22	3	320	CLA	MG-NA	5.92	2.20	2.06
22	1	311	CLA	MG-NA	5.91	2.20	2.06
22	9	305	CLA	MG-NA	5.89	2.20	2.06
24	3	306	BCR	C12-C13	5.89	1.58	1.45
38	4	802	LUT	C1-C6	-5.87	1.45	1.53
24	3	304	BCR	C12-C13	5.85	1.58	1.45
24	A	844	BCR	C12-C13	5.82	1.58	1.45
24	J	104	BCR	C12-C13	5.80	1.58	1.45
24	A	848	BCR	C12-C13	5.79	1.58	1.45
24	B	846	BCR	C12-C13	5.75	1.58	1.45
24	A	856	BCR	C12-C13	5.74	1.58	1.45
22	9	303	CLA	MG-NA	5.73	2.19	2.06
24	A	845	BCR	C12-C13	5.73	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	849	BCR	C12-C13	5.73	1.58	1.45
24	B	845	BCR	C12-C13	5.72	1.58	1.45
24	B	844	BCR	C12-C13	5.72	1.58	1.45
24	G	203	BCR	C12-C13	5.72	1.58	1.45
24	3	307	BCR	C12-C13	5.71	1.58	1.45
24	I	4001	BCR	C12-C13	5.71	1.58	1.45
24	F	303	BCR	C12-C13	5.71	1.58	1.45
24	7	303	BCR	C12-C13	5.71	1.58	1.45
24	3	305	BCR	C12-C13	5.68	1.58	1.45
24	6	305	BCR	C12-C13	5.68	1.58	1.45
24	4	804	BCR	C12-C13	5.68	1.58	1.45
24	8	304	BCR	C12-C13	5.68	1.58	1.45
24	B	853	BCR	C8-C9	5.67	1.58	1.45
24	5	304	BCR	C12-C13	5.67	1.58	1.45
24	B	847	BCR	C12-C13	5.65	1.58	1.45
24	5	305	BCR	C12-C13	5.64	1.58	1.45
24	L	204	BCR	C12-C13	5.62	1.58	1.45
24	A	846	BCR	C12-C13	5.62	1.58	1.45
24	K	206	BCR	C12-C13	5.62	1.58	1.45
24	A	847	BCR	C12-C13	5.60	1.58	1.45
24	B	848	BCR	C12-C13	5.60	1.58	1.45
24	6	306	BCR	C12-C13	5.59	1.58	1.45
24	B	844	BCR	C8-C9	5.56	1.57	1.45
24	4	804	BCR	C8-C9	5.52	1.57	1.45
24	I	4001	BCR	C8-C9	5.51	1.57	1.45
24	A	856	BCR	C8-C9	5.49	1.57	1.45
24	3	307	BCR	C8-C9	5.48	1.57	1.45
24	B	845	BCR	C8-C9	5.46	1.57	1.45
24	F	303	BCR	C8-C9	5.45	1.57	1.45
24	3	305	BCR	C8-C9	5.44	1.57	1.45
24	B	849	BCR	C8-C9	5.44	1.57	1.45
24	J	104	BCR	C8-C9	5.44	1.57	1.45
24	A	845	BCR	C8-C9	5.43	1.57	1.45
24	B	846	BCR	C8-C9	5.43	1.57	1.45
24	A	848	BCR	C8-C9	5.42	1.57	1.45
32	F	306	RRX	C1-C6	-5.41	1.46	1.53
24	L	204	BCR	C8-C9	5.41	1.57	1.45
24	3	306	BCR	C8-C9	5.41	1.57	1.45
36	5	306	C7Z	C1-C6	-5.41	1.46	1.53
24	5	305	BCR	C8-C9	5.40	1.57	1.45
24	B	853	BCR	C23-C22	5.40	1.57	1.45
24	B	848	BCR	C8-C9	5.40	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	303	BCR	C8-C9	5.39	1.57	1.45
24	6	305	BCR	C8-C9	5.39	1.57	1.45
24	8	304	BCR	C8-C9	5.38	1.57	1.45
24	A	846	BCR	C8-C9	5.37	1.57	1.45
24	A	856	BCR	C23-C22	5.37	1.57	1.45
24	8	304	BCR	C29-C30	5.35	1.66	1.54
24	3	304	BCR	C8-C9	5.35	1.57	1.45
24	3	305	BCR	C23-C22	5.35	1.57	1.45
24	5	304	BCR	C8-C9	5.34	1.57	1.45
24	A	847	BCR	C8-C9	5.34	1.57	1.45
24	K	206	BCR	C8-C9	5.34	1.57	1.45
24	A	856	BCR	C29-C30	5.33	1.66	1.54
24	B	847	BCR	C8-C9	5.32	1.57	1.45
24	5	304	BCR	C29-C30	5.32	1.66	1.54
24	G	203	BCR	C8-C9	5.32	1.57	1.45
24	8	304	BCR	C23-C22	5.31	1.57	1.45
24	B	846	BCR	C29-C30	5.31	1.66	1.54
24	G	203	BCR	C29-C30	5.31	1.66	1.54
24	F	303	BCR	C23-C22	5.31	1.57	1.45
24	B	849	BCR	C29-C30	5.30	1.66	1.54
24	J	104	BCR	C29-C30	5.30	1.66	1.54
24	A	848	BCR	C23-C22	5.30	1.57	1.45
24	B	849	BCR	C23-C22	5.29	1.57	1.45
24	A	844	BCR	C8-C9	5.29	1.57	1.45
24	6	306	BCR	C8-C9	5.29	1.57	1.45
24	K	206	BCR	C23-C22	5.28	1.57	1.45
24	3	304	BCR	C29-C30	5.28	1.66	1.54
32	F	306	RRX	C8-C9	5.28	1.57	1.45
24	3	305	BCR	C29-C30	5.28	1.66	1.54
24	A	845	BCR	C23-C22	5.28	1.57	1.45
24	7	303	BCR	C23-C22	5.27	1.57	1.45
24	I	4001	BCR	C29-C30	5.27	1.66	1.54
24	5	304	BCR	C23-C22	5.27	1.57	1.45
24	B	844	BCR	C23-C22	5.27	1.57	1.45
24	A	846	BCR	C29-C30	5.27	1.66	1.54
24	3	306	BCR	C23-C22	5.27	1.57	1.45
24	A	844	BCR	C29-C30	5.27	1.66	1.54
24	3	304	BCR	C23-C22	5.26	1.57	1.45
24	J	104	BCR	C23-C22	5.26	1.57	1.45
24	K	206	BCR	C29-C30	5.25	1.66	1.54
24	A	845	BCR	C29-C30	5.25	1.66	1.54
24	B	847	BCR	C29-C30	5.25	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	845	BCR	C23-C22	5.25	1.57	1.45
24	4	804	BCR	C23-C22	5.24	1.57	1.45
36	J	105	C7Z	C1-C6	-5.24	1.46	1.53
24	6	305	BCR	C29-C30	5.24	1.66	1.54
24	B	846	BCR	C23-C22	5.23	1.57	1.45
24	A	848	BCR	C29-C30	5.22	1.66	1.54
24	L	204	BCR	C29-C30	5.22	1.66	1.54
24	3	306	BCR	C29-C30	5.21	1.66	1.54
24	B	845	BCR	C29-C30	5.21	1.66	1.54
24	G	203	BCR	C23-C22	5.20	1.57	1.45
24	3	307	BCR	C29-C30	5.20	1.66	1.54
24	6	305	BCR	C23-C22	5.20	1.57	1.45
24	B	844	BCR	C29-C30	5.19	1.66	1.54
24	A	847	BCR	C23-C22	5.19	1.57	1.45
24	B	847	BCR	C23-C22	5.19	1.57	1.45
24	L	204	BCR	C23-C22	5.18	1.57	1.45
24	A	846	BCR	C23-C22	5.18	1.57	1.45
24	A	844	BCR	C23-C22	5.18	1.57	1.45
24	F	303	BCR	C29-C30	5.18	1.66	1.54
24	3	307	BCR	C23-C22	5.18	1.57	1.45
24	B	848	BCR	C23-C22	5.16	1.57	1.45
24	5	305	BCR	C23-C22	5.16	1.57	1.45
24	6	306	BCR	C29-C30	5.16	1.66	1.54
24	I	4001	BCR	C23-C22	5.15	1.57	1.45
21	A	801	CL0	O2D-CGD	5.15	1.45	1.33
24	4	804	BCR	C29-C30	5.14	1.66	1.54
24	7	303	BCR	C29-C30	5.11	1.65	1.54
24	B	848	BCR	C29-C30	5.10	1.65	1.54
21	A	801	CL0	O2A-C1	5.10	1.60	1.46
24	5	305	BCR	C29-C30	5.09	1.65	1.54
38	1	302	LUT	C8-C9	5.07	1.56	1.45
38	Z	301	LUT	C8-C9	5.03	1.56	1.45
38	6	303	LUT	C8-C9	5.02	1.56	1.45
32	F	306	RRX	C2-C1	5.02	1.65	1.54
36	5	306	C7Z	C24-C25	-5.01	1.43	1.51
24	B	853	BCR	C15-C14	5.01	1.59	1.43
38	7	302	LUT	C8-C9	4.99	1.56	1.45
38	Z	302	LUT	C8-C9	4.99	1.56	1.45
38	8	303	LUT	C8-C9	4.98	1.56	1.45
38	1	303	LUT	C8-C9	4.98	1.56	1.45
38	6	304	LUT	C8-C9	4.96	1.56	1.45
24	6	306	BCR	C23-C22	4.96	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	847	BCR	C29-C30	4.96	1.65	1.54
38	5	303	LUT	C8-C9	4.95	1.56	1.45
38	9	302	LUT	C8-C9	4.94	1.56	1.45
38	7	301	LUT	C8-C9	4.94	1.56	1.45
38	9	301	LUT	C8-C9	4.93	1.56	1.45
38	8	302	LUT	C8-C9	4.93	1.56	1.45
38	3	303	LUT	C8-C9	4.93	1.56	1.45
32	F	306	RRX	C23-C22	4.92	1.56	1.45
24	3	306	BCR	C15-C14	4.91	1.58	1.43
24	A	844	BCR	C15-C14	4.87	1.58	1.43
38	4	802	LUT	C8-C9	4.87	1.56	1.45
38	5	302	LUT	C8-C9	4.87	1.56	1.45
38	4	803	LUT	C8-C9	4.83	1.56	1.45
24	3	304	BCR	C15-C14	4.83	1.58	1.43
24	B	853	BCR	C19-C18	4.83	1.56	1.45
21	A	801	CL0	CHC-C1C	4.82	1.48	1.38
24	7	303	BCR	C15-C14	4.81	1.58	1.43
36	J	105	C7Z	C24-C25	-4.81	1.43	1.51
24	J	104	BCR	C15-C14	4.80	1.58	1.43
24	3	305	BCR	C15-C14	4.80	1.58	1.43
24	B	853	BCR	C29-C30	4.79	1.65	1.54
38	3	302	LUT	C8-C9	4.79	1.56	1.45
24	A	848	BCR	C15-C14	4.78	1.58	1.43
24	5	304	BCR	C15-C14	4.77	1.58	1.43
24	6	305	BCR	C15-C14	4.77	1.58	1.43
24	A	856	BCR	C15-C14	4.76	1.58	1.43
24	I	4001	BCR	C15-C14	4.76	1.58	1.43
24	8	304	BCR	C15-C14	4.76	1.58	1.43
24	B	849	BCR	C15-C14	4.75	1.58	1.43
24	3	307	BCR	C15-C14	4.74	1.58	1.43
24	F	303	BCR	C15-C14	4.74	1.58	1.43
24	B	848	BCR	C15-C14	4.74	1.58	1.43
24	4	804	BCR	C15-C14	4.73	1.58	1.43
24	G	203	BCR	C15-C14	4.73	1.58	1.43
24	7	303	BCR	C19-C18	4.73	1.56	1.45
24	B	845	BCR	C15-C14	4.73	1.58	1.43
24	B	846	BCR	C15-C14	4.72	1.58	1.43
24	5	305	BCR	C15-C14	4.72	1.58	1.43
24	5	305	BCR	C19-C18	4.72	1.56	1.45
24	A	845	BCR	C15-C14	4.72	1.58	1.43
24	A	847	BCR	C15-C14	4.72	1.58	1.43
21	A	801	CL0	CHD-C1D	4.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Z	301	LUT	C12-C13	4.71	1.56	1.45
24	3	307	BCR	C19-C18	4.71	1.56	1.45
24	B	844	BCR	C15-C14	4.71	1.58	1.43
24	7	303	BCR	C2-C1	4.69	1.64	1.54
38	1	302	LUT	C12-C13	4.69	1.56	1.45
24	A	848	BCR	C19-C18	4.69	1.56	1.45
24	4	804	BCR	C2-C1	4.69	1.64	1.54
24	A	856	BCR	C19-C18	4.68	1.56	1.45
24	J	104	BCR	C2-C1	4.68	1.64	1.54
38	9	302	LUT	C4-C5	-4.68	1.43	1.51
24	K	206	BCR	C15-C14	4.68	1.57	1.43
24	L	204	BCR	C15-C14	4.67	1.57	1.43
24	B	849	BCR	C19-C18	4.67	1.56	1.45
38	Z	302	LUT	C12-C13	4.67	1.56	1.45
24	3	306	BCR	C2-C1	4.67	1.64	1.54
24	B	848	BCR	C2-C1	4.67	1.64	1.54
24	8	304	BCR	C2-C1	4.66	1.64	1.54
24	G	203	BCR	C19-C18	4.65	1.55	1.45
24	A	846	BCR	C15-C14	4.65	1.57	1.43
36	5	306	C7Z	C28-C29	4.65	1.55	1.45
38	4	802	LUT	C4-C5	-4.65	1.43	1.51
24	B	845	BCR	C2-C1	4.65	1.64	1.54
24	B	847	BCR	C15-C14	4.65	1.57	1.43
24	4	804	BCR	C19-C18	4.64	1.55	1.45
24	A	847	BCR	C2-C1	4.64	1.64	1.54
24	8	304	BCR	C19-C18	4.64	1.55	1.45
32	F	306	RRX	C24-C25	4.64	1.61	1.45
24	J	104	BCR	C19-C18	4.64	1.55	1.45
36	J	105	C7Z	C28-C29	4.64	1.55	1.45
24	A	846	BCR	C2-C1	4.63	1.64	1.54
24	F	303	BCR	C19-C18	4.63	1.55	1.45
24	6	305	BCR	C2-C1	4.63	1.64	1.54
24	L	204	BCR	C2-C1	4.63	1.64	1.54
38	7	302	LUT	C12-C13	4.63	1.55	1.45
24	3	305	BCR	C19-C18	4.63	1.55	1.45
24	3	307	BCR	C2-C1	4.62	1.64	1.54
24	6	306	BCR	C15-C14	4.62	1.57	1.43
38	6	303	LUT	C12-C13	4.62	1.55	1.45
38	1	303	LUT	C12-C13	4.62	1.55	1.45
24	3	306	BCR	C19-C18	4.61	1.55	1.45
24	3	304	BCR	C19-C18	4.61	1.55	1.45
24	3	304	BCR	C2-C1	4.61	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	844	BCR	C2-C1	4.61	1.64	1.54
24	A	848	BCR	C2-C1	4.60	1.64	1.54
24	6	306	BCR	C2-C1	4.59	1.64	1.54
24	K	206	BCR	C19-C18	4.59	1.55	1.45
24	A	844	BCR	C19-C18	4.59	1.55	1.45
38	5	303	LUT	C12-C13	4.59	1.55	1.45
24	B	848	BCR	C19-C18	4.59	1.55	1.45
24	B	845	BCR	C19-C18	4.59	1.55	1.45
38	3	303	LUT	C12-C13	4.59	1.55	1.45
38	8	303	LUT	C12-C13	4.58	1.55	1.45
24	B	847	BCR	C19-C18	4.58	1.55	1.45
24	B	853	BCR	C28-C27	4.58	1.66	1.52
38	7	301	LUT	C12-C13	4.58	1.55	1.45
24	B	853	BCR	C2-C1	4.58	1.64	1.54
21	A	801	CL0	C3C-C2C	4.57	1.46	1.36
38	7	302	LUT	C4-C5	-4.57	1.44	1.51
38	4	803	LUT	C12-C13	4.57	1.55	1.45
24	A	845	BCR	C19-C18	4.56	1.55	1.45
38	6	304	LUT	C12-C13	4.56	1.55	1.45
24	B	844	BCR	C19-C18	4.56	1.55	1.45
24	I	4001	BCR	C19-C18	4.55	1.55	1.45
24	I	4001	BCR	C2-C1	4.54	1.64	1.54
24	B	849	BCR	C2-C1	4.54	1.64	1.54
24	L	204	BCR	C19-C18	4.54	1.55	1.45
24	5	304	BCR	C19-C18	4.54	1.55	1.45
24	B	846	BCR	C19-C18	4.54	1.55	1.45
24	6	305	BCR	C19-C18	4.54	1.55	1.45
36	5	306	C7Z	C31-C30	4.54	1.57	1.43
24	5	304	BCR	C2-C1	4.53	1.64	1.54
38	5	302	LUT	C12-C13	4.52	1.55	1.45
24	A	845	BCR	C2-C1	4.52	1.64	1.54
38	4	803	LUT	C4-C5	-4.52	1.44	1.51
24	5	305	BCR	C2-C1	4.52	1.64	1.54
24	B	846	BCR	C2-C1	4.52	1.64	1.54
38	7	301	LUT	C4-C5	-4.52	1.44	1.51
38	9	302	LUT	C12-C13	4.51	1.55	1.45
24	K	206	BCR	C2-C1	4.51	1.64	1.54
38	5	303	LUT	C4-C5	-4.51	1.44	1.51
38	8	302	LUT	C12-C13	4.51	1.55	1.45
38	9	301	LUT	C12-C13	4.51	1.55	1.45
38	3	303	LUT	C4-C5	-4.51	1.44	1.51
38	4	802	LUT	C12-C13	4.50	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	304	LUT	C4-C5	-4.50	1.44	1.51
38	9	301	LUT	C4-C5	-4.50	1.44	1.51
38	8	303	LUT	C4-C5	-4.50	1.44	1.51
24	A	856	BCR	C2-C1	4.49	1.64	1.54
24	A	846	BCR	C19-C18	4.49	1.55	1.45
24	B	844	BCR	C2-C1	4.48	1.64	1.54
24	A	847	BCR	C19-C18	4.48	1.55	1.45
38	Z	302	LUT	C4-C5	-4.48	1.44	1.51
24	F	303	BCR	C2-C1	4.47	1.64	1.54
38	5	302	LUT	C4-C5	-4.46	1.44	1.51
32	F	306	RRX	C12-C13	4.46	1.55	1.45
24	B	847	BCR	C2-C1	4.45	1.64	1.54
38	8	302	LUT	C4-C5	-4.45	1.44	1.51
36	J	105	C7Z	C31-C30	4.44	1.57	1.43
38	Z	301	LUT	C31-C30	4.41	1.57	1.43
38	3	302	LUT	C4-C5	-4.40	1.44	1.51
38	Z	301	LUT	C15-C14	4.40	1.57	1.43
38	1	302	LUT	C15-C14	4.40	1.57	1.43
24	G	203	BCR	C2-C1	4.40	1.64	1.54
24	3	305	BCR	C2-C1	4.38	1.64	1.54
38	1	303	LUT	C4-C5	-4.38	1.44	1.51
38	Z	302	LUT	C31-C30	4.37	1.57	1.43
38	Z	302	LUT	C15-C14	4.37	1.57	1.43
38	1	303	LUT	C15-C14	4.37	1.57	1.43
24	8	304	BCR	C20-C21	4.36	1.57	1.43
24	A	856	BCR	C20-C21	4.36	1.57	1.43
38	Z	301	LUT	C4-C5	-4.36	1.44	1.51
38	7	302	LUT	C15-C14	4.36	1.56	1.43
22	5	320	CLA	MG-ND	-4.36	1.97	2.05
38	6	303	LUT	C4-C5	-4.35	1.44	1.51
38	5	303	LUT	C31-C30	4.35	1.56	1.43
38	3	302	LUT	C31-C30	4.35	1.56	1.43
24	7	303	BCR	C20-C21	4.34	1.56	1.43
38	5	303	LUT	C15-C14	4.34	1.56	1.43
38	1	302	LUT	C35-C34	4.34	1.56	1.43
24	A	848	BCR	C20-C21	4.33	1.56	1.43
38	3	303	LUT	C15-C14	4.33	1.56	1.43
38	3	303	LUT	C31-C30	4.33	1.56	1.43
38	7	301	LUT	C15-C14	4.32	1.56	1.43
38	6	304	LUT	C15-C14	4.32	1.56	1.43
38	9	302	LUT	C31-C30	4.32	1.56	1.43
32	F	306	RRX	C3-C4	4.31	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	302	LUT	C31-C30	4.31	1.56	1.43
31	B	852	DGD	O1G-C1A	4.31	1.45	1.33
38	8	303	LUT	C31-C30	4.31	1.56	1.43
39	Z	312	CHL	CBB-CAB	4.31	1.51	1.30
22	A	817	CLA	CBB-CAB	4.31	1.51	1.30
22	K	205	CLA	MG-ND	-4.31	1.97	2.05
39	4	814	CHL	CBB-CAB	4.31	1.51	1.30
22	A	830	CLA	CBB-CAB	4.30	1.51	1.30
24	B	847	BCR	C28-C27	4.30	1.66	1.52
22	8	307	CLA	CBB-CAB	4.30	1.51	1.30
24	3	307	BCR	C20-C21	4.30	1.56	1.43
24	3	304	BCR	C20-C21	4.30	1.56	1.43
38	1	303	LUT	C31-C30	4.30	1.56	1.43
38	8	303	LUT	C15-C14	4.30	1.56	1.43
22	5	322	CLA	CBB-CAB	4.30	1.51	1.30
22	6	308	CLA	CBB-CAB	4.30	1.51	1.30
24	B	849	BCR	C20-C21	4.30	1.56	1.43
38	7	301	LUT	C31-C30	4.30	1.56	1.43
24	A	856	BCR	C28-C27	4.30	1.66	1.52
24	4	804	BCR	C20-C21	4.30	1.56	1.43
22	B	831	CLA	CBB-CAB	4.30	1.51	1.30
24	A	844	BCR	C28-C27	4.29	1.66	1.52
22	Z	306	CLA	CBB-CAB	4.29	1.51	1.30
39	4	816	CHL	CBB-CAB	4.29	1.51	1.30
39	6	318	CHL	CBB-CAB	4.29	1.51	1.30
38	Z	301	LUT	C35-C34	4.29	1.56	1.43
39	6	316	CHL	CBB-CAB	4.29	1.51	1.30
24	J	104	BCR	C28-C27	4.29	1.66	1.52
38	7	302	LUT	C31-C30	4.29	1.56	1.43
38	6	303	LUT	C15-C14	4.29	1.56	1.43
22	L	201	CLA	CBB-CAB	4.29	1.51	1.30
22	1	308	CLA	CBB-CAB	4.29	1.51	1.30
24	3	305	BCR	C20-C21	4.29	1.56	1.43
22	A	808	CLA	CBB-CAB	4.29	1.51	1.30
22	8	313	CLA	CBB-CAB	4.29	1.51	1.30
22	5	309	CLA	CBB-CAB	4.29	1.51	1.30
36	5	306	C7Z	C32-C33	4.29	1.55	1.45
38	6	304	LUT	C31-C30	4.29	1.56	1.43
22	B	834	CLA	CBB-CAB	4.29	1.51	1.30
24	B	853	BCR	C20-C21	4.29	1.56	1.43
22	B	808	CLA	CBB-CAB	4.29	1.51	1.30
22	Z	310	CLA	CBB-CAB	4.29	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	829	CLA	CBB-CAB	4.29	1.51	1.30
22	Z	304	CLA	CBB-CAB	4.29	1.51	1.30
22	B	822	CLA	CBB-CAB	4.29	1.51	1.30
22	6	321	CLA	CBB-CAB	4.29	1.51	1.30
22	4	809	CLA	CBB-CAB	4.29	1.51	1.30
22	5	318	CLA	CBB-CAB	4.29	1.51	1.30
22	2	301	CLA	CBB-CAB	4.29	1.51	1.30
22	7	304	CLA	CBB-CAB	4.29	1.51	1.30
22	Z	305	CLA	CBB-CAB	4.29	1.51	1.30
22	7	310	CLA	CBB-CAB	4.29	1.51	1.30
24	F	303	BCR	C20-C21	4.29	1.56	1.43
22	1	305	CLA	CBB-CAB	4.28	1.51	1.30
22	1	307	CLA	CBB-CAB	4.28	1.51	1.30
22	Z	308	CLA	CBB-CAB	4.28	1.51	1.30
22	7	311	CLA	CBB-CAB	4.28	1.51	1.30
22	8	310	CLA	CBB-CAB	4.28	1.51	1.30
22	3	314	CLA	CBB-CAB	4.28	1.51	1.30
24	5	304	BCR	C20-C21	4.28	1.56	1.43
39	1	312	CHL	CBB-CAB	4.28	1.51	1.30
22	A	820	CLA	CBB-CAB	4.28	1.51	1.30
31	3	301	DGD	O1G-C1A	4.28	1.45	1.33
22	1	309	CLA	CBB-CAB	4.28	1.51	1.30
22	8	306	CLA	CBB-CAB	4.28	1.51	1.30
22	5	307	CLA	CBB-CAB	4.28	1.51	1.30
22	B	826	CLA	CBB-CAB	4.28	1.51	1.30
22	A	821	CLA	CBB-CAB	4.28	1.51	1.30
22	A	807	CLA	CBB-CAB	4.28	1.51	1.30
22	3	313	CLA	CBB-CAB	4.28	1.51	1.30
22	4	810	CLA	CBB-CAB	4.28	1.51	1.30
22	5	313	CLA	CBB-CAB	4.28	1.51	1.30
22	9	311	CLA	CBB-CAB	4.28	1.51	1.30
36	J	105	C7Z	C32-C33	4.28	1.55	1.45
38	3	302	LUT	C12-C13	4.28	1.55	1.45
22	B	838	CLA	CBB-CAB	4.28	1.51	1.30
22	1	304	CLA	CBB-CAB	4.28	1.51	1.30
24	3	306	BCR	C20-C21	4.28	1.56	1.43
22	A	826	CLA	CBB-CAB	4.28	1.51	1.30
22	7	314	CLA	CBB-CAB	4.28	1.51	1.30
22	B	817	CLA	CBB-CAB	4.28	1.51	1.30
22	9	313	CLA	CBB-CAB	4.28	1.51	1.30
22	6	302	CLA	CBB-CAB	4.28	1.51	1.30
22	3	309	CLA	CBB-CAB	4.28	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	315	CLA	CBB-CAB	4.28	1.51	1.30
22	5	326	CLA	CBB-CAB	4.28	1.51	1.30
22	J	103	CLA	CBB-CAB	4.28	1.51	1.30
22	B	807	CLA	CBB-CAB	4.28	1.51	1.30
22	F	305	CLA	CBB-CAB	4.28	1.51	1.30
22	5	301	CLA	CBB-CAB	4.28	1.51	1.30
22	7	316	CLA	CBB-CAB	4.28	1.51	1.30
22	5	323	CLA	CBB-CAB	4.28	1.51	1.30
22	A	819	CLA	CBB-CAB	4.28	1.51	1.30
22	B	823	CLA	CBB-CAB	4.28	1.51	1.30
22	B	833	CLA	CBB-CAB	4.28	1.51	1.30
22	3	322	CLA	CBB-CAB	4.28	1.51	1.30
22	8	308	CLA	CBB-CAB	4.28	1.51	1.30
22	6	307	CLA	CBB-CAB	4.28	1.51	1.30
22	F	302	CLA	CBB-CAB	4.28	1.51	1.30
22	A	835	CLA	CBB-CAB	4.28	1.51	1.30
22	G	201	CLA	CBB-CAB	4.28	1.51	1.30
22	7	317	CLA	CBB-CAB	4.28	1.51	1.30
22	B	825	CLA	CBB-CAB	4.28	1.51	1.30
22	5	315	CLA	CBB-CAB	4.28	1.51	1.30
22	B	820	CLA	CBB-CAB	4.28	1.51	1.30
22	7	322	CLA	CBB-CAB	4.28	1.51	1.30
22	5	314	CLA	CBB-CAB	4.28	1.51	1.30
22	B	830	CLA	CBB-CAB	4.28	1.51	1.30
22	2	304	CLA	CBB-CAB	4.28	1.51	1.30
22	3	310	CLA	CBB-CAB	4.28	1.51	1.30
38	9	301	LUT	C15-C14	4.27	1.56	1.43
22	8	311	CLA	CBB-CAB	4.27	1.51	1.30
22	4	817	CLA	CBB-CAB	4.27	1.51	1.30
22	9	308	CLA	CBB-CAB	4.27	1.51	1.30
22	A	854	CLA	CBB-CAB	4.27	1.51	1.30
22	A	834	CLA	CBB-CAB	4.27	1.51	1.30
22	6	317	CLA	CBB-CAB	4.27	1.51	1.30
22	B	801	CLA	CBB-CAB	4.27	1.51	1.30
22	A	810	CLA	CBB-CAB	4.27	1.51	1.30
22	5	310	CLA	CBB-CAB	4.27	1.51	1.30
39	2	303	CHL	CBB-CAB	4.27	1.51	1.30
22	A	828	CLA	CBB-CAB	4.27	1.51	1.30
22	A	825	CLA	CBB-CAB	4.27	1.51	1.30
22	B	819	CLA	CBB-CAB	4.27	1.51	1.30
22	B	835	CLA	CBB-CAB	4.27	1.51	1.30
22	2	302	CLA	CBB-CAB	4.27	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	8	312	CHL	CBB-CAB	4.27	1.51	1.30
22	B	841	CLA	CBB-CAB	4.27	1.51	1.30
22	K	202	CLA	CBB-CAB	4.27	1.51	1.30
22	1	315	CLA	CBB-CAB	4.27	1.51	1.30
22	3	312	CLA	CBB-CAB	4.27	1.51	1.30
22	9	307	CLA	CBB-CAB	4.27	1.51	1.30
22	A	804	CLA	CBB-CAB	4.27	1.51	1.30
22	B	821	CLA	CBB-CAB	4.27	1.51	1.30
22	5	308	CLA	CBB-CAB	4.27	1.51	1.30
22	4	815	CLA	CBB-CAB	4.27	1.51	1.30
38	8	302	LUT	C15-C14	4.27	1.56	1.43
22	B	829	CLA	CBB-CAB	4.27	1.51	1.30
22	B	840	CLA	CBB-CAB	4.27	1.51	1.30
22	1	310	CLA	CBB-CAB	4.27	1.51	1.30
22	3	311	CLA	CBB-CAB	4.27	1.51	1.30
24	B	845	BCR	C28-C27	4.27	1.65	1.52
38	6	303	LUT	C31-C30	4.27	1.56	1.43
22	A	823	CLA	CBB-CAB	4.27	1.51	1.30
22	4	812	CLA	CBB-CAB	4.27	1.51	1.30
22	3	319	CLA	CBB-CAB	4.27	1.51	1.30
22	A	831	CLA	CBB-CAB	4.27	1.51	1.30
22	A	855	CLA	CBB-CAB	4.27	1.51	1.30
22	F	301	CLA	CBB-CAB	4.27	1.51	1.30
22	Z	313	CLA	CBB-CAB	4.27	1.51	1.30
22	B	836	CLA	CBB-CAB	4.27	1.51	1.30
22	8	314	CLA	CBB-CAB	4.27	1.51	1.30
22	7	323	CLA	CBB-CAB	4.27	1.51	1.30
22	B	809	CLA	CBB-CAB	4.27	1.51	1.30
22	Z	303	CLA	CBB-CAB	4.27	1.51	1.30
22	A	832	CLA	CBB-CAB	4.27	1.51	1.30
22	7	309	CLA	CBB-CAB	4.27	1.51	1.30
22	8	316	CLA	CBB-CAB	4.27	1.51	1.30
22	4	818	CLA	CBB-CAB	4.27	1.51	1.30
24	L	204	BCR	C28-C27	4.27	1.65	1.52
22	A	824	CLA	CBB-CAB	4.27	1.51	1.30
22	G	202	CLA	CBB-CAB	4.27	1.51	1.30
22	7	307	CLA	CBB-CAB	4.27	1.51	1.30
22	1	314	CLA	CBB-CAB	4.27	1.51	1.30
22	7	308	CLA	CBB-CAB	4.27	1.51	1.30
22	B	827	CLA	CBB-CAB	4.27	1.51	1.30
22	7	312	CLA	CBB-CAB	4.27	1.51	1.30
22	5	312	CLA	CBB-CAB	4.27	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	319	CLA	CBB-CAB	4.27	1.51	1.30
24	I	4001	BCR	C28-C27	4.27	1.65	1.52
22	A	818	CLA	CBB-CAB	4.27	1.51	1.30
39	4	813	CHL	CBB-CAB	4.27	1.51	1.30
22	7	324	CLA	CBB-CAB	4.27	1.51	1.30
39	8	315	CHL	CBB-CAB	4.27	1.51	1.30
22	B	813	CLA	CBB-CAB	4.26	1.51	1.30
22	3	318	CLA	CBB-CAB	4.26	1.51	1.30
22	B	812	CLA	CBB-CAB	4.26	1.51	1.30
24	5	304	BCR	C28-C27	4.26	1.65	1.52
38	9	301	LUT	C31-C30	4.26	1.56	1.43
22	A	833	CLA	CBB-CAB	4.26	1.51	1.30
22	B	832	CLA	CBB-CAB	4.26	1.51	1.30
22	6	301	CLA	CBB-CAB	4.26	1.51	1.30
24	K	206	BCR	C20-C21	4.26	1.56	1.43
22	A	815	CLA	CBB-CAB	4.26	1.51	1.30
22	1	313	CLA	CBB-CAB	4.26	1.51	1.30
22	3	308	CLA	CBB-CAB	4.26	1.51	1.30
22	A	805	CLA	CBB-CAB	4.26	1.51	1.30
22	B	842	CLA	CBB-CAB	4.26	1.51	1.30
22	A	814	CLA	CBB-CAB	4.26	1.51	1.30
22	A	822	CLA	CBB-CAB	4.26	1.51	1.30
22	L	202	CLA	CBB-CAB	4.26	1.51	1.30
24	J	104	BCR	C20-C21	4.26	1.56	1.43
22	A	802	CLA	CBB-CAB	4.26	1.51	1.30
22	6	311	CLA	CBB-CAB	4.26	1.51	1.30
22	3	316	CLA	CBB-CAB	4.26	1.51	1.30
22	A	841	CLA	CBB-CAB	4.26	1.51	1.30
22	1	306	CLA	CBB-CAB	4.26	1.51	1.30
22	Z	314	CLA	CBB-CAB	4.26	1.51	1.30
22	B	818	CLA	CBB-CAB	4.26	1.51	1.30
22	6	313	CLA	CBB-CAB	4.26	1.51	1.30
22	B	816	CLA	CBB-CAB	4.26	1.51	1.30
22	B	839	CLA	CBB-CAB	4.26	1.51	1.30
22	B	811	CLA	CBB-CAB	4.26	1.51	1.30
22	A	803	CLA	CBB-CAB	4.26	1.51	1.30
22	L	203	CLA	CBB-CAB	4.26	1.51	1.30
22	4	806	CLA	CBB-CAB	4.26	1.51	1.30
22	B	837	CLA	CBB-CAB	4.26	1.51	1.30
22	7	305	CLA	CBB-CAB	4.26	1.51	1.30
38	4	803	LUT	C15-C14	4.26	1.56	1.43
38	9	302	LUT	C15-C14	4.26	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	814	CLA	CBB-CAB	4.26	1.51	1.30
22	1	311	CLA	CBB-CAB	4.26	1.51	1.30
22	6	322	CLA	CBB-CAB	4.26	1.51	1.30
22	A	839	CLA	CBB-CAB	4.26	1.51	1.30
39	9	312	CHL	CBB-CAB	4.26	1.51	1.30
22	B	805	CLA	CBB-CAB	4.26	1.51	1.30
22	6	312	CLA	CBB-CAB	4.26	1.51	1.30
22	4	807	CLA	CBB-CAB	4.26	1.51	1.30
24	A	848	BCR	C28-C27	4.26	1.65	1.52
22	B	824	CLA	CBB-CAB	4.26	1.51	1.30
22	Z	307	CLA	CBB-CAB	4.26	1.51	1.30
22	A	816	CLA	CBB-CAB	4.26	1.51	1.30
22	4	811	CLA	CBB-CAB	4.26	1.51	1.30
22	9	306	CLA	CBB-CAB	4.26	1.51	1.30
22	3	315	CLA	CBB-CAB	4.26	1.51	1.30
38	1	303	LUT	C35-C34	4.26	1.56	1.43
22	A	812	CLA	CBB-CAB	4.25	1.51	1.30
22	6	314	CLA	CBB-CAB	4.25	1.51	1.30
22	A	809	CLA	CBB-CAB	4.25	1.51	1.30
22	Z	316	CLA	CBB-CAB	4.25	1.51	1.30
22	6	309	CLA	CBB-CAB	4.25	1.51	1.30
39	5	317	CHL	CBB-CAB	4.25	1.51	1.30
22	A	840	CLA	CBB-CAB	4.25	1.51	1.30
22	8	309	CLA	CBB-CAB	4.25	1.51	1.30
22	8	305	CLA	CBB-CAB	4.25	1.51	1.30
22	B	815	CLA	CBB-CAB	4.25	1.51	1.30
22	B	828	CLA	CBB-CAB	4.25	1.51	1.30
24	B	849	BCR	C28-C27	4.25	1.65	1.52
24	B	847	BCR	C20-C21	4.25	1.56	1.43
22	Z	309	CLA	CBB-CAB	4.25	1.51	1.30
22	F	304	CLA	CBB-CAB	4.25	1.51	1.30
22	4	805	CLA	CBB-CAB	4.25	1.51	1.30
38	4	802	LUT	C31-C30	4.25	1.56	1.43
24	B	844	BCR	C20-C21	4.25	1.56	1.43
24	I	4001	BCR	C20-C21	4.25	1.56	1.43
22	5	311	CLA	CBB-CAB	4.25	1.51	1.30
24	3	305	BCR	C28-C27	4.25	1.65	1.52
22	A	811	CLA	CBB-CAB	4.25	1.51	1.30
38	5	302	LUT	C15-C14	4.25	1.56	1.43
22	5	319	CLA	CBB-CAB	4.24	1.51	1.30
22	A	842	CLA	CBB-CAB	4.24	1.51	1.30
22	A	806	CLA	CBB-CAB	4.24	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	315	CLA	CBB-CAB	4.24	1.51	1.30
38	Z	302	LUT	C35-C34	4.24	1.56	1.43
22	A	837	CLA	CBB-CAB	4.24	1.51	1.30
39	9	314	CHL	CBB-CAB	4.24	1.51	1.30
22	A	813	CLA	CBB-CAB	4.24	1.51	1.30
38	5	303	LUT	C35-C34	4.24	1.56	1.43
21	A	801	CL0	C3D-C4D	-4.24	1.34	1.44
24	6	306	BCR	C19-C18	4.24	1.55	1.45
22	K	203	CLA	CBB-CAB	4.24	1.51	1.30
32	F	306	RRX	C11-C10	4.24	1.56	1.43
38	4	802	LUT	C15-C14	4.24	1.56	1.43
22	A	836	CLA	CBB-CAB	4.24	1.51	1.30
22	7	306	CLA	CBB-CAB	4.24	1.51	1.30
38	8	302	LUT	C31-C30	4.24	1.56	1.43
22	A	838	CLA	CBB-CAB	4.23	1.51	1.30
38	7	301	LUT	C35-C34	4.23	1.56	1.43
39	3	317	CHL	CBB-CAB	4.23	1.51	1.30
22	B	806	CLA	CBB-CAB	4.23	1.51	1.30
38	7	302	LUT	C35-C34	4.23	1.56	1.43
22	4	808	CLA	CBB-CAB	4.23	1.51	1.30
22	B	810	CLA	CBB-CAB	4.23	1.51	1.30
22	K	204	CLA	CBB-CAB	4.23	1.51	1.30
24	A	845	BCR	C20-C21	4.23	1.56	1.43
24	6	305	BCR	C20-C21	4.23	1.56	1.43
24	3	306	BCR	C28-C27	4.23	1.65	1.52
24	L	204	BCR	C20-C21	4.23	1.56	1.43
38	6	304	LUT	C35-C34	4.23	1.56	1.43
22	K	205	CLA	CBB-CAB	4.23	1.51	1.30
38	6	303	LUT	C35-C34	4.23	1.56	1.43
22	9	304	CLA	CBB-CAB	4.23	1.51	1.30
39	4	819	CHL	CBB-CAB	4.23	1.51	1.30
24	A	845	BCR	C28-C27	4.23	1.65	1.52
22	6	310	CLA	CBB-CAB	4.22	1.51	1.30
24	K	206	BCR	C28-C27	4.22	1.65	1.52
22	A	827	CLA	CBB-CAB	4.22	1.51	1.30
39	7	313	CHL	CBB-CAB	4.22	1.51	1.30
24	B	845	BCR	C20-C21	4.22	1.56	1.43
24	A	844	BCR	C20-C21	4.22	1.56	1.43
24	G	203	BCR	C20-C21	4.22	1.56	1.43
38	4	803	LUT	C31-C30	4.21	1.56	1.43
39	8	301	CHL	CBB-CAB	4.21	1.51	1.30
22	9	305	CLA	CBB-CAB	4.21	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	846	BCR	C20-C21	4.21	1.56	1.43
24	A	847	BCR	C20-C21	4.21	1.56	1.43
22	1	316	CLA	CBB-CAB	4.21	1.51	1.30
24	B	848	BCR	C20-C21	4.21	1.56	1.43
39	Z	311	CHL	CBB-CAB	4.20	1.51	1.30
39	6	315	CHL	CBB-CAB	4.20	1.51	1.30
24	A	847	BCR	C28-C27	4.20	1.65	1.52
39	5	321	CHL	CBB-CAB	4.20	1.51	1.30
24	5	305	BCR	C20-C21	4.20	1.56	1.43
38	8	302	LUT	C35-C34	4.19	1.56	1.43
22	9	310	CLA	CBB-CAB	4.19	1.51	1.30
38	8	303	LUT	C35-C34	4.19	1.56	1.43
38	5	302	LUT	C31-C30	4.19	1.56	1.43
38	Z	301	LUT	C28-C29	4.19	1.54	1.45
22	K	205	CLA	C1C-NC	-4.19	1.31	1.37
24	B	844	BCR	C28-C27	4.19	1.65	1.52
22	9	309	CLA	CBB-CAB	4.19	1.51	1.30
24	A	846	BCR	C20-C21	4.19	1.56	1.43
38	4	803	LUT	C35-C34	4.19	1.56	1.43
38	9	301	LUT	C35-C34	4.19	1.56	1.43
22	3	320	CLA	CBB-CAB	4.18	1.51	1.30
38	3	303	LUT	C35-C34	4.18	1.56	1.43
38	9	302	LUT	C35-C34	4.18	1.56	1.43
24	5	305	BCR	C28-C27	4.18	1.65	1.52
39	6	320	CHL	CBB-CAB	4.17	1.50	1.30
24	7	303	BCR	C28-C27	4.16	1.65	1.52
22	5	320	CLA	CBB-CAB	4.16	1.50	1.30
24	A	846	BCR	C28-C27	4.16	1.65	1.52
24	4	804	BCR	C28-C27	4.16	1.65	1.52
38	4	802	LUT	C35-C34	4.15	1.56	1.43
31	1	319	DGD	O1G-C1A	4.15	1.45	1.33
22	1	316	CLA	MG-ND	-4.14	1.97	2.05
24	3	307	BCR	C28-C27	4.14	1.65	1.52
39	5	316	CHL	CBB-CAB	4.14	1.50	1.30
24	3	304	BCR	C28-C27	4.14	1.65	1.52
32	F	306	RRX	C29-C30	4.14	1.67	1.54
24	B	846	BCR	C28-C27	4.13	1.65	1.52
38	3	302	LUT	C15-C14	4.13	1.56	1.43
38	3	302	LUT	C28-C29	4.13	1.54	1.45
24	F	303	BCR	C28-C27	4.13	1.65	1.52
38	1	302	LUT	C28-C29	4.13	1.54	1.45
24	B	848	BCR	C28-C27	4.11	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	306	BCR	C28-C27	4.10	1.65	1.52
38	5	302	LUT	C35-C34	4.10	1.56	1.43
32	F	306	RRX	C15-C14	4.10	1.56	1.43
24	G	203	BCR	C28-C27	4.09	1.65	1.52
24	8	304	BCR	C28-C27	4.08	1.65	1.52
38	3	302	LUT	C35-C34	4.08	1.56	1.43
22	9	303	CLA	CBB-CAB	4.08	1.50	1.30
24	6	305	BCR	C28-C27	4.07	1.65	1.52
25	3	321	LHG	O7-C5	-4.07	1.42	1.46
24	6	306	BCR	C20-C21	4.07	1.56	1.43
38	Z	301	LUT	C7-C6	4.07	1.59	1.45
38	Z	302	LUT	C28-C29	4.06	1.54	1.45
38	6	303	LUT	C7-C6	4.06	1.59	1.45
38	5	303	LUT	C28-C29	4.04	1.54	1.45
21	A	801	CL0	CHB-C1B	4.04	1.48	1.39
38	1	302	LUT	C7-C6	4.04	1.59	1.45
38	8	302	LUT	C28-C29	4.04	1.54	1.45
32	F	306	RRX	C16-C17	4.03	1.55	1.43
38	1	303	LUT	C28-C29	4.03	1.54	1.45
21	A	801	CL0	CHD-C4C	4.03	1.48	1.39
38	3	303	LUT	C28-C29	4.03	1.54	1.45
38	9	302	LUT	C28-C29	4.02	1.54	1.45
38	6	303	LUT	C28-C29	4.02	1.54	1.45
38	7	302	LUT	C7-C6	4.02	1.59	1.45
38	8	303	LUT	C28-C29	4.02	1.54	1.45
38	Z	302	LUT	C7-C6	4.02	1.59	1.45
22	9	309	CLA	MG-ND	-4.02	1.97	2.05
38	6	304	LUT	C28-C29	4.02	1.54	1.45
38	7	301	LUT	C28-C29	4.01	1.54	1.45
38	5	303	LUT	C7-C6	4.01	1.59	1.45
38	8	302	LUT	C21-C26	4.01	1.67	1.56
38	6	304	LUT	C7-C6	4.01	1.59	1.45
38	9	301	LUT	C28-C29	4.00	1.54	1.45
38	1	302	LUT	C4-C5	-4.00	1.44	1.51
38	9	301	LUT	C7-C6	4.00	1.59	1.45
22	3	315	CLA	MG-ND	-3.99	1.97	2.05
38	5	302	LUT	C7-C6	3.99	1.59	1.45
38	9	302	LUT	C7-C6	3.99	1.59	1.45
38	8	302	LUT	C7-C6	3.99	1.59	1.45
38	3	303	LUT	C7-C6	3.99	1.59	1.45
38	1	303	LUT	C7-C6	3.98	1.59	1.45
38	5	302	LUT	C28-C29	3.98	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	304	BCR	C3-C4	3.98	1.65	1.52
38	8	303	LUT	C7-C6	3.98	1.59	1.45
24	3	307	BCR	C3-C4	3.98	1.64	1.52
21	A	801	CL0	CHC-C4B	3.97	1.48	1.39
38	7	301	LUT	C7-C6	3.97	1.59	1.45
24	A	845	BCR	C3-C4	3.97	1.64	1.52
24	L	204	BCR	C3-C4	3.96	1.64	1.52
38	4	803	LUT	C7-C6	3.96	1.59	1.45
24	J	104	BCR	C3-C4	3.96	1.64	1.52
24	7	303	BCR	C3-C4	3.96	1.64	1.52
38	4	803	LUT	C28-C29	3.96	1.54	1.45
38	4	802	LUT	C7-C6	3.95	1.59	1.45
32	F	306	RRX	C20-C21	3.95	1.55	1.43
38	7	302	LUT	C28-C29	3.95	1.54	1.45
22	9	303	CLA	MG-ND	-3.95	1.98	2.05
24	A	848	BCR	C3-C4	3.95	1.64	1.52
38	4	802	LUT	C28-C29	3.94	1.54	1.45
22	9	304	CLA	MG-ND	-3.94	1.98	2.05
24	3	306	BCR	C11-C10	3.93	1.55	1.43
38	3	302	LUT	C7-C6	3.93	1.59	1.45
36	5	306	C7Z	C22-C21	3.93	1.67	1.54
24	I	4001	BCR	C3-C4	3.93	1.64	1.52
24	B	845	BCR	C3-C4	3.93	1.64	1.52
38	Z	301	LUT	C21-C26	3.93	1.67	1.56
38	9	302	LUT	C21-C26	3.92	1.67	1.56
38	9	301	LUT	C21-C26	3.92	1.67	1.56
24	A	856	BCR	C3-C4	3.92	1.64	1.52
38	Z	302	LUT	C21-C26	3.91	1.67	1.56
24	5	305	BCR	C11-C10	3.90	1.55	1.43
24	6	306	BCR	C3-C4	3.90	1.64	1.52
38	8	303	LUT	C21-C26	3.89	1.67	1.56
24	B	853	BCR	C3-C4	3.89	1.64	1.52
24	B	846	BCR	C3-C4	3.89	1.64	1.52
38	3	303	LUT	C21-C26	3.89	1.67	1.56
24	3	305	BCR	C3-C4	3.88	1.64	1.52
22	9	305	CLA	MG-ND	-3.88	1.98	2.05
24	G	203	BCR	C3-C4	3.88	1.64	1.52
22	1	316	CLA	C1C-NC	-3.88	1.32	1.37
22	9	310	CLA	MG-ND	-3.88	1.98	2.05
36	5	306	C7Z	C4-C5	-3.88	1.45	1.51
24	B	853	BCR	C16-C17	3.88	1.55	1.43
38	6	304	LUT	C21-C26	3.87	1.67	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	847	BCR	C3-C4	3.87	1.64	1.52
24	F	303	BCR	C3-C4	3.87	1.64	1.52
38	4	803	LUT	C21-C26	3.87	1.67	1.56
24	3	306	BCR	C3-C4	3.86	1.64	1.52
38	1	302	LUT	C21-C26	3.86	1.67	1.56
22	5	320	CLA	C4B-NB	-3.86	1.33	1.37
36	J	105	C7Z	C11-C10	3.86	1.55	1.43
36	5	306	C7Z	C15-C14	3.86	1.55	1.43
38	7	302	LUT	C21-C26	3.86	1.67	1.56
24	3	306	BCR	C16-C17	3.86	1.55	1.43
24	5	305	BCR	C3-C4	3.85	1.64	1.52
22	3	320	CLA	C1C-NC	-3.85	1.32	1.37
22	5	320	CLA	C1C-NC	-3.85	1.32	1.37
22	3	320	CLA	MG-ND	-3.85	1.98	2.05
36	J	105	C7Z	C15-C14	3.85	1.55	1.43
22	9	303	CLA	C4B-NB	-3.84	1.33	1.37
24	A	844	BCR	C16-C17	3.84	1.55	1.43
38	5	302	LUT	C21-C26	3.84	1.67	1.56
24	A	847	BCR	C3-C4	3.84	1.64	1.52
24	5	304	BCR	C3-C4	3.84	1.64	1.52
24	B	853	BCR	C11-C10	3.83	1.55	1.43
24	B	844	BCR	C3-C4	3.83	1.64	1.52
24	K	206	BCR	C3-C4	3.83	1.64	1.52
22	9	303	CLA	C1C-NC	-3.82	1.32	1.37
38	7	301	LUT	C21-C26	3.82	1.67	1.56
24	L	204	BCR	C11-C10	3.82	1.55	1.43
36	J	105	C7Z	C22-C21	3.81	1.66	1.54
24	3	304	BCR	C16-C17	3.81	1.55	1.43
24	B	848	BCR	C3-C4	3.81	1.64	1.52
24	B	849	BCR	C3-C4	3.80	1.64	1.52
38	Z	301	LUT	C11-C10	3.80	1.55	1.43
22	1	316	CLA	C4B-NB	-3.80	1.33	1.37
24	G	203	BCR	C11-C10	3.80	1.55	1.43
24	A	844	BCR	C11-C10	3.80	1.55	1.43
22	K	205	CLA	C4B-NB	-3.80	1.33	1.37
24	7	303	BCR	C16-C17	3.79	1.55	1.43
36	5	306	C7Z	C11-C10	3.79	1.55	1.43
38	3	302	LUT	C21-C26	3.79	1.66	1.56
38	1	303	LUT	C21-C26	3.79	1.66	1.56
24	A	846	BCR	C3-C4	3.79	1.64	1.52
24	A	848	BCR	C16-C17	3.79	1.55	1.43
32	F	306	RRX	C27-C26	-3.78	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	303	LUT	C11-C10	3.78	1.55	1.43
24	6	305	BCR	C3-C4	3.78	1.64	1.52
38	4	802	LUT	C21-C26	3.78	1.66	1.56
38	5	303	LUT	C21-C26	3.77	1.66	1.56
24	A	856	BCR	C16-C17	3.77	1.55	1.43
24	3	305	BCR	C16-C17	3.77	1.55	1.43
24	B	849	BCR	C11-C10	3.77	1.55	1.43
24	B	849	BCR	C16-C17	3.77	1.55	1.43
38	9	302	LUT	C38-C25	3.76	1.57	1.50
38	Z	302	LUT	C11-C10	3.76	1.55	1.43
24	J	104	BCR	C16-C17	3.76	1.55	1.43
24	I	4001	BCR	C16-C17	3.76	1.55	1.43
24	4	804	BCR	C3-C4	3.75	1.64	1.52
36	5	306	C7Z	C27-C26	3.75	1.58	1.45
24	3	307	BCR	C16-C17	3.75	1.55	1.43
24	F	303	BCR	C16-C17	3.75	1.55	1.43
24	5	305	BCR	C16-C17	3.74	1.55	1.43
38	1	303	LUT	C38-C25	3.74	1.57	1.50
38	1	302	LUT	C11-C10	3.74	1.55	1.43
38	6	303	LUT	C21-C26	3.74	1.66	1.56
22	3	315	CLA	C1C-NC	-3.74	1.32	1.37
38	7	301	LUT	C11-C10	3.74	1.55	1.43
24	A	845	BCR	C16-C17	3.73	1.55	1.43
24	A	856	BCR	C11-C10	3.73	1.55	1.43
24	G	203	BCR	C16-C17	3.73	1.55	1.43
24	4	804	BCR	C16-C17	3.73	1.55	1.43
24	B	845	BCR	C16-C17	3.73	1.55	1.43
38	7	302	LUT	C11-C10	3.73	1.55	1.43
24	B	846	BCR	C16-C17	3.73	1.55	1.43
24	A	844	BCR	C3-C4	3.73	1.64	1.52
38	1	303	LUT	C11-C10	3.73	1.55	1.43
24	F	303	BCR	C11-C10	3.72	1.55	1.43
38	5	303	LUT	C11-C10	3.72	1.55	1.43
38	8	303	LUT	C11-C10	3.72	1.55	1.43
36	J	105	C7Z	C4-C5	-3.72	1.45	1.51
24	B	844	BCR	C11-C10	3.72	1.55	1.43
24	A	848	BCR	C11-C10	3.72	1.55	1.43
21	A	801	CL0	OBD-CAD	3.72	1.28	1.22
38	9	301	LUT	C38-C25	3.72	1.57	1.50
24	K	206	BCR	C16-C17	3.72	1.55	1.43
24	6	305	BCR	C16-C17	3.71	1.55	1.43
24	J	104	BCR	C11-C10	3.71	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	105	C7Z	C27-C26	3.71	1.58	1.45
38	8	303	LUT	C38-C25	3.71	1.57	1.50
38	3	303	LUT	C11-C10	3.71	1.54	1.43
38	6	304	LUT	C11-C10	3.71	1.54	1.43
24	3	304	BCR	C3-C4	3.71	1.64	1.52
24	7	303	BCR	C11-C10	3.71	1.54	1.43
24	B	845	BCR	C11-C10	3.70	1.54	1.43
38	9	301	LUT	C11-C10	3.70	1.54	1.43
38	6	304	LUT	C38-C25	3.70	1.57	1.50
24	5	304	BCR	C16-C17	3.70	1.54	1.43
24	8	304	BCR	C16-C17	3.70	1.54	1.43
24	4	804	BCR	C11-C10	3.70	1.54	1.43
24	B	846	BCR	C11-C10	3.70	1.54	1.43
24	3	305	BCR	C11-C10	3.69	1.54	1.43
24	B	844	BCR	C16-C17	3.69	1.54	1.43
22	5	313	CLA	MG-ND	-3.68	1.98	2.05
38	1	302	LUT	C19-C9	3.68	1.58	1.50
24	I	4001	BCR	C11-C10	3.68	1.54	1.43
24	L	204	BCR	C16-C17	3.68	1.54	1.43
24	A	847	BCR	C16-C17	3.68	1.54	1.43
22	4	806	CLA	MG-ND	-3.68	1.98	2.05
38	7	302	LUT	C38-C25	3.68	1.57	1.50
38	4	803	LUT	C38-C25	3.68	1.57	1.50
22	G	201	CLA	MG-ND	-3.68	1.98	2.05
24	3	304	BCR	C11-C10	3.68	1.54	1.43
22	Z	305	CLA	MG-ND	-3.68	1.98	2.05
32	F	306	RRX	C7-C6	3.67	1.58	1.45
22	7	306	CLA	MG-ND	-3.67	1.98	2.05
38	5	302	LUT	C11-C10	3.67	1.54	1.43
22	A	820	CLA	MG-ND	-3.67	1.98	2.05
22	B	839	CLA	MG-ND	-3.67	1.98	2.05
38	4	802	LUT	C11-C10	3.67	1.54	1.43
24	B	848	BCR	C16-C17	3.67	1.54	1.43
22	A	816	CLA	MG-ND	-3.67	1.98	2.05
22	Z	313	CLA	MG-ND	-3.67	1.98	2.05
24	B	847	BCR	C16-C17	3.67	1.54	1.43
38	8	302	LUT	C11-C10	3.67	1.54	1.43
36	J	105	C7Z	C35-C34	3.67	1.54	1.43
22	6	312	CLA	MG-ND	-3.66	1.98	2.05
22	K	204	CLA	MG-ND	-3.66	1.98	2.05
22	1	305	CLA	MG-ND	-3.66	1.98	2.05
24	5	304	BCR	C11-C10	3.66	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	311	CLA	MG-ND	-3.66	1.98	2.05
22	5	308	CLA	MG-ND	-3.66	1.98	2.05
36	5	306	C7Z	C35-C34	3.66	1.54	1.43
24	A	845	BCR	C11-C10	3.66	1.54	1.43
38	4	803	LUT	C11-C10	3.65	1.54	1.43
22	6	309	CLA	MG-ND	-3.65	1.98	2.05
22	8	309	CLA	MG-ND	-3.65	1.98	2.05
38	8	302	LUT	C38-C25	3.65	1.57	1.50
38	3	302	LUT	C19-C9	3.65	1.58	1.50
22	3	315	CLA	C4B-NB	-3.65	1.33	1.37
22	A	839	CLA	MG-ND	-3.65	1.98	2.05
22	6	311	CLA	MG-ND	-3.65	1.98	2.05
24	A	846	BCR	C11-C10	3.64	1.54	1.43
22	1	311	CLA	C1C-NC	-3.64	1.32	1.37
22	9	308	CLA	MG-ND	-3.64	1.98	2.05
38	Z	302	LUT	C19-C9	3.64	1.58	1.50
24	B	847	BCR	C11-C10	3.64	1.54	1.43
22	4	818	CLA	MG-ND	-3.64	1.98	2.05
22	B	815	CLA	MG-ND	-3.63	1.98	2.05
22	5	309	CLA	MG-ND	-3.63	1.98	2.05
22	4	807	CLA	MG-ND	-3.63	1.98	2.05
22	B	817	CLA	MG-ND	-3.63	1.98	2.05
24	6	305	BCR	C11-C10	3.63	1.54	1.43
22	A	836	CLA	MG-ND	-3.63	1.98	2.05
22	5	311	CLA	MG-ND	-3.63	1.98	2.05
22	K	203	CLA	MG-ND	-3.63	1.98	2.05
22	7	308	CLA	MG-ND	-3.63	1.98	2.05
24	K	206	BCR	C11-C10	3.63	1.54	1.43
38	5	303	LUT	C38-C25	3.63	1.57	1.50
38	9	302	LUT	C11-C10	3.63	1.54	1.43
38	Z	302	LUT	C38-C25	3.63	1.57	1.50
24	B	848	BCR	C11-C10	3.63	1.54	1.43
22	6	302	CLA	MG-ND	-3.63	1.98	2.05
22	6	322	CLA	MG-ND	-3.63	1.98	2.05
24	A	856	BCR	C24-C25	3.63	1.58	1.45
22	1	304	CLA	MG-ND	-3.62	1.98	2.05
24	3	307	BCR	C11-C10	3.62	1.54	1.43
22	A	802	CLA	MG-ND	-3.62	1.98	2.05
22	A	842	CLA	MG-ND	-3.62	1.98	2.05
22	4	817	CLA	MG-ND	-3.62	1.98	2.05
22	B	834	CLA	MG-ND	-3.62	1.98	2.05
22	1	313	CLA	MG-ND	-3.62	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	808	CLA	MG-ND	-3.62	1.98	2.05
22	A	835	CLA	MG-ND	-3.62	1.98	2.05
22	8	306	CLA	MG-ND	-3.62	1.98	2.05
22	9	311	CLA	MG-ND	-3.62	1.98	2.05
38	5	302	LUT	C38-C25	3.62	1.57	1.50
38	6	303	LUT	C19-C9	3.62	1.58	1.50
22	4	809	CLA	MG-ND	-3.61	1.98	2.05
38	5	303	LUT	C19-C9	3.61	1.58	1.50
24	6	306	BCR	C11-C10	3.61	1.54	1.43
38	1	303	LUT	C19-C9	3.61	1.58	1.50
22	A	829	CLA	MG-ND	-3.61	1.98	2.05
22	K	202	CLA	MG-ND	-3.61	1.98	2.05
22	3	309	CLA	MG-ND	-3.61	1.98	2.05
38	9	301	LUT	C19-C9	3.61	1.58	1.50
24	8	304	BCR	C11-C10	3.61	1.54	1.43
22	A	804	CLA	MG-ND	-3.61	1.98	2.05
22	7	309	CLA	MG-ND	-3.61	1.98	2.05
22	6	319	CLA	MG-ND	-3.61	1.98	2.05
22	B	821	CLA	MG-ND	-3.61	1.98	2.05
22	B	822	CLA	MG-ND	-3.61	1.98	2.05
38	6	303	LUT	C38-C25	3.61	1.57	1.50
24	7	303	BCR	C24-C25	3.61	1.57	1.45
22	7	305	CLA	MG-ND	-3.61	1.98	2.05
24	A	847	BCR	C11-C10	3.61	1.54	1.43
22	5	315	CLA	MG-ND	-3.60	1.98	2.05
22	A	832	CLA	MG-ND	-3.60	1.98	2.05
22	B	806	CLA	MG-ND	-3.60	1.98	2.05
22	F	304	CLA	MG-ND	-3.60	1.98	2.05
22	1	315	CLA	MG-ND	-3.60	1.98	2.05
22	5	314	CLA	MG-ND	-3.60	1.98	2.05
24	A	846	BCR	C16-C17	3.60	1.54	1.43
24	B	844	BCR	C24-C25	3.60	1.57	1.45
22	6	313	CLA	MG-ND	-3.60	1.98	2.05
22	Z	304	CLA	MG-ND	-3.60	1.98	2.05
22	B	841	CLA	MG-ND	-3.60	1.98	2.05
22	9	305	CLA	C1C-NC	-3.60	1.32	1.37
22	3	310	CLA	MG-ND	-3.60	1.98	2.05
22	B	836	CLA	MG-ND	-3.60	1.98	2.05
24	A	845	BCR	C24-C25	3.60	1.57	1.45
38	4	802	LUT	C19-C9	3.60	1.58	1.50
22	B	807	CLA	MG-ND	-3.60	1.98	2.05
22	4	812	CLA	MG-ND	-3.60	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	203	CLA	MG-ND	-3.60	1.98	2.05
22	5	326	CLA	MG-ND	-3.60	1.98	2.05
22	8	313	CLA	MG-ND	-3.59	1.98	2.05
22	B	801	CLA	MG-ND	-3.59	1.98	2.05
24	A	848	BCR	C24-C25	3.59	1.57	1.45
22	A	831	CLA	MG-ND	-3.59	1.98	2.05
22	6	310	CLA	MG-ND	-3.59	1.98	2.05
22	2	302	CLA	MG-ND	-3.59	1.98	2.05
38	3	302	LUT	C38-C25	3.59	1.57	1.50
22	A	838	CLA	MG-ND	-3.59	1.98	2.05
38	6	304	LUT	C19-C9	3.59	1.58	1.50
22	A	814	CLA	MG-ND	-3.59	1.98	2.05
22	A	854	CLA	MG-ND	-3.59	1.98	2.05
22	5	310	CLA	MG-ND	-3.59	1.98	2.05
22	B	813	CLA	MG-ND	-3.59	1.98	2.05
22	2	301	CLA	MG-ND	-3.59	1.98	2.05
24	3	307	BCR	C24-C25	3.59	1.57	1.45
24	6	306	BCR	C16-C17	3.59	1.54	1.43
24	3	306	BCR	C24-C25	3.59	1.57	1.45
24	3	305	BCR	C24-C25	3.59	1.57	1.45
22	B	808	CLA	MG-ND	-3.59	1.98	2.05
22	3	308	CLA	MG-ND	-3.59	1.98	2.05
22	7	322	CLA	MG-ND	-3.59	1.98	2.05
22	8	305	CLA	MG-ND	-3.59	1.98	2.05
22	3	320	CLA	C4B-NB	-3.59	1.33	1.37
22	B	809	CLA	MG-ND	-3.59	1.98	2.05
22	3	322	CLA	MG-ND	-3.59	1.98	2.05
22	Z	307	CLA	MG-ND	-3.59	1.98	2.05
22	6	307	CLA	MG-ND	-3.59	1.98	2.05
38	4	803	LUT	C19-C9	3.58	1.58	1.50
24	J	104	BCR	C24-C25	3.58	1.57	1.45
24	8	304	BCR	C24-C25	3.58	1.57	1.45
22	J	103	CLA	MG-ND	-3.58	1.98	2.05
22	8	314	CLA	MG-ND	-3.58	1.98	2.05
22	5	312	CLA	MG-ND	-3.58	1.98	2.05
22	B	837	CLA	MG-ND	-3.58	1.98	2.05
22	3	312	CLA	MG-ND	-3.58	1.98	2.05
22	9	313	CLA	MG-ND	-3.58	1.98	2.05
22	3	314	CLA	MG-ND	-3.58	1.98	2.05
38	3	303	LUT	C38-C25	3.58	1.57	1.50
38	7	302	LUT	C19-C9	3.58	1.58	1.50
22	7	314	CLA	MG-ND	-3.58	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	315	CLA	MG-ND	-3.58	1.98	2.05
22	8	310	CLA	MG-ND	-3.58	1.98	2.05
22	6	317	CLA	MG-ND	-3.58	1.98	2.05
22	3	319	CLA	MG-ND	-3.58	1.98	2.05
38	5	302	LUT	C19-C9	3.58	1.58	1.50
22	B	826	CLA	MG-ND	-3.58	1.98	2.05
22	A	817	CLA	MG-ND	-3.57	1.98	2.05
22	B	832	CLA	MG-ND	-3.57	1.98	2.05
38	3	303	LUT	C19-C9	3.57	1.58	1.50
22	A	813	CLA	MG-ND	-3.57	1.98	2.05
22	A	821	CLA	MG-ND	-3.57	1.98	2.05
22	A	827	CLA	MG-ND	-3.57	1.98	2.05
22	7	323	CLA	MG-ND	-3.57	1.98	2.05
22	B	833	CLA	MG-ND	-3.57	1.98	2.05
22	1	306	CLA	MG-ND	-3.57	1.98	2.05
22	Z	310	CLA	MG-ND	-3.57	1.98	2.05
38	7	301	LUT	C19-C9	3.57	1.58	1.50
22	7	324	CLA	MG-ND	-3.57	1.98	2.05
38	3	302	LUT	C11-C10	3.57	1.54	1.43
38	9	302	LUT	C19-C9	3.57	1.58	1.50
22	6	308	CLA	MG-ND	-3.57	1.98	2.05
22	4	805	CLA	MG-ND	-3.57	1.98	2.05
24	G	203	BCR	C24-C25	3.57	1.57	1.45
22	1	307	CLA	MG-ND	-3.57	1.98	2.05
38	Z	301	LUT	C19-C9	3.57	1.58	1.50
22	B	828	CLA	MG-ND	-3.57	1.98	2.05
22	9	306	CLA	MG-ND	-3.57	1.98	2.05
22	6	321	CLA	MG-ND	-3.57	1.98	2.05
22	B	823	CLA	MG-ND	-3.57	1.98	2.05
22	7	307	CLA	MG-ND	-3.56	1.98	2.05
22	A	809	CLA	MG-ND	-3.56	1.98	2.05
22	L	202	CLA	MG-ND	-3.56	1.98	2.05
22	3	316	CLA	MG-ND	-3.56	1.98	2.05
22	8	307	CLA	MG-ND	-3.56	1.98	2.05
22	B	824	CLA	MG-ND	-3.56	1.98	2.05
22	Z	303	CLA	MG-ND	-3.56	1.98	2.05
22	A	828	CLA	MG-ND	-3.56	1.98	2.05
22	A	840	CLA	MG-ND	-3.56	1.98	2.05
22	4	811	CLA	MG-ND	-3.56	1.98	2.05
22	B	829	CLA	MG-ND	-3.56	1.98	2.05
22	3	311	CLA	MG-ND	-3.56	1.98	2.05
22	B	831	CLA	MG-ND	-3.56	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	317	CLA	MG-ND	-3.56	1.98	2.05
22	5	307	CLA	MG-ND	-3.56	1.98	2.05
22	B	825	CLA	MG-ND	-3.56	1.98	2.05
24	5	304	BCR	C24-C25	3.56	1.57	1.45
22	B	835	CLA	MG-ND	-3.56	1.98	2.05
22	B	816	CLA	MG-ND	-3.56	1.98	2.05
22	Z	306	CLA	MG-ND	-3.56	1.98	2.05
22	B	830	CLA	MG-ND	-3.56	1.98	2.05
38	8	302	LUT	C19-C9	3.56	1.58	1.50
22	B	811	CLA	MG-ND	-3.56	1.98	2.05
22	7	310	CLA	MG-ND	-3.56	1.98	2.05
22	9	307	CLA	MG-ND	-3.56	1.98	2.05
22	F	305	CLA	MG-ND	-3.55	1.98	2.05
22	7	304	CLA	MG-ND	-3.55	1.98	2.05
22	7	316	CLA	MG-ND	-3.55	1.98	2.05
22	2	304	CLA	MG-ND	-3.55	1.98	2.05
24	3	304	BCR	C24-C25	3.55	1.57	1.45
22	A	826	CLA	MG-ND	-3.55	1.98	2.05
22	B	840	CLA	MG-ND	-3.55	1.98	2.05
22	A	815	CLA	MG-ND	-3.55	1.98	2.05
22	5	301	CLA	MG-ND	-3.55	1.98	2.05
22	A	822	CLA	MG-ND	-3.55	1.98	2.05
22	A	825	CLA	MG-ND	-3.55	1.98	2.05
22	1	310	CLA	MG-ND	-3.55	1.98	2.05
22	A	812	CLA	MG-ND	-3.55	1.98	2.05
22	8	311	CLA	MG-ND	-3.55	1.98	2.05
24	5	305	BCR	C24-C25	3.55	1.57	1.45
24	B	849	BCR	C24-C25	3.55	1.57	1.45
24	4	804	BCR	C24-C25	3.55	1.57	1.45
22	5	322	CLA	MG-ND	-3.54	1.98	2.05
24	L	204	BCR	C24-C25	3.54	1.57	1.45
22	A	830	CLA	MG-ND	-3.54	1.98	2.05
22	B	810	CLA	MG-ND	-3.54	1.98	2.05
24	A	846	BCR	C24-C25	3.54	1.57	1.45
38	1	302	LUT	C38-C25	3.54	1.57	1.50
22	A	818	CLA	MG-ND	-3.54	1.98	2.05
22	5	323	CLA	MG-ND	-3.54	1.98	2.05
22	7	312	CLA	MG-ND	-3.54	1.98	2.05
22	7	315	CLA	MG-ND	-3.54	1.98	2.05
24	B	845	BCR	C24-C25	3.54	1.57	1.45
22	A	803	CLA	MG-ND	-3.54	1.98	2.05
22	6	301	CLA	MG-ND	-3.54	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	206	BCR	C24-C25	3.54	1.57	1.45
22	B	820	CLA	MG-ND	-3.54	1.98	2.05
22	A	806	CLA	MG-ND	-3.54	1.98	2.05
22	Z	309	CLA	MG-ND	-3.54	1.98	2.05
22	8	308	CLA	MG-ND	-3.53	1.98	2.05
22	Z	308	CLA	MG-ND	-3.53	1.98	2.05
22	9	310	CLA	C1C-NC	-3.53	1.32	1.37
36	J	105	C7Z	C2-C1	3.53	1.65	1.54
24	6	305	BCR	C4-C5	-3.53	1.44	1.51
22	4	815	CLA	MG-ND	-3.53	1.98	2.05
22	B	812	CLA	MG-ND	-3.53	1.98	2.05
22	G	202	CLA	MG-ND	-3.53	1.98	2.05
24	A	844	BCR	C24-C25	3.53	1.57	1.45
22	B	819	CLA	MG-ND	-3.53	1.98	2.05
22	F	302	CLA	MG-ND	-3.53	1.98	2.05
24	F	303	BCR	C24-C25	3.53	1.57	1.45
38	8	303	LUT	C19-C9	3.53	1.58	1.50
22	7	311	CLA	MG-ND	-3.53	1.98	2.05
22	6	314	CLA	MG-ND	-3.52	1.98	2.05
22	B	842	CLA	MG-ND	-3.52	1.98	2.05
22	A	819	CLA	MG-ND	-3.52	1.98	2.05
22	1	309	CLA	MG-ND	-3.52	1.98	2.05
22	Z	316	CLA	MG-ND	-3.52	1.98	2.05
21	A	801	CL0	MG-NC	3.52	2.14	2.06
22	A	823	CLA	MG-ND	-3.52	1.98	2.05
22	3	313	CLA	MG-ND	-3.52	1.98	2.05
22	A	824	CLA	MG-ND	-3.52	1.98	2.05
22	A	807	CLA	MG-ND	-3.52	1.98	2.05
22	A	805	CLA	MG-ND	-3.52	1.98	2.05
22	B	805	CLA	MG-ND	-3.52	1.98	2.05
22	A	841	CLA	MG-ND	-3.51	1.98	2.05
22	5	319	CLA	MG-ND	-3.51	1.98	2.05
24	6	305	BCR	C24-C25	3.51	1.57	1.45
22	A	810	CLA	MG-ND	-3.51	1.98	2.05
24	A	847	BCR	C24-C25	3.51	1.57	1.45
22	4	810	CLA	MG-ND	-3.51	1.98	2.05
22	A	834	CLA	MG-ND	-3.51	1.98	2.05
22	B	818	CLA	MG-ND	-3.51	1.98	2.05
24	B	847	BCR	C24-C25	3.50	1.57	1.45
22	A	811	CLA	MG-ND	-3.50	1.98	2.05
22	B	814	CLA	MG-ND	-3.50	1.98	2.05
22	A	833	CLA	MG-ND	-3.50	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	848	BCR	C24-C25	3.50	1.57	1.45
22	B	827	CLA	MG-ND	-3.50	1.98	2.05
22	8	316	CLA	MG-ND	-3.50	1.98	2.05
38	9	302	LUT	C2-C1	3.49	1.65	1.54
22	Z	314	CLA	MG-ND	-3.49	1.98	2.05
36	5	306	C7Z	C2-C1	3.49	1.65	1.54
22	5	318	CLA	MG-ND	-3.49	1.98	2.05
22	1	308	CLA	MG-ND	-3.49	1.98	2.05
22	3	318	CLA	MG-ND	-3.49	1.98	2.05
24	B	846	BCR	C24-C25	3.48	1.57	1.45
22	A	837	CLA	MG-ND	-3.48	1.98	2.05
22	1	311	CLA	C4B-NB	-3.48	1.33	1.37
22	B	838	CLA	MG-ND	-3.47	1.98	2.05
22	9	309	CLA	C4B-NB	-3.47	1.33	1.37
38	Z	302	LUT	C2-C1	3.47	1.65	1.54
22	9	309	CLA	C1C-NC	-3.47	1.32	1.37
24	B	846	BCR	C27-C26	-3.47	1.44	1.51
38	8	303	LUT	C2-C1	3.47	1.65	1.54
22	F	301	CLA	MG-ND	-3.46	1.98	2.05
38	7	301	LUT	C38-C25	3.46	1.57	1.50
22	A	855	CLA	MG-ND	-3.46	1.98	2.05
38	4	803	LUT	C2-C1	3.45	1.65	1.54
38	6	304	LUT	C2-C1	3.45	1.65	1.54
24	J	104	BCR	C27-C26	-3.45	1.44	1.51
38	3	303	LUT	C2-C1	3.45	1.65	1.54
24	B	845	BCR	C4-C5	-3.45	1.44	1.51
24	I	4001	BCR	C24-C25	3.45	1.57	1.45
22	1	314	CLA	MG-ND	-3.45	1.99	2.05
24	G	203	BCR	C27-C26	-3.44	1.44	1.51
22	4	805	CLA	C1C-NC	-3.44	1.32	1.37
38	7	301	LUT	C2-C1	3.44	1.65	1.54
24	B	845	BCR	C27-C26	-3.44	1.44	1.51
24	7	303	BCR	C4-C5	-3.43	1.44	1.51
24	L	204	BCR	C4-C5	-3.43	1.44	1.51
22	9	304	CLA	C1C-NC	-3.43	1.32	1.37
22	9	305	CLA	C4B-NB	-3.43	1.33	1.37
22	8	305	CLA	C1C-NC	-3.43	1.32	1.37
38	5	303	LUT	C2-C1	3.42	1.65	1.54
24	3	306	BCR	C4-C5	-3.42	1.44	1.51
38	1	303	LUT	C2-C1	3.42	1.65	1.54
24	3	304	BCR	C4-C5	-3.42	1.44	1.51
38	7	302	LUT	C2-C1	3.42	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	808	CLA	MG-ND	-3.42	1.99	2.05
36	J	105	C7Z	C18-C5	3.41	1.56	1.50
24	5	304	BCR	C27-C26	-3.41	1.44	1.51
22	L	201	CLA	MG-ND	-3.41	1.99	2.05
38	8	302	LUT	C2-C1	3.41	1.65	1.54
38	4	802	LUT	C2-C1	3.40	1.65	1.54
38	1	302	LUT	C2-C1	3.40	1.65	1.54
38	Z	301	LUT	C2-C1	3.40	1.65	1.54
38	8	303	LUT	C40-C33	3.40	1.57	1.50
27	A	852	DGA	OG2-CB1	3.40	1.43	1.34
38	6	303	LUT	C2-C1	3.40	1.65	1.54
24	8	304	BCR	C4-C5	-3.40	1.44	1.51
38	5	302	LUT	C2-C1	3.39	1.65	1.54
38	9	301	LUT	C2-C1	3.39	1.65	1.54
24	A	848	BCR	C4-C5	-3.39	1.44	1.51
24	6	306	BCR	C24-C25	3.39	1.57	1.45
24	A	844	BCR	C27-C26	-3.38	1.44	1.51
24	4	804	BCR	C4-C5	-3.38	1.44	1.51
24	8	304	BCR	C27-C26	-3.38	1.44	1.51
24	3	307	BCR	C4-C5	-3.38	1.44	1.51
38	Z	301	LUT	C38-C25	3.38	1.56	1.50
24	3	307	BCR	C27-C26	-3.38	1.44	1.51
38	6	304	LUT	C40-C33	3.38	1.57	1.50
38	7	302	LUT	C40-C33	3.37	1.57	1.50
24	A	856	BCR	C27-C26	-3.37	1.44	1.51
36	5	306	C7Z	C18-C5	3.37	1.56	1.50
38	8	302	LUT	C40-C33	3.37	1.57	1.50
24	B	848	BCR	C4-C5	-3.37	1.44	1.51
24	A	846	BCR	C27-C26	-3.36	1.44	1.51
24	I	4001	BCR	C27-C26	-3.36	1.44	1.51
22	9	310	CLA	C4B-NB	-3.36	1.33	1.37
38	Z	302	LUT	C40-C33	3.36	1.57	1.50
38	4	802	LUT	C38-C25	3.36	1.56	1.50
38	3	303	LUT	C40-C33	3.36	1.57	1.50
38	1	303	LUT	C40-C33	3.36	1.57	1.50
24	3	304	BCR	C27-C26	-3.36	1.44	1.51
24	5	304	BCR	C4-C5	-3.36	1.44	1.51
22	1	308	CLA	C1C-NC	-3.35	1.32	1.37
38	9	302	LUT	C40-C33	3.35	1.57	1.50
38	7	301	LUT	C40-C33	3.35	1.57	1.50
38	5	302	LUT	C40-C33	3.35	1.57	1.50
24	K	206	BCR	C27-C26	-3.35	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	305	BCR	C27-C26	-3.35	1.44	1.51
22	B	815	CLA	C1C-NC	-3.35	1.32	1.37
38	4	802	LUT	C40-C33	3.34	1.57	1.50
38	5	303	LUT	C40-C33	3.34	1.57	1.50
36	J	105	C7Z	C8-C9	3.34	1.53	1.45
24	A	846	BCR	C4-C5	-3.34	1.44	1.51
24	K	206	BCR	C4-C5	-3.34	1.44	1.51
24	6	305	BCR	C27-C26	-3.34	1.44	1.51
24	J	104	BCR	C4-C5	-3.34	1.44	1.51
24	B	853	BCR	C4-C5	-3.34	1.44	1.51
38	9	301	LUT	C40-C33	3.34	1.57	1.50
24	A	845	BCR	C4-C5	-3.34	1.44	1.51
38	Z	301	LUT	C40-C33	3.33	1.57	1.50
24	A	847	BCR	C4-C5	-3.33	1.44	1.51
24	B	848	BCR	C27-C26	-3.33	1.44	1.51
24	B	853	BCR	C24-C25	3.33	1.56	1.45
24	A	844	BCR	C4-C5	-3.33	1.44	1.51
24	6	306	BCR	C4-C5	-3.33	1.44	1.51
38	3	302	LUT	C40-C33	3.33	1.57	1.50
36	J	105	C7Z	C7-C6	3.33	1.56	1.45
24	6	306	BCR	C27-C26	-3.32	1.44	1.51
38	6	303	LUT	C40-C33	3.32	1.57	1.50
22	G	201	CLA	C1C-NC	-3.32	1.32	1.37
24	B	847	BCR	C4-C5	-3.31	1.44	1.51
24	B	849	BCR	C4-C5	-3.30	1.44	1.51
22	A	813	CLA	C1C-NC	-3.30	1.32	1.37
38	3	302	LUT	C2-C1	3.30	1.65	1.54
38	4	803	LUT	C40-C33	3.30	1.57	1.50
24	5	305	BCR	C4-C5	-3.30	1.44	1.51
24	L	204	BCR	C27-C26	-3.30	1.44	1.51
38	1	302	LUT	C40-C33	3.30	1.57	1.50
22	Z	304	CLA	C1C-NC	-3.29	1.32	1.37
24	B	844	BCR	C27-C26	-3.29	1.44	1.51
22	4	809	CLA	C1C-NC	-3.28	1.32	1.37
22	B	814	CLA	C1C-NC	-3.28	1.32	1.37
24	B	849	BCR	C27-C26	-3.28	1.44	1.51
24	B	844	BCR	C4-C5	-3.28	1.44	1.51
24	B	847	BCR	C27-C26	-3.28	1.44	1.51
36	J	105	C7Z	C21-C26	-3.28	1.49	1.53
31	B	852	DGD	CAA-C9A	-3.27	1.33	1.51
24	4	804	BCR	C27-C26	-3.27	1.44	1.51
31	B	852	DGD	CDB-CCB	-3.27	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	848	BCR	C27-C26	-3.27	1.44	1.51
24	I	4001	BCR	C4-C5	-3.26	1.44	1.51
22	6	302	CLA	C1C-NC	-3.26	1.32	1.37
22	B	818	CLA	C1C-NC	-3.26	1.32	1.37
22	A	827	CLA	C1C-NC	-3.26	1.32	1.37
27	A	852	DGA	OG1-CA1	3.26	1.42	1.33
31	B	852	DGD	CAB-C9B	-3.26	1.33	1.51
24	3	306	BCR	C27-C26	-3.26	1.44	1.51
36	5	306	C7Z	C7-C6	3.26	1.56	1.45
22	1	305	CLA	C1C-NC	-3.25	1.33	1.37
22	Z	303	CLA	C1C-NC	-3.25	1.33	1.37
22	8	306	CLA	C1C-NC	-3.25	1.33	1.37
24	A	845	BCR	C27-C26	-3.25	1.44	1.51
22	1	313	CLA	C1C-NC	-3.25	1.33	1.37
22	Z	305	CLA	C1C-NC	-3.24	1.33	1.37
22	3	312	CLA	C1C-NC	-3.24	1.33	1.37
22	Z	316	CLA	C1C-NC	-3.24	1.33	1.37
31	B	852	DGD	CGB-CFB	-3.23	1.33	1.51
22	A	805	CLA	C1C-NC	-3.23	1.33	1.37
31	1	319	DGD	CAA-C9A	-3.23	1.33	1.51
22	A	835	CLA	C1C-NC	-3.23	1.33	1.37
22	4	818	CLA	C1C-NC	-3.23	1.33	1.37
24	F	303	BCR	C4-C5	-3.23	1.44	1.51
22	A	823	CLA	C1C-NC	-3.23	1.33	1.37
31	3	301	DGD	CAA-C9A	-3.23	1.33	1.51
22	B	817	CLA	C1C-NC	-3.22	1.33	1.37
22	3	316	CLA	C1C-NC	-3.22	1.33	1.37
22	B	830	CLA	C1C-NC	-3.22	1.33	1.37
22	6	301	CLA	C1C-NC	-3.22	1.33	1.37
24	B	846	BCR	C4-C5	-3.22	1.44	1.51
22	2	304	CLA	C1C-NC	-3.21	1.33	1.37
22	A	812	CLA	C1C-NC	-3.21	1.33	1.37
22	3	311	CLA	C1C-NC	-3.21	1.33	1.37
22	6	307	CLA	C1C-NC	-3.21	1.33	1.37
22	1	304	CLA	C1C-NC	-3.21	1.33	1.37
22	Z	313	CLA	C1C-NC	-3.21	1.33	1.37
36	5	306	C7Z	C8-C9	3.21	1.52	1.45
22	5	314	CLA	C1C-NC	-3.21	1.33	1.37
22	A	855	CLA	C1C-NC	-3.20	1.33	1.37
22	8	305	CLA	C4B-NB	-3.20	1.33	1.37
32	F	306	RRX	C4-C5	-3.20	1.44	1.51
22	7	312	CLA	C1C-NC	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	311	CLA	C1C-NC	-3.20	1.33	1.37
22	5	309	CLA	C1C-NC	-3.20	1.33	1.37
38	9	301	LUT	C23-C24	-3.20	1.45	1.50
22	A	828	CLA	C1C-NC	-3.20	1.33	1.37
22	B	827	CLA	C1C-NC	-3.20	1.33	1.37
22	B	811	CLA	C1C-NC	-3.20	1.33	1.37
22	8	311	CLA	C1C-NC	-3.20	1.33	1.37
22	9	308	CLA	C1C-NC	-3.19	1.33	1.37
22	7	307	CLA	C1C-NC	-3.19	1.33	1.37
22	A	840	CLA	C1C-NC	-3.19	1.33	1.37
22	A	806	CLA	C1C-NC	-3.19	1.33	1.37
22	Z	309	CLA	C1C-NC	-3.19	1.33	1.37
22	F	301	CLA	C1C-NC	-3.19	1.33	1.37
22	K	203	CLA	C1C-NC	-3.19	1.33	1.37
22	8	316	CLA	C1C-NC	-3.19	1.33	1.37
24	A	847	BCR	C27-C26	-3.19	1.44	1.51
38	Z	301	LUT	C23-C24	-3.19	1.45	1.50
22	B	821	CLA	C1C-NC	-3.19	1.33	1.37
24	A	856	BCR	C4-C5	-3.19	1.44	1.51
24	7	303	BCR	C27-C26	-3.18	1.44	1.51
39	9	314	CHL	C3A-C2A	-3.18	1.51	1.54
22	6	311	CLA	C1C-NC	-3.18	1.33	1.37
22	1	307	CLA	C1C-NC	-3.18	1.33	1.37
22	B	823	CLA	C1C-NC	-3.18	1.33	1.37
22	5	301	CLA	C1C-NC	-3.18	1.33	1.37
22	G	202	CLA	C1C-NC	-3.18	1.33	1.37
22	7	305	CLA	C1C-NC	-3.18	1.33	1.37
22	B	834	CLA	C1C-NC	-3.18	1.33	1.37
22	2	302	CLA	C1C-NC	-3.18	1.33	1.37
24	F	303	BCR	C27-C26	-3.18	1.44	1.51
22	B	819	CLA	C1C-NC	-3.18	1.33	1.37
22	5	308	CLA	C1C-NC	-3.18	1.33	1.37
22	A	811	CLA	C1C-NC	-3.17	1.33	1.37
22	A	803	CLA	C1C-NC	-3.17	1.33	1.37
22	A	833	CLA	C1C-NC	-3.17	1.33	1.37
22	3	309	CLA	C1C-NC	-3.17	1.33	1.37
22	J	103	CLA	C1C-NC	-3.17	1.33	1.37
22	Z	315	CLA	C1C-NC	-3.17	1.33	1.37
22	A	821	CLA	C1C-NC	-3.17	1.33	1.37
22	9	306	CLA	C1C-NC	-3.17	1.33	1.37
22	9	313	CLA	C1C-NC	-3.17	1.33	1.37
22	B	828	CLA	C1C-NC	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	307	CLA	C1C-NC	-3.17	1.33	1.37
22	9	307	CLA	C1C-NC	-3.17	1.33	1.37
22	A	809	CLA	C1C-NC	-3.17	1.33	1.37
22	2	301	CLA	C1C-NC	-3.17	1.33	1.37
22	A	824	CLA	C1C-NC	-3.17	1.33	1.37
22	3	308	CLA	C1C-NC	-3.17	1.33	1.37
22	A	817	CLA	C1C-NC	-3.16	1.33	1.37
22	A	818	CLA	C1C-NC	-3.16	1.33	1.37
22	A	820	CLA	C1C-NC	-3.16	1.33	1.37
22	B	822	CLA	C1C-NC	-3.16	1.33	1.37
22	F	304	CLA	C1C-NC	-3.16	1.33	1.37
22	3	314	CLA	C1C-NC	-3.16	1.33	1.37
22	B	832	CLA	C1C-NC	-3.16	1.33	1.37
22	6	313	CLA	C1C-NC	-3.16	1.33	1.37
22	6	314	CLA	C1C-NC	-3.16	1.33	1.37
25	B	851	LHG	O7-C5	-3.16	1.43	1.46
22	5	326	CLA	C1C-NC	-3.16	1.33	1.37
24	G	203	BCR	C4-C5	-3.16	1.44	1.51
22	L	203	CLA	C1C-NC	-3.16	1.33	1.37
22	B	809	CLA	C1C-NC	-3.16	1.33	1.37
22	6	317	CLA	C1C-NC	-3.16	1.33	1.37
22	7	308	CLA	C1C-NC	-3.16	1.33	1.37
22	A	839	CLA	C1C-NC	-3.16	1.33	1.37
22	A	829	CLA	C1C-NC	-3.16	1.33	1.37
22	4	807	CLA	C1C-NC	-3.16	1.33	1.37
22	7	322	CLA	C1C-NC	-3.16	1.33	1.37
22	B	825	CLA	C1C-NC	-3.15	1.33	1.37
22	A	808	CLA	C1C-NC	-3.15	1.33	1.37
22	8	313	CLA	C1C-NC	-3.15	1.33	1.37
22	7	304	CLA	C1C-NC	-3.15	1.33	1.37
22	5	312	CLA	C1C-NC	-3.15	1.33	1.37
22	A	838	CLA	C1C-NC	-3.15	1.33	1.37
22	K	202	CLA	C1C-NC	-3.15	1.33	1.37
22	8	309	CLA	C1C-NC	-3.15	1.33	1.37
22	A	841	CLA	C1C-NC	-3.15	1.33	1.37
22	7	310	CLA	C1C-NC	-3.15	1.33	1.37
22	Z	310	CLA	C1C-NC	-3.15	1.33	1.37
22	A	836	CLA	C1C-NC	-3.15	1.33	1.37
22	F	302	CLA	C1C-NC	-3.15	1.33	1.37
22	L	201	CLA	C1C-NC	-3.15	1.33	1.37
22	4	811	CLA	C1C-NC	-3.15	1.33	1.37
24	5	305	BCR	C27-C26	-3.15	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	314	CLA	C1C-NC	-3.14	1.33	1.37
22	B	839	CLA	C1C-NC	-3.14	1.33	1.37
22	4	817	CLA	C1C-NC	-3.14	1.33	1.37
22	5	315	CLA	C1C-NC	-3.14	1.33	1.37
22	Z	314	CLA	C1C-NC	-3.14	1.33	1.37
22	B	836	CLA	C1C-NC	-3.14	1.33	1.37
22	A	804	CLA	C1C-NC	-3.14	1.33	1.37
22	A	842	CLA	C1C-NC	-3.14	1.33	1.37
22	5	319	CLA	C1C-NC	-3.14	1.33	1.37
24	B	853	BCR	C27-C26	-3.14	1.44	1.51
22	Z	307	CLA	C1C-NC	-3.14	1.33	1.37
22	B	829	CLA	C1C-NC	-3.14	1.33	1.37
22	1	310	CLA	C1C-NC	-3.14	1.33	1.37
22	3	313	CLA	C1C-NC	-3.14	1.33	1.37
22	8	310	CLA	C1C-NC	-3.14	1.33	1.37
22	A	830	CLA	C1C-NC	-3.14	1.33	1.37
22	Z	306	CLA	C1C-NC	-3.14	1.33	1.37
22	B	837	CLA	C1C-NC	-3.13	1.33	1.37
22	4	815	CLA	C1C-NC	-3.13	1.33	1.37
22	B	835	CLA	C1C-NC	-3.13	1.33	1.37
22	7	309	CLA	C1C-NC	-3.13	1.33	1.37
36	5	306	C7Z	C21-C26	-3.13	1.49	1.53
22	B	805	CLA	C1C-NC	-3.13	1.33	1.37
22	L	202	CLA	C1C-NC	-3.13	1.33	1.37
22	1	314	CLA	C1C-NC	-3.13	1.33	1.37
22	4	812	CLA	C1C-NC	-3.13	1.33	1.37
22	4	808	CLA	C1C-NC	-3.13	1.33	1.37
22	A	825	CLA	C1C-NC	-3.13	1.33	1.37
22	3	319	CLA	C1C-NC	-3.13	1.33	1.37
22	B	831	CLA	C1C-NC	-3.13	1.33	1.37
22	8	314	CLA	C1C-NC	-3.13	1.33	1.37
22	B	841	CLA	C1C-NC	-3.12	1.33	1.37
22	A	810	CLA	C1C-NC	-3.12	1.33	1.37
22	8	308	CLA	C1C-NC	-3.12	1.33	1.37
22	5	323	CLA	C1C-NC	-3.12	1.33	1.37
22	5	318	CLA	C1C-NC	-3.12	1.33	1.37
22	A	822	CLA	C1C-NC	-3.12	1.33	1.37
22	B	801	CLA	C1C-NC	-3.12	1.33	1.37
22	5	313	CLA	C1C-NC	-3.12	1.33	1.37
22	6	322	CLA	C1C-NC	-3.12	1.33	1.37
22	1	306	CLA	C1C-NC	-3.12	1.33	1.37
22	7	315	CLA	C1C-NC	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	302	LUT	C23-C24	-3.12	1.45	1.50
22	A	832	CLA	C1C-NC	-3.12	1.33	1.37
22	B	810	CLA	C1C-NC	-3.12	1.33	1.37
22	B	808	CLA	C1C-NC	-3.11	1.33	1.37
22	3	310	CLA	C1C-NC	-3.11	1.33	1.37
22	B	807	CLA	C1C-NC	-3.11	1.33	1.37
22	1	309	CLA	C1C-NC	-3.11	1.33	1.37
22	A	814	CLA	C1C-NC	-3.11	1.33	1.37
22	6	312	CLA	C1C-NC	-3.11	1.33	1.37
22	1	304	CLA	C4B-NB	-3.11	1.34	1.37
22	A	815	CLA	C1C-NC	-3.11	1.33	1.37
22	7	306	CLA	C1C-NC	-3.11	1.33	1.37
22	4	806	CLA	C1C-NC	-3.11	1.33	1.37
22	7	317	CLA	C1C-NC	-3.11	1.33	1.37
22	7	324	CLA	C1C-NC	-3.11	1.33	1.37
22	Z	313	CLA	C4B-NB	-3.11	1.34	1.37
22	B	840	CLA	C1C-NC	-3.10	1.33	1.37
22	K	204	CLA	C1C-NC	-3.10	1.33	1.37
22	3	318	CLA	C1C-NC	-3.10	1.33	1.37
22	A	831	CLA	C1C-NC	-3.10	1.33	1.37
22	Z	308	CLA	C1C-NC	-3.10	1.33	1.37
22	B	833	CLA	C1C-NC	-3.10	1.33	1.37
22	B	812	CLA	C1C-NC	-3.10	1.33	1.37
22	7	311	CLA	C1C-NC	-3.10	1.33	1.37
22	4	808	CLA	C4B-NB	-3.10	1.34	1.37
22	4	810	CLA	C1C-NC	-3.10	1.33	1.37
22	A	819	CLA	C1C-NC	-3.10	1.33	1.37
22	A	802	CLA	C1C-NC	-3.10	1.33	1.37
22	B	806	CLA	C1C-NC	-3.10	1.33	1.37
22	6	307	CLA	C4B-NB	-3.09	1.34	1.37
22	6	309	CLA	C1C-NC	-3.09	1.33	1.37
22	F	305	CLA	C1C-NC	-3.09	1.33	1.37
22	3	322	CLA	C1C-NC	-3.09	1.33	1.37
22	B	838	CLA	C1C-NC	-3.09	1.33	1.37
22	1	313	CLA	C4B-NB	-3.09	1.34	1.37
22	A	854	CLA	C1C-NC	-3.09	1.33	1.37
22	A	816	CLA	C1C-NC	-3.09	1.33	1.37
22	A	836	CLA	C4B-NB	-3.09	1.34	1.37
22	7	323	CLA	C1C-NC	-3.09	1.33	1.37
22	6	308	CLA	C1C-NC	-3.08	1.33	1.37
22	6	321	CLA	C1C-NC	-3.08	1.33	1.37
22	A	822	CLA	C4B-NB	-3.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	807	CLA	C1C-NC	-3.08	1.33	1.37
22	6	310	CLA	C1C-NC	-3.08	1.33	1.37
22	4	818	CLA	C4B-NB	-3.08	1.34	1.37
22	5	322	CLA	C1C-NC	-3.08	1.33	1.37
22	7	316	CLA	C1C-NC	-3.08	1.33	1.37
22	B	842	CLA	C1C-NC	-3.08	1.33	1.37
22	8	308	CLA	C4B-NB	-3.07	1.34	1.37
22	5	311	CLA	C1C-NC	-3.07	1.33	1.37
22	5	310	CLA	C1C-NC	-3.07	1.33	1.37
22	B	815	CLA	C4B-NB	-3.07	1.34	1.37
22	A	837	CLA	C1C-NC	-3.07	1.33	1.37
22	Z	303	CLA	C4B-NB	-3.07	1.34	1.37
38	4	802	LUT	C23-C24	-3.07	1.45	1.50
22	9	304	CLA	C4B-NB	-3.07	1.34	1.37
22	A	813	CLA	C4B-NB	-3.06	1.34	1.37
22	K	202	CLA	C4B-NB	-3.06	1.34	1.37
24	3	305	BCR	C4-C5	-3.06	1.45	1.51
22	G	202	CLA	C4B-NB	-3.06	1.34	1.37
22	B	824	CLA	C1C-NC	-3.06	1.33	1.37
22	7	307	CLA	C4B-NB	-3.06	1.34	1.37
22	3	308	CLA	C4B-NB	-3.06	1.34	1.37
38	1	302	LUT	C23-C24	-3.06	1.45	1.50
22	B	816	CLA	C1C-NC	-3.06	1.33	1.37
22	A	834	CLA	C1C-NC	-3.06	1.33	1.37
22	B	813	CLA	C1C-NC	-3.05	1.33	1.37
22	6	319	CLA	C1C-NC	-3.05	1.33	1.37
22	1	307	CLA	C4B-NB	-3.05	1.34	1.37
22	A	842	CLA	C4B-NB	-3.05	1.34	1.37
22	Z	306	CLA	C4B-NB	-3.05	1.34	1.37
22	6	317	CLA	C4B-NB	-3.05	1.34	1.37
22	7	309	CLA	C4B-NB	-3.04	1.34	1.37
22	9	306	CLA	C4B-NB	-3.04	1.34	1.37
22	B	820	CLA	C1C-NC	-3.04	1.33	1.37
22	4	805	CLA	C4B-NB	-3.04	1.34	1.37
22	1	315	CLA	C1C-NC	-3.04	1.33	1.37
22	A	838	CLA	C4B-NB	-3.04	1.34	1.37
22	3	309	CLA	C4B-NB	-3.03	1.34	1.37
22	B	826	CLA	C1C-NC	-3.03	1.33	1.37
22	A	835	CLA	C4B-NB	-3.03	1.34	1.37
22	B	831	CLA	C4B-NB	-3.03	1.34	1.37
22	6	321	CLA	C4B-NB	-3.03	1.34	1.37
22	5	307	CLA	C4B-NB	-3.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	810	CLA	C4B-NB	-3.02	1.34	1.37
21	A	801	CL0	C1D-ND	-3.02	1.34	1.37
22	Z	305	CLA	C4B-NB	-3.02	1.34	1.37
22	Z	307	CLA	C4B-NB	-3.02	1.34	1.37
22	4	817	CLA	C4B-NB	-3.02	1.34	1.37
38	7	301	LUT	C23-C24	-3.02	1.45	1.50
22	B	842	CLA	C4B-NB	-3.01	1.34	1.37
38	3	303	LUT	C23-C24	-3.01	1.45	1.50
22	6	311	CLA	C4B-NB	-3.01	1.34	1.37
22	A	818	CLA	C4B-NB	-3.01	1.34	1.37
22	A	827	CLA	C4B-NB	-3.01	1.34	1.37
22	B	827	CLA	C4B-NB	-3.01	1.34	1.37
22	B	836	CLA	C4B-NB	-3.01	1.34	1.37
22	A	821	CLA	C4B-NB	-3.01	1.34	1.37
22	A	839	CLA	C4B-NB	-3.00	1.34	1.37
22	5	312	CLA	C4B-NB	-3.00	1.34	1.37
22	8	307	CLA	C1C-NC	-3.00	1.33	1.37
22	3	311	CLA	C4B-NB	-3.00	1.34	1.37
22	B	806	CLA	C4B-NB	-2.99	1.34	1.37
22	7	322	CLA	C4B-NB	-2.99	1.34	1.37
22	K	203	CLA	C4B-NB	-2.99	1.34	1.37
22	8	314	CLA	C4B-NB	-2.99	1.34	1.37
22	5	310	CLA	C4B-NB	-2.99	1.34	1.37
21	A	801	CL0	C3D-C2D	2.99	1.47	1.39
22	B	809	CLA	C4B-NB	-2.99	1.34	1.37
22	A	831	CLA	C4B-NB	-2.99	1.34	1.37
22	A	816	CLA	C4B-NB	-2.99	1.34	1.37
22	3	318	CLA	C4B-NB	-2.99	1.34	1.37
22	4	812	CLA	C4B-NB	-2.99	1.34	1.37
22	A	826	CLA	C1C-NC	-2.99	1.33	1.37
22	B	817	CLA	C4B-NB	-2.99	1.34	1.37
22	4	815	CLA	C4B-NB	-2.98	1.34	1.37
22	A	832	CLA	C4B-NB	-2.98	1.34	1.37
22	9	307	CLA	C4B-NB	-2.98	1.34	1.37
22	A	840	CLA	C4B-NB	-2.98	1.34	1.37
22	8	310	CLA	C4B-NB	-2.97	1.34	1.37
22	6	322	CLA	C4B-NB	-2.97	1.34	1.37
38	3	302	LUT	C23-C24	-2.97	1.45	1.50
22	A	834	CLA	C4B-NB	-2.97	1.34	1.37
22	B	810	CLA	C4B-NB	-2.97	1.34	1.37
22	8	309	CLA	C4B-NB	-2.97	1.34	1.37
22	A	830	CLA	C4B-NB	-2.97	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	312	CLA	C4B-NB	-2.97	1.34	1.37
22	L	203	CLA	C4B-NB	-2.97	1.34	1.37
22	4	807	CLA	C4B-NB	-2.97	1.34	1.37
22	B	833	CLA	C4B-NB	-2.97	1.34	1.37
22	B	841	CLA	C4B-NB	-2.97	1.34	1.37
22	Z	315	CLA	C4B-NB	-2.96	1.34	1.37
22	8	313	CLA	C4B-NB	-2.96	1.34	1.37
22	B	812	CLA	C4B-NB	-2.96	1.34	1.37
22	B	835	CLA	C4B-NB	-2.96	1.34	1.37
22	7	316	CLA	C4B-NB	-2.96	1.34	1.37
22	B	838	CLA	C4B-NB	-2.96	1.34	1.37
22	5	319	CLA	C4B-NB	-2.96	1.34	1.37
22	A	805	CLA	C4B-NB	-2.96	1.34	1.37
22	A	804	CLA	C4B-NB	-2.96	1.34	1.37
22	B	837	CLA	C4B-NB	-2.96	1.34	1.37
22	6	309	CLA	C4B-NB	-2.95	1.34	1.37
22	9	308	CLA	C4B-NB	-2.95	1.34	1.37
22	B	834	CLA	C4B-NB	-2.95	1.34	1.37
22	B	839	CLA	C4B-NB	-2.95	1.34	1.37
22	A	826	CLA	C4B-NB	-2.95	1.34	1.37
22	1	315	CLA	C4B-NB	-2.95	1.34	1.37
22	J	103	CLA	C4B-NB	-2.95	1.34	1.37
22	7	306	CLA	C4B-NB	-2.95	1.34	1.37
22	B	822	CLA	C4B-NB	-2.95	1.34	1.37
22	3	313	CLA	C4B-NB	-2.94	1.34	1.37
22	B	832	CLA	C4B-NB	-2.94	1.34	1.37
22	5	318	CLA	C4B-NB	-2.94	1.34	1.37
22	B	824	CLA	C4B-NB	-2.94	1.34	1.37
22	6	310	CLA	C4B-NB	-2.94	1.34	1.37
22	B	825	CLA	C4B-NB	-2.94	1.34	1.37
38	Z	302	LUT	C23-C24	-2.94	1.46	1.50
22	B	808	CLA	C4B-NB	-2.94	1.34	1.37
22	7	324	CLA	C4B-NB	-2.94	1.34	1.37
22	L	202	CLA	C4B-NB	-2.94	1.34	1.37
22	F	305	CLA	C4B-NB	-2.93	1.34	1.37
22	5	311	CLA	C4B-NB	-2.93	1.34	1.37
22	7	304	CLA	C4B-NB	-2.93	1.34	1.37
22	5	323	CLA	C4B-NB	-2.93	1.34	1.37
22	A	815	CLA	C4B-NB	-2.93	1.34	1.37
38	6	304	LUT	C23-C24	-2.93	1.46	1.50
22	B	816	CLA	C4B-NB	-2.93	1.34	1.37
22	K	204	CLA	C4B-NB	-2.93	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	303	LUT	C23-C24	-2.93	1.46	1.50
22	A	819	CLA	C4B-NB	-2.93	1.34	1.37
22	7	310	CLA	C4B-NB	-2.93	1.34	1.37
22	B	820	CLA	C4B-NB	-2.93	1.34	1.37
22	6	313	CLA	C4B-NB	-2.92	1.34	1.37
22	A	810	CLA	C4B-NB	-2.92	1.34	1.37
22	A	811	CLA	C4B-NB	-2.92	1.34	1.37
22	A	828	CLA	C4B-NB	-2.92	1.34	1.37
22	A	854	CLA	C4B-NB	-2.92	1.34	1.37
22	3	319	CLA	C4B-NB	-2.92	1.34	1.37
22	A	817	CLA	C4B-NB	-2.92	1.34	1.37
22	7	308	CLA	C4B-NB	-2.92	1.34	1.37
22	1	306	CLA	C4B-NB	-2.91	1.34	1.37
22	1	314	CLA	C4B-NB	-2.91	1.34	1.37
22	8	307	CLA	C4B-NB	-2.91	1.34	1.37
22	B	829	CLA	C4B-NB	-2.91	1.34	1.37
22	B	813	CLA	C4B-NB	-2.90	1.34	1.37
22	5	308	CLA	C4B-NB	-2.90	1.34	1.37
22	3	310	CLA	C4B-NB	-2.90	1.34	1.37
21	A	801	CL0	C1B-C2B	2.90	1.50	1.43
22	A	802	CLA	C4B-NB	-2.90	1.34	1.37
22	B	807	CLA	C4B-NB	-2.90	1.34	1.37
22	9	311	CLA	C4B-NB	-2.89	1.34	1.37
22	B	801	CLA	C4B-NB	-2.89	1.34	1.37
22	7	323	CLA	C4B-NB	-2.89	1.34	1.37
22	A	814	CLA	C4B-NB	-2.89	1.34	1.37
24	L	204	BCR	C34-C9	2.88	1.56	1.50
22	2	302	CLA	C4B-NB	-2.87	1.34	1.37
22	A	825	CLA	C4B-NB	-2.87	1.34	1.37
22	G	201	CLA	C4B-NB	-2.87	1.34	1.37
24	5	305	BCR	C34-C9	2.87	1.56	1.50
22	7	314	CLA	C4B-NB	-2.87	1.34	1.37
22	5	301	CLA	C4B-NB	-2.87	1.34	1.37
24	B	853	BCR	C34-C9	2.87	1.56	1.50
22	6	301	CLA	C4B-NB	-2.87	1.34	1.37
22	B	840	CLA	C4B-NB	-2.86	1.34	1.37
22	F	304	CLA	C4B-NB	-2.86	1.34	1.37
22	B	814	CLA	C4B-NB	-2.86	1.34	1.37
22	6	302	CLA	C4B-NB	-2.85	1.34	1.37
22	Z	308	CLA	C4B-NB	-2.85	1.34	1.37
38	7	302	LUT	C23-C24	-2.85	1.46	1.50
24	A	845	BCR	C34-C9	2.85	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	313	CLA	C4B-NB	-2.85	1.34	1.37
22	5	322	CLA	C4B-NB	-2.85	1.34	1.37
24	B	849	BCR	C34-C9	2.85	1.56	1.50
22	4	806	CLA	C4B-NB	-2.85	1.34	1.37
22	Z	304	CLA	C4B-NB	-2.85	1.34	1.37
22	2	301	CLA	C4B-NB	-2.85	1.34	1.37
22	7	315	CLA	C4B-NB	-2.84	1.34	1.37
24	B	847	BCR	C34-C9	2.84	1.56	1.50
22	7	305	CLA	C4B-NB	-2.84	1.34	1.37
22	B	826	CLA	C4B-NB	-2.84	1.34	1.37
24	A	846	BCR	C34-C9	2.84	1.56	1.50
24	F	303	BCR	C34-C9	2.84	1.56	1.50
22	A	855	CLA	C4B-NB	-2.84	1.34	1.37
38	5	302	LUT	C23-C24	-2.84	1.46	1.50
22	8	311	CLA	C4B-NB	-2.83	1.34	1.37
22	Z	310	CLA	C4B-NB	-2.83	1.34	1.37
22	A	833	CLA	C4B-NB	-2.83	1.34	1.37
22	B	823	CLA	C4B-NB	-2.83	1.34	1.37
22	5	314	CLA	C4B-NB	-2.83	1.34	1.37
22	3	322	CLA	C4B-NB	-2.82	1.34	1.37
22	4	811	CLA	C4B-NB	-2.82	1.34	1.37
22	5	309	CLA	C4B-NB	-2.82	1.34	1.37
24	A	847	BCR	C34-C9	2.82	1.56	1.50
24	5	304	BCR	C34-C9	2.82	1.56	1.50
24	6	306	BCR	C34-C9	2.82	1.56	1.50
22	1	309	CLA	C4B-NB	-2.82	1.34	1.37
22	5	315	CLA	C4B-NB	-2.82	1.34	1.37
24	B	844	BCR	C34-C9	2.82	1.56	1.50
22	B	821	CLA	C4B-NB	-2.82	1.34	1.37
22	5	326	CLA	C4B-NB	-2.82	1.34	1.37
22	7	311	CLA	C4B-NB	-2.82	1.34	1.37
22	3	314	CLA	C4B-NB	-2.81	1.34	1.37
24	B	853	BCR	C7-C6	2.81	1.55	1.45
24	B	845	BCR	C34-C9	2.81	1.56	1.50
24	3	307	BCR	C34-C9	2.81	1.56	1.50
22	7	312	CLA	C4B-NB	-2.81	1.34	1.37
24	6	305	BCR	C34-C9	2.81	1.56	1.50
21	A	801	CL0	C4D-CHA	2.81	1.48	1.38
22	7	317	CLA	C4B-NB	-2.81	1.34	1.37
22	6	308	CLA	C4B-NB	-2.81	1.34	1.37
22	Z	316	CLA	C4B-NB	-2.80	1.34	1.37
22	B	819	CLA	C4B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	803	LUT	C23-C24	-2.80	1.46	1.50
24	A	856	BCR	C34-C9	2.80	1.56	1.50
24	I	4001	BCR	C34-C9	2.80	1.56	1.50
24	3	305	BCR	C34-C9	2.79	1.56	1.50
22	6	319	CLA	C4B-NB	-2.79	1.34	1.37
24	5	305	BCR	C7-C6	2.79	1.55	1.45
22	A	807	CLA	C4B-NB	-2.79	1.34	1.37
22	A	806	CLA	C4B-NB	-2.78	1.34	1.37
22	B	811	CLA	C4B-NB	-2.78	1.34	1.37
22	1	305	CLA	C4B-NB	-2.78	1.34	1.37
38	9	302	LUT	C23-C24	-2.78	1.46	1.50
24	K	206	BCR	C34-C9	2.78	1.56	1.50
22	8	316	CLA	C4B-NB	-2.78	1.34	1.37
24	8	304	BCR	C34-C9	2.78	1.56	1.50
24	J	104	BCR	C34-C9	2.78	1.56	1.50
24	B	848	BCR	C34-C9	2.78	1.56	1.50
24	3	304	BCR	C34-C9	2.78	1.56	1.50
24	4	804	BCR	C34-C9	2.77	1.56	1.50
24	A	848	BCR	C34-C9	2.77	1.56	1.50
22	A	837	CLA	C4B-NB	-2.77	1.34	1.37
24	7	303	BCR	C34-C9	2.77	1.56	1.50
24	G	203	BCR	C34-C9	2.76	1.56	1.50
22	F	301	CLA	C4B-NB	-2.76	1.34	1.37
22	A	841	CLA	C4B-NB	-2.75	1.34	1.37
22	2	304	CLA	C4B-NB	-2.75	1.34	1.37
22	B	818	CLA	C4B-NB	-2.75	1.34	1.37
24	3	306	BCR	C7-C6	2.75	1.54	1.45
22	1	310	CLA	C4B-NB	-2.75	1.34	1.37
22	A	809	CLA	C4B-NB	-2.75	1.34	1.37
24	F	303	BCR	C7-C6	2.74	1.54	1.45
22	B	830	CLA	C4B-NB	-2.74	1.34	1.37
38	5	303	LUT	C23-C24	-2.74	1.46	1.50
22	3	312	CLA	C4B-NB	-2.74	1.34	1.37
24	B	848	BCR	C7-C6	2.73	1.54	1.45
22	6	314	CLA	C4B-NB	-2.73	1.34	1.37
22	Z	309	CLA	C4B-NB	-2.73	1.34	1.37
24	B	844	BCR	C7-C6	2.73	1.54	1.45
24	B	846	BCR	C34-C9	2.73	1.56	1.50
21	A	801	CL0	C1B-NB	-2.72	1.34	1.37
22	1	308	CLA	C4B-NB	-2.72	1.34	1.37
22	A	820	CLA	C4B-NB	-2.72	1.34	1.37
24	3	306	BCR	C34-C9	2.72	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	803	CLA	C4B-NB	-2.72	1.34	1.37
24	3	305	BCR	C7-C6	2.72	1.54	1.45
22	Z	314	CLA	C4B-NB	-2.72	1.34	1.37
22	A	823	CLA	C4B-NB	-2.71	1.34	1.37
22	A	829	CLA	C4B-NB	-2.71	1.34	1.37
22	4	809	CLA	C4B-NB	-2.70	1.34	1.37
24	A	856	BCR	C7-C6	2.70	1.54	1.45
24	4	804	BCR	C7-C6	2.70	1.54	1.45
38	1	302	LUT	C18-C5	2.70	1.55	1.50
24	7	303	BCR	C7-C6	2.69	1.54	1.45
24	J	104	BCR	C7-C6	2.69	1.54	1.45
38	9	301	LUT	C18-C5	2.69	1.55	1.50
38	6	303	LUT	C23-C24	-2.69	1.46	1.50
38	6	303	LUT	C18-C5	2.69	1.55	1.50
38	Z	301	LUT	C18-C5	2.69	1.55	1.50
24	A	845	BCR	C7-C6	2.69	1.54	1.45
22	A	812	CLA	C4B-NB	-2.69	1.34	1.37
22	B	828	CLA	C4B-NB	-2.69	1.34	1.37
38	4	802	LUT	C18-C5	2.69	1.55	1.50
24	B	845	BCR	C7-C6	2.68	1.54	1.45
22	A	824	CLA	C4B-NB	-2.68	1.34	1.37
22	9	313	CLA	C4B-NB	-2.68	1.34	1.37
24	B	853	BCR	C36-C18	2.68	1.56	1.50
24	B	849	BCR	C7-C6	2.67	1.54	1.45
38	7	301	LUT	C18-C5	2.67	1.55	1.50
22	F	302	CLA	C4B-NB	-2.67	1.34	1.37
22	B	805	CLA	C4B-NB	-2.66	1.34	1.37
22	L	201	CLA	C4B-NB	-2.66	1.34	1.37
24	A	844	BCR	C34-C9	2.66	1.56	1.50
24	B	846	BCR	C7-C6	2.66	1.54	1.45
38	5	302	LUT	C18-C5	2.66	1.55	1.50
24	B	847	BCR	C7-C6	2.65	1.54	1.45
38	3	302	LUT	C18-C5	2.64	1.55	1.50
24	A	848	BCR	C7-C6	2.64	1.54	1.45
24	6	305	BCR	C7-C6	2.64	1.54	1.45
38	8	302	LUT	O23-C23	-2.64	1.38	1.43
22	3	316	CLA	C4B-NB	-2.63	1.34	1.37
24	B	853	BCR	C38-C26	2.63	1.55	1.50
24	G	203	BCR	C7-C6	2.63	1.54	1.45
24	I	4001	BCR	C7-C6	2.63	1.54	1.45
38	6	304	LUT	C18-C5	2.63	1.55	1.50
38	8	302	LUT	C18-C5	2.63	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	808	CLA	C4B-NB	-2.62	1.34	1.37
22	8	306	CLA	C4B-NB	-2.62	1.34	1.37
24	3	307	BCR	C7-C6	2.62	1.54	1.45
38	4	802	LUT	O23-C23	-2.62	1.38	1.43
24	A	847	BCR	C7-C6	2.61	1.54	1.45
24	L	204	BCR	C7-C6	2.61	1.54	1.45
24	6	306	BCR	C7-C6	2.61	1.54	1.45
24	8	304	BCR	C7-C6	2.61	1.54	1.45
24	A	846	BCR	C7-C6	2.61	1.54	1.45
24	A	844	BCR	C7-C6	2.59	1.54	1.45
24	3	304	BCR	C7-C6	2.59	1.54	1.45
38	1	303	LUT	C23-C24	-2.59	1.46	1.50
38	9	301	LUT	O23-C23	-2.59	1.38	1.43
24	5	304	BCR	C7-C6	2.58	1.54	1.45
41	5	325	3PH	O21-C2	-2.58	1.40	1.46
38	7	302	LUT	C18-C5	2.58	1.55	1.50
24	K	206	BCR	C7-C6	2.58	1.54	1.45
38	3	303	LUT	C18-C5	2.58	1.55	1.50
38	5	303	LUT	C18-C5	2.57	1.55	1.50
35	J	102	T7X	O16-C8	-2.56	1.40	1.46
38	4	803	LUT	C18-C5	2.56	1.55	1.50
38	5	303	LUT	O23-C23	-2.55	1.39	1.43
38	1	303	LUT	C18-C5	2.55	1.55	1.50
38	9	302	LUT	C18-C5	2.55	1.55	1.50
38	Z	301	LUT	O23-C23	-2.54	1.39	1.43
38	3	303	LUT	O23-C23	-2.53	1.39	1.43
38	7	301	LUT	O23-C23	-2.52	1.39	1.43
38	8	303	LUT	C18-C5	2.51	1.55	1.50
38	Z	302	LUT	C18-C5	2.50	1.55	1.50
38	3	302	LUT	O23-C23	-2.49	1.39	1.43
41	7	319	3PH	O21-C2	-2.48	1.40	1.46
38	Z	302	LUT	O23-C23	-2.48	1.39	1.43
21	A	801	CL0	C1D-C2D	2.48	1.50	1.45
38	6	303	LUT	O23-C23	-2.48	1.39	1.43
38	4	803	LUT	O23-C23	-2.48	1.39	1.43
41	8	320	3PH	O21-C2	-2.47	1.40	1.46
38	1	302	LUT	O23-C23	-2.47	1.39	1.43
38	6	304	LUT	O23-C23	-2.47	1.39	1.43
38	1	303	LUT	O23-C23	-2.46	1.39	1.43
21	A	801	CL0	C4B-NB	-2.46	1.34	1.37
22	1	308	CLA	C1C-C2C	2.45	1.49	1.44
41	6	324	3PH	O21-C2	-2.44	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	303	BCR	C36-C18	2.44	1.55	1.50
38	5	302	LUT	O23-C23	-2.43	1.39	1.43
41	6	324	3PH	O31-C31	2.43	1.40	1.33
38	8	303	LUT	O23-C23	-2.43	1.39	1.43
38	9	302	LUT	O23-C23	-2.43	1.39	1.43
38	Z	301	LUT	C26-C27	2.43	1.53	1.50
24	F	303	BCR	C36-C18	2.43	1.55	1.50
24	5	305	BCR	C36-C18	2.43	1.55	1.50
24	J	104	BCR	C36-C18	2.42	1.55	1.50
38	8	302	LUT	C30-C29	-2.42	1.32	1.35
21	A	801	CL0	C1C-NC	-2.42	1.34	1.37
32	F	306	RRX	C34-C9	2.42	1.55	1.50
36	J	105	C7Z	C20-C13	2.41	1.55	1.50
24	3	307	BCR	C36-C18	2.40	1.55	1.50
24	B	853	BCR	C39-C30	-2.40	1.49	1.53
39	4	816	CHL	C1B-NB	-2.40	1.34	1.37
38	7	302	LUT	O23-C23	-2.39	1.39	1.43
24	B	849	BCR	C36-C18	2.39	1.55	1.50
24	G	203	BCR	C36-C18	2.39	1.55	1.50
41	8	320	3PH	O31-C31	2.39	1.40	1.33
21	A	801	CL0	C3B-C4B	2.39	1.48	1.42
36	5	306	C7Z	C20-C13	2.39	1.55	1.50
24	A	848	BCR	C36-C18	2.39	1.55	1.50
36	5	306	C7Z	C38-C25	2.38	1.54	1.50
24	A	856	BCR	C36-C18	2.38	1.55	1.50
38	1	302	LUT	C26-C27	2.38	1.53	1.50
24	I	4001	BCR	C36-C18	2.38	1.55	1.50
32	F	306	RRX	C17-C18	-2.38	1.32	1.35
41	5	325	3PH	O31-C31	2.38	1.40	1.33
24	A	847	BCR	C36-C18	2.38	1.55	1.50
24	5	304	BCR	C36-C18	2.38	1.55	1.50
24	3	306	BCR	C36-C18	2.37	1.55	1.50
22	9	305	CLA	C1A-CHA	2.37	1.52	1.43
24	3	305	BCR	C36-C18	2.37	1.55	1.50
24	8	304	BCR	C36-C18	2.37	1.55	1.50
24	6	305	BCR	C36-C18	2.37	1.55	1.50
35	J	102	T7X	O18-C11	2.37	1.40	1.33
24	3	307	BCR	C39-C30	-2.36	1.49	1.53
24	B	847	BCR	C36-C18	2.36	1.55	1.50
24	B	845	BCR	C36-C18	2.36	1.55	1.50
24	K	206	BCR	C36-C18	2.36	1.55	1.50
24	4	804	BCR	C36-C18	2.35	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	105	C7Z	C40-C33	2.35	1.55	1.50
24	B	848	BCR	C36-C18	2.35	1.55	1.50
24	B	846	BCR	C36-C18	2.35	1.55	1.50
36	J	105	C7Z	C38-C25	2.34	1.54	1.50
24	6	306	BCR	C36-C18	2.33	1.55	1.50
24	L	204	BCR	C36-C18	2.33	1.55	1.50
38	9	301	LUT	C30-C29	-2.33	1.32	1.35
24	8	304	BCR	C39-C30	-2.33	1.49	1.53
38	7	301	LUT	C30-C29	-2.32	1.32	1.35
24	A	844	BCR	C36-C18	2.32	1.55	1.50
24	A	846	BCR	C36-C18	2.32	1.55	1.50
38	6	303	LUT	C30-C29	-2.31	1.32	1.35
39	5	317	CHL	C1B-NB	-2.31	1.34	1.37
38	3	302	LUT	C34-C33	-2.30	1.32	1.35
24	3	306	BCR	C39-C30	-2.30	1.49	1.53
36	5	306	C7Z	C40-C33	2.30	1.55	1.50
41	7	319	3PH	O31-C31	2.29	1.40	1.33
38	Z	302	LUT	C26-C27	2.29	1.53	1.50
24	3	304	BCR	C36-C18	2.29	1.55	1.50
24	A	845	BCR	C36-C18	2.28	1.55	1.50
38	3	303	LUT	C26-C27	2.27	1.53	1.50
22	3	315	CLA	C3D-C4D	-2.27	1.39	1.44
38	5	302	LUT	C30-C29	-2.27	1.32	1.35
36	J	105	C7Z	C19-C9	2.26	1.55	1.50
24	A	856	BCR	C39-C30	-2.25	1.49	1.53
38	4	802	LUT	C30-C29	-2.25	1.32	1.35
22	9	303	CLA	C3D-C4D	-2.25	1.39	1.44
22	Z	306	CLA	C1C-C2C	2.25	1.48	1.44
22	B	824	CLA	C1C-C2C	2.25	1.48	1.44
38	8	303	LUT	C26-C27	2.25	1.53	1.50
38	6	304	LUT	C26-C27	2.24	1.53	1.50
22	K	205	CLA	C1A-CHA	2.24	1.52	1.43
36	5	306	C7Z	C19-C9	2.24	1.55	1.50
24	B	844	BCR	C39-C30	-2.23	1.49	1.53
38	9	302	LUT	C26-C27	2.23	1.53	1.50
38	1	302	LUT	C30-C29	-2.22	1.32	1.35
22	A	826	CLA	C1C-C2C	2.22	1.48	1.44
38	4	803	LUT	C30-C29	-2.22	1.32	1.35
38	7	302	LUT	C26-C27	2.22	1.53	1.50
24	3	304	BCR	C39-C30	-2.22	1.49	1.53
24	K	206	BCR	C39-C30	-2.22	1.49	1.53
24	6	305	BCR	C39-C30	-2.21	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	5	303	LUT	C26-C27	2.21	1.53	1.50
22	3	320	CLA	C3D-C4D	-2.21	1.39	1.44
22	4	806	CLA	C1C-C2C	2.21	1.48	1.44
38	8	302	LUT	C26-C27	2.21	1.53	1.50
22	7	305	CLA	C1C-C2C	2.21	1.48	1.44
22	7	307	CLA	C1C-C2C	2.21	1.48	1.44
22	6	310	CLA	C1C-C2C	2.21	1.48	1.44
22	6	313	CLA	C1C-C2C	2.21	1.48	1.44
24	A	847	BCR	C39-C30	-2.21	1.49	1.53
24	I	4001	BCR	C38-C26	2.21	1.54	1.50
38	7	301	LUT	C26-C27	2.21	1.53	1.50
39	8	312	CHL	C1B-NB	-2.20	1.35	1.37
24	F	303	BCR	C39-C30	-2.20	1.49	1.53
38	9	302	LUT	C30-C29	-2.20	1.32	1.35
22	B	807	CLA	C1C-C2C	2.20	1.48	1.44
38	3	302	LUT	C30-C29	-2.20	1.32	1.35
22	4	815	CLA	C1C-C2C	2.20	1.48	1.44
22	F	302	CLA	C1C-C2C	2.20	1.48	1.44
22	1	316	CLA	C3D-C4D	-2.20	1.39	1.44
27	A	852	DGA	OG2-CG2	-2.19	1.41	1.46
24	5	305	BCR	C39-C30	-2.19	1.49	1.53
22	B	828	CLA	C1C-C2C	2.19	1.48	1.44
24	7	303	BCR	C39-C30	-2.19	1.49	1.53
24	L	204	BCR	C39-C30	-2.19	1.49	1.53
22	K	205	CLA	C3D-C4D	-2.19	1.39	1.44
22	1	313	CLA	C1C-C2C	2.19	1.48	1.44
24	5	305	BCR	C38-C26	2.19	1.54	1.50
22	B	808	CLA	C1C-C2C	2.19	1.48	1.44
22	F	301	CLA	C1C-C2C	2.18	1.48	1.44
24	3	305	BCR	C39-C30	-2.18	1.49	1.53
41	6	324	3PH	O21-C21	2.18	1.40	1.34
22	4	811	CLA	C1C-C2C	2.18	1.48	1.44
22	5	322	CLA	C1C-C2C	2.18	1.48	1.44
38	4	802	LUT	C26-C27	2.18	1.53	1.50
38	3	303	LUT	C30-C29	-2.18	1.32	1.35
41	7	319	3PH	O31-C3	-2.18	1.40	1.45
22	J	103	CLA	C1C-C2C	2.18	1.48	1.44
22	9	307	CLA	C1C-C2C	2.18	1.48	1.44
24	4	804	BCR	C39-C30	-2.18	1.49	1.53
22	5	310	CLA	C1C-C2C	2.17	1.48	1.44
35	J	102	T7X	O18-C9	-2.17	1.40	1.45
24	B	845	BCR	C39-C30	-2.17	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	803	LUT	C26-C27	2.17	1.53	1.50
38	8	303	LUT	C30-C29	-2.17	1.32	1.35
39	6	316	CHL	C1B-NB	-2.17	1.35	1.37
39	4	819	CHL	C1B-NB	-2.17	1.35	1.37
22	7	322	CLA	C1C-C2C	2.17	1.48	1.44
22	1	315	CLA	C1C-C2C	2.17	1.48	1.44
22	Z	308	CLA	C1C-C2C	2.17	1.48	1.44
24	A	846	BCR	C39-C30	-2.17	1.49	1.53
22	6	319	CLA	C1C-C2C	2.17	1.48	1.44
22	B	813	CLA	C1C-C2C	2.16	1.48	1.44
22	A	823	CLA	C1C-C2C	2.16	1.48	1.44
22	7	311	CLA	C1C-C2C	2.16	1.48	1.44
22	3	318	CLA	C1C-C2C	2.16	1.48	1.44
41	6	324	3PH	O31-C3	-2.16	1.40	1.45
22	Z	314	CLA	C1C-C2C	2.16	1.48	1.44
22	A	833	CLA	C1C-C2C	2.16	1.48	1.44
22	A	841	CLA	C1C-C2C	2.16	1.48	1.44
22	7	315	CLA	C1C-C2C	2.16	1.48	1.44
22	B	825	CLA	C1C-C2C	2.16	1.48	1.44
22	B	805	CLA	C1C-C2C	2.16	1.48	1.44
22	B	831	CLA	C1C-C2C	2.16	1.48	1.44
39	6	315	CHL	C1B-NB	-2.16	1.35	1.37
22	8	311	CLA	C1C-C2C	2.16	1.48	1.44
38	7	302	LUT	C30-C29	-2.16	1.32	1.35
22	Z	313	CLA	C1C-C2C	2.16	1.48	1.44
22	A	834	CLA	C1C-C2C	2.16	1.48	1.44
24	B	846	BCR	C39-C30	-2.15	1.49	1.53
22	1	307	CLA	C1C-C2C	2.15	1.48	1.44
24	6	306	BCR	C39-C30	-2.15	1.49	1.53
22	L	203	CLA	C1C-C2C	2.15	1.48	1.44
24	8	304	BCR	C38-C26	2.15	1.54	1.50
22	7	324	CLA	C1C-C2C	2.15	1.48	1.44
24	A	846	BCR	C38-C26	2.15	1.54	1.50
22	A	812	CLA	C1C-C2C	2.15	1.48	1.44
24	K	206	BCR	C38-C26	2.15	1.54	1.50
41	5	325	3PH	O31-C3	-2.15	1.40	1.45
22	A	824	CLA	C1C-C2C	2.15	1.48	1.44
22	A	818	CLA	C1C-C2C	2.15	1.48	1.44
24	B	847	BCR	C39-C30	-2.15	1.49	1.53
32	F	306	RRX	C33-C5	2.14	1.54	1.50
22	A	825	CLA	C1C-C2C	2.14	1.48	1.44
22	B	829	CLA	C1C-C2C	2.14	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	848	BCR	C38-C26	2.14	1.54	1.50
41	8	320	3PH	O21-C21	2.14	1.40	1.34
22	7	310	CLA	C1C-C2C	2.14	1.48	1.44
22	6	317	CLA	C1C-C2C	2.14	1.48	1.44
41	7	319	3PH	O21-C21	2.14	1.40	1.34
22	8	306	CLA	C1C-C2C	2.14	1.48	1.44
22	5	314	CLA	C1C-C2C	2.14	1.48	1.44
22	B	837	CLA	C1C-C2C	2.14	1.48	1.44
38	6	304	LUT	C30-C29	-2.14	1.32	1.35
24	B	848	BCR	C39-C30	-2.14	1.49	1.53
22	B	826	CLA	C1C-C2C	2.14	1.48	1.44
22	B	801	CLA	C1C-C2C	2.14	1.48	1.44
24	B	853	BCR	C37-C22	2.14	1.55	1.50
22	A	835	CLA	C1C-C2C	2.14	1.48	1.44
22	B	822	CLA	C1C-C2C	2.14	1.48	1.44
22	B	823	CLA	C1C-C2C	2.14	1.48	1.44
22	3	319	CLA	C1C-C2C	2.14	1.48	1.44
22	8	316	CLA	C1C-C2C	2.14	1.48	1.44
24	J	104	BCR	C39-C30	-2.14	1.49	1.53
22	B	838	CLA	C1C-C2C	2.14	1.48	1.44
22	4	817	CLA	C1C-C2C	2.14	1.48	1.44
24	3	306	BCR	C38-C26	2.14	1.54	1.50
22	9	311	CLA	C1C-C2C	2.14	1.48	1.44
22	B	833	CLA	C1C-C2C	2.14	1.48	1.44
39	8	315	CHL	C1B-NB	-2.14	1.35	1.37
22	A	829	CLA	C1C-C2C	2.14	1.48	1.44
22	B	820	CLA	C1C-C2C	2.14	1.48	1.44
22	4	808	CLA	C1C-C2C	2.14	1.48	1.44
22	A	819	CLA	C1C-C2C	2.13	1.48	1.44
24	B	847	BCR	C38-C26	2.13	1.54	1.50
38	1	303	LUT	C26-C27	2.13	1.53	1.50
24	A	848	BCR	C39-C30	-2.13	1.49	1.53
22	3	311	CLA	C1C-C2C	2.13	1.48	1.44
22	1	304	CLA	C1C-C2C	2.13	1.48	1.44
38	9	301	LUT	C26-C27	2.13	1.53	1.50
24	B	849	BCR	C39-C30	-2.13	1.49	1.53
22	Z	309	CLA	C1C-C2C	2.13	1.48	1.44
24	A	844	BCR	C39-C30	-2.13	1.49	1.53
22	7	308	CLA	C1C-C2C	2.13	1.48	1.44
24	G	203	BCR	C39-C30	-2.13	1.49	1.53
41	8	320	3PH	O31-C3	-2.13	1.40	1.45
38	5	302	LUT	C26-C27	2.13	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	821	CLA	C1C-C2C	2.13	1.48	1.44
22	5	311	CLA	C1C-C2C	2.13	1.48	1.44
39	4	814	CHL	C1B-NB	-2.13	1.35	1.37
24	B	845	BCR	C38-C26	2.13	1.54	1.50
22	3	314	CLA	C1C-C2C	2.13	1.48	1.44
22	B	816	CLA	C1C-C2C	2.13	1.48	1.44
22	B	836	CLA	C1C-C2C	2.13	1.48	1.44
22	8	309	CLA	C1C-C2C	2.13	1.48	1.44
24	B	849	BCR	C37-C22	2.13	1.55	1.50
22	A	830	CLA	C1C-C2C	2.13	1.48	1.44
39	6	320	CHL	C1B-NB	-2.13	1.35	1.37
22	8	307	CLA	C1C-C2C	2.12	1.48	1.44
24	B	844	BCR	C38-C26	2.12	1.54	1.50
24	A	845	BCR	C39-C30	-2.12	1.49	1.53
38	4	802	LUT	C34-C33	-2.12	1.33	1.35
22	A	809	CLA	C1C-C2C	2.12	1.48	1.44
24	B	848	BCR	C38-C26	2.12	1.54	1.50
22	3	316	CLA	C1C-C2C	2.12	1.48	1.44
22	Z	304	CLA	C1C-C2C	2.12	1.48	1.44
22	K	202	CLA	C1C-C2C	2.12	1.48	1.44
22	8	308	CLA	C1C-C2C	2.12	1.48	1.44
22	1	305	CLA	C3D-C4D	-2.12	1.39	1.44
22	Z	303	CLA	C1C-C2C	2.12	1.48	1.44
24	I	4001	BCR	C39-C30	-2.12	1.49	1.53
22	A	831	CLA	C1C-C2C	2.12	1.48	1.44
38	6	303	LUT	C26-C27	2.12	1.53	1.50
24	6	305	BCR	C38-C26	2.12	1.54	1.50
22	A	806	CLA	C1C-C2C	2.12	1.48	1.44
38	4	803	LUT	C34-C33	-2.12	1.33	1.35
22	B	811	CLA	C1C-C2C	2.12	1.48	1.44
22	A	810	CLA	C1C-C2C	2.12	1.48	1.44
22	B	835	CLA	C1C-C2C	2.12	1.48	1.44
22	3	322	CLA	C1C-C2C	2.12	1.48	1.44
22	A	820	CLA	C1C-C2C	2.12	1.48	1.44
22	1	309	CLA	C1C-C2C	2.12	1.48	1.44
22	2	304	CLA	C1C-C2C	2.12	1.48	1.44
22	B	806	CLA	C1C-C2C	2.12	1.48	1.44
22	A	811	CLA	C1C-C2C	2.11	1.48	1.44
22	F	305	CLA	C1C-C2C	2.11	1.48	1.44
22	5	315	CLA	C1C-C2C	2.11	1.48	1.44
24	A	844	BCR	C38-C26	2.11	1.54	1.50
38	5	302	LUT	C34-C33	-2.11	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	9	302	LUT	C34-C33	-2.11	1.33	1.35
22	A	836	CLA	C1C-C2C	2.11	1.48	1.44
22	9	305	CLA	CAA-C2A	-2.11	1.50	1.54
22	3	313	CLA	C1C-C2C	2.11	1.48	1.44
39	9	314	CHL	C1B-NB	-2.11	1.35	1.37
38	9	301	LUT	C34-C33	-2.11	1.33	1.35
41	5	325	3PH	O21-C21	2.11	1.40	1.34
24	B	846	BCR	C38-C26	2.11	1.54	1.50
22	4	805	CLA	C1C-C2C	2.11	1.48	1.44
22	1	311	CLA	C3D-C4D	-2.11	1.39	1.44
24	5	304	BCR	C39-C30	-2.11	1.49	1.53
22	Z	316	CLA	C1C-C2C	2.11	1.48	1.44
24	B	844	BCR	C37-C22	2.11	1.55	1.50
22	A	808	CLA	C1C-C2C	2.11	1.48	1.44
22	A	855	CLA	C1C-C2C	2.11	1.48	1.44
22	6	322	CLA	C1C-C2C	2.11	1.48	1.44
22	A	807	CLA	C1C-C2C	2.11	1.48	1.44
22	Z	307	CLA	C1C-C2C	2.11	1.48	1.44
24	3	306	BCR	C37-C22	2.10	1.55	1.50
38	3	302	LUT	C26-C27	2.10	1.53	1.50
22	6	311	CLA	C1C-C2C	2.10	1.48	1.44
22	5	309	CLA	C1C-C2C	2.10	1.48	1.44
22	B	832	CLA	C1C-C2C	2.10	1.48	1.44
24	A	845	BCR	C37-C22	2.10	1.55	1.50
24	A	847	BCR	C37-C22	2.10	1.55	1.50
22	A	803	CLA	C1C-C2C	2.10	1.48	1.44
22	6	321	CLA	C1C-C2C	2.10	1.48	1.44
24	A	847	BCR	C38-C26	2.10	1.54	1.50
22	Z	310	CLA	C1C-C2C	2.10	1.48	1.44
24	6	306	BCR	C38-C26	2.10	1.54	1.50
38	7	301	LUT	C34-C33	-2.10	1.33	1.35
22	8	310	CLA	C1C-C2C	2.10	1.48	1.44
24	K	206	BCR	C37-C22	2.10	1.55	1.50
22	B	817	CLA	C1C-C2C	2.10	1.48	1.44
22	L	201	CLA	C1C-C2C	2.10	1.48	1.44
22	7	316	CLA	C1C-C2C	2.10	1.48	1.44
22	B	841	CLA	C1C-C2C	2.09	1.48	1.44
22	3	308	CLA	C1C-C2C	2.09	1.48	1.44
22	8	314	CLA	C1C-C2C	2.09	1.48	1.44
22	7	317	CLA	C1C-C2C	2.09	1.48	1.44
22	5	313	CLA	C1A-CHA	2.09	1.51	1.43
24	G	203	BCR	C37-C22	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	326	CLA	C1C-C2C	2.09	1.48	1.44
22	5	313	CLA	C1C-C2C	2.09	1.48	1.44
22	Z	315	CLA	C1C-C2C	2.09	1.48	1.44
22	9	306	CLA	C1C-C2C	2.09	1.48	1.44
24	L	204	BCR	C38-C26	2.09	1.54	1.50
22	7	304	CLA	C1C-C2C	2.09	1.48	1.44
22	A	814	CLA	C1C-C2C	2.09	1.48	1.44
22	1	306	CLA	C1C-C2C	2.09	1.48	1.44
22	6	312	CLA	C1C-C2C	2.09	1.48	1.44
22	G	202	CLA	C1C-C2C	2.09	1.48	1.44
38	7	302	LUT	C34-C33	-2.09	1.33	1.35
24	F	303	BCR	C37-C22	2.09	1.55	1.50
24	3	305	BCR	C37-C22	2.09	1.55	1.50
22	B	827	CLA	C1C-C2C	2.08	1.48	1.44
39	9	312	CHL	C1B-NB	-2.08	1.35	1.37
22	B	830	CLA	C1C-C2C	2.08	1.48	1.44
22	B	809	CLA	C1C-C2C	2.08	1.48	1.44
22	L	202	CLA	C1C-C2C	2.08	1.48	1.44
24	3	307	BCR	C38-C26	2.08	1.54	1.50
22	4	805	CLA	MG-NC	2.08	2.11	2.06
24	3	304	BCR	C37-C22	2.08	1.55	1.50
24	B	845	BCR	C37-C22	2.08	1.55	1.50
22	9	309	CLA	C1A-CHA	2.08	1.51	1.43
22	A	815	CLA	C1C-C2C	2.08	1.48	1.44
22	7	307	CLA	C3D-C4D	-2.08	1.39	1.44
22	5	320	CLA	C1A-CHA	2.08	1.51	1.43
22	B	818	CLA	C1C-C2C	2.08	1.48	1.44
24	3	304	BCR	C38-C26	2.08	1.54	1.50
22	A	839	CLA	C1C-C2C	2.08	1.48	1.44
22	B	819	CLA	C1C-C2C	2.08	1.48	1.44
22	7	309	CLA	C1C-C2C	2.08	1.48	1.44
24	G	203	BCR	C38-C26	2.08	1.54	1.50
22	6	309	CLA	C1A-CHA	2.08	1.51	1.43
22	4	807	CLA	C1C-C2C	2.08	1.48	1.44
22	A	827	CLA	C1C-C2C	2.08	1.48	1.44
22	3	310	CLA	C1C-C2C	2.08	1.48	1.44
22	B	840	CLA	C1C-C2C	2.08	1.48	1.44
38	1	303	LUT	C30-C29	-2.08	1.33	1.35
24	J	104	BCR	C38-C26	2.07	1.54	1.50
24	A	848	BCR	C37-C22	2.07	1.55	1.50
22	6	307	CLA	C1C-C2C	2.07	1.48	1.44
22	F	304	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	C1C-C2C	2.07	1.48	1.44
22	1	314	CLA	C1C-C2C	2.07	1.48	1.44
24	A	846	BCR	C37-C22	2.07	1.55	1.50
22	1	310	CLA	C1C-C2C	2.07	1.48	1.44
22	4	812	CLA	C1C-C2C	2.07	1.48	1.44
22	6	302	CLA	C1C-C2C	2.07	1.48	1.44
22	9	313	CLA	C1C-C2C	2.07	1.48	1.44
39	Z	312	CHL	C1B-NB	-2.07	1.35	1.37
22	5	312	CLA	C1C-C2C	2.07	1.48	1.44
22	9	304	CLA	C3D-C4D	-2.07	1.39	1.44
22	9	310	CLA	C1A-CHA	2.07	1.51	1.43
22	A	832	CLA	C1C-C2C	2.07	1.48	1.44
22	3	312	CLA	C1C-C2C	2.07	1.48	1.44
22	5	307	CLA	C1C-C2C	2.07	1.48	1.44
24	J	104	BCR	C37-C22	2.07	1.55	1.50
22	K	205	CLA	C1D-ND	-2.07	1.35	1.37
22	3	310	CLA	C1A-CHA	2.07	1.51	1.43
22	A	838	CLA	C1C-C2C	2.06	1.48	1.44
22	K	203	CLA	C1C-C2C	2.06	1.48	1.44
22	6	308	CLA	C1C-C2C	2.06	1.48	1.44
22	7	308	CLA	C3D-C4D	-2.06	1.39	1.44
22	B	812	CLA	C1C-C2C	2.06	1.48	1.44
22	4	809	CLA	C1C-C2C	2.06	1.48	1.44
22	5	319	CLA	C1C-C2C	2.06	1.48	1.44
22	6	301	CLA	C1C-C2C	2.06	1.48	1.44
24	3	307	BCR	C37-C22	2.06	1.55	1.50
22	A	816	CLA	C1C-C2C	2.06	1.48	1.44
22	7	323	CLA	C1C-C2C	2.06	1.48	1.44
22	8	309	CLA	C3D-C4D	-2.06	1.39	1.44
22	A	854	CLA	C1C-C2C	2.06	1.48	1.44
22	5	323	CLA	C1C-C2C	2.06	1.48	1.44
22	A	802	CLA	C1C-C2C	2.06	1.48	1.44
38	5	303	LUT	C34-C33	-2.06	1.33	1.35
39	5	321	CHL	C1B-NB	-2.06	1.35	1.37
22	8	307	CLA	C1A-CHA	2.06	1.51	1.43
35	J	102	T7X	O16-C10	2.06	1.40	1.34
24	7	303	BCR	C37-C22	2.06	1.55	1.50
22	A	804	CLA	C1C-C2C	2.06	1.48	1.44
22	5	301	CLA	C1C-C2C	2.06	1.48	1.44
22	7	312	CLA	C1C-C2C	2.06	1.48	1.44
24	B	849	BCR	C38-C26	2.06	1.54	1.50
24	B	846	BCR	C37-C22	2.06	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	302	CLA	C1C-C2C	2.06	1.48	1.44
22	5	308	CLA	C1C-C2C	2.06	1.48	1.44
24	A	845	BCR	C38-C26	2.05	1.54	1.50
22	9	310	CLA	C3D-C4D	-2.05	1.39	1.44
22	A	828	CLA	C1C-C2C	2.05	1.48	1.44
24	6	306	BCR	C37-C22	2.05	1.55	1.50
22	9	305	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	848	BCR	C37-C22	2.05	1.55	1.50
24	I	4001	BCR	C37-C22	2.05	1.55	1.50
24	B	847	BCR	C37-C22	2.05	1.55	1.50
22	7	315	CLA	C1A-CHA	2.05	1.51	1.43
22	B	842	CLA	C1C-C2C	2.05	1.48	1.44
22	A	822	CLA	C1C-C2C	2.05	1.48	1.44
22	A	840	CLA	C1C-C2C	2.05	1.48	1.44
22	5	308	CLA	C3D-C4D	-2.05	1.39	1.44
22	8	313	CLA	C1C-C2C	2.05	1.48	1.44
22	3	309	CLA	C1C-C2C	2.05	1.48	1.44
38	1	303	LUT	C34-C33	-2.05	1.33	1.35
22	A	842	CLA	C1C-C2C	2.05	1.48	1.44
24	5	305	BCR	C37-C22	2.05	1.55	1.50
22	B	831	CLA	C3D-C4D	-2.04	1.39	1.44
24	A	856	BCR	C38-C26	2.04	1.54	1.50
22	4	807	CLA	C1A-CHA	2.04	1.51	1.43
24	L	204	BCR	C37-C22	2.04	1.55	1.50
22	K	204	CLA	C1C-C2C	2.04	1.48	1.44
38	5	303	LUT	C30-C29	-2.04	1.33	1.35
22	4	805	CLA	CHD-C1D	2.04	1.42	1.38
22	5	309	CLA	C1A-CHA	2.04	1.51	1.43
22	4	818	CLA	C1C-C2C	2.04	1.48	1.44
38	Z	301	LUT	C28-C27	2.04	1.37	1.32
22	B	834	CLA	C1C-C2C	2.04	1.48	1.44
39	8	301	CHL	C1B-NB	-2.04	1.35	1.37
22	1	308	CLA	C3D-C4D	-2.04	1.39	1.44
22	9	307	CLA	C3D-C4D	-2.04	1.39	1.44
22	2	301	CLA	C3D-C4D	-2.04	1.39	1.44
22	4	810	CLA	C1C-C2C	2.04	1.48	1.44
22	5	318	CLA	C1C-C2C	2.04	1.48	1.44
39	4	813	CHL	C1B-NB	-2.04	1.35	1.37
22	A	823	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	836	CLA	C3D-C4D	-2.03	1.39	1.44
22	1	311	CLA	C1A-CHA	2.03	1.51	1.43
22	Z	306	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	308	CLA	C3D-C4D	-2.03	1.39	1.44
22	6	314	CLA	C1C-C2C	2.03	1.48	1.44
24	F	303	BCR	C38-C26	2.03	1.54	1.50
38	8	303	LUT	C34-C33	-2.03	1.33	1.35
22	1	309	CLA	C3D-C4D	-2.03	1.39	1.44
22	A	816	CLA	C1A-CHA	2.03	1.51	1.43
38	6	304	LUT	C34-C33	-2.03	1.33	1.35
39	6	318	CHL	C1B-NB	-2.03	1.35	1.37
22	A	821	CLA	C1C-C2C	2.03	1.48	1.44
21	A	801	CL0	C4C-C3C	2.03	1.48	1.45
22	4	809	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	814	CLA	C3D-C4D	-2.03	1.39	1.44
22	B	839	CLA	C3D-C4D	-2.03	1.39	1.44
22	6	309	CLA	C1C-C2C	2.03	1.48	1.44
22	4	806	CLA	C3D-C4D	-2.03	1.39	1.44
22	1	316	CLA	C1A-CHA	2.02	1.51	1.43
22	B	809	CLA	C3D-C4D	-2.02	1.39	1.44
22	Z	305	CLA	C1C-C2C	2.02	1.48	1.44
38	Z	302	LUT	C30-C29	-2.02	1.33	1.35
22	A	811	CLA	C3D-C4D	-2.02	1.39	1.44
22	3	309	CLA	C3D-C4D	-2.02	1.39	1.44
22	B	818	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	817	CLA	C1C-C2C	2.02	1.48	1.44
24	7	303	BCR	C38-C26	2.02	1.54	1.50
38	1	302	LUT	C28-C27	2.02	1.37	1.32
22	B	835	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	818	CLA	C3D-C4D	-2.02	1.39	1.44
22	A	842	CLA	C3D-C4D	-2.02	1.39	1.44
22	1	310	CLA	C1A-CHA	2.02	1.51	1.43
22	F	305	CLA	C3D-C4D	-2.01	1.39	1.44
22	1	307	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	822	CLA	C1A-CHA	2.01	1.51	1.43
39	7	313	CHL	C1B-NB	-2.01	1.35	1.37
24	8	304	BCR	C37-C22	2.01	1.55	1.50
38	3	303	LUT	C34-C33	-2.01	1.33	1.35
38	8	302	LUT	C34-C33	-2.01	1.33	1.35
22	6	312	CLA	C1A-CHA	2.01	1.51	1.43
22	3	312	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	839	CLA	C1C-C2C	2.01	1.48	1.44
22	5	311	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	839	CLA	C3D-C4D	-2.01	1.39	1.44
22	5	307	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	306	CLA	C1A-CHA	2.01	1.51	1.43
22	6	310	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	805	CLA	C3D-C4D	-2.01	1.39	1.44
22	3	322	CLA	C3D-C4D	-2.01	1.39	1.44
24	3	305	BCR	C38-C26	2.01	1.54	1.50
31	B	852	DGD	CDA-CCA	-2.01	1.33	1.49
22	A	840	CLA	C3D-C4D	-2.01	1.39	1.44
22	8	316	CLA	C3D-C4D	-2.01	1.39	1.44
22	5	320	CLA	C3D-C4D	-2.01	1.39	1.44
22	9	308	CLA	C1C-C2C	2.01	1.48	1.44
22	A	812	CLA	C3D-C4D	-2.01	1.39	1.44
22	1	305	CLA	C1C-C2C	2.01	1.48	1.44
22	6	307	CLA	C3D-C4D	-2.01	1.39	1.44
22	A	817	CLA	C3D-C4D	-2.01	1.39	1.44
22	B	823	CLA	C3D-C4D	-2.01	1.39	1.44
22	F	302	CLA	C3D-C4D	-2.01	1.39	1.44
42	7	321	SPH	C3-C4	2.00	1.53	1.50
24	A	856	BCR	C37-C22	2.00	1.55	1.50
22	4	808	CLA	C3D-C4D	-2.00	1.39	1.44
24	4	804	BCR	C38-C26	2.00	1.54	1.50
22	6	301	CLA	C3D-C4D	-2.00	1.39	1.44
24	A	844	BCR	C37-C22	2.00	1.55	1.50
22	A	805	CLA	C1C-C2C	2.00	1.48	1.44
22	A	810	CLA	C3D-C4D	-2.00	1.39	1.44

All (5260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	848	BCR	C37-C22-C21	-29.76	81.23	122.92
24	B	848	BCR	C23-C22-C21	28.06	162.01	118.94
24	B	848	BCR	C37-C22-C23	-23.62	80.87	118.08
24	3	304	BCR	C11-C10-C9	-11.56	110.82	127.31
22	K	205	CLA	C4A-NA-C1A	11.24	111.76	106.71
22	9	309	CLA	C4A-NA-C1A	10.90	111.61	106.71
22	9	305	CLA	C4A-NA-C1A	10.78	111.55	106.71
24	A	844	BCR	C15-C14-C13	-10.68	112.06	127.31
22	1	311	CLA	C4A-NA-C1A	10.16	111.27	106.71
22	3	320	CLA	C4A-NA-C1A	9.77	111.10	106.71
22	9	310	CLA	C4A-NA-C1A	9.65	111.05	106.71
24	3	307	BCR	C20-C21-C22	-9.52	113.73	127.31
22	8	307	CLA	C4A-NA-C1A	9.46	110.96	106.71
22	5	320	CLA	C4A-NA-C1A	9.44	110.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	822	CLA	C4A-NA-C1A	9.39	110.93	106.71
22	1	316	CLA	C4A-NA-C1A	9.38	110.92	106.71
22	3	315	CLA	C4A-NA-C1A	9.35	110.91	106.71
22	5	323	CLA	C4A-NA-C1A	9.31	110.89	106.71
24	3	307	BCR	C15-C14-C13	-9.30	114.04	127.31
22	6	307	CLA	C4A-NA-C1A	9.29	110.88	106.71
22	7	306	CLA	C4A-NA-C1A	9.18	110.83	106.71
22	4	807	CLA	C4A-NA-C1A	9.17	110.83	106.71
22	B	815	CLA	C4A-NA-C1A	9.16	110.82	106.71
22	9	304	CLA	C4A-NA-C1A	9.16	110.82	106.71
22	A	813	CLA	C4A-NA-C1A	9.12	110.81	106.71
22	3	313	CLA	C4A-NA-C1A	9.12	110.81	106.71
22	A	818	CLA	C4A-NA-C1A	9.07	110.78	106.71
22	A	816	CLA	C4A-NA-C1A	9.07	110.78	106.71
24	A	844	BCR	C7-C8-C9	-9.06	112.55	126.23
22	A	838	CLA	C4A-NA-C1A	9.05	110.77	106.71
22	1	309	CLA	C4A-NA-C1A	9.04	110.77	106.71
22	L	201	CLA	C4A-NA-C1A	9.02	110.76	106.71
22	7	310	CLA	C4A-NA-C1A	9.01	110.75	106.71
22	6	317	CLA	C4A-NA-C1A	8.99	110.75	106.71
22	A	808	CLA	C4A-NA-C1A	8.98	110.75	106.71
22	B	810	CLA	C4A-NA-C1A	8.98	110.74	106.71
22	B	827	CLA	C4A-NA-C1A	8.97	110.74	106.71
22	A	815	CLA	C4A-NA-C1A	8.96	110.73	106.71
22	A	826	CLA	C4A-NA-C1A	8.95	110.73	106.71
22	K	202	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	4	815	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	Z	305	CLA	C4A-NA-C1A	8.93	110.72	106.71
22	B	805	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	A	832	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	8	305	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	A	827	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	7	314	CLA	C4A-NA-C1A	8.88	110.70	106.71
22	5	326	CLA	C4A-NA-C1A	8.87	110.70	106.71
22	5	309	CLA	C4A-NA-C1A	8.87	110.69	106.71
22	B	817	CLA	C4A-NA-C1A	8.86	110.69	106.71
22	7	309	CLA	C4A-NA-C1A	8.85	110.69	106.71
22	5	313	CLA	C4A-NA-C1A	8.85	110.68	106.71
22	B	841	CLA	C4A-NA-C1A	8.84	110.68	106.71
22	5	318	CLA	C4A-NA-C1A	8.82	110.67	106.71
22	A	817	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	B	833	CLA	C4A-NA-C1A	8.80	110.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	834	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	A	839	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	Z	314	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	7	304	CLA	C4A-NA-C1A	8.80	110.66	106.71
22	7	315	CLA	C4A-NA-C1A	8.79	110.66	106.71
22	4	810	CLA	C4A-NA-C1A	8.79	110.66	106.71
22	A	842	CLA	C4A-NA-C1A	8.78	110.65	106.71
22	B	837	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	B	811	CLA	C4A-NA-C1A	8.77	110.65	106.71
22	7	311	CLA	C4A-NA-C1A	8.76	110.65	106.71
22	Z	313	CLA	C4A-NA-C1A	8.76	110.64	106.71
22	6	308	CLA	C4A-NA-C1A	8.76	110.64	106.71
22	8	313	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	6	313	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	A	807	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	A	812	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	3	310	CLA	C4A-NA-C1A	8.75	110.64	106.71
22	3	314	CLA	C4A-NA-C1A	8.74	110.64	106.71
22	1	304	CLA	C4A-NA-C1A	8.74	110.64	106.71
22	L	203	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	Z	303	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	6	322	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	6	309	CLA	C4A-NA-C1A	8.73	110.63	106.71
24	B	844	BCR	C11-C10-C9	-8.72	114.86	127.31
22	B	813	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	1	313	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	5	314	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	A	833	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	2	304	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	8	308	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	5	312	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	A	836	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	4	811	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	A	831	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	A	840	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	B	819	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	K	203	CLA	C4A-NA-C1A	8.70	110.62	106.71
22	Z	308	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	1	310	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	A	825	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	G	201	CLA	C4A-NA-C1A	8.68	110.61	106.71
22	A	828	CLA	C4A-NA-C1A	8.68	110.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	311	CLA	C4A-NA-C1A	8.68	110.61	106.71
22	F	304	CLA	C4A-NA-C1A	8.67	110.61	106.71
22	1	314	CLA	C4A-NA-C1A	8.67	110.61	106.71
22	G	202	CLA	C4A-NA-C1A	8.67	110.60	106.71
22	7	324	CLA	C4A-NA-C1A	8.67	110.60	106.71
22	3	318	CLA	C4A-NA-C1A	8.67	110.60	106.71
22	B	830	CLA	C4A-NA-C1A	8.66	110.60	106.71
22	6	321	CLA	C4A-NA-C1A	8.66	110.60	106.71
22	A	805	CLA	C4A-NA-C1A	8.65	110.60	106.71
22	3	308	CLA	C4A-NA-C1A	8.65	110.60	106.71
22	B	826	CLA	C4A-NA-C1A	8.65	110.60	106.71
22	3	311	CLA	C4A-NA-C1A	8.65	110.60	106.71
22	F	302	CLA	C4A-NA-C1A	8.65	110.59	106.71
22	A	804	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	B	842	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	8	316	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	B	838	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	5	310	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	5	315	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	A	837	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	1	307	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	6	312	CLA	C4A-NA-C1A	8.64	110.59	106.71
22	B	818	CLA	C4A-NA-C1A	8.63	110.59	106.71
22	1	315	CLA	C4A-NA-C1A	8.63	110.59	106.71
22	3	319	CLA	C4A-NA-C1A	8.63	110.58	106.71
22	A	814	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	6	301	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	B	839	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	7	316	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	5	322	CLA	C4A-NA-C1A	8.62	110.58	106.71
22	5	311	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	4	812	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	B	820	CLA	C4A-NA-C1A	8.61	110.58	106.71
22	B	832	CLA	C4A-NA-C1A	8.60	110.57	106.71
22	A	830	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	4	818	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	5	307	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	B	808	CLA	C4A-NA-C1A	8.59	110.57	106.71
22	4	808	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	A	841	CLA	C4A-NA-C1A	8.58	110.56	106.71
22	2	302	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	6	319	CLA	C4A-NA-C1A	8.57	110.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	306	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	Z	315	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	A	802	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	A	810	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	B	806	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	L	202	CLA	C4A-NA-C1A	8.57	110.56	106.71
22	B	829	CLA	C4A-NA-C1A	8.56	110.55	106.71
22	A	821	CLA	C4A-NA-C1A	8.56	110.55	106.71
22	Z	309	CLA	C4A-NA-C1A	8.56	110.55	106.71
22	5	319	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	9	313	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	9	306	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	1	305	CLA	C4A-NA-C1A	8.55	110.55	106.71
22	F	301	CLA	C4A-NA-C1A	8.54	110.54	106.71
22	9	311	CLA	C4A-NA-C1A	8.54	110.54	106.71
22	B	807	CLA	C4A-NA-C1A	8.53	110.54	106.71
22	A	824	CLA	C4A-NA-C1A	8.53	110.54	106.71
22	B	840	CLA	C4A-NA-C1A	8.52	110.54	106.71
22	K	204	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	Z	304	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	A	803	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	A	854	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	B	831	CLA	C4A-NA-C1A	8.51	110.53	106.71
22	7	323	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	5	308	CLA	C4A-NA-C1A	8.50	110.53	106.71
22	A	823	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	4	817	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	B	835	CLA	C4A-NA-C1A	8.49	110.52	106.71
22	B	836	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	5	301	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	2	301	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	B	814	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	3	309	CLA	C4A-NA-C1A	8.48	110.52	106.71
22	6	302	CLA	C4A-NA-C1A	8.47	110.51	106.71
22	B	824	CLA	C4A-NA-C1A	8.47	110.51	106.71
22	B	823	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	7	322	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	8	309	CLA	C4A-NA-C1A	8.44	110.50	106.71
22	Z	310	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	J	103	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	A	819	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	4	806	CLA	C4A-NA-C1A	8.43	110.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	314	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	9	308	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	7	312	CLA	C4A-NA-C1A	8.43	110.49	106.71
22	A	820	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	A	834	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	F	305	CLA	C4A-NA-C1A	8.41	110.49	106.71
22	B	801	CLA	C4A-NA-C1A	8.40	110.48	106.71
22	8	310	CLA	C4A-NA-C1A	8.39	110.48	106.71
22	A	829	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	B	816	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	Z	316	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	7	305	CLA	C4A-NA-C1A	8.38	110.47	106.71
22	B	821	CLA	C4A-NA-C1A	8.37	110.47	106.71
22	7	308	CLA	C4A-NA-C1A	8.37	110.47	106.71
22	3	316	CLA	C4A-NA-C1A	8.37	110.47	106.71
22	B	812	CLA	C4A-NA-C1A	8.36	110.46	106.71
22	A	811	CLA	C4A-NA-C1A	8.35	110.46	106.71
22	A	835	CLA	C4A-NA-C1A	8.33	110.45	106.71
22	B	822	CLA	C4A-NA-C1A	8.33	110.45	106.71
22	8	306	CLA	C4A-NA-C1A	8.30	110.44	106.71
22	1	306	CLA	C4A-NA-C1A	8.29	110.43	106.71
22	A	855	CLA	C4A-NA-C1A	8.29	110.43	106.71
24	5	305	BCR	C20-C21-C22	-8.28	115.49	127.31
22	6	310	CLA	C4A-NA-C1A	8.27	110.42	106.71
22	7	307	CLA	C4A-NA-C1A	8.27	110.42	106.71
22	7	317	CLA	C4A-NA-C1A	8.27	110.42	106.71
22	B	825	CLA	C4A-NA-C1A	8.25	110.42	106.71
22	6	314	CLA	C4A-NA-C1A	8.25	110.42	106.71
22	3	322	CLA	C4A-NA-C1A	8.24	110.41	106.71
22	B	828	CLA	C4A-NA-C1A	8.23	110.41	106.71
22	4	809	CLA	C4A-NA-C1A	8.22	110.40	106.71
22	Z	307	CLA	C4A-NA-C1A	8.20	110.39	106.71
22	A	806	CLA	C4A-NA-C1A	8.19	110.39	106.71
22	6	311	CLA	C4A-NA-C1A	8.19	110.39	106.71
22	9	307	CLA	C4A-NA-C1A	8.19	110.39	106.71
24	6	306	BCR	C24-C23-C22	-8.19	113.87	126.23
24	B	848	BCR	C20-C21-C22	-8.17	115.65	127.31
22	3	312	CLA	C4A-NA-C1A	8.17	110.38	106.71
22	B	809	CLA	C4A-NA-C1A	8.12	110.36	106.71
22	1	308	CLA	C4A-NA-C1A	8.10	110.35	106.71
24	3	304	BCR	C7-C8-C9	-8.03	114.10	126.23
22	9	303	CLA	C4A-NA-C1A	8.02	110.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	809	CLA	C4A-NA-C1A	8.01	110.31	106.71
21	A	801	CL0	CMD-C2D-C1D	7.95	138.73	124.71
22	4	805	CLA	C4A-NA-C1A	7.80	110.21	106.71
24	6	306	BCR	C16-C17-C18	-7.58	116.49	127.31
24	3	307	BCR	C24-C23-C22	-7.48	114.93	126.23
24	6	306	BCR	C11-C10-C9	-7.35	116.82	127.31
22	9	305	CLA	CAA-C2A-C3A	-7.25	92.94	112.78
24	5	305	BCR	C15-C14-C13	-7.24	116.98	127.31
24	B	847	BCR	C15-C14-C13	-7.16	117.09	127.31
24	I	4001	BCR	C16-C17-C18	-7.15	117.11	127.31
24	A	846	BCR	C15-C14-C13	-7.14	117.12	127.31
32	F	306	RRX	C11-C10-C9	-6.88	117.49	127.31
24	3	304	BCR	C15-C16-C17	-6.66	109.82	123.47
21	A	801	CL0	C4A-NA-C1A	6.60	109.67	106.71
24	5	305	BCR	C11-C10-C9	-6.40	118.18	127.31
36	5	306	C7Z	C11-C10-C9	-6.35	118.25	127.31
24	3	307	BCR	C11-C10-C9	-6.31	118.30	127.31
24	G	203	BCR	C20-C21-C22	-6.30	118.31	127.31
24	5	304	BCR	C20-C21-C22	-6.28	118.34	127.31
24	B	844	BCR	C20-C21-C22	-6.26	118.38	127.31
24	K	206	BCR	C11-C10-C9	-6.22	118.43	127.31
21	A	801	CL0	C2D-C1D-ND	6.19	114.67	110.10
22	1	308	CLA	CMD-C2D-C1D	6.07	135.42	124.71
21	A	801	CL0	C2C-C1C-NC	6.06	115.65	109.97
24	A	848	BCR	C20-C21-C22	-6.06	118.66	127.31
24	6	305	BCR	C20-C21-C22	-6.06	118.67	127.31
24	B	848	BCR	C33-C5-C6	-6.03	117.76	124.53
24	A	856	BCR	C20-C21-C22	-6.03	118.71	127.31
24	3	307	BCR	C38-C26-C25	-6.01	117.78	124.53
24	B	849	BCR	C20-C21-C22	-5.99	118.77	127.31
38	5	302	LUT	C35-C34-C33	-5.98	118.78	127.31
22	7	304	CLA	O2A-C1-C2	5.97	124.34	108.64
22	9	305	CLA	O2D-CGD-CBD	5.96	121.86	111.27
24	A	845	BCR	C16-C17-C18	-5.95	118.81	127.31
24	5	304	BCR	C16-C17-C18	-5.94	118.83	127.31
24	B	846	BCR	C15-C14-C13	-5.93	118.85	127.31
22	B	831	CLA	CMD-C2D-C1D	5.93	135.16	124.71
38	4	803	LUT	C35-C34-C33	-5.92	118.86	127.31
22	7	307	CLA	CMD-C2D-C1D	5.86	135.03	124.71
25	3	321	LHG	O7-C7-O9	-5.85	118.12	125.57
22	B	835	CLA	CMD-C2D-C1D	5.85	135.02	124.71
24	I	4001	BCR	C24-C23-C22	-5.84	117.41	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	305	BCR	C33-C5-C6	-5.84	117.97	124.53
38	6	303	LUT	C35-C34-C33	-5.83	118.99	127.31
24	B	845	BCR	C1-C6-C5	-5.83	114.41	122.61
24	F	303	BCR	C16-C17-C18	-5.80	119.04	127.31
22	9	303	CLA	O2A-C1-C2	5.78	123.81	108.64
22	5	307	CLA	CMD-C2D-C1D	5.77	134.89	124.71
22	A	818	CLA	CMD-C2D-C1D	5.77	134.88	124.71
22	6	322	CLA	O2D-CGD-CBD	5.77	121.51	111.27
22	2	301	CLA	CMD-C2D-C1D	5.76	134.86	124.71
22	B	838	CLA	CMD-C2D-C1D	5.73	134.82	124.71
36	5	306	C7Z	C15-C14-C13	-5.73	119.13	127.31
22	1	309	CLA	CMD-C2D-C1D	5.72	134.79	124.71
24	A	847	BCR	C38-C26-C25	-5.71	118.11	124.53
22	B	816	CLA	CMD-C2D-C1D	5.70	134.76	124.71
32	F	306	RRX	C12-C13-C14	5.70	127.69	118.94
22	7	315	CLA	O2D-CGD-CBD	5.69	121.39	111.27
22	B	824	CLA	CMD-C2D-C1D	5.69	134.74	124.71
22	5	323	CLA	CMD-C2D-C1D	5.68	134.73	124.71
22	A	825	CLA	CMD-C2D-C1D	5.68	134.73	124.71
22	A	811	CLA	CMD-C2D-C1D	5.68	134.72	124.71
22	F	304	CLA	CMD-C2D-C1D	5.67	134.70	124.71
22	Z	306	CLA	CMD-C2D-C1D	5.66	134.69	124.71
22	A	807	CLA	CMD-C2D-C1D	5.66	134.68	124.71
22	B	826	CLA	CMD-C2D-C1D	5.66	134.68	124.71
22	A	823	CLA	CMD-C2D-C1D	5.65	134.67	124.71
22	6	309	CLA	CMD-C2D-C1D	5.65	134.67	124.71
22	Z	307	CLA	CMD-C2D-C1D	5.65	134.67	124.71
22	K	204	CLA	O2A-C1-C2	5.64	122.16	108.97
22	A	805	CLA	CMD-C2D-C1D	5.64	134.65	124.71
24	J	104	BCR	C27-C26-C25	-5.64	114.55	122.73
38	Z	301	LUT	C11-C10-C9	-5.63	119.27	127.31
22	8	305	CLA	CMD-C2D-C1D	5.63	134.64	124.71
22	Z	303	CLA	CMD-C2D-C1D	5.63	134.64	124.71
22	1	307	CLA	CMD-C2D-C1D	5.63	134.63	124.71
38	1	302	LUT	C11-C10-C9	-5.62	119.29	127.31
22	A	810	CLA	CMD-C2D-C1D	5.62	134.61	124.71
22	4	818	CLA	O2A-C1-C2	5.61	123.38	108.64
22	9	306	CLA	CMD-C2D-C1D	5.61	134.59	124.71
22	B	832	CLA	CMD-C2D-C1D	5.61	134.59	124.71
22	1	315	CLA	CMD-C2D-C1D	5.61	134.59	124.71
22	5	310	CLA	CMD-C2D-C1D	5.61	134.59	124.71
38	4	802	LUT	C7-C8-C9	-5.61	117.77	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	F	306	RRX	C20-C21-C22	-5.60	119.31	127.31
22	1	305	CLA	CMD-C2D-C1D	5.60	134.59	124.71
24	5	304	BCR	C11-C10-C9	-5.60	119.32	127.31
22	B	840	CLA	CMD-C2D-C1D	5.59	134.57	124.71
22	1	313	CLA	CMD-C2D-C1D	5.59	134.57	124.71
22	A	827	CLA	CMD-C2D-C1D	5.59	134.57	124.71
22	3	322	CLA	CMD-C2D-C1D	5.59	134.56	124.71
22	B	814	CLA	CMD-C2D-C1D	5.59	134.56	124.71
22	B	828	CLA	CMD-C2D-C1D	5.59	134.56	124.71
22	8	309	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	A	812	CLA	CMD-C2D-C1D	5.58	134.55	124.71
22	A	832	CLA	CMD-C2D-C1D	5.58	134.55	124.71
24	A	847	BCR	C16-C17-C18	-5.58	119.35	127.31
22	4	812	CLA	CMD-C2D-C1D	5.58	134.54	124.71
22	4	809	CLA	CMD-C2D-C1D	5.58	134.54	124.71
22	B	818	CLA	CMD-C2D-C1D	5.57	134.54	124.71
22	A	809	CLA	CMD-C2D-C1D	5.57	134.54	124.71
22	A	839	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	5	301	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	3	313	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	F	305	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	3	308	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	A	819	CLA	CMD-C2D-C1D	5.57	134.53	124.71
22	5	309	CLA	CMD-C2D-C1D	5.57	134.52	124.71
22	5	308	CLA	CMD-C2D-C1D	5.56	134.52	124.71
22	6	322	CLA	CMD-C2D-C1D	5.56	134.52	124.71
22	6	310	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	3	309	CLA	CMD-C2D-C1D	5.56	134.51	124.71
22	Z	308	CLA	CMD-C2D-C1D	5.56	134.51	124.71
24	A	848	BCR	C7-C8-C9	-5.56	117.84	126.23
22	A	833	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	7	304	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	3	318	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	A	840	CLA	CMD-C2D-C1D	5.55	134.50	124.71
22	7	323	CLA	CMD-C2D-C1D	5.55	134.49	124.71
22	A	802	CLA	O2A-C1-C2	5.55	123.22	108.64
22	Z	315	CLA	CMD-C2D-C1D	5.55	134.49	124.71
22	B	815	CLA	CMD-C2D-C1D	5.55	134.49	124.71
22	G	201	CLA	CMD-C2D-C1D	5.54	134.49	124.71
22	7	324	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	A	822	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	A	837	CLA	CMD-C2D-C1D	5.54	134.48	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	842	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	B	813	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	Z	316	CLA	CMD-C2D-C1D	5.54	134.47	124.71
22	K	203	CLA	CMD-C2D-C1D	5.54	134.47	124.71
22	G	202	CLA	CMD-C2D-C1D	5.53	134.47	124.71
22	L	201	CLA	CMD-C2D-C1D	5.53	134.47	124.71
22	B	836	CLA	CMD-C2D-C1D	5.53	134.47	124.71
24	I	4001	BCR	C20-C21-C22	-5.53	119.41	127.31
22	5	309	CLA	O2A-C1-C2	5.53	123.17	108.64
22	7	309	CLA	CMD-C2D-C1D	5.53	134.46	124.71
22	7	305	CLA	CMD-C2D-C1D	5.53	134.46	124.71
24	A	846	BCR	C11-C10-C9	-5.53	119.42	127.31
22	B	829	CLA	CMD-C2D-C1D	5.53	134.46	124.71
22	B	810	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	B	819	CLA	CMD-C2D-C1D	5.53	134.45	124.71
22	B	835	CLA	O2D-CGD-CBD	5.53	121.09	111.27
22	5	326	CLA	CMD-C2D-C1D	5.52	134.44	124.71
22	B	808	CLA	CMD-C2D-C1D	5.52	134.44	124.71
24	B	849	BCR	C16-C17-C18	-5.52	119.44	127.31
22	4	810	CLA	CMD-C2D-C1D	5.52	134.44	124.71
22	8	308	CLA	CMD-C2D-C1D	5.52	134.44	124.71
22	A	831	CLA	CMD-C2D-C1D	5.52	134.43	124.71
22	2	302	CLA	CMD-C2D-C1D	5.51	134.43	124.71
22	3	316	CLA	CMD-C2D-C1D	5.51	134.43	124.71
22	7	308	CLA	CMD-C2D-C1D	5.51	134.43	124.71
22	A	838	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	6	312	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	B	825	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	B	817	CLA	O2D-CGD-CBD	5.51	121.05	111.27
22	B	833	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	7	314	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	A	841	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	A	834	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	6	307	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	A	802	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	K	204	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	B	823	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	F	301	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	4	817	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	B	827	CLA	CMD-C2D-C1D	5.50	134.41	124.71
22	A	836	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	3	319	CLA	CMD-C2D-C1D	5.50	134.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	311	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	3	312	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	B	834	CLA	CMD-C2D-C1D	5.50	134.40	124.71
22	8	307	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	F	302	CLA	CMD-C2D-C1D	5.49	134.40	124.71
24	A	845	BCR	C15-C14-C13	-5.49	119.47	127.31
22	4	818	CLA	CMD-C2D-C1D	5.49	134.40	124.71
22	7	312	CLA	CMD-C2D-C1D	5.49	134.39	124.71
22	A	815	CLA	CMD-C2D-C1D	5.49	134.39	124.71
22	A	817	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	B	811	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	A	821	CLA	CMD-C2D-C1D	5.49	134.38	124.71
22	A	813	CLA	CMD-C2D-C1D	5.48	134.38	124.71
22	A	855	CLA	CMD-C2D-C1D	5.48	134.38	124.71
22	2	302	CLA	O2D-CGD-CBD	5.48	121.01	111.27
22	9	308	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	B	809	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	8	310	CLA	CMD-C2D-C1D	5.48	134.37	124.71
22	B	821	CLA	CMD-C2D-C1D	5.47	134.36	124.71
22	7	323	CLA	O2D-CGD-CBD	5.47	121.00	111.27
38	7	301	LUT	C35-C34-C33	-5.47	119.50	127.31
22	L	203	CLA	CMD-C2D-C1D	5.47	134.35	124.71
22	6	301	CLA	CMD-C2D-C1D	5.47	134.35	124.71
38	7	302	LUT	C11-C10-C9	-5.47	119.51	127.31
24	I	4001	BCR	C30-C25-C26	-5.47	114.91	122.61
21	A	801	CL0	C1C-C2C-C3C	-5.47	101.21	106.96
22	6	311	CLA	CMD-C2D-C1D	5.47	134.35	124.71
22	B	806	CLA	CMD-C2D-C1D	5.46	134.34	124.71
22	4	808	CLA	CMD-C2D-C1D	5.46	134.34	124.71
22	A	816	CLA	CMD-C2D-C1D	5.46	134.34	124.71
22	5	312	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	6	319	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	8	310	CLA	O2A-C1-C2	5.46	122.97	108.64
22	7	311	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	J	103	CLA	CMD-C2D-C1D	5.46	134.33	124.71
22	9	311	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	7	316	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	K	202	CLA	CMD-C2D-C1D	5.45	134.32	124.71
22	6	319	CLA	O2D-CGD-CBD	5.45	120.95	111.27
24	6	305	BCR	C11-C10-C9	-5.44	119.54	127.31
22	A	803	CLA	CMD-C2D-C1D	5.44	134.30	124.71
22	1	306	CLA	CMD-C2D-C1D	5.44	134.30	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	322	CLA	CMD-C2D-C1D	5.44	134.30	124.71
22	4	806	CLA	CMD-C2D-C1D	5.43	134.29	124.71
22	B	826	CLA	O2D-CGD-CBD	5.43	120.92	111.27
22	B	820	CLA	CMD-C2D-C1D	5.43	134.28	124.71
22	A	828	CLA	CMD-C2D-C1D	5.43	134.28	124.71
22	3	314	CLA	O2A-C1-C2	5.43	122.90	108.64
22	5	319	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	3	310	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	B	839	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	4	807	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	7	317	CLA	CMD-C2D-C1D	5.42	134.27	124.71
32	F	306	RRX	C11-C12-C13	-5.41	111.21	126.42
22	8	316	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	A	826	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	A	814	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	6	314	CLA	CMD-C2D-C1D	5.41	134.25	124.71
24	B	847	BCR	C11-C10-C9	-5.41	119.59	127.31
22	4	805	CLA	CMD-C2D-C1D	5.41	134.25	124.71
22	A	842	CLA	CMD-C2D-C1D	5.41	134.25	124.71
24	G	203	BCR	C16-C17-C18	-5.41	119.59	127.31
22	A	830	CLA	CMD-C2D-C1D	5.41	134.25	124.71
24	A	856	BCR	C27-C26-C25	-5.41	114.88	122.73
22	6	308	CLA	CMD-C2D-C1D	5.41	134.24	124.71
22	1	304	CLA	CMD-C2D-C1D	5.40	134.24	124.71
22	A	820	CLA	CMD-C2D-C1D	5.40	134.24	124.71
22	B	812	CLA	CMD-C2D-C1D	5.40	134.23	124.71
22	A	808	CLA	CMD-C2D-C1D	5.40	134.23	124.71
22	6	321	CLA	CMD-C2D-C1D	5.39	134.22	124.71
22	8	313	CLA	CMD-C2D-C1D	5.39	134.22	124.71
24	3	306	BCR	C1-C6-C5	-5.39	115.02	122.61
22	A	824	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	1	310	CLA	CMD-C2D-C1D	5.39	134.20	124.71
22	L	202	CLA	CMD-C2D-C1D	5.38	134.20	124.71
24	3	307	BCR	C15-C16-C17	-5.38	112.45	123.47
22	5	318	CLA	CMD-C2D-C1D	5.38	134.20	124.71
24	A	847	BCR	C20-C21-C22	-5.38	119.63	127.31
22	Z	303	CLA	O2D-CGD-CBD	5.38	120.82	111.27
22	B	837	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	3	311	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	B	807	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	5	308	CLA	O2D-CGD-CBD	5.37	120.82	111.27
24	B	853	BCR	C1-C6-C5	-5.37	115.05	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	307	CLA	CMD-C2D-C1D	5.37	134.18	124.71
22	5	322	CLA	CMD-C2D-C1D	5.37	134.17	124.71
22	8	306	CLA	CMD-C2D-C1D	5.36	134.17	124.71
22	A	804	CLA	CMD-C2D-C1D	5.36	134.16	124.71
22	4	815	CLA	O2D-CGD-CBD	5.36	120.79	111.27
22	1	314	CLA	CMD-C2D-C1D	5.36	134.16	124.71
22	9	305	CLA	CMD-C2D-C1D	5.35	134.15	124.71
22	A	806	CLA	CMD-C2D-C1D	5.35	134.14	124.71
22	A	803	CLA	O2D-CGD-CBD	5.35	120.77	111.27
22	B	841	CLA	CMD-C2D-C1D	5.35	134.13	124.71
24	G	203	BCR	C33-C5-C6	-5.34	118.53	124.53
22	7	306	CLA	CMD-C2D-C1D	5.33	134.12	124.71
22	Z	307	CLA	O2D-CGD-CBD	5.33	120.75	111.27
22	A	854	CLA	CMD-C2D-C1D	5.33	134.11	124.71
24	K	206	BCR	C15-C14-C13	-5.33	119.70	127.31
38	9	302	LUT	C35-C34-C33	-5.33	119.71	127.31
22	4	811	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	7	323	CLA	O2A-C1-C2	5.32	122.61	108.64
22	7	324	CLA	O2A-C1-C2	5.32	122.61	108.64
22	B	805	CLA	CMD-C2D-C1D	5.32	134.08	124.71
24	B	846	BCR	C24-C23-C22	-5.31	118.20	126.23
22	B	801	CLA	CMD-C2D-C1D	5.31	134.07	124.71
22	A	804	CLA	O2D-CGD-CBD	5.31	120.69	111.27
24	5	304	BCR	C38-C26-C25	-5.30	118.57	124.53
22	B	822	CLA	CMD-C2D-C1D	5.30	134.05	124.71
22	5	313	CLA	O2A-C1-C2	5.30	122.56	108.64
22	A	816	CLA	O2D-CGD-CBD	5.29	120.67	111.27
22	Z	310	CLA	CMD-C2D-C1D	5.29	134.04	124.71
22	1	308	CLA	O2D-CGD-CBD	5.29	120.67	111.27
38	3	302	LUT	C35-C34-C33	-5.29	119.76	127.31
22	8	306	CLA	O2D-CGD-CBD	5.29	120.66	111.27
22	A	809	CLA	O2D-CGD-CBD	5.28	120.65	111.27
22	A	834	CLA	O2D-CGD-CBD	5.28	120.64	111.27
22	4	811	CLA	O2A-C1-C2	5.27	122.50	108.64
22	1	306	CLA	O2A-C1-C2	5.27	122.49	108.64
22	6	309	CLA	O2A-C1-C2	5.27	122.49	108.64
22	9	313	CLA	CMD-C2D-C1D	5.27	134.00	124.71
36	J	105	C7Z	C35-C34-C33	-5.27	119.79	127.31
38	8	303	LUT	C35-C34-C33	-5.27	119.79	127.31
22	Z	313	CLA	O2A-C1-C2	5.27	122.48	108.64
38	8	302	LUT	C35-C34-C33	-5.27	119.79	127.31
36	J	105	C7Z	C27-C28-C29	-5.26	118.28	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	306	CLA	O2A-C1-C2	5.25	122.44	108.64
22	A	818	CLA	O2A-C1-C2	5.25	122.44	108.64
22	A	833	CLA	O2D-CGD-CBD	5.25	120.60	111.27
22	6	308	CLA	O2D-CGD-CBD	5.25	120.59	111.27
22	B	831	CLA	O2D-CGD-CBD	5.24	120.58	111.27
22	5	313	CLA	CMD-C2D-C1D	5.24	133.95	124.71
22	B	820	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	A	856	BCR	C16-C17-C18	-5.24	119.83	127.31
22	9	308	CLA	O2D-CGD-CBD	5.23	120.56	111.27
22	A	835	CLA	CMD-C2D-C1D	5.23	133.93	124.71
22	9	303	CLA	CMD-C2D-C1D	5.23	133.93	124.71
24	6	305	BCR	C7-C8-C9	-5.23	118.34	126.23
22	B	810	CLA	O2D-CGD-CBD	5.22	120.55	111.27
22	1	311	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	A	829	CLA	CMD-C2D-C1D	5.22	133.91	124.71
22	A	814	CLA	O2A-C1-C2	5.22	122.35	108.64
22	1	313	CLA	O2A-C1-C2	5.22	122.35	108.64
22	Z	313	CLA	O2D-CGD-CBD	5.22	120.54	111.27
22	8	314	CLA	CMD-C2D-C1D	5.20	133.89	124.71
22	9	313	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	7	307	CLA	O2D-CGD-CBD	5.20	120.51	111.27
38	7	302	LUT	C15-C14-C13	-5.20	119.89	127.31
24	A	847	BCR	C24-C23-C22	-5.20	118.38	126.23
22	5	314	CLA	CMD-C2D-C1D	5.19	133.87	124.71
22	7	305	CLA	O2D-CGD-CBD	5.19	120.50	111.27
22	B	834	CLA	O2D-CGD-CBD	5.19	120.49	111.27
22	B	811	CLA	O2D-CGD-CBD	5.19	120.49	111.27
24	3	306	BCR	C15-C14-C13	-5.19	119.91	127.31
22	5	319	CLA	O2A-C1-C2	5.18	122.26	108.64
22	B	837	CLA	O2D-CGD-CBD	5.18	120.48	111.27
24	7	303	BCR	C11-C10-C9	-5.18	119.91	127.31
22	B	814	CLA	O2D-CGD-CBD	5.18	120.47	111.27
22	7	310	CLA	CMD-C2D-C1D	5.18	133.84	124.71
22	6	314	CLA	O2D-CGD-CBD	5.18	120.47	111.27
21	A	801	CL0	O2D-CGD-CBD	5.18	120.47	111.27
22	5	311	CLA	O2D-CGD-CBD	5.17	120.46	111.27
22	5	301	CLA	O2A-C1-C2	5.17	122.23	108.64
24	B	853	BCR	C7-C8-C9	-5.17	118.42	126.23
24	7	303	BCR	C38-C26-C25	-5.17	118.72	124.53
22	A	841	CLA	O2A-C1-C2	5.17	122.22	108.64
22	3	308	CLA	O2D-CGD-CBD	5.17	120.45	111.27
38	3	303	LUT	C7-C8-C9	-5.16	118.43	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	314	CLA	CMD-C2D-C1D	5.16	133.81	124.71
22	B	839	CLA	O2D-CGD-CBD	5.16	120.44	111.27
22	B	813	CLA	O2A-C1-C2	5.16	122.20	108.64
22	8	305	CLA	O2D-CGD-CBD	5.16	120.44	111.27
22	B	817	CLA	CMD-C2D-C1D	5.16	133.81	124.71
22	B	830	CLA	CMD-C2D-C1D	5.16	133.81	124.71
22	3	320	CLA	CMD-C2D-C1D	5.16	133.80	124.71
22	4	818	CLA	O2D-CGD-CBD	5.15	120.43	111.27
22	A	838	CLA	O2D-CGD-CBD	5.15	120.42	111.27
25	B	851	LHG	O7-C7-O9	-5.15	119.01	125.57
22	6	302	CLA	CMD-C2D-C1D	5.15	133.79	124.71
22	Z	314	CLA	CMD-C2D-C1D	5.15	133.79	124.71
22	3	316	CLA	O2D-CGD-CBD	5.15	120.42	111.27
22	A	813	CLA	O2D-CGD-CBD	5.15	120.41	111.27
22	B	827	CLA	O2D-CGD-CBD	5.15	120.41	111.27
22	B	819	CLA	O2D-CGD-CBD	5.14	120.41	111.27
22	2	304	CLA	CMD-C2D-C1D	5.14	133.78	124.71
22	5	326	CLA	O2D-CGD-CBD	5.14	120.41	111.27
22	6	301	CLA	O2D-CGD-CBD	5.14	120.40	111.27
38	1	302	LUT	C7-C8-C9	-5.14	118.47	126.23
24	7	303	BCR	C1-C6-C5	-5.14	115.38	122.61
38	1	302	LUT	C1-C6-C5	-5.14	115.38	122.61
22	K	202	CLA	O2D-CGD-CBD	5.13	120.39	111.27
21	A	801	CL0	CHD-C1D-ND	-5.13	119.74	124.45
22	B	822	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	5	315	CLA	CMD-C2D-C1D	5.13	133.75	124.71
22	Z	305	CLA	O2D-CGD-CBD	5.13	120.38	111.27
22	B	829	CLA	O2A-C1-C2	5.12	122.10	108.64
22	8	311	CLA	CMD-C2D-C1D	5.12	133.74	124.71
22	A	810	CLA	O2A-C1-C2	5.12	122.10	108.64
22	F	301	CLA	O2D-CGD-CBD	5.12	120.36	111.27
22	5	310	CLA	O2D-CGD-CBD	5.12	120.36	111.27
22	1	313	CLA	O2D-CGD-CBD	5.12	120.36	111.27
22	B	815	CLA	O2D-CGD-CBD	5.11	120.36	111.27
24	B	845	BCR	C27-C26-C25	-5.11	115.31	122.73
22	G	201	CLA	O2D-CGD-CBD	5.11	120.35	111.27
36	J	105	C7Z	C31-C30-C29	-5.11	120.01	127.31
22	A	839	CLA	O2D-CGD-CBD	5.11	120.35	111.27
22	A	817	CLA	O2A-C1-C2	5.11	122.06	108.64
22	6	317	CLA	CMD-C2D-C1D	5.11	133.71	124.71
36	5	306	C7Z	C35-C34-C33	-5.11	120.02	127.31
32	F	306	RRX	C33-C5-C6	-5.10	118.80	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	312	CLA	O2D-CGD-CBD	5.10	120.33	111.27
22	A	837	CLA	O2D-CGD-CBD	5.10	120.33	111.27
22	8	313	CLA	O2D-CGD-CBD	5.10	120.33	111.27
24	B	848	BCR	C7-C8-C9	-5.10	118.54	126.23
22	9	306	CLA	O2D-CGD-CBD	5.09	120.32	111.27
22	B	840	CLA	O2D-CGD-CBD	5.09	120.31	111.27
22	B	841	CLA	O2D-CGD-CBD	5.09	120.31	111.27
24	7	303	BCR	C4-C5-C6	-5.09	115.34	122.73
22	7	307	CLA	O2A-C1-C2	5.09	122.00	108.64
22	B	824	CLA	O2D-CGD-CBD	5.09	120.30	111.27
22	B	828	CLA	O2D-CGD-CBD	5.09	120.30	111.27
22	B	832	CLA	O2D-CGD-CBD	5.08	120.30	111.27
24	F	303	BCR	C20-C21-C22	-5.08	120.06	127.31
22	A	808	CLA	O2D-CGD-CBD	5.08	120.30	111.27
22	4	812	CLA	O2D-CGD-CBD	5.08	120.30	111.27
22	7	315	CLA	CMD-C2D-C1D	5.08	133.67	124.71
22	A	841	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	3	318	CLA	O2D-CGD-CBD	5.08	120.29	111.27
22	4	817	CLA	O2D-CGD-CBD	5.08	120.29	111.27
38	3	303	LUT	C15-C14-C13	-5.07	120.07	127.31
22	Z	309	CLA	CMD-C2D-C1D	5.07	133.65	124.71
22	A	818	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	4	808	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	4	815	CLA	CMD-C2D-C1D	5.07	133.65	124.71
22	7	316	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	A	819	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	A	831	CLA	O2D-CGD-CBD	5.07	120.27	111.27
22	A	802	CLA	O2D-CGD-CBD	5.06	120.27	111.27
22	A	814	CLA	O2D-CGD-CBD	5.06	120.27	111.27
22	8	307	CLA	O2D-CGD-CBD	5.06	120.27	111.27
22	5	322	CLA	O2A-C1-C2	5.06	121.94	108.64
22	6	319	CLA	O2A-C1-C2	5.06	121.94	108.64
22	7	304	CLA	O2D-CGD-CBD	5.06	120.26	111.27
22	B	805	CLA	O2D-CGD-CBD	5.06	120.25	111.27
22	G	202	CLA	O2D-CGD-CBD	5.06	120.25	111.27
22	1	305	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	4	806	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	6	317	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	B	818	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	B	808	CLA	O2D-CGD-CBD	5.05	120.25	111.27
21	A	801	CL0	C3D-C2D-C1D	-5.05	98.94	105.83
22	7	314	CLA	O2D-CGD-CBD	5.05	120.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	838	CLA	O2A-C1-C2	5.05	121.90	108.64
22	3	319	CLA	O2D-CGD-CBD	5.05	120.24	111.27
22	B	806	CLA	O2D-CGD-CBD	5.05	120.24	111.27
24	5	305	BCR	C1-C6-C5	-5.05	115.50	122.61
24	6	305	BCR	C16-C17-C18	-5.05	120.11	127.31
21	A	801	CL0	O2A-CGA-O1A	-5.04	110.86	123.59
34	F	308	LMG	O7-C10-C11	5.04	122.36	111.50
22	B	841	CLA	O2A-C1-C2	5.04	121.88	108.64
22	6	310	CLA	O2D-CGD-CBD	5.04	120.22	111.27
24	6	306	BCR	C38-C26-C25	-5.04	118.87	124.53
22	4	811	CLA	O2D-CGD-CBD	5.04	120.22	111.27
24	8	304	BCR	C15-C14-C13	-5.04	120.12	127.31
22	5	319	CLA	O2D-CGD-CBD	5.03	120.21	111.27
22	3	311	CLA	O2D-CGD-CBD	5.03	120.21	111.27
24	A	845	BCR	C11-C10-C9	-5.03	120.13	127.31
22	6	313	CLA	CMD-C2D-C1D	5.03	133.57	124.71
24	7	303	BCR	C20-C21-C22	-5.03	120.14	127.31
22	A	822	CLA	O2A-C1-C2	5.03	121.85	108.64
22	A	825	CLA	O2D-CGD-CBD	5.03	120.20	111.27
24	K	206	BCR	C20-C21-C22	-5.02	120.14	127.31
22	3	322	CLA	O2D-CGD-CBD	5.02	120.19	111.27
24	A	848	BCR	C15-C14-C13	-5.02	120.14	127.31
24	3	307	BCR	C4-C5-C6	-5.02	115.44	122.73
22	A	829	CLA	O2A-C1-C2	5.02	121.83	108.64
38	1	303	LUT	C35-C34-C33	-5.02	120.14	127.31
22	B	809	CLA	O2A-C1-C2	5.02	121.83	108.64
22	8	308	CLA	O2D-CGD-CBD	5.02	120.19	111.27
22	1	310	CLA	O2A-C1-C2	5.02	121.83	108.64
22	6	301	CLA	O2A-C1-C2	5.02	121.82	108.64
22	A	855	CLA	O2D-CGD-CBD	5.01	120.18	111.27
22	A	807	CLA	O2D-CGD-CBD	5.01	120.17	111.27
22	5	301	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	B	844	BCR	C20-C19-C18	-5.01	112.34	126.42
22	B	836	CLA	O2D-CGD-CBD	5.01	120.17	111.27
22	8	307	CLA	O2A-C1-C2	5.01	121.80	108.64
22	B	816	CLA	O2D-CGD-CBD	5.00	120.16	111.27
38	Z	302	LUT	C11-C10-C9	-5.00	120.17	127.31
22	3	315	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	A	835	CLA	O2D-CGD-CBD	5.00	120.16	111.27
22	Z	308	CLA	O2D-CGD-CBD	5.00	120.16	111.27
24	B	849	BCR	C7-C8-C9	-5.00	118.68	126.23
22	K	205	CLA	O2A-C1-C2	5.00	121.78	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	812	CLA	O2D-CGD-CBD	5.00	120.15	111.27
22	1	309	CLA	O2D-CGD-CBD	5.00	120.15	111.27
24	4	804	BCR	C16-C17-C18	-5.00	120.18	127.31
22	A	805	CLA	O2D-CGD-CBD	5.00	120.15	111.27
22	5	315	CLA	O2D-CGD-CBD	5.00	120.15	111.27
22	1	308	CLA	O2A-C1-C2	5.00	121.76	108.64
24	K	206	BCR	C16-C17-C18	-5.00	120.18	127.31
22	F	304	CLA	O2A-C1-C2	4.99	121.75	108.64
22	F	305	CLA	O2D-CGD-CBD	4.99	120.14	111.27
22	Z	309	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	A	830	CLA	O2A-C1-C2	4.99	121.74	108.64
22	4	809	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	A	822	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	B	807	CLA	O2D-CGD-CBD	4.99	120.13	111.27
22	4	806	CLA	O2A-C1-C2	4.99	121.74	108.64
22	5	310	CLA	O2A-C1-C2	4.99	121.74	108.64
24	A	845	BCR	C20-C21-C22	-4.98	120.20	127.31
22	A	827	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	6	321	CLA	O2D-CGD-CBD	4.98	120.12	111.27
22	G	201	CLA	O2A-C1-C2	4.98	121.72	108.64
22	5	307	CLA	O2D-CGD-CBD	4.98	120.11	111.27
22	B	815	CLA	O2A-C1-C2	4.97	121.71	108.64
24	4	804	BCR	C24-C23-C22	-4.97	118.72	126.23
22	J	103	CLA	O2D-CGD-CBD	4.97	120.11	111.27
22	L	202	CLA	O2D-CGD-CBD	4.97	120.11	111.27
22	Z	313	CLA	CMD-C2D-C1D	4.97	133.48	124.71
38	9	301	LUT	C35-C34-C33	-4.97	120.22	127.31
24	A	845	BCR	C33-C5-C6	-4.97	118.95	124.53
38	4	803	LUT	C7-C8-C9	-4.97	118.73	126.23
22	1	306	CLA	O2D-CGD-CBD	4.97	120.09	111.27
22	2	304	CLA	O2D-CGD-CBD	4.97	120.09	111.27
22	7	324	CLA	O2D-CGD-CBD	4.97	120.09	111.27
22	A	806	CLA	O2D-CGD-CBD	4.96	120.09	111.27
22	4	810	CLA	O2D-CGD-CBD	4.96	120.09	111.27
24	L	204	BCR	C1-C6-C5	-4.96	115.63	122.61
22	F	302	CLA	O2D-CGD-CBD	4.96	120.08	111.27
39	9	312	CHL	C4A-NA-C1A	4.96	108.94	106.71
22	5	314	CLA	O2D-CGD-CBD	4.96	120.08	111.27
22	1	304	CLA	O2D-CGD-CBD	4.96	120.07	111.27
22	1	315	CLA	O2D-CGD-CBD	4.96	120.07	111.27
22	Z	304	CLA	CMD-C2D-C1D	4.95	133.44	124.71
22	A	815	CLA	O2D-CGD-CBD	4.95	120.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	314	CLA	O2D-CGD-CBD	4.95	120.07	111.27
22	A	832	CLA	O2D-CGD-CBD	4.95	120.07	111.27
24	B	846	BCR	C33-C5-C6	-4.95	118.97	124.53
22	8	309	CLA	O2A-C1-C2	4.95	121.64	108.64
22	A	821	CLA	O2D-CGD-CBD	4.95	120.06	111.27
38	8	302	LUT	C18-C5-C6	-4.95	118.97	124.53
22	F	304	CLA	O2D-CGD-CBD	4.94	120.05	111.27
22	7	322	CLA	O2D-CGD-CBD	4.94	120.05	111.27
38	4	802	LUT	C35-C34-C33	-4.94	120.26	127.31
22	B	828	CLA	O2A-C1-C2	4.94	121.61	108.64
22	Z	315	CLA	O2D-CGD-CBD	4.94	120.04	111.27
22	L	201	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	1	307	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	B	842	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	8	314	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	B	823	CLA	O2D-CGD-CBD	4.93	120.02	111.27
22	3	308	CLA	O2A-C1-C2	4.93	121.58	108.64
22	B	806	CLA	O2A-C1-C2	4.93	121.58	108.64
22	Z	314	CLA	O2A-C1-C2	4.93	121.58	108.64
21	A	801	CL0	C3B-C2B-C1B	-4.93	101.22	107.16
38	1	303	LUT	C11-C10-C9	-4.92	120.28	127.31
22	B	814	CLA	O2A-C1-C2	4.92	121.58	108.64
22	K	205	CLA	O2D-CGD-CBD	4.92	120.02	111.27
22	F	301	CLA	O2A-C1-C2	4.92	121.57	108.64
22	7	308	CLA	O2D-CGD-CBD	4.92	120.01	111.27
38	1	303	LUT	C7-C8-C9	-4.92	118.80	126.23
22	Z	308	CLA	O2A-C1-C2	4.92	121.56	108.64
22	1	310	CLA	O2D-CGD-CBD	4.92	120.01	111.27
22	B	811	CLA	O2A-C1-C2	4.92	121.56	108.64
24	B	847	BCR	C7-C8-C9	-4.92	118.81	126.23
22	A	836	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	5	309	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	B	833	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	A	820	CLA	O2D-CGD-CBD	4.91	120.00	111.27
22	9	307	CLA	O2A-C1-C2	4.91	121.54	108.64
22	B	830	CLA	O2A-C1-C2	4.91	121.54	108.64
22	6	313	CLA	O2D-CGD-CBD	4.91	119.99	111.27
22	B	831	CLA	O2A-C1-C2	4.91	121.53	108.64
22	B	809	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	B	837	CLA	O2A-C1-C2	4.90	121.53	108.64
22	B	835	CLA	O2A-C1-C2	4.90	121.52	108.64
22	Z	314	CLA	O2D-CGD-CBD	4.90	119.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	840	CLA	O2A-C1-C2	4.90	121.52	108.64
22	8	310	CLA	O2D-CGD-CBD	4.90	119.98	111.27
22	7	312	CLA	O2D-CGD-CBD	4.90	119.97	111.27
22	A	817	CLA	O2D-CGD-CBD	4.89	119.97	111.27
24	B	848	BCR	C11-C10-C9	-4.89	120.33	127.31
38	6	304	LUT	C15-C14-C13	-4.89	120.33	127.31
22	B	839	CLA	O2A-C1-C2	4.89	121.49	108.64
24	3	306	BCR	C30-C25-C26	-4.89	115.72	122.61
22	A	830	CLA	O2D-CGD-CBD	4.89	119.96	111.27
22	B	813	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	5	313	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	A	828	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	A	823	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	7	311	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	6	309	CLA	O2D-CGD-CBD	4.89	119.95	111.27
22	3	310	CLA	O2A-C1-C2	4.88	121.47	108.64
22	B	838	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	A	824	CLA	O2D-CGD-CBD	4.88	119.94	111.27
22	A	810	CLA	O2D-CGD-CBD	4.87	119.93	111.27
22	2	301	CLA	O2A-C1-C2	4.87	121.44	108.64
22	7	309	CLA	O2A-C1-C2	4.87	121.43	108.64
38	6	304	LUT	C35-C34-C33	-4.87	120.36	127.31
22	B	801	CLA	O2D-CGD-CBD	4.87	119.92	111.27
24	6	306	BCR	C7-C8-C9	-4.87	118.88	126.23
22	3	310	CLA	O2D-CGD-CBD	4.87	119.92	111.27
22	7	308	CLA	O2A-C1-C2	4.87	121.43	108.64
24	J	104	BCR	C20-C21-C22	-4.87	120.37	127.31
22	6	302	CLA	O2D-CGD-CBD	4.86	119.91	111.27
22	B	824	CLA	O2A-C1-C2	4.86	121.41	108.64
22	6	313	CLA	O2A-C1-C2	4.86	121.41	108.64
22	B	816	CLA	O2A-C1-C2	4.86	121.41	108.64
22	3	318	CLA	O2A-C1-C2	4.86	121.40	108.64
22	B	812	CLA	O2A-C1-C2	4.86	121.40	108.64
22	L	203	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	6	311	CLA	O2A-C1-C2	4.86	121.40	108.64
24	A	844	BCR	C33-C5-C6	-4.86	119.08	124.53
24	8	304	BCR	C11-C10-C9	-4.85	120.38	127.31
22	7	305	CLA	O2A-C1-C2	4.85	121.39	108.64
22	A	826	CLA	O2A-C1-C2	4.85	121.39	108.64
22	9	311	CLA	O2D-CGD-CBD	4.85	119.89	111.27
22	B	810	CLA	O2A-C1-C2	4.85	121.39	108.64
24	A	844	BCR	C12-C13-C14	4.85	126.39	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	317	CLA	O2A-C1-C2	4.85	121.38	108.64
22	5	308	CLA	O2A-C1-C2	4.85	121.38	108.64
22	K	203	CLA	O2D-CGD-CBD	4.85	119.88	111.27
22	2	301	CLA	O2D-CGD-CBD	4.85	119.88	111.27
22	L	203	CLA	O2A-C1-C2	4.85	121.37	108.64
32	F	306	RRX	C1-C6-C5	-4.84	115.79	122.61
22	B	821	CLA	O2D-CGD-CBD	4.84	119.88	111.27
21	A	801	CL0	O2A-C1-C2	4.84	121.37	108.64
38	5	303	LUT	C11-C10-C9	-4.84	120.40	127.31
24	I	4001	BCR	C1-C6-C5	-4.84	115.80	122.61
24	G	203	BCR	C38-C26-C25	-4.84	119.10	124.53
24	K	206	BCR	C7-C8-C9	-4.84	118.93	126.23
24	A	844	BCR	C38-C26-C25	-4.83	119.10	124.53
22	3	322	CLA	O2A-C1-C2	4.83	121.34	108.64
22	K	204	CLA	O2D-CGD-CBD	4.83	119.86	111.27
39	9	312	CHL	CMA-C3A-C4A	4.83	124.75	111.77
36	5	306	C7Z	C38-C25-C26	-4.83	119.11	124.53
22	7	309	CLA	O2D-CGD-CBD	4.83	119.84	111.27
22	A	842	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	A	842	CLA	O2A-C1-C2	4.82	121.31	108.64
22	B	829	CLA	O2D-CGD-CBD	4.82	119.84	111.27
22	5	323	CLA	O2D-CGD-CBD	4.82	119.83	111.27
24	A	844	BCR	C8-C9-C10	4.82	126.33	118.94
22	A	854	CLA	O2D-CGD-CBD	4.82	119.83	111.27
24	A	844	BCR	C15-C16-C17	-4.81	113.61	123.47
22	6	322	CLA	O2A-C1-C2	4.81	121.28	108.64
38	Z	301	LUT	C15-C14-C13	-4.81	120.45	127.31
22	B	812	CLA	O2D-CGD-CBD	4.81	119.81	111.27
24	B	845	BCR	C16-C17-C18	-4.81	120.45	127.31
22	4	815	CLA	O2A-C1-C2	4.81	121.27	108.64
22	1	316	CLA	CMD-C2D-C1D	4.81	133.18	124.71
24	B	846	BCR	C7-C8-C9	-4.80	118.98	126.23
22	Z	310	CLA	O2D-CGD-CBD	4.80	119.80	111.27
22	B	826	CLA	O2A-C1-C2	4.80	121.25	108.64
24	A	845	BCR	C1-C6-C5	-4.80	115.86	122.61
24	B	844	BCR	C19-C18-C17	4.80	126.30	118.94
22	1	314	CLA	O2D-CGD-CBD	4.79	119.78	111.27
22	7	306	CLA	O2D-CGD-CBD	4.79	119.78	111.27
22	6	311	CLA	O2D-CGD-CBD	4.79	119.78	111.27
22	Z	304	CLA	O2D-CGD-CBD	4.79	119.78	111.27
24	J	104	BCR	C38-C26-C25	-4.79	119.15	124.53
22	6	317	CLA	O2A-C1-C2	4.79	121.22	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	311	CLA	O2D-CGD-CBD	4.79	119.77	111.27
22	9	309	CLA	O2A-C1-C2	4.78	121.21	108.64
38	Z	302	LUT	C7-C8-C9	-4.78	119.01	126.23
38	6	304	LUT	C7-C8-C9	-4.78	119.01	126.23
24	A	856	BCR	C38-C26-C25	-4.78	119.16	124.53
22	B	825	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	A	815	CLA	O2A-C1-C2	4.78	121.20	108.64
22	A	855	CLA	O2A-C1-C2	4.78	121.19	108.64
24	B	853	BCR	C20-C21-C22	-4.78	120.49	127.31
22	B	818	CLA	O2A-C1-C2	4.78	121.19	108.64
24	J	104	BCR	C4-C5-C6	-4.78	115.80	122.73
24	8	304	BCR	C7-C8-C9	-4.77	119.02	126.23
22	9	313	CLA	O2A-C1-C2	4.77	121.18	108.64
24	3	305	BCR	C27-C26-C25	-4.77	115.80	122.73
22	4	807	CLA	O2A-C1-C2	4.77	121.18	108.64
22	7	317	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	3	309	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	8	308	CLA	O2A-C1-C2	4.77	121.16	108.64
22	9	307	CLA	O2D-CGD-CBD	4.76	119.73	111.27
22	6	312	CLA	O2A-C1-C2	4.76	121.16	108.64
22	A	839	CLA	O2A-C1-C2	4.76	121.14	108.64
22	A	840	CLA	O2D-CGD-CBD	4.76	119.72	111.27
24	7	303	BCR	C15-C14-C13	-4.76	120.52	127.31
22	B	819	CLA	O2A-C1-C2	4.75	121.13	108.64
22	A	816	CLA	O2A-C1-C2	4.75	121.12	108.64
24	8	304	BCR	C4-C5-C6	-4.75	115.83	122.73
22	Z	316	CLA	O2A-C1-C2	4.75	121.12	108.64
36	J	105	C7Z	C11-C10-C9	-4.75	120.53	127.31
22	6	307	CLA	O2D-CGD-CBD	4.75	119.71	111.27
22	A	835	CLA	O2A-C1-C2	4.75	121.11	108.64
24	5	305	BCR	C38-C26-C25	-4.75	119.20	124.53
22	9	304	CLA	CMD-C2D-C1D	4.75	133.08	124.71
24	6	305	BCR	C24-C23-C22	-4.74	119.07	126.23
38	5	303	LUT	C15-C14-C13	-4.74	120.54	127.31
22	3	319	CLA	O2A-C1-C2	4.74	121.09	108.64
22	A	826	CLA	O2D-CGD-CBD	4.73	119.67	111.27
38	7	302	LUT	C7-C8-C9	-4.73	119.09	126.23
22	7	309	CLA	C1-C2-C3	-4.73	117.86	126.04
22	1	314	CLA	O2A-C1-C2	4.73	121.06	108.64
22	9	310	CLA	O2D-CGD-CBD	4.73	119.67	111.27
22	8	316	CLA	O2D-CGD-CBD	4.72	119.66	111.27
24	3	305	BCR	C30-C25-C26	-4.72	115.96	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	3	302	LUT	C11-C10-C9	-4.72	120.57	127.31
24	4	804	BCR	C15-C14-C13	-4.72	120.58	127.31
22	A	809	CLA	O2A-C1-C2	4.71	121.02	108.64
22	8	309	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	5	312	CLA	O2D-CGD-CBD	4.71	119.64	111.27
22	Z	316	CLA	O2D-CGD-CBD	4.71	119.63	111.27
22	A	817	CLA	C1-C2-C3	-4.70	117.91	126.04
22	B	808	CLA	O2A-C1-C2	4.70	120.99	108.64
24	3	307	BCR	C7-C8-C9	-4.70	119.13	126.23
38	5	302	LUT	C18-C5-C6	-4.70	119.25	124.53
22	B	840	CLA	O2A-C1-C2	4.70	120.98	108.64
24	4	804	BCR	C38-C26-C25	-4.69	119.26	124.53
22	B	805	CLA	O2A-C1-C2	4.69	120.97	108.64
22	Z	306	CLA	O2D-CGD-CBD	4.69	119.61	111.27
22	A	803	CLA	O2A-C1-C2	4.69	120.96	108.64
22	7	314	CLA	O2A-C1-C2	4.69	120.96	108.64
22	3	312	CLA	O2A-C1-C2	4.69	120.96	108.64
38	4	802	LUT	C15-C14-C13	-4.69	120.62	127.31
24	L	204	BCR	C38-C26-C25	-4.69	119.26	124.53
22	9	304	CLA	O2D-CGD-CBD	4.69	119.60	111.27
31	1	319	DGD	O2G-C1B-C2B	4.69	121.60	111.50
38	5	303	LUT	C7-C8-C9	-4.69	119.15	126.23
22	Z	307	CLA	O2A-C1-C2	4.69	120.95	108.64
22	8	310	CLA	C1-C2-C3	-4.68	117.94	126.04
22	L	202	CLA	O2A-C1-C2	4.68	120.94	108.64
22	6	314	CLA	O2A-C1-C2	4.68	120.94	108.64
22	Z	305	CLA	CMD-C2D-C1D	4.68	132.96	124.71
22	6	302	CLA	O2A-C1-C2	4.68	120.93	108.64
22	A	829	CLA	O2D-CGD-CBD	4.68	119.58	111.27
38	Z	302	LUT	C15-C14-C13	-4.67	120.64	127.31
22	B	827	CLA	O2A-C1-C2	4.67	120.90	108.64
22	1	307	CLA	O2A-C1-C2	4.67	120.90	108.64
24	B	844	BCR	C33-C5-C6	-4.66	119.29	124.53
22	A	811	CLA	O2D-CGD-CBD	4.66	119.55	111.27
24	L	204	BCR	C27-C26-C25	-4.66	115.97	122.73
22	5	322	CLA	O2D-CGD-CBD	4.66	119.54	111.27
22	3	313	CLA	O2D-CGD-CBD	4.65	119.54	111.27
22	3	312	CLA	O2D-CGD-CBD	4.65	119.53	111.27
24	8	304	BCR	C16-C17-C18	-4.65	120.67	127.31
38	7	302	LUT	C35-C34-C33	-4.65	120.68	127.31
24	B	847	BCR	C27-C26-C25	-4.64	115.99	122.73
24	6	305	BCR	C38-C26-C25	-4.64	119.32	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	306	CLA	O2A-C1-C2	4.64	120.82	108.64
22	Z	309	CLA	O2A-C1-C2	4.64	120.82	108.64
24	3	305	BCR	C38-C26-C25	-4.63	119.33	124.53
22	6	308	CLA	O2A-C1-C2	4.63	120.80	108.64
38	3	302	LUT	C7-C8-C9	-4.63	119.24	126.23
22	1	311	CLA	CMD-C2D-C1D	4.62	132.86	124.71
22	L	201	CLA	O2A-C1-C2	4.62	120.78	108.64
24	A	856	BCR	C33-C5-C6	-4.62	119.34	124.53
36	5	306	C7Z	C7-C8-C9	-4.62	119.26	126.23
22	B	821	CLA	O2A-C1-C2	4.62	120.77	108.64
22	A	805	CLA	O2A-C1-C2	4.62	120.77	108.64
22	K	203	CLA	O2A-C1-C2	4.62	120.76	108.64
22	A	825	CLA	O2A-C1-C2	4.61	120.76	108.64
22	B	825	CLA	O2A-C1-C2	4.61	120.75	108.64
24	3	305	BCR	C24-C23-C22	-4.61	119.27	126.23
22	B	822	CLA	O2A-C1-C2	4.61	120.74	108.64
24	B	844	BCR	C7-C8-C9	-4.60	119.28	126.23
24	F	303	BCR	C33-C5-C6	-4.60	119.37	124.53
22	B	830	CLA	O2D-CGD-CBD	4.59	119.43	111.27
38	3	303	LUT	C11-C10-C9	-4.59	120.76	127.31
22	6	307	CLA	O2A-C1-C2	4.59	120.69	108.64
22	4	810	CLA	O2A-C1-C2	4.59	120.69	108.64
38	4	803	LUT	C11-C10-C9	-4.59	120.77	127.31
22	9	308	CLA	O2A-C1-C2	4.58	120.69	108.64
22	A	834	CLA	O2A-C1-C2	4.58	120.68	108.64
31	3	301	DGD	O2G-C1B-C2B	4.58	121.37	111.50
24	5	305	BCR	C15-C16-C17	-4.58	114.09	123.47
22	7	310	CLA	O2A-C1-C2	4.58	120.67	108.64
24	B	844	BCR	C11-C12-C13	-4.58	113.56	126.42
22	B	842	CLA	O2A-C1-C2	4.57	120.65	108.64
38	1	303	LUT	C15-C14-C13	-4.57	120.79	127.31
22	Z	305	CLA	O2A-C1-C2	4.57	120.64	108.64
24	L	204	BCR	C4-C5-C6	-4.57	116.10	122.73
24	B	849	BCR	C38-C26-C25	-4.57	119.40	124.53
24	A	844	BCR	C27-C26-C25	-4.56	116.11	122.73
38	9	301	LUT	C31-C30-C29	-4.56	120.80	127.31
22	1	304	CLA	O2A-C1-C2	4.56	120.62	108.64
24	J	104	BCR	C33-C5-C6	-4.56	119.41	124.53
22	A	819	CLA	O2A-C1-C2	4.56	120.61	108.64
22	A	854	CLA	O2A-C1-C2	4.55	120.60	108.64
22	B	833	CLA	O2A-C1-C2	4.55	120.60	108.64
24	3	306	BCR	C16-C17-C18	-4.55	120.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	833	CLA	O2A-C1-C2	4.55	120.59	108.64
24	A	848	BCR	C1-C6-C5	-4.55	116.21	122.61
24	5	304	BCR	C24-C23-C22	-4.54	119.37	126.23
22	5	318	CLA	O2A-C1-C2	4.54	120.57	108.64
22	7	315	CLA	O2A-C1-C2	4.54	120.57	108.64
24	A	856	BCR	C15-C14-C13	-4.54	120.83	127.31
22	6	310	CLA	O2A-C1-C2	4.54	120.57	108.64
38	9	301	LUT	C7-C8-C9	-4.54	119.38	126.23
22	7	312	CLA	O2A-C1-C2	4.54	120.56	108.64
22	B	834	CLA	O2A-C1-C2	4.54	120.56	108.64
24	A	844	BCR	C20-C21-C22	-4.54	120.83	127.31
22	5	318	CLA	O2D-CGD-CBD	4.54	119.33	111.27
22	7	322	CLA	O2A-C1-C2	4.53	120.55	108.64
22	A	806	CLA	O2A-C1-C2	4.53	120.54	108.64
38	Z	302	LUT	C35-C34-C33	-4.53	120.85	127.31
38	5	303	LUT	C35-C34-C33	-4.53	120.85	127.31
39	3	317	CHL	CHD-C1D-ND	-4.52	120.30	124.45
24	A	856	BCR	C24-C23-C22	-4.52	119.41	126.23
22	A	823	CLA	O2A-C1-C2	4.52	120.50	108.64
22	8	313	CLA	O2A-C1-C2	4.52	120.50	108.64
24	B	848	BCR	C38-C26-C25	-4.51	119.46	124.53
22	8	306	CLA	O2A-C1-C2	4.51	120.49	108.64
24	G	203	BCR	C15-C14-C13	-4.51	120.87	127.31
38	Z	301	LUT	C35-C34-C33	-4.51	120.87	127.31
22	8	311	CLA	O2A-C1-C2	4.51	120.48	108.64
24	K	206	BCR	C30-C25-C26	-4.50	116.27	122.61
22	4	807	CLA	O2D-CGD-CBD	4.50	119.27	111.27
22	Z	303	CLA	O2A-C1-C2	4.50	120.46	108.64
22	5	312	CLA	O2A-C1-C2	4.50	120.46	108.64
24	5	305	BCR	C33-C5-C6	-4.50	119.48	124.53
24	B	845	BCR	C38-C26-C25	-4.50	119.48	124.53
24	A	846	BCR	C24-C23-C22	-4.50	119.44	126.23
22	A	837	CLA	O2A-C1-C2	4.49	120.44	108.64
24	B	848	BCR	C24-C23-C22	-4.49	119.45	126.23
22	A	821	CLA	O2A-C1-C2	4.49	120.43	108.64
24	3	304	BCR	C33-C5-C6	-4.49	119.49	124.53
22	B	801	CLA	O2A-C1-C2	4.49	120.43	108.64
22	5	311	CLA	O2A-C1-C2	4.48	120.42	108.64
22	9	305	CLA	O2A-C1-C2	4.48	120.42	108.64
24	A	856	BCR	C1-C6-C5	-4.48	116.30	122.61
22	5	315	CLA	O2A-C1-C2	4.48	120.41	108.64
22	A	808	CLA	O2A-C1-C2	4.48	120.40	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	808	CLA	O2A-C1-C2	4.48	120.40	108.64
22	9	310	CLA	CMD-C2D-C1D	4.47	132.60	124.71
22	A	811	CLA	O2A-C1-C2	4.47	120.38	108.64
24	B	847	BCR	C33-C5-C6	-4.47	119.51	124.53
22	A	831	CLA	O2A-C1-C2	4.46	120.36	108.64
22	B	835	CLA	C1-C2-C3	-4.46	119.53	126.75
24	J	104	BCR	C1-C6-C5	-4.46	116.33	122.61
32	F	306	RRX	C7-C8-C9	-4.46	119.50	126.23
22	A	813	CLA	O2A-C1-C2	4.46	120.35	108.64
24	8	304	BCR	C33-C5-C6	-4.46	119.52	124.53
22	3	316	CLA	O2A-C1-C2	4.45	120.34	108.64
22	A	828	CLA	O2A-C1-C2	4.45	120.34	108.64
22	B	832	CLA	O2A-C1-C2	4.45	120.33	108.64
22	3	311	CLA	O2A-C1-C2	4.45	120.33	108.64
22	5	320	CLA	O2A-C1-C2	4.45	120.33	108.64
22	4	809	CLA	O2A-C1-C2	4.45	120.33	108.64
25	B	803	LHG	O7-C7-C8	4.44	121.08	111.50
22	3	313	CLA	O2A-C1-C2	4.44	120.31	108.64
39	8	315	CHL	CHD-C1D-ND	-4.44	120.37	124.45
24	B	853	BCR	C16-C17-C18	-4.44	120.97	127.31
22	A	820	CLA	O2A-C1-C2	4.44	120.31	108.64
22	1	306	CLA	C1-C2-C3	-4.44	118.37	126.04
24	B	853	BCR	C27-C26-C25	-4.44	116.29	122.73
24	3	304	BCR	C12-C13-C14	-4.43	112.14	118.94
24	A	846	BCR	C7-C8-C9	-4.43	119.54	126.23
22	A	827	CLA	O2A-C1-C2	4.43	120.28	108.64
39	6	318	CHL	CHD-C1D-ND	-4.42	120.39	124.45
22	3	320	CLA	O2D-CGD-CBD	4.42	119.13	111.27
24	B	847	BCR	C38-C26-C25	-4.42	119.56	124.53
22	Z	310	CLA	O2A-C1-C2	4.42	120.25	108.64
22	8	305	CLA	O2A-C1-C2	4.42	120.24	108.64
38	4	802	LUT	C11-C10-C9	-4.41	121.02	127.31
24	7	303	BCR	C16-C17-C18	-4.41	121.02	127.31
25	6	323	LHG	O7-C7-C8	4.41	121.00	111.50
21	A	801	CL0	C2B-C1B-NB	4.41	113.19	110.23
24	B	846	BCR	C16-C17-C18	-4.40	121.03	127.31
22	5	320	CLA	CMD-C2D-C1D	4.40	132.47	124.71
24	B	844	BCR	C38-C26-C25	-4.40	119.59	124.53
22	1	316	CLA	O2D-CGD-CBD	4.40	119.08	111.27
22	1	309	CLA	O2A-C1-C2	4.40	120.19	108.64
24	A	847	BCR	C7-C8-C9	-4.40	119.59	126.23
24	4	804	BCR	C20-C21-C22	-4.39	121.04	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	812	CLA	O2A-C1-C2	4.39	120.18	108.64
22	F	302	CLA	O2A-C1-C2	4.39	120.17	108.64
22	A	824	CLA	O2A-C1-C2	4.39	120.17	108.64
22	A	836	CLA	O2A-C1-C2	4.38	120.16	108.64
38	1	302	LUT	C35-C34-C33	-4.37	121.07	127.31
24	8	304	BCR	C24-C23-C22	-4.37	119.64	126.23
38	7	301	LUT	C15-C14-C13	-4.36	121.08	127.31
22	A	807	CLA	O2A-C1-C2	4.36	120.09	108.64
24	F	303	BCR	C38-C26-C25	-4.35	119.64	124.53
24	B	845	BCR	C11-C10-C9	-4.35	121.10	127.31
24	5	304	BCR	C30-C25-C26	-4.35	116.49	122.61
24	L	204	BCR	C33-C5-C6	-4.35	119.65	124.53
24	L	204	BCR	C16-C17-C18	-4.35	121.11	127.31
39	5	321	CHL	CHD-C1D-ND	-4.34	120.46	124.45
22	B	813	CLA	C1-C2-C3	-4.34	118.54	126.04
24	A	844	BCR	C35-C13-C14	-4.34	116.84	122.92
24	6	305	BCR	C15-C14-C13	-4.34	121.12	127.31
22	4	805	CLA	O2D-CGD-CBD	4.33	118.97	111.27
39	6	320	CHL	CHD-C1D-ND	-4.33	120.47	124.45
24	3	306	BCR	C27-C26-C25	-4.33	116.45	122.73
24	B	853	BCR	C38-C26-C25	-4.32	119.68	124.53
24	A	846	BCR	C33-C5-C6	-4.32	119.68	124.53
39	4	819	CHL	CHD-C1D-ND	-4.32	120.49	124.45
24	B	853	BCR	C38-C26-C27	4.31	121.90	113.62
22	7	310	CLA	O2D-CGD-CBD	4.31	118.93	111.27
24	B	845	BCR	C15-C14-C13	-4.31	121.16	127.31
24	I	4001	BCR	C7-C8-C9	-4.30	119.73	126.23
24	I	4001	BCR	C11-C10-C9	-4.30	121.17	127.31
39	Z	312	CHL	CHD-C1D-ND	-4.30	120.50	124.45
24	8	304	BCR	C1-C6-C5	-4.30	116.56	122.61
22	B	837	CLA	C1-C2-C3	-4.29	118.62	126.04
39	4	816	CHL	CHD-C1D-ND	-4.29	120.51	124.45
39	4	813	CHL	CHD-C1D-ND	-4.29	120.51	124.45
22	9	303	CLA	O2D-CGD-CBD	4.29	118.89	111.27
22	5	307	CLA	C1-C2-C3	-4.28	118.63	126.04
24	L	204	BCR	C15-C14-C13	-4.28	121.20	127.31
39	2	303	CHL	CHD-C1D-ND	-4.27	120.53	124.45
24	B	848	BCR	C16-C17-C18	-4.27	121.22	127.31
24	A	846	BCR	C20-C21-C22	-4.27	121.22	127.31
24	3	307	BCR	C33-C5-C6	-4.26	119.74	124.53
24	3	304	BCR	C27-C26-C25	-4.26	116.54	122.73
22	5	307	CLA	O2A-C1-C2	4.26	119.84	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	306	C7Z	C1-C6-C5	-4.26	116.61	122.61
24	L	204	BCR	C30-C25-C26	-4.26	116.62	122.61
25	1	317	LHG	O7-C7-C8	4.26	120.67	111.50
39	8	301	CHL	CHD-C1D-ND	-4.25	120.55	124.45
22	B	838	CLA	O2A-C1-C2	4.25	119.81	108.64
25	Z	317	LHG	O7-C7-C8	4.25	120.67	111.50
22	4	806	CLA	C1-C2-C3	-4.25	118.69	126.04
22	K	203	CLA	C1-C2-C3	-4.25	118.69	126.04
22	L	203	CLA	C1-C2-C3	-4.25	119.88	126.75
22	7	305	CLA	C1-C2-C3	-4.25	119.88	126.75
24	3	307	BCR	C1-C6-C5	-4.25	116.63	122.61
22	4	812	CLA	O2A-C1-C2	4.24	119.79	108.64
24	F	303	BCR	C24-C23-C22	-4.24	119.82	126.23
24	I	4001	BCR	C38-C26-C27	4.24	121.76	113.62
24	A	856	BCR	C11-C10-C9	-4.24	121.26	127.31
38	7	301	LUT	C7-C8-C9	-4.24	119.83	126.23
22	4	810	CLA	C1-C2-C3	-4.24	119.90	126.75
22	B	817	CLA	O2A-C1-C2	4.23	119.75	108.64
22	B	820	CLA	O2A-C1-C2	4.23	119.75	108.64
36	J	105	C7Z	C18-C5-C6	-4.23	119.78	124.53
24	G	203	BCR	C27-C26-C25	-4.23	116.60	122.73
22	7	310	CLA	C1-C2-C3	-4.22	118.75	126.04
38	4	803	LUT	C18-C5-C6	-4.21	119.80	124.53
22	A	826	CLA	C1-C2-C3	-4.21	119.94	126.75
22	B	823	CLA	O2A-C1-C2	4.21	119.71	108.64
24	A	848	BCR	C4-C5-C6	-4.21	116.62	122.73
24	K	206	BCR	C24-C23-C22	-4.21	119.88	126.23
39	9	312	CHL	CHD-C1D-ND	-4.20	120.59	124.45
22	7	306	CLA	C1-C2-C3	-4.20	118.77	126.04
24	B	845	BCR	C4-C5-C6	-4.20	116.63	122.73
22	9	309	CLA	CMD-C2D-C1D	4.20	132.11	124.71
24	A	848	BCR	C30-C25-C26	-4.20	116.70	122.61
39	1	312	CHL	CHD-C1D-ND	-4.19	120.60	124.45
22	3	315	CLA	CMD-C2D-C1D	4.19	132.10	124.71
24	A	846	BCR	C38-C26-C25	-4.19	119.82	124.53
39	6	316	CHL	CHD-C1D-ND	-4.19	120.60	124.45
22	5	326	CLA	O2A-C1-C2	4.19	119.65	108.64
24	5	304	BCR	C33-C5-C6	-4.19	119.83	124.53
39	Z	311	CHL	CHD-C1D-ND	-4.18	120.61	124.45
22	9	306	CLA	C1-C2-C3	-4.18	118.82	126.04
38	7	301	LUT	C11-C10-C9	-4.17	121.35	127.31
24	A	844	BCR	C30-C25-C26	-4.17	116.73	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	Z	302	LUT	C18-C5-C6	-4.17	119.84	124.53
22	A	806	CLA	C1-C2-C3	-4.17	118.83	126.04
24	3	304	BCR	C8-C9-C10	4.17	125.34	118.94
36	5	306	C7Z	C31-C30-C29	-4.17	121.36	127.31
22	A	814	CLA	C1-C2-C3	-4.17	118.84	126.04
24	B	849	BCR	C24-C23-C22	-4.16	119.95	126.23
38	1	303	LUT	C18-C5-C6	-4.16	119.86	124.53
38	6	304	LUT	C11-C10-C9	-4.16	121.38	127.31
22	Z	306	CLA	O2A-C1-C2	4.16	119.56	108.64
24	I	4001	BCR	C4-C5-C6	-4.15	116.70	122.73
39	9	314	CHL	CHD-C1D-ND	-4.15	120.64	124.45
24	I	4001	BCR	C27-C26-C25	-4.15	116.71	122.73
22	6	319	CLA	C1-C2-C3	-4.15	118.87	126.04
36	J	105	C7Z	C38-C25-C26	-4.15	119.87	124.53
22	4	815	CLA	C1-C2-C3	-4.15	120.05	126.75
24	8	304	BCR	C20-C21-C22	-4.14	121.40	127.31
36	J	105	C7Z	C1-C6-C5	-4.14	116.78	122.61
22	7	315	CLA	C1-C2-C3	-4.14	120.05	126.75
22	Z	307	CLA	C1-C2-C3	-4.14	118.89	126.04
39	5	316	CHL	CHD-C1D-ND	-4.14	120.65	124.45
38	3	302	LUT	C18-C5-C6	-4.14	119.88	124.53
38	4	803	LUT	C15-C14-C13	-4.14	121.41	127.31
21	A	801	CL0	O2A-CGA-CBA	4.13	124.88	111.91
24	B	845	BCR	C7-C8-C9	-4.13	119.99	126.23
24	3	307	BCR	C27-C26-C25	-4.12	116.75	122.73
22	7	314	CLA	C1-C2-C3	-4.12	120.09	126.75
24	A	847	BCR	C15-C14-C13	-4.12	121.43	127.31
39	8	312	CHL	CHD-C1D-ND	-4.12	120.67	124.45
22	4	805	CLA	O2A-C1-C2	4.11	119.44	108.64
24	6	306	BCR	C33-C5-C6	-4.11	119.91	124.53
33	4	822	LMT	C1B-O1B-C4'	-4.10	107.81	117.96
22	5	320	CLA	C2C-C1C-NC	4.10	113.82	109.97
22	6	317	CLA	C1-C2-C3	-4.10	120.11	126.75
22	7	317	CLA	C1-C2-C3	-4.10	118.95	126.04
38	8	303	LUT	C18-C5-C6	-4.10	119.92	124.53
24	A	847	BCR	C11-C10-C9	-4.10	121.46	127.31
22	A	825	CLA	C1-C2-C3	-4.09	118.97	126.04
38	Z	301	LUT	C1-C6-C5	-4.09	116.86	122.61
25	A	850	LHG	O7-C7-C8	4.08	120.30	111.50
38	4	803	LUT	C1-C6-C5	-4.08	116.87	122.61
24	L	204	BCR	C24-C23-C22	-4.08	120.07	126.23
41	5	325	3PH	O21-C21-C22	4.07	120.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	318	LHG	O7-C7-C8	4.06	120.26	111.50
21	A	801	CL0	C1D-ND-C4D	-4.06	103.45	106.33
24	3	306	BCR	C4-C5-C6	-4.06	116.83	122.73
22	1	308	CLA	C1-C2-C3	-4.06	119.02	126.04
24	6	306	BCR	C15-C14-C13	-4.06	121.52	127.31
22	A	828	CLA	C1-C2-C3	-4.06	119.02	126.04
36	5	306	C7Z	C27-C28-C29	-4.06	120.10	126.23
24	3	306	BCR	C38-C26-C25	-4.06	119.97	124.53
24	B	845	BCR	C30-C25-C26	-4.05	116.90	122.61
22	1	316	CLA	O2A-C1-C2	4.05	119.28	108.64
24	A	856	BCR	C30-C25-C26	-4.05	116.91	122.61
24	3	306	BCR	C7-C8-C9	-4.05	120.12	126.23
39	4	814	CHL	CHD-C1D-ND	-4.03	120.75	124.45
22	B	810	CLA	C1-C2-C3	-4.02	119.08	126.04
22	9	308	CLA	C1-C2-C3	-4.02	120.25	126.75
24	G	203	BCR	C1-C6-C5	-4.02	116.95	122.61
22	9	313	CLA	C1-C2-C3	-4.01	120.26	126.75
22	9	304	CLA	C2D-C1D-ND	4.01	113.06	110.10
38	9	301	LUT	C11-C10-C9	-4.00	121.60	127.31
22	1	307	CLA	C1-C2-C3	-4.00	119.12	126.04
38	3	303	LUT	C18-C5-C6	-4.00	120.04	124.53
25	B	850	LHG	O7-C7-C8	4.00	120.12	111.50
22	7	307	CLA	C1-C2-C3	-3.99	119.13	126.04
32	F	306	RRX	C16-C15-C14	-3.99	115.30	123.47
22	4	807	CLA	C1-C2-C3	-3.99	119.14	126.04
22	8	311	CLA	C1-C2-C3	-3.99	120.30	126.75
24	6	306	BCR	C4-C5-C6	-3.99	116.94	122.73
39	8	301	CHL	C1-C2-C3	-3.99	119.15	126.04
24	8	304	BCR	C29-C30-C25	3.98	116.61	110.48
22	B	824	CLA	C1-C2-C3	-3.98	119.16	126.04
22	B	825	CLA	C1-C2-C3	-3.98	119.16	126.04
24	3	304	BCR	C38-C26-C25	-3.97	120.07	124.53
24	B	849	BCR	C27-C26-C25	-3.97	116.97	122.73
34	J	101	LMG	O7-C10-C11	3.97	120.05	111.50
22	A	831	CLA	C1-C2-C3	-3.97	120.33	126.75
25	A	849	LHG	O7-C7-C8	3.96	120.04	111.50
24	6	306	BCR	C11-C12-C13	-3.96	115.29	126.42
24	7	303	BCR	C24-C23-C22	-3.96	120.26	126.23
39	7	313	CHL	CHD-C1D-ND	-3.96	120.82	124.45
24	B	847	BCR	C30-C25-C26	-3.95	117.05	122.61
24	B	853	BCR	C33-C5-C6	-3.95	120.10	124.53
24	J	104	BCR	C30-C25-C26	-3.94	117.06	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	316	CLA	C2C-C1C-NC	3.94	113.66	109.97
38	8	303	LUT	C1-C6-C5	-3.94	117.07	122.61
24	B	847	BCR	C24-C23-C22	-3.94	120.29	126.23
22	G	201	CLA	C1-C2-C3	-3.94	120.39	126.75
22	B	841	CLA	C1-C2-C3	-3.93	119.24	126.04
22	3	312	CLA	C1-C2-C3	-3.93	119.25	126.04
22	9	310	CLA	C2D-C1D-ND	3.93	113.00	110.10
32	F	306	RRX	C38-C26-C25	-3.93	120.12	124.53
24	I	4001	BCR	C33-C5-C6	-3.92	120.12	124.53
24	A	844	BCR	C24-C23-C22	-3.92	120.31	126.23
38	9	302	LUT	C15-C14-C13	-3.92	121.71	127.31
22	5	313	CLA	C1-C2-C3	-3.92	119.26	126.04
41	6	324	3PH	O21-C21-C22	3.92	119.95	111.50
38	5	302	LUT	C7-C8-C9	-3.92	120.32	126.23
22	2	301	CLA	C1-C2-C3	-3.91	119.27	126.04
36	5	306	C7Z	C18-C5-C6	-3.91	120.13	124.53
24	B	844	BCR	C12-C13-C14	3.91	124.94	118.94
24	A	845	BCR	C4-C5-C6	-3.91	117.06	122.73
22	9	309	CLA	O2D-CGD-CBD	3.90	118.21	111.27
24	3	304	BCR	C34-C9-C10	-3.90	117.45	122.92
24	3	304	BCR	C16-C15-C14	3.90	131.46	123.47
39	5	317	CHL	CHD-C1D-ND	-3.89	120.88	124.45
22	Z	316	CLA	C1-C2-C3	-3.89	119.31	126.04
24	A	845	BCR	C38-C26-C25	-3.89	120.16	124.53
24	6	305	BCR	C33-C5-C6	-3.89	120.16	124.53
22	5	312	CLA	C1-C2-C3	-3.89	120.46	126.75
24	A	844	BCR	C10-C11-C12	-3.88	111.09	123.22
24	6	306	BCR	C27-C26-C25	-3.88	117.10	122.73
24	3	307	BCR	C11-C12-C13	-3.88	115.53	126.42
24	A	847	BCR	C4-C5-C6	-3.87	117.11	122.73
38	5	303	LUT	C18-C5-C6	-3.87	120.18	124.53
24	6	305	BCR	C4-C5-C6	-3.87	117.11	122.73
24	A	844	BCR	C1-C6-C5	-3.87	117.17	122.61
22	9	303	CLA	C2D-C1D-ND	3.86	112.95	110.10
38	6	304	LUT	C18-C5-C6	-3.86	120.20	124.53
24	5	304	BCR	C4-C5-C6	-3.86	117.13	122.73
24	K	206	BCR	C33-C5-C6	-3.86	120.20	124.53
38	1	303	LUT	C31-C30-C29	-3.86	121.81	127.31
24	F	303	BCR	C11-C12-C13	-3.86	115.59	126.42
24	7	303	BCR	C33-C5-C6	-3.85	120.20	124.53
24	J	104	BCR	C24-C23-C22	-3.85	120.41	126.23
24	A	848	BCR	C33-C5-C4	3.85	121.02	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	820	LHG	O7-C7-C8	3.85	119.79	111.50
24	3	307	BCR	C30-C25-C26	-3.84	117.20	122.61
22	B	839	CLA	C1-C2-C3	-3.84	119.40	126.04
24	B	846	BCR	C20-C21-C22	-3.84	121.83	127.31
22	8	305	CLA	C1-C2-C3	-3.84	119.40	126.04
22	A	832	CLA	O2A-C1-C2	3.84	118.73	108.64
24	B	853	BCR	C24-C23-C22	-3.84	120.44	126.23
24	B	846	BCR	C15-C16-C17	-3.84	115.62	123.47
22	B	832	CLA	C1-C2-C3	-3.82	120.58	126.75
22	Z	308	CLA	C1-C2-C3	-3.81	119.45	126.04
22	6	309	CLA	C1-C2-C3	-3.81	119.46	126.04
38	8	303	LUT	C21-C26-C27	-3.81	107.89	112.70
22	5	309	CLA	C1-C2-C3	-3.80	119.46	126.04
22	F	301	CLA	C1-C2-C3	-3.80	119.46	126.04
38	6	304	LUT	C31-C30-C29	-3.80	121.88	127.31
24	5	304	BCR	C27-C26-C25	-3.80	117.21	122.73
24	A	847	BCR	C33-C5-C6	-3.80	120.26	124.53
24	A	845	BCR	C30-C25-C26	-3.79	117.28	122.61
38	8	303	LUT	C11-C10-C9	-3.79	121.90	127.31
22	Z	310	CLA	C1-C2-C3	-3.79	120.62	126.75
35	J	102	T7X	O16-C10-C12	3.78	119.66	111.50
24	B	846	BCR	C38-C26-C27	3.78	120.89	113.62
22	B	821	CLA	C1-C2-C3	-3.78	119.50	126.04
24	A	846	BCR	C16-C17-C18	-3.78	121.92	127.31
25	5	324	LHG	O7-C7-C8	3.78	119.64	111.50
38	1	302	LUT	C15-C14-C13	-3.76	121.94	127.31
27	A	852	DGA	CDB-CCB-CBB	-3.76	80.39	115.30
24	3	304	BCR	C2-C1-C6	3.76	116.27	110.48
24	L	204	BCR	C7-C8-C9	-3.75	120.56	126.23
38	Z	301	LUT	C7-C8-C9	-3.75	120.57	126.23
24	A	845	BCR	C7-C8-C9	-3.75	120.57	126.23
24	A	844	BCR	C34-C9-C10	-3.75	117.68	122.92
38	6	303	LUT	C18-C5-C6	-3.74	120.33	124.53
22	A	841	CLA	C1-C2-C3	-3.74	119.58	126.04
38	6	304	LUT	C21-C26-C27	-3.74	107.98	112.70
22	5	319	CLA	C1-C2-C3	-3.73	119.58	126.04
39	6	315	CHL	CHD-C1D-ND	-3.73	121.02	124.45
24	B	849	BCR	C15-C14-C13	-3.73	121.98	127.31
22	3	315	CLA	C2D-C1D-ND	3.73	112.85	110.10
38	3	303	LUT	C35-C34-C33	-3.73	121.99	127.31
32	F	306	RRX	C35-C13-C14	-3.73	117.70	122.92
24	K	206	BCR	C4-C5-C6	-3.73	117.32	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	308	CLA	C1-C2-C3	-3.73	119.60	126.04
39	5	321	CHL	CMA-C3A-C4A	3.73	121.79	111.77
22	A	816	CLA	C1-C2-C3	-3.73	119.60	126.04
27	A	852	DGA	OG2-CB1-CB2	3.72	119.52	111.50
24	3	304	BCR	C15-C14-C13	3.72	132.62	127.31
22	8	313	CLA	C1-C2-C3	-3.72	120.74	126.75
22	A	830	CLA	C1-C2-C3	-3.71	119.63	126.04
22	9	309	CLA	C2D-C1D-ND	3.71	112.84	110.10
38	Z	302	LUT	C31-C30-C29	-3.70	122.03	127.31
38	3	302	LUT	C31-C30-C29	-3.70	122.03	127.31
24	J	104	BCR	C11-C10-C9	-3.70	122.03	127.31
24	B	848	BCR	C15-C16-C17	-3.69	115.91	123.47
25	4	821	LHG	O7-C7-C8	3.69	119.46	111.50
24	A	848	BCR	C38-C26-C27	3.69	120.70	113.62
22	K	205	CLA	C2C-C1C-NC	3.68	113.42	109.97
22	A	808	CLA	C1-C2-C3	-3.68	119.67	126.04
22	7	322	CLA	C1-C2-C3	-3.68	119.67	126.04
24	A	846	BCR	C15-C16-C17	-3.68	115.93	123.47
22	5	310	CLA	C1-C2-C3	-3.68	119.68	126.04
22	B	809	CLA	C1-C2-C3	-3.68	119.68	126.04
38	4	802	LUT	C31-C30-C29	-3.68	122.06	127.31
24	K	206	BCR	C38-C26-C25	-3.68	120.40	124.53
22	6	302	CLA	C1-C2-C3	-3.67	119.69	126.04
39	Z	311	CHL	C1-C2-C3	-3.67	120.81	126.75
24	4	804	BCR	C11-C10-C9	-3.67	122.07	127.31
22	5	308	CLA	C1-C2-C3	-3.67	119.70	126.04
22	A	842	CLA	C1-C2-C3	-3.67	119.70	126.04
39	9	312	CHL	C1-O2A-CGA	3.67	126.06	116.44
21	A	801	CL0	C1-C2-C3	-3.67	119.70	126.04
22	B	828	CLA	C1-C2-C3	-3.66	119.70	126.04
24	J	104	BCR	C15-C14-C13	-3.66	122.09	127.31
22	7	312	CLA	C1-C2-C3	-3.65	119.72	126.04
22	B	815	CLA	C1-C2-C3	-3.65	119.73	126.04
39	6	318	CHL	C1-C2-C3	-3.64	119.75	126.04
22	A	809	CLA	C1-C2-C3	-3.64	119.75	126.04
24	L	204	BCR	C20-C21-C22	-3.64	122.12	127.31
24	3	304	BCR	C35-C13-C12	3.64	123.81	118.08
22	7	308	CLA	C1-C2-C3	-3.63	119.76	126.04
22	B	830	CLA	C1-C2-C3	-3.63	119.76	126.04
24	B	845	BCR	C33-C5-C4	3.63	120.59	113.62
24	B	847	BCR	C20-C21-C22	-3.63	122.13	127.31
22	6	309	CLA	CAA-C2A-C3A	-3.63	102.84	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	317	LHG	O7-C7-C8	3.63	119.32	111.50
24	A	848	BCR	C27-C26-C25	-3.63	117.47	122.73
22	5	320	CLA	O2D-CGD-CBD	3.62	117.71	111.27
22	8	307	CLA	C1-C2-C3	-3.62	119.78	126.04
41	7	319	3PH	O21-C21-C22	3.62	119.30	111.50
24	8	304	BCR	C38-C26-C27	3.62	120.57	113.62
22	A	840	CLA	C1-C2-C3	-3.62	119.78	126.04
22	7	304	CLA	C1-C2-C3	-3.61	119.80	126.04
38	7	302	LUT	C18-C5-C6	-3.61	120.47	124.53
38	9	302	LUT	C31-C30-C29	-3.61	122.16	127.31
24	B	849	BCR	C15-C16-C17	-3.61	116.09	123.47
38	9	301	LUT	C18-C5-C6	-3.60	120.48	124.53
24	J	104	BCR	C16-C17-C18	-3.60	122.17	127.31
22	9	310	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
22	3	310	CLA	CAA-C2A-C3A	-3.60	102.92	112.78
22	3	320	CLA	C2D-C1D-ND	3.60	112.75	110.10
24	5	304	BCR	C1-C6-C5	-3.60	117.55	122.61
22	1	310	CLA	C1-C2-C3	-3.60	119.83	126.04
38	5	302	LUT	C11-C10-C9	-3.59	122.18	127.31
24	J	104	BCR	C7-C8-C9	-3.59	120.81	126.23
22	6	308	CLA	C1-C2-C3	-3.59	119.84	126.04
22	8	308	CLA	C1-C2-C3	-3.59	119.84	126.04
38	3	302	LUT	C15-C14-C13	-3.58	122.20	127.31
24	K	206	BCR	C38-C26-C27	3.58	120.49	113.62
40	1	318	SQD	O7-S-C6	-3.58	102.69	106.94
22	A	803	CLA	C1-C2-C3	-3.58	119.86	126.04
24	B	846	BCR	C29-C30-C25	3.57	115.98	110.48
22	Z	309	CLA	C1-C2-C3	-3.57	119.86	126.04
22	B	818	CLA	C1-C2-C3	-3.57	119.87	126.04
32	F	306	RRX	C4-C5-C6	-3.57	117.55	122.73
24	5	305	BCR	C24-C23-C22	-3.57	120.84	126.23
24	5	304	BCR	C8-C7-C6	-3.56	117.19	127.20
22	K	205	CLA	C2D-C1D-ND	3.56	112.73	110.10
38	4	803	LUT	C21-C26-C27	-3.56	108.20	112.70
24	6	306	BCR	C20-C21-C22	-3.56	122.23	127.31
22	4	818	CLA	C1-C2-C3	-3.56	119.89	126.04
24	B	847	BCR	C15-C16-C17	-3.56	116.19	123.47
24	B	845	BCR	C24-C23-C22	-3.56	120.86	126.23
22	B	827	CLA	C1-C2-C3	-3.55	119.89	126.04
24	3	305	BCR	C11-C12-C13	-3.55	116.43	126.42
22	6	311	CLA	C1-C2-C3	-3.55	119.90	126.04
22	3	315	CLA	O2D-CGD-O1D	-3.55	116.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	852	DGD	O2G-C1B-C2B	3.55	119.16	111.50
22	A	838	CLA	C1-C2-C3	-3.55	119.91	126.04
24	F	303	BCR	C1-C6-C5	-3.55	117.62	122.61
39	Z	311	CHL	C3C-C4C-NC	-3.54	106.60	110.57
24	F	303	BCR	C15-C14-C13	-3.54	122.26	127.31
22	A	807	CLA	C1-C2-C3	-3.54	119.92	126.04
22	4	812	CLA	C1-C2-C3	-3.54	119.92	126.04
24	A	845	BCR	C27-C26-C25	-3.54	117.59	122.73
39	4	814	CHL	C1-C2-C3	-3.53	121.03	126.75
22	1	309	CLA	C1-C2-C3	-3.53	119.93	126.04
24	A	846	BCR	C4-C5-C6	-3.53	117.61	122.73
24	5	304	BCR	C11-C12-C13	-3.53	116.51	126.42
38	8	302	LUT	C21-C26-C27	-3.52	108.25	112.70
24	B	846	BCR	C4-C5-C6	-3.52	117.62	122.73
24	A	845	BCR	C24-C23-C22	-3.52	120.92	126.23
22	1	308	CLA	CHD-C1D-ND	-3.51	121.22	124.45
22	9	305	CLA	C2D-C1D-ND	3.51	112.69	110.10
24	B	844	BCR	C4-C5-C6	-3.51	117.63	122.73
24	B	849	BCR	C1-C6-C5	-3.51	117.67	122.61
22	3	313	CLA	C2D-C1D-ND	3.51	112.69	110.10
24	K	206	BCR	C1-C6-C5	-3.51	117.67	122.61
22	5	322	CLA	C1-C2-C3	-3.51	119.97	126.04
22	A	822	CLA	C1-C2-C3	-3.51	119.98	126.04
24	B	848	BCR	C15-C14-C13	-3.49	122.32	127.31
38	9	302	LUT	C18-C5-C6	-3.49	120.61	124.53
32	F	306	RRX	C16-C17-C18	-3.49	122.33	127.31
24	4	804	BCR	C2-C1-C6	3.49	115.85	110.48
22	B	834	CLA	C1-C2-C3	-3.48	120.02	126.04
22	9	305	CLA	C2C-C1C-NC	3.48	113.23	109.97
22	A	818	CLA	C1-C2-C3	-3.48	120.03	126.04
24	B	846	BCR	C38-C26-C25	-3.47	120.63	124.53
22	8	309	CLA	C1-C2-C3	-3.47	120.04	126.04
24	3	306	BCR	C33-C5-C6	-3.47	120.63	124.53
24	A	845	BCR	C38-C26-C27	3.46	120.27	113.62
22	1	311	CLA	C2C-C1C-NC	3.46	113.22	109.97
22	5	309	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
38	1	302	LUT	C18-C5-C4	3.46	120.77	114.36
22	B	835	CLA	CHD-C1D-ND	-3.45	121.28	124.45
24	7	303	BCR	C33-C5-C4	3.45	120.24	113.62
24	B	844	BCR	C34-C9-C10	-3.45	118.09	122.92
38	8	303	LUT	C7-C8-C9	-3.44	121.03	126.23
38	Z	302	LUT	C21-C26-C27	-3.44	108.35	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	805	CLA	C2C-C1C-NC	3.44	113.19	109.97
38	3	303	LUT	C31-C30-C29	-3.44	122.41	127.31
22	3	310	CLA	C1-C2-C3	-3.44	120.10	126.04
24	3	304	BCR	C24-C23-C22	-3.44	121.04	126.23
39	6	320	CHL	C4D-CHA-C1A	3.43	125.43	121.25
39	3	317	CHL	C2C-C3C-C4C	3.43	108.94	106.49
22	B	822	CLA	C1-C2-C3	-3.43	120.11	126.04
22	A	813	CLA	C2C-C1C-NC	3.43	113.19	109.97
22	B	805	CLA	C1-C2-C3	-3.43	120.11	126.04
22	B	806	CLA	C1-C2-C3	-3.43	120.11	126.04
39	8	315	CHL	C4D-CHA-C1A	3.43	125.42	121.25
38	9	302	LUT	C11-C10-C9	-3.43	122.42	127.31
22	B	816	CLA	C1-C2-C3	-3.42	120.12	126.04
24	G	203	BCR	C29-C30-C25	3.42	115.75	110.48
22	1	308	CLA	C1D-ND-C4D	-3.42	103.90	106.33
22	6	308	CLA	C6-C5-C3	-3.42	109.02	114.62
24	6	305	BCR	C29-C30-C25	3.42	115.75	110.48
24	G	203	BCR	C11-C12-C13	-3.42	116.82	126.42
24	L	204	BCR	C33-C5-C4	3.42	120.18	113.62
38	4	803	LUT	C31-C30-C29	-3.42	122.44	127.31
24	K	206	BCR	C27-C26-C25	-3.41	117.78	122.73
24	B	844	BCR	C1-C6-C5	-3.41	117.81	122.61
22	B	829	CLA	C1-C2-C3	-3.41	120.15	126.04
22	A	823	CLA	C1-C2-C3	-3.40	120.16	126.04
38	5	303	LUT	C31-C30-C29	-3.40	122.45	127.31
22	9	303	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
38	6	303	LUT	C1-C6-C5	-3.40	117.83	122.61
22	A	815	CLA	C1-C2-C3	-3.40	120.17	126.04
24	4	804	BCR	C33-C5-C4	3.39	120.14	113.62
22	7	304	CLA	CHD-C1D-ND	-3.39	121.33	124.45
38	4	802	LUT	C18-C5-C6	-3.39	120.72	124.53
24	4	804	BCR	C7-C8-C9	-3.39	121.11	126.23
22	7	306	CLA	C2C-C1C-NC	3.39	113.15	109.97
24	B	848	BCR	C11-C12-C13	-3.39	116.90	126.42
24	B	844	BCR	C27-C26-C25	-3.38	117.82	122.73
38	Z	302	LUT	C1-C6-C5	-3.38	117.85	122.61
22	5	315	CLA	C1-C2-C3	-3.38	120.20	126.04
22	3	311	CLA	C1-C2-C3	-3.38	120.20	126.04
24	B	849	BCR	C30-C25-C26	-3.38	117.86	122.61
22	B	842	CLA	C1-C2-C3	-3.38	120.20	126.04
22	9	303	CLA	C1D-ND-C4D	-3.37	103.94	106.33
24	3	305	BCR	C20-C21-C22	-3.37	122.50	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	848	BCR	C38-C26-C25	-3.37	120.74	124.53
24	A	846	BCR	C29-C30-C25	3.37	115.67	110.48
22	B	831	CLA	C1-C2-C3	-3.37	120.21	126.04
22	6	313	CLA	C1-C2-C3	-3.37	120.22	126.04
38	5	303	LUT	C1-C6-C5	-3.36	117.87	122.61
24	B	844	BCR	C36-C18-C17	-3.36	118.21	122.92
22	B	815	CLA	C2C-C1C-NC	3.36	113.12	109.97
39	4	813	CHL	C1-C2-C3	-3.36	121.32	126.75
24	6	305	BCR	C15-C16-C17	-3.36	116.60	123.47
22	Z	303	CLA	C1-C2-C3	-3.35	120.24	126.04
38	Z	301	LUT	C18-C5-C4	3.35	120.57	114.36
39	3	317	CHL	C3C-C4C-NC	-3.35	106.81	110.57
22	G	201	CLA	C2C-C1C-NC	3.35	113.11	109.97
22	9	305	CLA	C1-C2-C3	-3.35	120.25	126.04
22	9	309	CLA	C2C-C1C-NC	3.35	113.11	109.97
22	A	805	CLA	CHD-C1D-ND	-3.34	121.38	124.45
24	B	853	BCR	C4-C5-C6	-3.34	117.88	122.73
22	5	320	CLA	C2D-C1D-ND	3.34	112.57	110.10
22	4	806	CLA	C6-C5-C3	-3.34	109.16	114.62
24	G	203	BCR	C24-C23-C22	-3.34	121.19	126.23
24	A	848	BCR	C16-C17-C18	-3.34	122.55	127.31
22	F	302	CLA	C1-C2-C3	-3.34	120.27	126.04
22	3	318	CLA	C1-C2-C3	-3.33	120.28	126.04
39	4	819	CHL	C4D-CHA-C1A	3.33	125.31	121.25
22	7	311	CLA	C2D-C1D-ND	3.33	112.56	110.10
41	8	320	3PH	O21-C21-C22	3.33	120.08	110.80
22	6	308	CLA	C2D-C1D-ND	3.33	112.56	110.10
22	3	313	CLA	CHD-C1D-ND	-3.32	121.40	124.45
22	B	824	CLA	C2D-C1D-ND	3.32	112.55	110.10
22	6	301	CLA	C1-C2-C3	-3.32	120.30	126.04
24	3	307	BCR	C35-C13-C14	-3.32	118.27	122.92
32	F	306	RRX	C24-C23-C22	-3.32	121.22	126.23
22	Z	315	CLA	C2C-C1C-NC	3.32	113.08	109.97
22	4	807	CLA	C2C-C1C-NC	3.32	113.08	109.97
22	7	307	CLA	CHD-C1D-ND	-3.32	121.41	124.45
22	L	201	CLA	C2D-C1D-ND	3.32	112.55	110.10
22	4	808	CLA	C1-C2-C3	-3.31	120.31	126.04
22	5	313	CLA	C2C-C1C-NC	3.31	113.08	109.97
24	3	305	BCR	C15-C14-C13	-3.31	122.59	127.31
39	8	301	CHL	C3C-C4C-NC	-3.30	106.87	110.57
38	5	302	LUT	C35-C15-C14	-3.30	116.71	123.47
22	7	309	CLA	C2D-C1D-ND	3.30	112.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	202	CLA	CHD-C1D-ND	-3.30	121.42	124.45
38	8	302	LUT	C15-C14-C13	-3.30	122.60	127.31
22	3	315	CLA	C3B-C4B-NB	-3.30	107.46	110.52
22	L	202	CLA	C1-C2-C3	-3.29	120.35	126.04
22	6	312	CLA	C1-C2-C3	-3.29	120.35	126.04
39	4	816	CHL	C3B-C4B-NB	-3.29	107.46	110.52
22	Z	309	CLA	C2D-C1D-ND	3.29	112.53	110.10
24	B	845	BCR	C20-C21-C22	-3.29	122.62	127.31
22	1	304	CLA	C1-C2-C3	-3.29	120.36	126.04
22	9	307	CLA	C1-C2-C3	-3.29	120.36	126.04
24	6	305	BCR	C11-C12-C13	-3.29	117.19	126.42
24	A	856	BCR	C4-C5-C6	-3.28	117.96	122.73
22	A	816	CLA	C2C-C1C-NC	3.28	113.05	109.97
22	Z	307	CLA	CHD-C1D-ND	-3.28	121.44	124.45
22	L	201	CLA	C1-C2-C3	-3.28	120.37	126.04
38	8	303	LUT	C15-C14-C13	-3.28	122.63	127.31
22	1	308	CLA	C2D-C1D-ND	3.28	112.52	110.10
22	A	833	CLA	C1-C2-C3	-3.28	120.38	126.04
22	4	805	CLA	CMA-C3A-C4A	3.27	120.57	111.77
22	3	318	CLA	CHD-C1D-ND	-3.27	121.45	124.45
38	8	302	LUT	C11-C10-C9	-3.27	122.64	127.31
22	5	307	CLA	CHD-C1D-ND	-3.27	121.45	124.45
22	7	305	CLA	C2D-C1D-ND	3.27	112.51	110.10
38	1	303	LUT	C1-C6-C5	-3.27	118.01	122.61
22	A	805	CLA	C2D-C1D-ND	3.26	112.51	110.10
22	B	805	CLA	C2D-C1D-ND	3.26	112.51	110.10
24	A	847	BCR	C1-C6-C5	-3.26	118.02	122.61
22	K	204	CLA	CHD-C1D-ND	-3.26	121.45	124.45
22	7	304	CLA	C2D-C1D-ND	3.26	112.51	110.10
22	1	313	CLA	C2D-C1D-ND	3.26	112.51	110.10
36	J	105	C7Z	C31-C32-C33	-3.26	117.26	126.42
22	7	322	CLA	C2D-C1D-ND	3.26	112.51	110.10
22	A	839	CLA	C1-C2-C3	-3.26	120.41	126.04
22	A	842	CLA	C2C-C1C-NC	3.25	113.02	109.97
22	A	842	CLA	C6-C5-C3	-3.25	109.30	114.62
38	4	802	LUT	C21-C26-C27	-3.25	108.59	112.70
22	Z	308	CLA	CHD-C1D-ND	-3.25	121.47	124.45
22	B	834	CLA	C2C-C1C-NC	3.25	113.01	109.97
24	B	853	BCR	C30-C25-C26	-3.25	118.04	122.61
39	Z	311	CHL	C2C-C3C-C4C	3.24	108.80	106.49
22	B	838	CLA	CHD-C1D-ND	-3.24	121.47	124.45
22	1	316	CLA	C2D-C1D-ND	3.24	112.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	2	303	CHL	C4D-CHA-C1A	3.24	125.19	121.25
24	6	306	BCR	C33-C5-C4	3.24	119.84	113.62
39	2	303	CHL	C1-C2-C3	-3.24	121.51	126.75
22	1	308	CLA	C3B-C4B-NB	-3.24	107.51	110.52
22	B	839	CLA	C2C-C1C-NC	3.24	113.00	109.97
22	8	306	CLA	C1-C2-C3	-3.24	120.44	126.04
24	F	303	BCR	C38-C26-C27	3.24	119.83	113.62
24	B	846	BCR	C1-C6-C5	-3.23	118.06	122.61
22	7	310	CLA	C2D-C1D-ND	3.23	112.49	110.10
24	L	204	BCR	C11-C10-C9	-3.23	122.70	127.31
22	A	814	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	A	817	CLA	CMA-C3A-C4A	3.23	120.46	111.77
22	K	203	CLA	C2C-C1C-NC	3.23	113.00	109.97
39	5	317	CHL	C1-C2-C3	-3.23	121.53	126.75
22	9	308	CLA	C2C-C1C-NC	3.23	113.00	109.97
22	1	314	CLA	CHD-C1D-ND	-3.23	121.49	124.45
22	A	812	CLA	C2D-C1D-ND	3.23	112.48	110.10
22	6	310	CLA	C1-C2-C3	-3.23	120.47	126.04
24	3	306	BCR	C24-C23-C22	-3.22	121.36	126.23
22	A	818	CLA	C2D-C1D-ND	3.22	112.48	110.10
22	5	322	CLA	C2D-C1D-ND	3.22	112.48	110.10
22	F	302	CLA	C2D-C1D-ND	3.22	112.48	110.10
22	B	833	CLA	C1-C2-C3	-3.22	120.47	126.04
22	5	323	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	6	310	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	B	810	CLA	C2C-C1C-NC	3.22	112.99	109.97
22	5	326	CLA	C2D-C1D-ND	3.22	112.47	110.10
24	4	804	BCR	C30-C25-C26	-3.21	118.08	122.61
22	Z	305	CLA	C2C-C1C-NC	3.21	112.98	109.97
22	B	824	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	4	805	CLA	CHD-C1D-ND	-3.21	121.50	124.45
22	6	314	CLA	C2C-C1C-NC	3.21	112.98	109.97
24	A	848	BCR	C24-C23-C22	-3.21	121.39	126.23
38	9	302	LUT	C7-C8-C9	-3.21	121.39	126.23
22	A	827	CLA	C2D-C1D-ND	3.21	112.47	110.10
24	I	4001	BCR	C33-C5-C4	3.21	119.78	113.62
22	F	301	CLA	C2D-C1D-ND	3.21	112.47	110.10
24	5	305	BCR	C4-C5-C6	-3.21	118.08	122.73
22	A	833	CLA	C2D-C1D-ND	3.21	112.47	110.10
22	Z	313	CLA	C2D-C1D-ND	3.21	112.47	110.10
22	3	308	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	B	823	CLA	C1-C2-C3	-3.20	120.50	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	313	CLA	C1D-ND-C4D	-3.20	104.06	106.33
22	5	301	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	6	312	CLA	C2C-C1C-NC	3.20	112.97	109.97
22	2	304	CLA	C2D-C1D-ND	3.20	112.46	110.10
22	B	806	CLA	C2C-C1C-NC	3.20	112.97	109.97
38	8	302	LUT	C7-C8-C9	-3.20	121.40	126.23
24	5	305	BCR	C33-C5-C4	3.20	119.76	113.62
24	6	306	BCR	C1-C6-C5	-3.20	118.11	122.61
22	2	301	CLA	CHD-C1D-ND	-3.20	121.52	124.45
22	Z	303	CLA	C2D-C1D-ND	3.20	112.46	110.10
38	9	301	LUT	C15-C14-C13	-3.20	122.75	127.31
22	B	809	CLA	CHD-C1D-ND	-3.19	121.52	124.45
22	A	855	CLA	C1-C2-C3	-3.19	120.52	126.04
22	9	304	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	7	305	CLA	CHD-C1D-ND	-3.19	121.52	124.45
24	G	203	BCR	C7-C8-C9	-3.19	121.41	126.23
22	A	839	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	5	309	CLA	C2C-C1C-NC	3.19	112.96	109.97
38	8	302	LUT	C31-C30-C29	-3.19	122.76	127.31
22	9	303	CLA	C3B-C4B-NB	-3.19	107.56	110.52
22	A	810	CLA	C1-C2-C3	-3.19	120.53	126.04
22	5	315	CLA	C2D-C1D-ND	3.19	112.45	110.10
22	A	827	CLA	C1-C2-C3	-3.19	120.53	126.04
22	A	823	CLA	C1D-ND-C4D	-3.18	104.07	106.33
22	B	818	CLA	C2D-C1D-ND	3.18	112.45	110.10
24	3	307	BCR	C33-C5-C4	3.18	119.73	113.62
22	5	320	CLA	C1-C2-C3	-3.18	121.60	126.75
24	B	847	BCR	C38-C26-C27	3.18	119.73	113.62
22	Z	308	CLA	C2D-C1D-ND	3.18	112.45	110.10
22	A	822	CLA	C2C-C1C-NC	3.18	112.95	109.97
22	B	806	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	5	304	BCR	C38-C26-C27	3.18	119.73	113.62
24	B	844	BCR	C30-C25-C26	-3.18	118.13	122.61
22	A	812	CLA	C1-C2-C3	-3.18	120.54	126.04
38	8	303	LUT	C31-C30-C29	-3.18	122.77	127.31
22	1	307	CLA	CHD-C1D-ND	-3.18	121.53	124.45
22	B	815	CLA	CMA-C3A-C4A	3.18	120.31	111.77
22	Z	305	CLA	C2D-C1D-ND	3.18	112.45	110.10
22	6	309	CLA	C2C-C1C-NC	3.18	112.95	109.97
22	9	305	CLA	CMA-C3A-C4A	3.18	120.31	111.77
22	A	824	CLA	C2D-C1D-ND	3.18	112.44	110.10
22	4	812	CLA	C2C-C1C-NC	3.18	112.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	314	CLA	C2D-C1D-ND	3.18	112.44	110.10
24	5	304	BCR	C15-C16-C17	-3.18	116.97	123.47
22	A	817	CLA	C2C-C1C-NC	3.17	112.95	109.97
22	B	811	CLA	C2C-C1C-NC	3.17	112.95	109.97
22	6	311	CLA	C2C-C1C-NC	3.17	112.95	109.97
22	B	811	CLA	C1-C2-C3	-3.17	120.55	126.04
22	A	802	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	2	301	CLA	CMA-C3A-C4A	3.17	120.30	111.77
22	Z	304	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	Z	305	CLA	C1-C2-C3	-3.17	120.56	126.04
22	A	810	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	A	819	CLA	C1-C2-C3	-3.17	120.56	126.04
22	A	823	CLA	C2D-C1D-ND	3.17	112.44	110.10
24	8	304	BCR	C33-C5-C4	3.17	119.71	113.62
22	K	204	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	Z	310	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	5	319	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	7	312	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	3	310	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	B	813	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	6	311	CLA	CHD-C1D-ND	-3.17	121.54	124.45
22	1	310	CLA	C2C-C1C-NC	3.17	112.94	109.97
22	4	807	CLA	C2D-C1D-ND	3.17	112.44	110.10
24	8	304	BCR	C38-C26-C25	-3.16	120.97	124.53
24	B	849	BCR	C33-C5-C4	3.16	119.69	113.62
22	6	314	CLA	C1-C2-C3	-3.16	120.57	126.04
22	Z	303	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	4	811	CLA	C2D-C1D-ND	3.16	112.43	110.10
22	3	322	CLA	CHD-C1D-ND	-3.16	121.55	124.45
24	B	849	BCR	C33-C5-C6	-3.16	120.98	124.53
22	A	839	CLA	CHD-C1D-ND	-3.16	121.55	124.45
22	B	832	CLA	CHD-C1D-ND	-3.16	121.55	124.45
39	5	321	CHL	C3C-C4C-NC	-3.16	107.03	110.57
36	5	306	C7Z	C21-C26-C25	-3.16	118.16	122.61
22	A	837	CLA	C1-C2-C3	-3.16	120.58	126.04
22	8	307	CLA	C2C-C1C-NC	3.16	112.93	109.97
22	B	821	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	A	823	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	3	319	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	5	309	CLA	C2D-C1D-ND	3.15	112.43	110.10
22	3	319	CLA	C2C-C1C-NC	3.15	112.92	109.97
22	B	819	CLA	C1-C2-C3	-3.15	120.59	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	318	CLA	C2D-C1D-ND	3.15	112.43	110.10
22	3	312	CLA	C2C-C1C-NC	3.15	112.92	109.97
22	A	803	CLA	C2D-C1D-ND	3.15	112.42	110.10
24	B	844	BCR	C24-C23-C22	-3.15	121.48	126.23
22	B	842	CLA	C2C-C1C-NC	3.15	112.92	109.97
22	B	841	CLA	C2D-C1D-ND	3.15	112.42	110.10
22	B	801	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	K	204	CLA	C2D-C1D-ND	3.15	112.42	110.10
22	J	103	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	5	323	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	Z	316	CLA	CHD-C1D-ND	-3.14	121.56	124.45
24	G	203	BCR	C8-C7-C6	-3.14	118.37	127.20
22	B	830	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	2	302	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	B	836	CLA	CHD-C1D-ND	-3.14	121.57	124.45
25	9	315	LHG	O7-C7-C8	3.14	118.27	111.50
22	7	311	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	A	827	CLA	C2C-C1C-NC	3.14	112.92	109.97
22	B	811	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	6	317	CLA	C2D-C1D-ND	3.14	112.42	110.10
39	6	316	CHL	C4D-CHA-C1A	3.14	125.07	121.25
22	5	301	CLA	C1-C2-C3	-3.14	120.61	126.04
22	9	303	CLA	O2A-CGA-CBA	3.14	121.76	111.91
38	7	301	LUT	C31-C30-C29	-3.14	122.83	127.31
22	B	808	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	7	314	CLA	CHD-C1D-ND	-3.14	121.57	124.45
22	8	313	CLA	C2D-C1D-ND	3.14	112.42	110.10
22	4	809	CLA	C2C-C1C-NC	3.14	112.91	109.97
22	6	302	CLA	C2C-C1C-NC	3.14	112.91	109.97
24	A	848	BCR	C33-C5-C6	-3.14	121.01	124.53
22	Z	307	CLA	CMA-C3A-C4A	3.14	120.20	111.77
24	B	849	BCR	C11-C10-C9	-3.13	122.84	127.31
22	B	817	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	8	310	CLA	CHD-C1D-ND	-3.13	121.58	124.45
38	7	302	LUT	C21-C26-C27	-3.13	108.74	112.70
22	B	812	CLA	C2C-C1C-NC	3.13	112.91	109.97
22	8	305	CLA	C2C-C1C-NC	3.13	112.91	109.97
24	A	848	BCR	C20-C19-C18	-3.13	117.62	126.42
22	A	854	CLA	CHD-C1D-ND	-3.13	121.58	124.45
22	1	305	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	7	312	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	4	808	CLA	C2C-C1C-NC	3.13	112.90	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	825	CLA	CHD-C1D-ND	-3.13	121.58	124.45
39	6	316	CHL	CMA-C3A-C4A	3.13	120.18	111.77
22	8	307	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	4	815	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	Z	307	CLA	C2C-C1C-NC	3.13	112.90	109.97
38	7	301	LUT	C18-C5-C4	3.13	120.15	114.36
23	A	843	PQN	C11-C12-C13	-3.13	121.59	126.79
22	8	308	CLA	C2D-C1D-ND	3.13	112.41	110.10
24	6	305	BCR	C33-C5-C4	3.13	119.62	113.62
24	3	307	BCR	C23-C22-C21	3.13	123.74	118.94
22	A	834	CLA	C1-C2-C3	-3.13	120.64	126.04
22	A	838	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	3	320	CLA	C2C-C1C-NC	3.13	112.90	109.97
22	A	825	CLA	CMA-C3A-C4A	3.12	120.17	111.77
22	A	805	CLA	C1-C2-C3	-3.12	120.64	126.04
22	A	808	CLA	C2C-C1C-NC	3.12	112.90	109.97
24	3	307	BCR	C37-C22-C21	-3.12	118.55	122.92
22	A	808	CLA	C2D-C1D-ND	3.12	112.41	110.10
22	2	304	CLA	C2C-C1C-NC	3.12	112.90	109.97
39	1	312	CHL	CMA-C3A-C4A	3.12	120.16	111.77
22	1	307	CLA	CMA-C3A-C4A	3.12	120.16	111.77
22	6	322	CLA	C2C-C1C-NC	3.12	112.90	109.97
22	B	828	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	6	302	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	8	305	CLA	CMA-C3A-C4A	3.12	120.16	111.77
22	B	811	CLA	CMA-C3A-C4A	3.12	120.16	111.77
22	6	314	CLA	CMA-C3A-C4A	3.12	120.16	111.77
22	Z	310	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	3	316	CLA	C2C-C1C-NC	3.12	112.89	109.97
22	3	310	CLA	CMA-C3A-C4A	3.12	120.15	111.77
39	6	316	CHL	C1-C2-C3	-3.12	121.71	126.75
22	A	809	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	B	819	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	B	823	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	9	311	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	Z	313	CLA	C2C-C1C-NC	3.12	112.89	109.97
22	B	819	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	8	305	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	B	836	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	5	311	CLA	C2D-C1D-ND	3.12	112.40	110.10
22	A	837	CLA	CHD-C1D-ND	-3.11	121.59	124.45
22	A	823	CLA	C3B-C4B-NB	-3.11	107.63	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	812	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	A	816	CLA	CMA-C3A-C4A	3.11	120.14	111.77
22	A	829	CLA	C2C-C1C-NC	3.11	112.89	109.97
22	A	809	CLA	CHD-C1D-ND	-3.11	121.59	124.45
22	9	308	CLA	CMA-C3A-C4A	3.11	120.14	111.77
22	A	811	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	A	841	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	B	827	CLA	C2C-C1C-NC	3.11	112.89	109.97
22	B	807	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	B	808	CLA	C2D-C1D-ND	3.11	112.40	110.10
22	B	813	CLA	C2C-C1C-NC	3.11	112.89	109.97
22	7	310	CLA	C2C-C1C-NC	3.11	112.89	109.97
24	5	305	BCR	C36-C18-C19	3.11	122.97	118.08
22	B	820	CLA	C2C-C1C-NC	3.11	112.88	109.97
22	2	302	CLA	C2C-C1C-NC	3.11	112.88	109.97
22	A	819	CLA	CHD-C1D-ND	-3.11	121.60	124.45
39	4	819	CHL	C3C-C4C-NC	-3.11	107.09	110.57
22	A	829	CLA	C2D-C1D-ND	3.11	112.39	110.10
22	3	309	CLA	C2D-C1D-ND	3.11	112.39	110.10
22	B	829	CLA	C2C-C1C-NC	3.11	112.88	109.97
39	8	301	CHL	C2C-C3C-C4C	3.11	108.70	106.49
22	1	309	CLA	CHD-C1D-ND	-3.11	121.60	124.45
22	8	313	CLA	CHD-C1D-ND	-3.11	121.60	124.45
38	3	303	LUT	C1-C6-C5	-3.11	118.24	122.61
23	B	843	PQN	C14-C13-C15	3.11	120.50	115.27
22	B	840	CLA	C1-C2-C3	-3.10	120.67	126.04
39	4	816	CHL	C3C-C4C-NC	-3.10	107.09	110.57
22	A	838	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	A	832	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	B	840	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	8	308	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	9	303	CLA	C4B-CHC-C1C	3.10	133.70	126.34
22	9	307	CLA	CMA-C3A-C4A	3.10	120.11	111.77
22	A	826	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	B	817	CLA	C1-C2-C3	-3.10	120.68	126.04
24	3	306	BCR	C33-C5-C4	3.10	119.58	113.62
22	A	836	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	7	316	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	4	809	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	3	316	CLA	C6-C5-C3	-3.10	109.55	114.62
22	7	309	CLA	CHD-C1D-ND	-3.10	121.60	124.45
22	3	312	CLA	C2D-C1D-ND	3.10	112.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	811	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	B	829	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	A	840	CLA	C2C-C1C-NC	3.10	112.88	109.97
22	7	323	CLA	C2C-C1C-NC	3.10	112.88	109.97
24	B	847	BCR	C11-C12-C13	-3.10	117.71	126.42
24	B	848	BCR	C38-C26-C27	3.10	119.57	113.62
22	A	802	CLA	C2C-C1C-NC	3.10	112.87	109.97
38	6	304	LUT	C1-C6-C5	-3.10	118.25	122.61
38	5	302	LUT	C21-C26-C27	-3.10	108.79	112.70
24	B	853	BCR	C33-C5-C4	3.10	119.56	113.62
22	A	820	CLA	C2C-C1C-NC	3.10	112.87	109.97
22	5	314	CLA	C2C-C1C-NC	3.10	112.87	109.97
22	3	311	CLA	C2D-C1D-ND	3.10	112.39	110.10
22	7	304	CLA	CMA-C3A-C4A	3.10	120.09	111.77
22	4	808	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	5	314	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	A	818	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	A	837	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	B	839	CLA	CHD-C1D-ND	-3.09	121.61	124.45
22	6	307	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	1	315	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	5	318	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	9	313	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	9	310	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	A	806	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	B	833	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	7	305	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	1	311	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	B	833	CLA	CHD-C1D-ND	-3.09	121.62	124.45
38	6	303	LUT	C11-C10-C9	-3.09	122.90	127.31
22	B	825	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	4	817	CLA	C2D-C1D-ND	3.09	112.38	110.10
39	6	315	CHL	C4D-CHA-C1A	3.09	125.00	121.25
22	1	313	CLA	CHD-C1D-ND	-3.09	121.62	124.45
22	3	314	CLA	C2C-C1C-NC	3.09	112.86	109.97
22	6	301	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	5	301	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	A	804	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	Z	316	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	B	807	CLA	CHD-C1D-ND	-3.08	121.62	124.45
22	4	810	CLA	CHD-C1D-ND	-3.08	121.62	124.45
22	5	318	CLA	CHD-C1D-ND	-3.08	121.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	323	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	B	812	CLA	C1-C2-C3	-3.08	120.71	126.04
24	B	847	BCR	C16-C17-C18	-3.08	122.91	127.31
38	6	303	LUT	C22-C23-C24	3.08	115.25	111.74
22	9	305	CLA	C2A-C1A-CHA	3.08	129.25	123.86
22	6	322	CLA	C1-C2-C3	-3.08	120.72	126.04
22	Z	310	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	5	308	CLA	CHD-C1D-ND	-3.08	121.62	124.45
22	B	840	CLA	C2C-C1C-NC	3.08	112.86	109.97
22	A	831	CLA	CHD-C1D-ND	-3.08	121.63	124.45
22	7	312	CLA	CHD-C1D-ND	-3.08	121.63	124.45
22	B	841	CLA	C2C-C1C-NC	3.08	112.85	109.97
22	5	311	CLA	C2C-C1C-NC	3.08	112.85	109.97
22	8	311	CLA	C2D-C1D-ND	3.08	112.37	110.10
22	B	818	CLA	CHD-C1D-ND	-3.08	121.63	124.45
22	L	203	CLA	CHD-C1D-ND	-3.08	121.63	124.45
22	8	311	CLA	C2C-C1C-NC	3.08	112.85	109.97
22	B	823	CLA	CHD-C1D-ND	-3.08	121.63	124.45
24	A	846	BCR	C33-C5-C4	3.07	119.52	113.62
22	6	310	CLA	C2D-C1D-ND	3.07	112.37	110.10
38	7	301	LUT	C18-C5-C6	-3.07	121.08	124.53
22	5	308	CLA	C2D-C1D-ND	3.07	112.37	110.10
22	8	308	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	5	301	CLA	C2C-C1C-NC	3.07	112.85	109.97
36	5	306	C7Z	C11-C12-C13	-3.07	117.78	126.42
22	A	836	CLA	C1-C2-C3	-3.07	120.73	126.04
22	4	812	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	2	301	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	7	314	CLA	C2D-C1D-ND	3.07	112.37	110.10
22	4	818	CLA	C2D-C1D-ND	3.07	112.37	110.10
22	A	828	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	5	320	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	B	825	CLA	CMA-C3A-C4A	3.07	120.02	111.77
22	B	835	CLA	C2D-C1D-ND	3.07	112.37	110.10
22	4	808	CLA	C2D-C1D-ND	3.07	112.37	110.10
22	5	319	CLA	CHD-C1D-ND	-3.07	121.63	124.45
22	F	304	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	9	306	CLA	CHD-C1D-ND	-3.07	121.64	124.45
22	A	807	CLA	C2C-C1C-NC	3.07	112.84	109.97
22	A	837	CLA	C2D-C1D-ND	3.07	112.36	110.10
22	B	833	CLA	C2D-C1D-ND	3.07	112.36	110.10
22	A	821	CLA	CHD-C1D-ND	-3.07	121.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	322	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	9	311	CLA	C2C-C1C-NC	3.06	112.84	109.97
36	5	306	C7Z	C18-C5-C4	3.06	120.03	114.36
22	6	321	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	L	201	CLA	CHD-C1D-ND	-3.06	121.64	124.45
38	1	302	LUT	C18-C5-C6	-3.06	121.09	124.53
22	1	306	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	6	313	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	7	322	CLA	CHD-C1D-ND	-3.06	121.64	124.45
22	K	205	CLA	CMD-C2D-C1D	3.06	130.11	124.71
22	B	829	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	A	825	CLA	CHD-C1D-ND	-3.06	121.64	124.45
39	4	814	CHL	C3C-C4C-NC	-3.06	107.14	110.57
22	1	304	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	9	310	CLA	C3B-C4B-NB	-3.06	107.68	110.52
22	3	319	CLA	C1-C2-C3	-3.06	120.75	126.04
22	L	203	CLA	C2C-C1C-NC	3.06	112.84	109.97
22	A	834	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	A	836	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	7	315	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	7	305	CLA	CMA-C3A-C4A	3.06	119.99	111.77
22	4	806	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	A	835	CLA	CHD-C1D-ND	-3.06	121.65	124.45
39	1	312	CHL	C4D-CHA-C1A	3.06	124.97	121.25
24	B	845	BCR	C38-C26-C27	3.05	119.48	113.62
22	B	821	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	G	202	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	7	309	CLA	C2C-C1C-NC	3.05	112.83	109.97
24	A	844	BCR	C38-C26-C27	3.05	119.48	113.62
39	6	320	CHL	C3C-C4C-NC	-3.05	107.15	110.57
22	B	809	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	A	811	CLA	C3B-C4B-NB	-3.05	107.68	110.52
22	7	317	CLA	CHD-C1D-ND	-3.05	121.65	124.45
22	Z	309	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	F	305	CLA	CHD-C1D-ND	-3.05	121.65	124.45
22	Z	304	CLA	C2C-C1C-NC	3.05	112.83	109.97
24	A	846	BCR	C1-C6-C5	-3.05	118.32	122.61
22	K	204	CLA	CMA-C3A-C4A	3.05	119.97	111.77
22	B	835	CLA	C1D-ND-C4D	-3.05	104.17	106.33
22	B	827	CLA	CHD-C1D-ND	-3.05	121.65	124.45
22	1	314	CLA	C1-C2-C3	-3.05	120.77	126.04
24	3	306	BCR	C38-C26-C27	3.05	119.47	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	319	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	K	202	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	5	312	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	6	317	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	A	835	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	K	202	CLA	C2D-C1D-ND	3.05	112.35	110.10
22	A	834	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	B	837	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	1	307	CLA	C2C-C1C-NC	3.04	112.82	109.97
24	A	844	BCR	C4-C5-C6	-3.04	118.31	122.73
24	6	305	BCR	C38-C26-C27	3.04	119.46	113.62
22	6	312	CLA	C2D-C1D-ND	3.04	112.35	110.10
22	6	314	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	A	832	CLA	C2D-C1D-ND	3.04	112.35	110.10
22	1	304	CLA	C2D-C1D-ND	3.04	112.35	110.10
22	8	314	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	4	811	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	Z	314	CLA	C1-C2-C3	-3.04	120.78	126.04
24	3	305	BCR	C1-C6-C5	-3.04	118.33	122.61
22	B	816	CLA	CHD-C1D-ND	-3.04	121.66	124.45
39	6	318	CHL	C4D-CHA-C1A	3.04	124.95	121.25
22	8	310	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	4	810	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	A	831	CLA	C2D-C1D-ND	3.04	112.34	110.10
22	B	827	CLA	C2D-C1D-ND	3.04	112.34	110.10
22	J	103	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	5	310	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	9	308	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	1	313	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	3	313	CLA	C1-C2-C3	-3.04	120.79	126.04
22	K	203	CLA	C2D-C1D-ND	3.04	112.34	110.10
22	7	324	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	A	805	CLA	CMA-C3A-C4A	3.04	119.94	111.77
22	A	832	CLA	C2C-C1C-NC	3.04	112.82	109.97
22	6	301	CLA	C2C-C1C-NC	3.04	112.82	109.97
24	B	853	BCR	C36-C18-C17	-3.04	118.67	122.92
39	Z	311	CHL	CMA-C3A-C4A	3.04	119.93	111.77
24	3	307	BCR	C36-C18-C19	3.04	122.86	118.08
22	3	309	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	7	324	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	B	801	CLA	C2D-C1D-ND	3.04	112.34	110.10
22	B	810	CLA	C2D-C1D-ND	3.04	112.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	832	CLA	C2D-C1D-ND	3.04	112.34	110.10
22	A	842	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	Z	315	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	A	825	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	7	304	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	A	807	CLA	C2D-C1D-ND	3.03	112.34	110.10
22	1	306	CLA	CHD-C1D-ND	-3.03	121.67	124.45
24	4	804	BCR	C33-C5-C6	-3.03	121.12	124.53
22	L	201	CLA	C1D-ND-C4D	-3.03	104.18	106.33
24	B	853	BCR	C11-C10-C9	-3.03	122.98	127.31
22	B	834	CLA	C2D-C1D-ND	3.03	112.34	110.10
22	K	202	CLA	CMA-C3A-C4A	3.03	119.92	111.77
39	2	303	CHL	C3C-C4C-NC	-3.03	107.17	110.57
22	6	321	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	9	306	CLA	C2C-C1C-NC	3.03	112.81	109.97
24	7	303	BCR	C7-C8-C9	-3.03	121.66	126.23
22	A	802	CLA	C2D-C1D-ND	3.03	112.34	110.10
22	G	201	CLA	C2D-C1D-ND	3.03	112.34	110.10
22	A	808	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	8	309	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	8	313	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	5	326	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	A	855	CLA	CHD-C1D-ND	-3.03	121.67	124.45
36	J	105	C7Z	C38-C25-C24	3.03	119.96	114.36
22	L	201	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	5	307	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	5	322	CLA	C2C-C1C-NC	3.03	112.81	109.97
22	8	309	CLA	C2D-C1D-ND	3.03	112.33	110.10
22	B	831	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	A	803	CLA	CHD-C1D-ND	-3.02	121.67	124.45
22	7	308	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	9	313	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	3	316	CLA	C1-C2-C3	-3.02	120.81	126.04
39	Z	312	CHL	C4D-CHA-C1A	3.02	124.93	121.25
22	L	202	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	7	324	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	A	831	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	A	814	CLA	CHD-C1D-ND	-3.02	121.68	124.45
22	2	304	CLA	CMA-C3A-C4A	3.02	119.89	111.77
22	A	821	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	F	304	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	5	315	CLA	C3B-C4B-NB	-3.02	107.71	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	313	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	5	315	CLA	CMA-C3A-C4A	3.02	119.89	111.77
22	B	822	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	3	319	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	5	312	CLA	CHD-C1D-ND	-3.02	121.68	124.45
21	A	801	CL0	CMC-C2C-C1C	3.02	129.63	125.04
22	6	308	CLA	CHD-C1D-ND	-3.02	121.68	124.45
24	3	305	BCR	C16-C17-C18	-3.02	123.00	127.31
22	A	822	CLA	CMA-C3A-C4A	3.02	119.88	111.77
22	1	309	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	7	308	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	B	832	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	J	103	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	9	306	CLA	C2D-C1D-ND	3.02	112.33	110.10
22	8	311	CLA	C3B-C4B-NB	-3.01	107.72	110.52
22	B	828	CLA	CHD-C1D-ND	-3.01	121.68	124.45
22	7	304	CLA	C1D-ND-C4D	-3.01	104.19	106.33
22	B	830	CLA	CMA-C3A-C4A	3.01	119.87	111.77
24	3	306	BCR	C20-C21-C22	-3.01	123.01	127.31
22	6	308	CLA	C2C-C1C-NC	3.01	112.80	109.97
22	A	838	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	A	815	CLA	C2D-C1D-ND	3.01	112.32	110.10
22	B	830	CLA	C2C-C1C-NC	3.01	112.79	109.97
22	B	812	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	B	813	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	7	323	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	9	307	CLA	C2C-C1C-NC	3.01	112.79	109.97
24	A	846	BCR	C27-C26-C25	-3.01	118.36	122.73
24	8	304	BCR	C27-C26-C25	-3.01	118.36	122.73
22	A	806	CLA	C2D-C1D-ND	3.01	112.32	110.10
22	B	823	CLA	CMA-C3A-C4A	3.01	119.86	111.77
38	4	803	LUT	C18-C5-C4	3.01	119.93	114.36
22	A	823	CLA	CMA-C3A-C4A	3.01	119.86	111.77
39	5	316	CHL	C4D-CHA-C1A	3.01	124.91	121.25
22	F	302	CLA	CMA-C3A-C4A	3.01	119.86	111.77
22	A	824	CLA	C2C-C1C-NC	3.01	112.79	109.97
38	7	302	LUT	C31-C30-C29	-3.01	123.02	127.31
22	1	306	CLA	CMA-C3A-C4A	3.01	119.85	111.77
22	F	301	CLA	C2C-C1C-NC	3.01	112.79	109.97
22	7	306	CLA	C2D-C1D-ND	3.01	112.32	110.10
22	A	841	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	4	817	CLA	CHD-C1D-ND	-3.01	121.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	818	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	A	841	CLA	C1D-ND-C4D	-3.01	104.20	106.33
22	4	806	CLA	C3B-C4B-NB	-3.01	107.73	110.52
22	5	309	CLA	CMA-C3A-C4A	3.00	119.85	111.77
24	B	848	BCR	C33-C5-C4	3.00	119.39	113.62
22	7	316	CLA	CHD-C1D-ND	-3.00	121.69	124.45
22	B	831	CLA	C2C-C1C-NC	3.00	112.79	109.97
22	B	814	CLA	CHD-C1D-ND	-3.00	121.69	124.45
22	5	319	CLA	C2D-C1D-ND	3.00	112.32	110.10
22	B	842	CLA	CHD-C1D-ND	-3.00	121.69	124.45
22	6	313	CLA	C2D-C1D-ND	3.00	112.32	110.10
22	A	818	CLA	C1D-ND-C4D	-3.00	104.20	106.33
22	B	818	CLA	C1D-ND-C4D	-3.00	104.20	106.33
39	5	316	CHL	C3B-C4B-NB	-3.00	107.73	110.52
22	A	820	CLA	C2D-C1D-ND	3.00	112.31	110.10
22	B	826	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	1	304	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	6	310	CLA	C3B-C4B-NB	-3.00	107.73	110.52
22	B	826	CLA	C2C-C1C-NC	3.00	112.78	109.97
22	4	806	CLA	C2C-C1C-NC	3.00	112.78	109.97
22	B	807	CLA	CMA-C3A-C4A	3.00	119.83	111.77
38	5	302	LUT	C1-C6-C5	-3.00	118.39	122.61
22	4	811	CLA	C1-C2-C3	-3.00	120.86	126.04
22	A	825	CLA	C2D-C1D-ND	3.00	112.31	110.10
22	3	314	CLA	C2D-C1D-ND	3.00	112.31	110.10
22	A	838	CLA	CMA-C3A-C4A	3.00	119.83	111.77
22	F	302	CLA	C2C-C1C-NC	3.00	112.78	109.97
22	6	309	CLA	CMA-C3A-C4A	3.00	119.83	111.77
22	B	824	CLA	C1D-ND-C4D	-3.00	104.21	106.33
22	F	301	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	6	312	CLA	CHD-C1D-ND	-3.00	121.70	124.45
22	A	814	CLA	C2D-C1D-ND	3.00	112.31	110.10
22	L	203	CLA	C2D-C1D-ND	2.99	112.31	110.10
22	9	303	CLA	CHD-C1D-ND	-2.99	121.70	124.45
22	A	841	CLA	C3B-C4B-NB	-2.99	107.74	110.52
22	Z	314	CLA	C2C-C1C-NC	2.99	112.78	109.97
22	8	316	CLA	C2C-C1C-NC	2.99	112.78	109.97
22	B	823	CLA	C1D-ND-C4D	-2.99	104.21	106.33
22	7	311	CLA	C1D-ND-C4D	-2.99	104.21	106.33
22	A	830	CLA	CMA-C3A-C4A	2.99	119.82	111.77
22	B	815	CLA	CHD-C1D-ND	-2.99	121.70	124.45
22	A	818	CLA	CMA-C3A-C4A	2.99	119.82	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	811	CLA	C1D-ND-C4D	-2.99	104.21	106.33
22	B	823	CLA	C3B-C4B-NB	-2.99	107.74	110.52
22	A	818	CLA	C2C-C1C-NC	2.99	112.78	109.97
22	7	311	CLA	C2C-C1C-NC	2.99	112.78	109.97
22	1	308	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
22	A	829	CLA	CMA-C3A-C4A	2.99	119.81	111.77
22	A	807	CLA	CHD-C1D-ND	-2.99	121.70	124.45
22	L	202	CLA	CHD-C1D-ND	-2.99	121.70	124.45
39	6	320	CHL	C3B-C4B-NB	-2.99	107.74	110.52
22	6	321	CLA	CMA-C3A-C4A	2.99	119.81	111.77
22	A	830	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	6	322	CLA	CHD-C1D-ND	-2.99	121.71	124.45
22	9	310	CLA	CMA-C3A-C4A	2.99	119.81	111.77
22	A	828	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	B	810	CLA	CMA-C3A-C4A	2.99	119.81	111.77
22	A	833	CLA	CHD-C1D-ND	-2.99	121.71	124.45
22	B	805	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	L	202	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	7	314	CLA	C2C-C1C-NC	2.99	112.77	109.97
39	8	315	CHL	C3C-C4C-NC	-2.99	107.22	110.57
22	A	813	CLA	C1-C2-C3	-2.99	120.88	126.04
22	7	314	CLA	CMA-C3A-C4A	2.99	119.80	111.77
22	A	836	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	A	828	CLA	C2D-C1D-ND	2.99	112.31	110.10
22	3	310	CLA	C2D-C1D-ND	2.99	112.31	110.10
22	Z	308	CLA	C1D-ND-C4D	-2.99	104.21	106.33
22	4	815	CLA	CMA-C3A-C4A	2.99	119.80	111.77
22	Z	306	CLA	CHD-C1D-ND	-2.98	121.71	124.45
39	8	312	CHL	C4D-CHA-C1A	2.98	124.88	121.25
22	A	805	CLA	C1D-ND-C4D	-2.98	104.22	106.33
24	B	846	BCR	C34-C9-C10	-2.98	118.74	122.92
22	4	810	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	5	308	CLA	C2C-C1C-NC	2.98	112.77	109.97
22	B	836	CLA	CMA-C3A-C4A	2.98	119.79	111.77
22	B	838	CLA	C2C-C1C-NC	2.98	112.77	109.97
22	A	811	CLA	C1-C2-C3	-2.98	120.89	126.04
22	7	306	CLA	CMA-C3A-C4A	2.98	119.79	111.77
39	6	320	CHL	C4B-CHC-C1C	2.98	133.41	126.34
22	8	309	CLA	CHD-C1D-ND	-2.98	121.71	124.45
22	A	826	CLA	C2C-C1C-NC	2.98	112.77	109.97
22	3	308	CLA	C2C-C1C-NC	2.98	112.77	109.97
22	5	323	CLA	C2C-C1C-NC	2.98	112.77	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	844	BCR	C33-C5-C4	2.98	119.34	113.62
22	A	830	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	K	203	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	A	815	CLA	C2C-C1C-NC	2.98	112.76	109.97
22	7	317	CLA	C2C-C1C-NC	2.98	112.76	109.97
22	A	854	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	9	308	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	B	808	CLA	C1-C2-C3	-2.98	120.89	126.04
22	B	819	CLA	C2C-C1C-NC	2.98	112.76	109.97
24	K	206	BCR	C33-C5-C4	2.98	119.34	113.62
22	A	813	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	A	840	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	3	316	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	Z	316	CLA	C2C-C1C-NC	2.98	112.76	109.97
22	7	307	CLA	C2C-C1C-NC	2.98	112.76	109.97
38	1	302	LUT	C31-C30-C29	-2.98	123.06	127.31
22	6	301	CLA	CHD-C1D-ND	-2.98	121.72	124.45
22	A	834	CLA	C2C-C1C-NC	2.98	112.76	109.97
39	9	314	CHL	C4D-CHA-C1A	2.98	124.87	121.25
22	B	814	CLA	C1-C2-C3	-2.98	120.89	126.04
22	A	810	CLA	CMA-C3A-C4A	2.98	119.77	111.77
22	A	819	CLA	CMA-C3A-C4A	2.98	119.77	111.77
38	7	301	LUT	C21-C26-C27	-2.98	108.94	112.70
39	Z	311	CHL	C3B-C4B-NB	-2.98	107.75	110.52
22	3	322	CLA	CMA-C3A-C4A	2.97	119.77	111.77
39	6	315	CHL	C3C-C4C-NC	-2.97	107.24	110.57
22	1	305	CLA	C2D-C1D-ND	2.97	112.30	110.10
39	7	313	CHL	C3C-C4C-NC	-2.97	107.24	110.57
22	A	824	CLA	C3B-C4B-NB	-2.97	107.76	110.52
24	A	856	BCR	C38-C26-C27	2.97	119.33	113.62
22	6	321	CLA	C2D-C1D-ND	2.97	112.29	110.10
22	A	855	CLA	CMA-C3A-C4A	2.97	119.76	111.77
22	3	311	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	5	309	CLA	CHD-C1D-ND	-2.97	121.72	124.45
38	9	302	LUT	C21-C26-C27	-2.97	108.95	112.70
22	K	205	CLA	C1-C2-C3	-2.97	120.91	126.04
39	4	813	CHL	C4D-CHA-C1A	2.97	124.86	121.25
22	1	305	CLA	CHD-C1D-ND	-2.97	121.72	124.45
39	8	315	CHL	C4B-CHC-C1C	2.97	133.38	126.34
23	B	843	PQN	C11-C12-C13	-2.97	121.85	126.79
39	8	312	CHL	CMA-C3A-C4A	2.97	119.75	111.77
22	1	304	CLA	CMA-C3A-C4A	2.97	119.75	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	301	CLA	C3B-C4B-NB	-2.97	107.76	110.52
22	A	827	CLA	CHD-C1D-ND	-2.97	121.73	124.45
22	A	809	CLA	C3B-C4B-NB	-2.97	107.76	110.52
22	A	819	CLA	C2C-C1C-NC	2.97	112.75	109.97
22	1	309	CLA	C2C-C1C-NC	2.97	112.75	109.97
22	5	326	CLA	C1-C2-C3	-2.97	120.91	126.04
39	4	819	CHL	C4B-CHC-C1C	2.97	133.38	126.34
24	B	847	BCR	C4-C5-C6	-2.97	118.42	122.73
22	B	817	CLA	C2C-C1C-NC	2.97	112.75	109.97
22	1	314	CLA	C2C-C1C-NC	2.97	112.75	109.97
22	7	316	CLA	C2C-C1C-NC	2.97	112.75	109.97
22	B	837	CLA	CMA-C3A-C4A	2.97	119.75	111.77
22	7	310	CLA	CMA-C3A-C4A	2.97	119.75	111.77
36	J	105	C7Z	C35-C15-C14	-2.97	117.40	123.47
39	6	318	CHL	CMA-C3A-C4A	2.96	119.74	111.77
24	B	846	BCR	C27-C26-C25	-2.96	118.43	122.73
22	A	854	CLA	C1-C2-C3	-2.96	120.92	126.04
22	A	809	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	3	311	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	8	316	CLA	CHD-C1D-ND	-2.96	121.73	124.45
24	6	305	BCR	C27-C26-C25	-2.96	118.43	122.73
22	Z	306	CLA	C2D-C1D-ND	2.96	112.29	110.10
22	3	316	CLA	C2D-C1D-ND	2.96	112.29	110.10
22	A	854	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	9	305	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
38	9	301	LUT	C1-C6-C5	-2.96	118.44	122.61
22	4	818	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	5	310	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	B	820	CLA	CHD-C1D-ND	-2.96	121.73	124.45
24	G	203	BCR	C33-C5-C4	2.96	119.31	113.62
22	6	319	CLA	C2C-C1C-NC	2.96	112.75	109.97
22	B	840	CLA	C2D-C1D-ND	2.96	112.29	110.10
22	B	820	CLA	CMA-C3A-C4A	2.96	119.73	111.77
22	B	810	CLA	CHD-C1D-ND	-2.96	121.73	124.45
22	B	841	CLA	CHD-C1D-ND	-2.96	121.73	124.45
24	B	853	BCR	C23-C24-C25	-2.96	118.89	127.20
24	3	307	BCR	C12-C13-C14	2.96	123.48	118.94
22	9	313	CLA	CMA-C3A-C4A	2.96	119.73	111.77
22	Z	315	CLA	CMA-C3A-C4A	2.96	119.72	111.77
22	3	308	CLA	CMA-C3A-C4A	2.96	119.72	111.77
22	A	806	CLA	CHD-C1D-ND	-2.96	121.74	124.45
22	6	319	CLA	CHD-C1D-ND	-2.96	121.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	306	CLA	C2D-C1D-ND	2.96	112.28	110.10
22	4	817	CLA	C2C-C1C-NC	2.96	112.74	109.97
22	1	315	CLA	CHD-C1D-ND	-2.96	121.74	124.45
39	9	314	CHL	C3C-C4C-NC	-2.95	107.26	110.57
22	3	309	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	B	813	CLA	CMA-C3A-C4A	2.95	119.71	111.77
22	B	840	CLA	CMA-C3A-C4A	2.95	119.71	111.77
22	4	812	CLA	CMA-C3A-C4A	2.95	119.71	111.77
22	7	315	CLA	C2C-C1C-NC	2.95	112.74	109.97
39	6	318	CHL	C4B-CHC-C1C	2.95	133.34	126.34
22	4	806	CLA	CMA-C3A-C4A	2.95	119.71	111.77
22	K	202	CLA	CHD-C1D-ND	-2.95	121.74	124.45
22	1	310	CLA	C2D-C1D-ND	2.95	112.28	110.10
22	1	309	CLA	C1D-ND-C4D	-2.95	104.24	106.33
22	A	833	CLA	CMA-C3A-C4A	2.95	119.70	111.77
39	7	313	CHL	C3B-C4B-NB	-2.95	107.78	110.52
22	A	824	CLA	C1D-ND-C4D	-2.95	104.24	106.33
22	A	826	CLA	CHD-C1D-ND	-2.95	121.74	124.45
24	B	849	BCR	C4-C5-C6	-2.95	118.45	122.73
22	A	815	CLA	CHD-C1D-ND	-2.95	121.75	124.45
22	3	318	CLA	C1D-ND-C4D	-2.95	104.24	106.33
22	1	315	CLA	CMA-C3A-C4A	2.95	119.69	111.77
22	8	314	CLA	C2D-C1D-ND	2.95	112.28	110.10
39	8	301	CHL	CMA-C3A-C4A	2.95	119.69	111.77
22	3	312	CLA	C1D-ND-C4D	-2.95	104.24	106.33
22	F	305	CLA	C2C-C1C-NC	2.95	112.73	109.97
22	A	810	CLA	C2D-C1D-ND	2.95	112.28	110.10
22	A	809	CLA	CMA-C3A-C4A	2.95	119.69	111.77
22	G	202	CLA	C2C-C1C-NC	2.95	112.73	109.97
22	J	103	CLA	CMA-C3A-C4A	2.94	119.69	111.77
25	4	821	LHG	C5-O7-C7	-2.94	110.54	117.79
22	A	824	CLA	CHD-C1D-ND	-2.94	121.75	124.45
22	8	311	CLA	CMA-C3A-C4A	2.94	119.69	111.77
22	8	306	CLA	CMA-C3A-C4A	2.94	119.68	111.77
22	B	833	CLA	CMA-C3A-C4A	2.94	119.68	111.77
36	J	105	C7Z	C8-C7-C6	-2.94	118.94	127.20
22	A	855	CLA	C2D-C1D-ND	2.94	112.27	110.10
22	A	824	CLA	CMA-C3A-C4A	2.94	119.67	111.77
39	3	317	CHL	C4D-CHA-C1A	2.94	124.83	121.25
22	Z	316	CLA	C3B-C4B-NB	-2.94	107.79	110.52
22	9	313	CLA	C1D-ND-C4D	-2.94	104.25	106.33
22	B	837	CLA	C2D-C1D-ND	2.94	112.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	802	CLA	C1-C2-C3	-2.94	120.96	126.04
22	5	314	CLA	CMA-C3A-C4A	2.94	119.67	111.77
24	A	844	BCR	C2-C1-C6	2.94	115.00	110.48
22	7	315	CLA	CMA-C3A-C4A	2.94	119.67	111.77
22	5	312	CLA	C2D-C1D-ND	2.94	112.27	110.10
22	1	311	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
22	A	802	CLA	CMA-C3A-C4A	2.94	119.67	111.77
22	Z	310	CLA	CMA-C3A-C4A	2.94	119.67	111.77
22	A	806	CLA	C3B-C4B-NB	-2.94	107.79	110.52
22	5	318	CLA	CMA-C3A-C4A	2.94	119.66	111.77
24	B	853	BCR	C34-C9-C10	-2.94	118.81	122.92
23	A	843	PQN	C14-C13-C15	2.94	120.21	115.27
22	8	306	CLA	C3B-C4B-NB	-2.94	107.79	110.52
38	8	302	LUT	C8-C7-C6	-2.93	118.96	127.20
22	8	310	CLA	C2D-C1D-ND	2.93	112.27	110.10
22	Z	304	CLA	CMA-C3A-C4A	2.93	119.66	111.77
22	8	314	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	2	302	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	Z	309	CLA	C1D-ND-C4D	-2.93	104.25	106.33
22	Z	316	CLA	C1D-ND-C4D	-2.93	104.25	106.33
22	B	824	CLA	CMA-C3A-C4A	2.93	119.66	111.77
24	3	306	BCR	C11-C12-C13	-2.93	118.18	126.42
22	B	806	CLA	CMA-C3A-C4A	2.93	119.65	111.77
36	J	105	C7Z	C15-C14-C13	-2.93	123.13	127.31
22	2	302	CLA	CMA-C3A-C4A	2.93	119.65	111.77
22	A	830	CLA	C2D-C1D-ND	2.93	112.26	110.10
22	1	307	CLA	C2D-C1D-ND	2.93	112.26	110.10
39	8	301	CHL	C3B-C4B-NB	-2.93	107.80	110.52
22	Z	314	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	B	842	CLA	CMA-C3A-C4A	2.93	119.65	111.77
22	B	823	CLA	C2C-C1C-NC	2.93	112.72	109.97
22	8	306	CLA	C2C-C1C-NC	2.93	112.72	109.97
22	9	309	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
22	5	307	CLA	CMA-C3A-C4A	2.93	119.64	111.77
22	A	839	CLA	C2D-C1D-ND	2.93	112.26	110.10
22	B	834	CLA	CHD-C1D-ND	-2.93	121.76	124.45
22	L	202	CLA	CMA-C3A-C4A	2.93	119.64	111.77
22	B	814	CLA	C2C-C1C-NC	2.93	112.72	109.97
22	B	805	CLA	C1D-ND-C4D	-2.93	104.25	106.33
22	Z	313	CLA	CMA-C3A-C4A	2.93	119.64	111.77
22	4	811	CLA	CMA-C3A-C4A	2.93	119.64	111.77
39	9	312	CHL	C4B-CHC-C1C	2.93	133.28	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	816	CLA	C2C-C1C-NC	2.93	112.71	109.97
22	B	822	CLA	C2C-C1C-NC	2.93	112.71	109.97
22	A	837	CLA	CMA-C3A-C4A	2.93	119.64	111.77
24	5	304	BCR	C33-C5-C4	2.92	119.23	113.62
22	B	825	CLA	C2C-C1C-NC	2.92	112.71	109.97
36	J	105	C7Z	C18-C5-C4	2.92	119.77	114.36
22	B	808	CLA	C1D-ND-C4D	-2.92	104.26	106.33
39	6	316	CHL	C4B-CHC-C1C	2.92	133.27	126.34
24	A	856	BCR	C33-C5-C4	2.92	119.23	113.62
39	1	312	CHL	C4B-CHC-C1C	2.92	133.27	126.34
22	B	805	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	5	322	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	Z	303	CLA	C2C-C1C-NC	2.92	112.71	109.97
22	A	803	CLA	C1D-ND-C4D	-2.92	104.26	106.33
22	3	312	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	2	304	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	A	855	CLA	C2C-C1C-NC	2.92	112.71	109.97
22	A	821	CLA	C2D-C1D-ND	2.92	112.26	110.10
22	5	323	CLA	CMA-C3A-C4A	2.92	119.62	111.77
22	9	311	CLA	CMA-C3A-C4A	2.92	119.62	111.77
22	B	837	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	A	812	CLA	CMA-C3A-C4A	2.92	119.62	111.77
22	Z	309	CLA	CMA-C3A-C4A	2.92	119.62	111.77
39	4	816	CHL	C4B-CHC-C1C	2.92	133.26	126.34
22	Z	309	CLA	C3B-C4B-NB	-2.92	107.81	110.52
22	1	313	CLA	CMA-C3A-C4A	2.92	119.61	111.77
22	B	828	CLA	C3B-C4B-NB	-2.92	107.81	110.52
22	A	809	CLA	C1D-ND-C4D	-2.92	104.26	106.33
22	A	812	CLA	C1D-ND-C4D	-2.92	104.26	106.33
24	B	849	BCR	C38-C26-C27	2.92	119.22	113.62
39	4	816	CHL	C4D-CHA-C1A	2.92	124.80	121.25
22	A	814	CLA	CMA-C3A-C4A	2.92	119.61	111.77
22	7	309	CLA	C1D-ND-C4D	-2.92	104.26	106.33
39	1	312	CHL	C3C-C4C-NC	-2.91	107.30	110.57
22	Z	307	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	7	317	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	A	810	CLA	C2C-C1C-NC	2.91	112.70	109.97
22	5	315	CLA	C2C-C1C-NC	2.91	112.70	109.97
22	B	811	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	7	310	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	B	839	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	2	304	CLA	C3B-C4B-NB	-2.91	107.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	816	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	1	311	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
22	A	812	CLA	C3B-C4B-NB	-2.91	107.81	110.52
22	A	803	CLA	CMA-C3A-C4A	2.91	119.60	111.77
22	4	808	CLA	CMA-C3A-C4A	2.91	119.60	111.77
22	3	313	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
22	4	807	CLA	CMA-C3A-C4A	2.91	119.59	111.77
24	5	305	BCR	C23-C24-C25	-2.91	119.03	127.20
22	A	813	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	3	322	CLA	C2D-C1D-ND	2.91	112.25	110.10
39	3	317	CHL	C1-C2-C3	-2.91	121.01	126.04
22	B	838	CLA	CMA-C3A-C4A	2.91	119.59	111.77
22	1	310	CLA	CMA-C3A-C4A	2.91	119.59	111.77
22	5	310	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	A	835	CLA	C2C-C1C-NC	2.91	112.70	109.97
22	B	814	CLA	C1D-ND-C4D	-2.91	104.27	106.33
22	A	803	CLA	C2C-C1C-NC	2.91	112.69	109.97
22	Z	308	CLA	C2C-C1C-NC	2.91	112.69	109.97
22	8	316	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	3	312	CLA	CMA-C3A-C4A	2.91	119.58	111.77
22	A	807	CLA	C3B-C4B-NB	-2.91	107.82	110.52
22	B	835	CLA	C2C-C1C-NC	2.91	112.69	109.97
22	F	302	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	B	821	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	B	826	CLA	C2D-C1D-ND	2.91	112.25	110.10
22	A	855	CLA	C3B-C4B-NB	-2.90	107.82	110.52
22	B	815	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	1	315	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	8	306	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	B	829	CLA	CMA-C3A-C4A	2.90	119.58	111.77
22	A	805	CLA	C2C-C1C-NC	2.90	112.69	109.97
22	6	313	CLA	CMA-C3A-C4A	2.90	119.58	111.77
22	Z	314	CLA	C1D-ND-C4D	-2.90	104.27	106.33
22	B	814	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	B	818	CLA	C3B-C4B-NB	-2.90	107.82	110.52
22	6	313	CLA	C3B-C4B-NB	-2.90	107.82	110.52
22	2	301	CLA	C1D-ND-C4D	-2.90	104.27	106.33
39	Z	311	CHL	C4B-CHC-C1C	2.90	133.22	126.34
22	7	307	CLA	CMA-C3A-C4A	2.90	119.57	111.77
22	A	813	CLA	CMA-C3A-C4A	2.90	119.57	111.77
24	A	848	BCR	C34-C9-C10	-2.90	118.86	122.92
22	3	308	CLA	C2D-C1D-ND	2.90	112.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	315	CHL	C4B-CHC-C1C	2.90	133.21	126.34
24	J	104	BCR	C33-C5-C4	2.90	119.18	113.62
22	F	301	CLA	C3B-C4B-NB	-2.90	107.83	110.52
22	5	326	CLA	C3B-C4B-NB	-2.90	107.83	110.52
22	1	314	CLA	C2D-C1D-ND	2.90	112.24	110.10
22	A	832	CLA	CMA-C3A-C4A	2.90	119.56	111.77
22	3	314	CLA	CMA-C3A-C4A	2.90	119.56	111.77
22	8	316	CLA	CMA-C3A-C4A	2.90	119.56	111.77
22	9	311	CLA	CHD-C1D-ND	-2.90	121.79	124.45
22	B	824	CLA	C3B-C4B-NB	-2.90	107.83	110.52
22	K	204	CLA	C3B-C4B-NB	-2.90	107.83	110.52
39	5	317	CHL	C3C-C4C-NC	-2.90	107.32	110.57
22	A	833	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	3	315	CLA	CMA-C3A-C4A	2.89	119.55	111.77
22	7	307	CLA	C2D-C1D-ND	2.89	112.24	110.10
22	Z	306	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	7	309	CLA	CMA-C3A-C4A	2.89	119.55	111.77
22	A	837	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	Z	307	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	A	829	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	A	842	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	B	838	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	6	314	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	B	832	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	7	307	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	A	820	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	A	812	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	B	806	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	B	842	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	B	828	CLA	CMA-C3A-C4A	2.89	119.54	111.77
22	7	305	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	B	807	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	6	301	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	A	841	CLA	C2C-C1C-NC	2.89	112.68	109.97
22	5	314	CLA	CHD-C1D-ND	-2.89	121.80	124.45
22	B	831	CLA	CMA-C3A-C4A	2.89	119.53	111.77
24	F	303	BCR	C8-C7-C6	-2.89	119.09	127.20
22	6	311	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	Z	306	CLA	CMA-C3A-C4A	2.89	119.53	111.77
24	J	104	BCR	C38-C26-C27	2.89	119.16	113.62
39	Z	312	CHL	C3C-C4C-NC	-2.89	107.33	110.57
22	8	311	CLA	CHD-C1D-ND	-2.89	121.80	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	304	BCR	C29-C30-C25	2.89	114.92	110.48
22	Z	303	CLA	CMA-C3A-C4A	2.89	119.53	111.77
22	A	811	CLA	C1D-ND-C4D	-2.89	104.28	106.33
22	7	310	CLA	C1D-ND-C4D	-2.89	104.28	106.33
24	B	845	BCR	C23-C24-C25	-2.89	119.10	127.20
22	B	828	CLA	C2C-C1C-NC	2.89	112.67	109.97
39	6	315	CHL	C1-O2A-CGA	2.88	124.01	116.44
22	A	808	CLA	CMA-C3A-C4A	2.88	119.53	111.77
22	9	311	CLA	C3B-C4B-NB	-2.88	107.84	110.52
22	7	314	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	B	838	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	6	310	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	A	834	CLA	CMA-C3A-C4A	2.88	119.52	111.77
22	B	819	CLA	CMA-C3A-C4A	2.88	119.52	111.77
22	5	318	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	5	323	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	5	314	CLA	C3B-C4B-NB	-2.88	107.84	110.52
22	Z	305	CLA	CMA-C3A-C4A	2.88	119.52	111.77
22	B	812	CLA	C2D-C1D-ND	2.88	112.23	110.10
22	F	305	CLA	C2D-C1D-ND	2.88	112.23	110.10
22	A	804	CLA	CHD-C1D-ND	-2.88	121.81	124.45
22	J	103	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	L	202	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	B	830	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	A	842	CLA	CMA-C3A-C4A	2.88	119.51	111.77
22	Z	314	CLA	CMA-C3A-C4A	2.88	119.51	111.77
22	2	301	CLA	C3B-C4B-NB	-2.88	107.84	110.52
38	Z	301	LUT	C11-C12-C13	-2.88	118.33	126.42
39	2	303	CHL	C4B-CHC-C1C	2.88	133.16	126.34
22	A	822	CLA	CHD-C1D-ND	-2.88	121.81	124.45
24	F	303	BCR	C33-C5-C4	2.88	119.14	113.62
39	8	312	CHL	C3C-C4C-NC	-2.88	107.34	110.57
22	L	203	CLA	CMA-C3A-C4A	2.88	119.50	111.77
22	Z	304	CLA	C3B-C4B-NB	-2.88	107.85	110.52
22	Z	303	CLA	C1D-ND-C4D	-2.88	104.29	106.33
38	3	302	LUT	C18-C5-C4	2.88	119.68	114.36
22	B	808	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	5	319	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
22	A	811	CLA	C2C-C1C-NC	2.87	112.67	109.97
38	1	303	LUT	C18-C5-C4	2.87	119.68	114.36
24	A	856	BCR	C7-C8-C9	-2.87	121.89	126.23
22	5	310	CLA	CMA-C3A-C4A	2.87	119.50	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	313	CLA	C1-C2-C3	-2.87	121.07	126.04
22	5	313	CLA	CMA-C3A-C4A	2.87	119.49	111.77
39	Z	312	CHL	CMA-C3A-C4A	2.87	119.49	111.77
22	4	809	CLA	C1-C2-C3	-2.87	121.08	126.04
22	A	807	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	4	818	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	9	303	CLA	CBA-CAA-C2A	2.87	122.34	113.86
22	9	307	CLA	CHD-C1D-ND	-2.87	121.81	124.45
22	5	313	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	7	308	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	3	314	CLA	C3B-C4B-NB	-2.87	107.85	110.52
22	4	811	CLA	C3B-C4B-NB	-2.87	107.85	110.52
39	4	813	CHL	C3B-C4B-NB	-2.87	107.85	110.52
22	Z	310	CLA	C1D-ND-C4D	-2.87	104.30	106.33
22	L	201	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	A	840	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	Z	315	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	4	817	CLA	CMA-C3A-C4A	2.87	119.49	111.77
22	K	203	CLA	CMA-C3A-C4A	2.87	119.48	111.77
22	8	313	CLA	C1D-ND-C4D	-2.87	104.30	106.33
22	A	839	CLA	CMA-C3A-C4A	2.87	119.48	111.77
24	6	306	BCR	C21-C20-C19	-2.87	114.27	123.22
22	6	310	CLA	C2C-C1C-NC	2.87	112.66	109.97
22	5	318	CLA	C1D-ND-C4D	-2.87	104.30	106.33
22	6	301	CLA	CMA-C3A-C4A	2.87	119.48	111.77
22	5	319	CLA	C3B-C4B-NB	-2.87	107.86	110.52
22	5	301	CLA	CMA-C3A-C4A	2.87	119.48	111.77
22	B	809	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	F	302	CLA	C3B-C4B-NB	-2.87	107.86	110.52
22	8	316	CLA	C3B-C4B-NB	-2.87	107.86	110.52
22	1	308	CLA	CMA-C3A-C4A	2.86	119.47	111.77
22	5	322	CLA	CMA-C3A-C4A	2.86	119.47	111.77
34	F	308	LMG	C9-C8-C7	-2.86	105.01	111.79
22	B	822	CLA	CHD-C1D-ND	-2.86	121.82	124.45
24	B	847	BCR	C23-C24-C25	-2.86	119.16	127.20
24	K	206	BCR	C11-C12-C13	-2.86	118.37	126.42
24	B	844	BCR	C35-C13-C14	-2.86	118.91	122.92
22	B	821	CLA	C3B-C4B-NB	-2.86	107.86	110.52
22	B	820	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	6	322	CLA	C2D-C1D-ND	2.86	112.21	110.10
38	9	302	LUT	C18-C5-C4	2.86	119.66	114.36
22	4	809	CLA	CHD-C1D-ND	-2.86	121.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	836	CLA	C2C-C1C-NC	2.86	112.65	109.97
22	A	804	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	A	820	CLA	CMA-C3A-C4A	2.86	119.46	111.77
22	A	833	CLA	C1D-ND-C4D	-2.86	104.30	106.33
22	Z	304	CLA	C1D-ND-C4D	-2.86	104.30	106.33
22	A	835	CLA	C1-C2-C3	-2.86	121.10	126.04
22	A	837	CLA	C3B-C4B-NB	-2.86	107.86	110.52
22	5	320	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
22	F	304	CLA	C3B-C4B-NB	-2.86	107.86	110.52
22	7	323	CLA	CMA-C3A-C4A	2.86	119.45	111.77
22	1	314	CLA	CMA-C3A-C4A	2.86	119.45	111.77
22	6	312	CLA	CMA-C3A-C4A	2.86	119.45	111.77
22	2	301	CLA	C2D-C1D-ND	2.86	112.21	110.10
22	B	841	CLA	CMA-C3A-C4A	2.86	119.45	111.77
24	4	804	BCR	C29-C30-C25	2.86	114.88	110.48
22	9	313	CLA	C3B-C4B-NB	-2.86	107.87	110.52
22	4	815	CLA	C2C-C1C-NC	2.86	112.65	109.97
22	7	308	CLA	CHD-C1D-ND	-2.86	121.83	124.45
24	A	845	BCR	C33-C5-C4	2.86	119.10	113.62
22	9	305	CLA	C1D-ND-C4D	-2.85	104.31	106.33
24	G	203	BCR	C38-C26-C27	2.85	119.10	113.62
22	A	840	CLA	CMA-C3A-C4A	2.85	119.44	111.77
22	8	306	CLA	C1D-ND-C4D	-2.85	104.31	106.33
38	6	303	LUT	C35-C15-C14	-2.85	117.63	123.47
39	5	321	CHL	C3B-C4B-NB	-2.85	107.87	110.52
22	Z	305	CLA	CHD-C1D-ND	-2.85	121.83	124.45
22	6	308	CLA	C1D-ND-C4D	-2.85	104.31	106.33
22	7	317	CLA	C3B-C4B-NB	-2.85	107.87	110.52
22	6	307	CLA	C2D-C1D-ND	2.85	112.20	110.10
22	4	809	CLA	CMA-C3A-C4A	2.85	119.43	111.77
39	8	312	CHL	C4B-CHC-C1C	2.85	133.10	126.34
22	3	318	CLA	C2C-C1C-NC	2.85	112.64	109.97
22	A	803	CLA	C3B-C4B-NB	-2.85	107.87	110.52
22	7	312	CLA	C3B-C4B-NB	-2.85	107.87	110.52
22	9	303	CLA	C1-C2-C3	-2.85	121.11	126.04
24	I	4001	BCR	C20-C19-C18	-2.85	118.41	126.42
22	B	818	CLA	CMA-C3A-C4A	2.85	119.43	111.77
39	Z	311	CHL	C4D-CHA-C1A	2.85	124.72	121.25
39	5	321	CHL	C4D-CHA-C1A	2.85	124.71	121.25
24	A	844	BCR	C23-C24-C25	-2.85	119.21	127.20
22	5	307	CLA	C2D-C1D-ND	2.85	112.20	110.10
22	5	313	CLA	C3B-C4B-NB	-2.85	107.87	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	820	LHG	O8-C23-C24	2.85	120.84	111.91
22	7	305	CLA	C1D-ND-C4D	-2.85	104.31	106.33
22	6	313	CLA	C1D-ND-C4D	-2.85	104.31	106.33
22	1	313	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
39	5	321	CHL	C4B-CHC-C1C	2.85	133.09	126.34
22	3	318	CLA	CMA-C3A-C4A	2.85	119.42	111.77
22	Z	309	CLA	CHD-C1D-ND	-2.85	121.84	124.45
39	6	316	CHL	C3C-C4C-NC	-2.85	107.38	110.57
22	1	313	CLA	C1D-ND-C4D	-2.84	104.31	106.33
22	F	301	CLA	CMA-C3A-C4A	2.84	119.41	111.77
22	4	811	CLA	CHD-C1D-ND	-2.84	121.84	124.45
22	7	311	CLA	CMA-C3A-C4A	2.84	119.41	111.77
22	A	838	CLA	C1D-ND-C4D	-2.84	104.32	106.33
39	Z	312	CHL	C4B-CHC-C1C	2.84	133.08	126.34
22	7	324	CLA	CMA-C3A-C4A	2.84	119.41	111.77
22	A	806	CLA	CMA-C3A-C4A	2.84	119.41	111.77
22	7	312	CLA	C1D-ND-C4D	-2.84	104.32	106.33
22	B	808	CLA	CMA-C3A-C4A	2.84	119.40	111.77
24	B	844	BCR	C38-C26-C27	2.84	119.07	113.62
22	9	304	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	F	302	CLA	C1D-ND-C4D	-2.84	104.32	106.33
22	7	311	CLA	C3B-C4B-NB	-2.84	107.88	110.52
24	L	204	BCR	C15-C16-C17	-2.84	117.66	123.47
22	3	313	CLA	C2C-C1C-NC	2.84	112.63	109.97
38	3	303	LUT	C18-C5-C4	2.84	119.61	114.36
22	B	816	CLA	CMA-C3A-C4A	2.84	119.39	111.77
22	A	836	CLA	C1D-ND-C4D	-2.84	104.32	106.33
22	4	807	CLA	CHD-C1D-ND	-2.83	121.85	124.45
24	3	304	BCR	C38-C26-C27	2.83	119.06	113.62
22	6	319	CLA	CMA-C3A-C4A	2.83	119.39	111.77
39	4	816	CHL	CMA-C3A-C4A	2.83	119.39	111.77
22	A	827	CLA	CMA-C3A-C4A	2.83	119.39	111.77
22	B	801	CLA	C2C-C1C-NC	2.83	112.62	109.97
38	9	301	LUT	C18-C5-C4	2.83	119.60	114.36
22	8	309	CLA	CMA-C3A-C4A	2.83	119.38	111.77
22	A	819	CLA	C2D-C1D-ND	2.83	112.19	110.10
38	6	303	LUT	C7-C8-C9	-2.83	121.96	126.23
22	B	826	CLA	C1-C2-C3	-2.83	121.15	126.04
39	6	316	CHL	C1-O2A-CGA	2.83	123.87	116.44
22	Z	310	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	3	316	CLA	CMA-C3A-C4A	2.83	119.38	111.77
24	3	306	BCR	C23-C24-C25	-2.83	119.26	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	307	CLA	CHD-C1D-ND	-2.83	121.86	124.45
22	A	807	CLA	C1D-ND-C4D	-2.83	104.33	106.33
22	A	828	CLA	C1D-ND-C4D	-2.83	104.33	106.33
22	7	322	CLA	C2C-C1C-NC	2.83	112.62	109.97
24	G	203	BCR	C23-C24-C25	-2.83	119.26	127.20
24	B	844	BCR	C15-C16-C17	-2.83	117.68	123.47
38	6	304	LUT	C18-C5-C4	2.83	119.59	114.36
22	8	310	CLA	CMA-C3A-C4A	2.83	119.37	111.77
22	F	304	CLA	C1-C2-C3	-2.82	121.16	126.04
22	A	822	CLA	C2D-C1D-ND	2.82	112.19	110.10
22	2	302	CLA	C1D-ND-C4D	-2.82	104.33	106.33
39	3	317	CHL	C3B-C4B-NB	-2.82	107.90	110.52
22	B	822	CLA	CMA-C3A-C4A	2.82	119.36	111.77
22	F	302	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
39	4	813	CHL	C4B-CHC-C1C	2.82	133.03	126.34
22	B	814	CLA	C3B-C4B-NB	-2.82	107.90	110.52
22	A	829	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	Z	304	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	5	326	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	B	819	CLA	C1D-ND-C4D	-2.82	104.33	106.33
22	3	308	CLA	C1D-ND-C4D	-2.82	104.33	106.33
22	B	830	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	6	302	CLA	CHD-C1D-ND	-2.82	121.86	124.45
39	8	312	CHL	C1-C2-C3	-2.82	121.17	126.04
22	B	842	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
22	F	304	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	9	303	CLA	CMA-C3A-C4A	2.82	119.35	111.77
24	3	304	BCR	C33-C5-C4	2.82	119.03	113.62
22	1	307	CLA	C1D-ND-C4D	-2.82	104.33	106.33
22	5	310	CLA	C1D-ND-C4D	-2.82	104.33	106.33
22	3	316	CLA	C3B-C4B-NB	-2.82	107.90	110.52
22	7	312	CLA	CMA-C3A-C4A	2.82	119.34	111.77
22	A	820	CLA	CHD-C1D-ND	-2.82	121.87	124.45
22	6	317	CLA	CMA-C3A-C4A	2.82	119.34	111.77
22	A	810	CLA	C1D-ND-C4D	-2.82	104.33	106.33
22	Z	306	CLA	C1-C2-C3	-2.81	121.17	126.04
22	4	809	CLA	C1D-ND-C4D	-2.81	104.34	106.33
22	4	810	CLA	C1D-ND-C4D	-2.81	104.34	106.33
22	B	820	CLA	C3B-C4B-NB	-2.81	107.91	110.52
22	3	320	CLA	C3B-C4B-NB	-2.81	107.91	110.52
31	B	852	DGD	C2G-O2G-C1B	-2.81	110.86	117.79
25	4	821	LHG	O8-C23-C24	2.81	120.73	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	306	CLA	C2C-C1C-NC	2.81	112.61	109.97
22	F	301	CLA	C1D-ND-C4D	-2.81	104.34	106.33
24	I	4001	BCR	C38-C26-C25	-2.81	121.37	124.53
22	A	812	CLA	CHD-C1D-ND	-2.81	121.87	124.45
22	B	805	CLA	C3B-C4B-NB	-2.81	107.91	110.52
22	3	322	CLA	C3B-C4B-NB	-2.81	107.91	110.52
22	8	308	CLA	C1D-ND-C4D	-2.81	104.34	106.33
22	Z	314	CLA	C3B-C4B-NB	-2.81	107.91	110.52
24	6	305	BCR	C2-C1-C6	2.81	114.81	110.48
22	F	305	CLA	CMA-C3A-C4A	2.81	119.32	111.77
22	B	816	CLA	C2D-C1D-ND	2.81	112.17	110.10
22	A	811	CLA	CMA-C3A-C4A	2.81	119.32	111.77
39	9	314	CHL	CMA-C3A-C2A	2.81	122.65	116.10
22	A	840	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
24	A	847	BCR	C33-C5-C4	2.81	119.01	113.62
22	5	301	CLA	C1D-ND-C4D	-2.81	104.34	106.33
22	5	307	CLA	C1D-ND-C4D	-2.81	104.34	106.33
38	1	302	LUT	C11-C12-C13	-2.81	118.53	126.42
22	6	302	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	5	326	CLA	CMA-C3A-C4A	2.80	119.31	111.77
22	3	312	CLA	C3B-C4B-NB	-2.80	107.91	110.52
39	Z	311	CHL	CHD-C4C-C3C	2.80	128.96	124.84
38	8	303	LUT	C8-C7-C6	-2.80	119.33	127.20
22	A	823	CLA	C2C-C1C-NC	2.80	112.60	109.97
22	B	813	CLA	C1D-ND-C4D	-2.80	104.34	106.33
22	7	322	CLA	C1D-ND-C4D	-2.80	104.34	106.33
22	1	310	CLA	CHD-C1D-ND	-2.80	121.88	124.45
39	4	813	CHL	C3C-C4C-NC	-2.80	107.43	110.57
22	8	311	CLA	C1D-ND-C4D	-2.80	104.34	106.33
22	9	309	CLA	C3B-C4B-NB	-2.80	107.92	110.52
22	3	319	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
22	A	826	CLA	C1D-ND-C4D	-2.80	104.35	106.33
22	4	808	CLA	C1D-ND-C4D	-2.80	104.35	106.33
39	5	316	CHL	C3C-C4C-NC	-2.80	107.43	110.57
22	4	818	CLA	C1D-ND-C4D	-2.80	104.35	106.33
38	9	302	LUT	C8-C7-C6	-2.80	119.35	127.20
22	5	311	CLA	CHD-C1D-ND	-2.79	121.89	124.45
22	2	304	CLA	C1D-ND-C4D	-2.79	104.35	106.33
22	8	305	CLA	C2D-C1D-ND	2.79	112.16	110.10
22	6	311	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
22	6	314	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
39	5	317	CHL	C4D-CHA-C1A	2.79	124.65	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	832	CLA	C1D-ND-C4D	-2.79	104.35	106.33
22	A	806	CLA	C1D-ND-C4D	-2.79	104.35	106.33
22	F	304	CLA	C1D-ND-C4D	-2.79	104.35	106.33
22	9	307	CLA	C2D-C1D-ND	2.79	112.16	110.10
24	3	305	BCR	C38-C26-C27	2.79	118.98	113.62
22	B	830	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	4	809	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	4	819	CHL	C3B-C4B-NB	-2.79	107.93	110.52
24	B	844	BCR	C33-C5-C4	2.79	118.98	113.62
22	8	314	CLA	CMA-C3A-C4A	2.79	119.27	111.77
22	A	815	CLA	C1D-ND-C4D	-2.79	104.35	106.33
22	K	204	CLA	C1D-ND-C4D	-2.79	104.35	106.33
22	1	310	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	2	302	CLA	C3B-C4B-NB	-2.79	107.93	110.52
39	4	814	CHL	C4D-CHA-C1A	2.79	124.64	121.25
22	8	313	CLA	CMA-C3A-C4A	2.79	119.27	111.77
22	6	314	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	B	848	BCR	C30-C25-C26	-2.79	118.69	122.61
39	6	318	CHL	C3C-C4C-NC	-2.79	107.44	110.57
22	L	203	CLA	C1D-ND-C4D	-2.79	104.36	106.33
22	A	826	CLA	CMA-C3A-C4A	2.79	119.26	111.77
22	6	309	CLA	CHD-C1D-ND	-2.79	121.89	124.45
22	1	309	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	L	202	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	4	807	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
22	7	306	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
35	J	102	T7X	C12-C13-C14	-2.79	108.26	113.23
22	7	324	CLA	C1-C2-C3	-2.78	121.23	126.04
22	7	308	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	A	833	CLA	C3B-C4B-NB	-2.78	107.93	110.52
22	3	320	CLA	CHD-C1D-ND	-2.78	121.90	124.45
22	6	309	CLA	C2D-C1D-ND	2.78	112.16	110.10
22	A	808	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	A	827	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	A	829	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	3	319	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	5	314	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	3	310	CLA	CHD-C1D-ND	-2.78	121.90	124.45
22	6	302	CLA	C3B-C4B-NB	-2.78	107.94	110.52
24	4	804	BCR	C4-C5-C6	-2.78	118.69	122.73
22	9	310	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	B	832	CLA	CMA-C3A-C4A	2.78	119.25	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	8	301	CHL	C4D-CHA-C1A	2.78	124.63	121.25
22	B	817	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	A	808	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
22	A	802	CLA	C1D-ND-C4D	-2.78	104.36	106.33
24	L	204	BCR	C8-C7-C6	-2.78	119.40	127.20
39	7	313	CHL	C4D-CHA-C1A	2.78	124.63	121.25
22	B	817	CLA	CMA-C3A-C4A	2.78	119.23	111.77
22	B	833	CLA	C1D-ND-C4D	-2.78	104.36	106.33
22	7	324	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	A	842	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
21	A	801	CL0	C4-C3-C5	2.77	119.94	115.27
22	9	305	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
25	5	324	LHG	O8-C23-C24	2.77	120.61	111.91
22	1	304	CLA	C1D-ND-C4D	-2.77	104.36	106.33
22	B	805	CLA	CMA-C3A-C4A	2.77	119.23	111.77
22	7	304	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	3	314	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	4	818	CLA	C1-O2A-CGA	2.77	123.72	116.44
22	Z	305	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
22	B	825	CLA	C1D-ND-C4D	-2.77	104.37	106.33
22	7	323	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	Z	315	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
39	5	316	CHL	C4B-CHC-C1C	2.77	132.91	126.34
22	A	841	CLA	CMA-C3A-C4A	2.77	119.22	111.77
22	B	807	CLA	C2C-C1C-NC	2.77	112.57	109.97
22	4	817	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	A	839	CLA	C1D-ND-C4D	-2.77	104.37	106.33
22	4	815	CLA	C1D-ND-C4D	-2.77	104.37	106.33
22	3	322	CLA	C1-C2-C3	-2.77	121.25	126.04
22	A	828	CLA	CMA-C3A-C4A	2.77	119.21	111.77
22	A	832	CLA	C1-C2-C3	-2.77	121.26	126.04
22	B	810	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	6	308	CLA	CMA-C3A-C4A	2.77	119.21	111.77
22	8	308	CLA	CMA-C3A-C4A	2.77	119.21	111.77
22	7	310	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
38	6	303	LUT	C15-C14-C13	-2.76	123.36	127.31
22	A	820	CLA	C1D-ND-C4D	-2.76	104.37	106.33
22	B	831	CLA	C1D-ND-C4D	-2.76	104.37	106.33
22	6	317	CLA	C1D-ND-C4D	-2.76	104.37	106.33
22	A	816	CLA	CHD-C1D-ND	-2.76	121.91	124.45
22	A	817	CLA	CHD-C1D-ND	-2.76	121.91	124.45
22	B	817	CLA	CHD-C1D-ND	-2.76	121.91	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	201	CLA	CHD-C1D-ND	-2.76	121.91	124.45
38	6	304	LUT	C11-C12-C13	-2.76	118.66	126.42
22	3	316	CLA	C1D-ND-C4D	-2.76	104.37	106.33
39	4	813	CHL	CMA-C3A-C4A	2.76	119.20	111.77
39	3	317	CHL	C4B-CHC-C1C	2.76	132.89	126.34
22	6	309	CLA	O2A-CGA-CBA	2.76	120.57	111.91
22	9	306	CLA	CMA-C3A-C4A	2.76	119.19	111.77
22	B	811	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	B	818	CLA	C2C-C1C-NC	2.76	112.56	109.97
24	A	848	BCR	C11-C10-C9	-2.76	123.37	127.31
38	7	302	LUT	C1-C6-C5	-2.76	118.73	122.61
22	B	836	CLA	C1D-ND-C4D	-2.76	104.38	106.33
22	Z	305	CLA	C1D-ND-C4D	-2.76	104.38	106.33
22	A	823	CLA	C4B-CHC-C1C	2.76	132.88	126.34
24	3	304	BCR	C23-C24-C25	-2.76	119.45	127.20
22	9	311	CLA	C1D-ND-C4D	-2.76	104.38	106.33
22	4	815	CLA	CHD-C1D-ND	-2.76	121.92	124.45
24	5	304	BCR	C15-C14-C13	-2.76	123.38	127.31
22	A	854	CLA	O2A-CGA-CBA	2.76	120.56	111.91
22	5	323	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
22	5	322	CLA	C1D-ND-C4D	-2.76	104.38	106.33
22	1	305	CLA	C3B-C4B-NB	-2.76	107.96	110.52
22	A	829	CLA	C1-C2-C3	-2.75	121.28	126.04
22	B	807	CLA	C3B-C4B-NB	-2.75	107.96	110.52
22	6	307	CLA	CMA-C3A-C4A	2.75	119.17	111.77
22	Z	307	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
22	3	311	CLA	C1D-ND-C4D	-2.75	104.38	106.33
38	8	302	LUT	C35-C15-C14	-2.75	117.84	123.47
22	A	814	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
24	5	305	BCR	C8-C9-C10	2.75	123.16	118.94
22	8	307	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
39	2	303	CHL	C3B-C4B-NB	-2.75	107.97	110.52
24	A	856	BCR	C37-C22-C21	-2.75	119.07	122.92
22	9	304	CLA	C1D-ND-C4D	-2.75	104.38	106.33
22	A	802	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	6	308	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
22	6	319	CLA	C3B-C4B-NB	-2.75	107.97	110.52
24	I	4001	BCR	C15-C14-C13	-2.75	123.39	127.31
24	5	305	BCR	C37-C22-C21	-2.75	119.08	122.92
22	B	801	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	A	835	CLA	C1D-ND-C4D	-2.74	104.39	106.33
22	B	841	CLA	C1D-ND-C4D	-2.74	104.39	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	812	CLA	C1D-ND-C4D	-2.74	104.39	106.33
24	4	804	BCR	C27-C26-C25	-2.74	118.75	122.73
22	5	320	CLA	C3B-C4B-NB	-2.74	107.97	110.52
22	A	831	CLA	C1D-ND-C4D	-2.74	104.39	106.33
22	A	855	CLA	C1D-ND-C4D	-2.74	104.39	106.33
39	8	301	CHL	C4B-CHC-C1C	2.74	132.84	126.34
22	Z	306	CLA	C3B-C4B-NB	-2.74	107.97	110.52
24	A	847	BCR	C15-C16-C17	-2.74	117.86	123.47
22	B	813	CLA	C3B-C4B-NB	-2.74	107.97	110.52
22	5	301	CLA	C3B-C4B-NB	-2.74	107.97	110.52
22	B	834	CLA	CMA-C3A-C4A	2.74	119.14	111.77
22	8	307	CLA	CHD-C1D-ND	-2.74	121.94	124.45
24	A	848	BCR	C23-C24-C25	-2.74	119.51	127.20
24	B	844	BCR	C23-C24-C25	-2.74	119.51	127.20
39	6	315	CHL	C2C-C3C-C4C	2.74	108.44	106.49
22	B	834	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	4	811	CLA	C1D-ND-C4D	-2.74	104.39	106.33
39	7	313	CHL	C4B-CHC-C1C	2.74	132.84	126.34
24	3	307	BCR	C19-C18-C17	-2.74	114.74	118.94
22	L	202	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	5	313	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	6	322	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
22	7	316	CLA	C1D-ND-C4D	-2.74	104.39	106.33
22	6	317	CLA	CHD-C1D-ND	-2.74	121.94	124.45
22	8	309	CLA	C1D-ND-C4D	-2.74	104.39	106.33
22	B	819	CLA	C3B-C4B-NB	-2.73	107.98	110.52
39	5	317	CHL	C4B-CHC-C1C	2.73	132.82	126.34
24	A	856	BCR	C8-C7-C6	-2.73	119.52	127.20
22	1	314	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
22	1	308	CLA	CMD-C2D-C3D	-2.73	121.33	127.61
24	F	303	BCR	C29-C30-C25	2.73	114.69	110.48
39	6	316	CHL	C3B-C4B-NB	-2.73	107.98	110.52
22	7	315	CLA	CHD-C1D-ND	-2.73	121.94	124.45
24	8	304	BCR	C11-C12-C13	-2.73	118.74	126.42
22	A	817	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	L	201	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	7	315	CLA	C3B-C4B-NB	-2.73	107.98	110.52
24	A	846	BCR	C38-C26-C27	2.73	118.86	113.62
23	A	843	PQN	C2M-C2-C3	-2.73	119.95	124.40
39	4	814	CHL	C4B-CHC-C1C	2.73	132.81	126.34
22	8	307	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	Z	314	CLA	C1C-C2C-C3C	-2.73	104.09	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	844	BCR	C16-C17-C18	-2.73	123.42	127.31
22	B	839	CLA	C1D-ND-C4D	-2.73	104.40	106.33
22	6	302	CLA	C1D-ND-C4D	-2.73	104.40	106.33
22	A	838	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
22	A	830	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
22	B	841	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	B	823	CLA	C4B-CHC-C1C	2.73	132.81	126.34
22	3	309	CLA	C1D-ND-C4D	-2.73	104.40	106.33
38	3	303	LUT	C15-C35-C34	-2.73	117.89	123.47
22	B	809	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
22	1	305	CLA	CMA-C3A-C4A	2.73	119.10	111.77
22	9	308	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
22	A	854	CLA	C1D-ND-C4D	-2.73	104.40	106.33
22	7	305	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	B	809	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	6	321	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	A	802	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	A	816	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	B	811	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	Z	315	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	B	821	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	8	316	CLA	C1D-ND-C4D	-2.72	104.40	106.33
32	F	306	RRX	C38-C26-C27	2.72	119.40	114.36
22	Z	313	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	7	323	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	B	829	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	8	307	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	B	839	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	3	312	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	7	312	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	B	828	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	5	315	CLA	CHD-C1D-ND	-2.72	121.95	124.45
22	K	203	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	5	323	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	5	315	CLA	C1D-ND-C4D	-2.72	104.40	106.33
22	4	808	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	B	812	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	4	812	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	9	306	CLA	C1D-ND-C4D	-2.72	104.41	106.33
38	7	301	LUT	C1-C6-C5	-2.72	118.79	122.61
22	4	806	CLA	CHD-C1D-ND	-2.72	121.96	124.45
39	7	313	CHL	C1-O2A-CGA	2.72	123.57	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	812	CLA	CMA-C3A-C4A	2.72	119.07	111.77
22	8	305	CLA	C1D-ND-C4D	-2.72	104.41	106.33
22	5	309	CLA	C3B-C4B-NB	-2.72	108.00	110.52
22	3	311	CLA	CMA-C3A-C4A	2.71	119.07	111.77
22	F	305	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	1	315	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	5	309	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	A	839	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
22	Z	313	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
22	B	827	CLA	CMA-C3A-C4A	2.71	119.07	111.77
22	7	316	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	5	311	CLA	CMA-C3A-C4A	2.71	119.06	111.77
22	B	840	CLA	C1D-ND-C4D	-2.71	104.41	106.33
25	6	323	LHG	C5-O7-C7	-2.71	111.11	117.79
22	8	313	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	4	818	CLA	O2A-CGA-CBA	2.71	120.42	111.91
22	B	806	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	A	808	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	F	303	BCR	C4-C5-C6	-2.71	118.80	122.73
22	A	830	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	B	816	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	3	310	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	B	813	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	A	825	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	3	314	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	1	304	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	9	305	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	3	305	BCR	C20-C19-C18	-2.71	118.81	126.42
39	9	314	CHL	C3B-C4B-NB	-2.71	108.00	110.52
22	3	315	CLA	C1D-ND-C4D	-2.71	104.41	106.33
22	4	808	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
22	A	854	CLA	C3B-C4B-NB	-2.70	108.01	110.52
22	6	309	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
24	5	305	BCR	C35-C13-C14	-2.70	119.14	122.92
22	B	831	CLA	C2D-C1D-ND	2.70	112.10	110.10
39	5	316	CHL	CMA-C3A-C4A	2.70	119.04	111.77
22	B	826	CLA	O2A-CGA-CBA	2.70	120.39	111.91
22	6	307	CLA	C1D-ND-C4D	-2.70	104.42	106.33
22	B	821	CLA	CMA-C3A-C4A	2.70	119.04	111.77
22	K	204	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
22	3	320	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
22	6	302	CLA	C1C-C2C-C3C	-2.70	104.11	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	306	BCR	C30-C25-C26	-2.70	118.81	122.61
22	4	815	CLA	C3B-C4B-NB	-2.70	108.01	110.52
22	4	812	CLA	C3B-C4B-NB	-2.70	108.01	110.52
25	6	323	LHG	O8-C23-C24	2.70	120.38	111.91
22	A	831	CLA	CMA-C3A-C4A	2.70	119.03	111.77
22	B	814	CLA	C4B-CHC-C1C	2.70	132.74	126.34
22	7	316	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
39	6	315	CHL	C3B-C4B-NB	-2.70	108.01	110.52
22	1	309	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	8	314	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	B	827	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
38	6	303	LUT	C8-C7-C6	-2.70	119.63	127.20
38	7	302	LUT	C18-C5-C4	2.70	119.35	114.36
22	8	307	CLA	CMA-C3A-C4A	2.70	119.02	111.77
22	8	310	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
22	A	834	CLA	C1D-ND-C4D	-2.70	104.42	106.33
22	4	817	CLA	C1D-ND-C4D	-2.70	104.42	106.33
22	6	319	CLA	C1D-ND-C4D	-2.70	104.42	106.33
22	4	818	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	3	304	BCR	C1-C6-C5	-2.69	118.82	122.61
22	5	309	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	8	310	CLA	C1D-ND-C4D	-2.69	104.42	106.33
22	A	836	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	5	307	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	6	313	CLA	CHD-C1D-ND	-2.69	121.98	124.45
24	5	305	BCR	C27-C26-C25	-2.69	118.82	122.73
24	B	844	BCR	C8-C9-C10	2.69	123.07	118.94
24	3	304	BCR	C21-C20-C19	-2.69	114.82	123.22
22	7	317	CLA	C1D-ND-C4D	-2.69	104.42	106.33
22	B	806	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	B	822	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	7	306	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	B	805	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	5	315	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
22	7	310	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	3	322	CLA	C1D-ND-C4D	-2.69	104.43	106.33
22	7	323	CLA	C1D-ND-C4D	-2.69	104.43	106.33
22	B	821	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
39	9	314	CHL	C4B-CHC-C1C	2.69	132.71	126.34
22	6	310	CLA	CMA-C3A-C4A	2.69	118.99	111.77
22	Z	313	CLA	C1D-ND-C4D	-2.69	104.43	106.33
22	9	308	CLA	C1D-ND-C4D	-2.69	104.43	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	311	CLA	C1-C2-C3	-2.69	121.40	126.04
22	B	841	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
24	B	847	BCR	C1-C6-C5	-2.68	118.83	122.61
22	B	826	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	6	314	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	4	809	CLA	C4B-CHC-C1C	2.68	132.70	126.34
22	F	304	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	Z	316	CLA	C4B-CHC-C1C	2.68	132.70	126.34
22	B	816	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	8	309	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	B	810	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	B	827	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	A	807	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	8	311	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	5	311	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	1	308	CLA	C4B-CHC-C1C	2.68	132.70	126.34
22	5	326	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	A	832	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	9	311	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	G	202	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	B	838	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	6	307	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	8	306	CLA	C4B-CHC-C1C	2.68	132.69	126.34
24	A	845	BCR	C23-C24-C25	-2.68	119.68	127.20
22	1	306	CLA	C1D-ND-C4D	-2.68	104.43	106.33
22	7	324	CLA	C1D-ND-C4D	-2.68	104.43	106.33
24	7	303	BCR	C15-C16-C17	-2.68	117.99	123.47
22	A	817	CLA	C2D-C1D-ND	2.68	112.08	110.10
22	B	840	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
24	B	846	BCR	C11-C10-C9	-2.68	123.49	127.31
38	8	303	LUT	C18-C5-C4	2.67	119.31	114.36
22	8	308	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
22	1	314	CLA	C1D-ND-C4D	-2.67	104.44	106.33
22	5	301	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	A	820	CLA	C4B-CHC-C1C	2.67	132.68	126.34
36	J	105	C7Z	C21-C26-C25	-2.67	118.85	122.61
22	A	812	CLA	C4B-CHC-C1C	2.67	132.67	126.34
22	B	801	CLA	C1D-ND-C4D	-2.67	104.44	106.33
22	1	314	CLA	C3B-C4B-NB	-2.67	108.04	110.52
22	4	817	CLA	CAA-C2A-C3A	-2.67	109.87	116.10
22	A	806	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	3	316	CLA	C1C-C2C-C3C	-2.67	104.15	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	305	BCR	C1-C6-C5	-2.67	118.86	122.61
22	A	840	CLA	C1D-ND-C4D	-2.67	104.44	106.33
22	A	833	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	7	307	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	4	811	CLA	O2A-CGA-CBA	2.67	120.27	111.91
22	A	819	CLA	C1D-ND-C4D	-2.66	104.44	106.33
22	5	312	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	G	201	CLA	C4B-CHC-C1C	2.66	132.66	126.34
25	1	317	LHG	O8-C23-C24	2.66	120.27	111.91
22	8	314	CLA	C3B-C4B-NB	-2.66	108.04	110.52
22	9	304	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	8	314	CLA	C1D-ND-C4D	-2.66	104.44	106.33
22	A	809	CLA	C4B-CHC-C1C	2.66	132.65	126.34
22	B	826	CLA	CMA-C3A-C4A	2.66	118.93	111.77
22	1	316	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	5	320	CLA	CMA-C3A-C4A	2.66	118.93	111.77
24	6	306	BCR	C16-C15-C14	-2.66	118.02	123.47
22	B	822	CLA	C1D-ND-C4D	-2.66	104.44	106.33
22	B	811	CLA	C4B-CHC-C1C	2.66	132.65	126.34
22	Z	316	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	3	309	CLA	CMA-C3A-C4A	2.66	118.92	111.77
22	B	831	CLA	CMD-C2D-C3D	-2.66	121.49	127.61
22	B	820	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	1	315	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	Z	308	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
38	8	302	LUT	C1-C6-C5	-2.66	118.87	122.61
22	A	818	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	4	810	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	1	310	CLA	C4B-CHC-C1C	2.66	132.64	126.34
22	B	809	CLA	CMA-C3A-C4A	2.66	118.92	111.77
22	A	824	CLA	C4B-CHC-C1C	2.66	132.64	126.34
22	G	201	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
22	5	308	CLA	C1D-ND-C4D	-2.66	104.45	106.33
22	6	311	CLA	CMA-C3A-C4A	2.66	118.92	111.77
22	5	309	CLA	O2A-CGA-CBA	2.66	120.25	111.91
24	5	304	BCR	C37-C22-C21	-2.66	119.20	122.92
22	K	202	CLA	C1D-ND-C4D	-2.66	104.45	106.33
22	A	808	CLA	C4B-CHC-C1C	2.66	132.64	126.34
22	A	815	CLA	CMA-C3A-C4A	2.66	118.91	111.77
24	4	804	BCR	C38-C26-C27	2.66	118.72	113.62
22	L	201	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	4	817	CLA	C1C-C2C-C3C	-2.65	104.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	310	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	A	837	CLA	C4B-CHC-C1C	2.65	132.63	126.34
22	A	821	CLA	C1D-ND-C4D	-2.65	104.45	106.33
22	Z	306	CLA	C4B-CHC-C1C	2.65	132.63	126.34
39	8	315	CHL	CMA-C3A-C4A	2.65	118.90	111.77
22	J	103	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	5	314	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	832	CLA	C3B-C4B-NB	-2.65	108.05	110.52
22	5	311	CLA	C3B-C4B-NB	-2.65	108.05	110.52
22	L	203	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	6	313	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	2	301	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	835	CLA	CMA-C3A-C4A	2.65	118.90	111.77
22	3	322	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	7	309	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	7	324	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	6	312	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	A	821	CLA	C1-C2-C3	-2.65	121.46	126.04
22	A	811	CLA	C4B-CHC-C1C	2.65	132.62	126.34
22	Z	309	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	3	308	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	830	CLA	C4B-CHC-C1C	2.65	132.62	126.34
22	F	304	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	B	848	BCR	C2-C1-C6	2.65	114.56	110.48
22	A	826	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	801	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	831	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	4	809	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
39	4	814	CHL	C1-O2A-CGA	2.65	123.39	116.44
22	A	835	CLA	C3B-C4B-NB	-2.65	108.06	110.52
22	7	307	CLA	C4B-CHC-C1C	2.65	132.61	126.34
24	B	846	BCR	C33-C5-C4	2.65	118.70	113.62
24	A	848	BCR	C36-C18-C17	-2.65	119.22	122.92
22	A	831	CLA	C3B-C4B-NB	-2.65	108.06	110.52
22	B	829	CLA	C3B-C4B-NB	-2.65	108.06	110.52
22	A	842	CLA	C1D-ND-C4D	-2.65	104.46	106.33
22	B	833	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	G	201	CLA	C3B-C4B-NB	-2.64	108.06	110.52
22	G	202	CLA	CMA-C3A-C4A	2.64	118.88	111.77
38	4	802	LUT	C18-C5-C4	2.64	119.25	114.36
22	3	314	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
24	3	304	BCR	C30-C25-C26	-2.64	118.89	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	103	CLA	C3B-C4B-NB	-2.64	108.06	110.52
39	9	312	CHL	CHB-C4A-NA	2.64	128.16	124.51
22	F	301	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	7	308	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	5	322	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	1	308	CLA	C2C-C1C-NC	2.64	112.45	109.97
22	A	827	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	2	304	CLA	C4B-CHC-C1C	2.64	132.60	126.34
22	A	806	CLA	C4B-CHC-C1C	2.64	132.60	126.34
39	6	318	CHL	C3B-C4B-NB	-2.64	108.07	110.52
22	3	318	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	B	839	CLA	C6-C5-C3	-2.64	110.30	114.62
22	Z	307	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
38	6	303	LUT	C18-C5-C4	2.64	119.24	114.36
22	B	819	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	K	203	CLA	C1D-ND-C4D	-2.64	104.46	106.33
22	Z	304	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	B	817	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	4	806	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
36	J	105	C7Z	C7-C8-C9	-2.64	122.25	126.23
22	1	305	CLA	C1D-ND-C4D	-2.64	104.46	106.33
22	2	304	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
22	6	321	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
22	1	305	CLA	C4B-CHC-C1C	2.63	132.59	126.34
22	1	306	CLA	C3B-C4B-NB	-2.63	108.07	110.52
22	3	316	CLA	C4B-CHC-C1C	2.63	132.59	126.34
22	7	322	CLA	CMA-C3A-C4A	2.63	118.85	111.77
24	A	846	BCR	C8-C7-C6	-2.63	119.81	127.20
22	Z	310	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
38	7	302	LUT	C11-C12-C13	-2.63	119.02	126.42
22	B	824	CLA	C2C-C1C-NC	2.63	112.44	109.97
22	3	315	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
22	1	307	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	5	308	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	6	314	CLA	C4B-CHC-C1C	2.63	132.58	126.34
24	7	303	BCR	C8-C7-C6	-2.63	119.81	127.20
22	Z	304	CLA	C4B-CHC-C1C	2.63	132.58	126.34
22	A	819	CLA	C3B-C4B-NB	-2.63	108.08	110.52
22	1	311	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	Z	313	CLA	C4B-CHC-C1C	2.63	132.58	126.34
22	7	312	CLA	C4B-CHC-C1C	2.63	132.57	126.34
22	3	311	CLA	C1C-C2C-C3C	-2.63	104.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	9	306	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
22	B	805	CLA	C4B-CHC-C1C	2.63	132.57	126.34
22	7	315	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
24	B	848	BCR	C27-C26-C25	-2.63	118.92	122.73
22	7	315	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	5	313	CLA	CHD-C1D-ND	-2.63	122.04	124.45
22	6	312	CLA	C1D-ND-C4D	-2.63	104.47	106.33
22	F	302	CLA	C4B-CHC-C1C	2.63	132.57	126.34
22	A	803	CLA	C4B-CHC-C1C	2.63	132.57	126.34
22	A	835	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
22	1	305	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
22	A	822	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	7	317	CLA	CMA-C3A-C4A	2.63	118.83	111.77
38	Z	301	LUT	C18-C5-C6	-2.63	121.58	124.53
22	4	815	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
39	Z	312	CHL	C3B-C4B-NB	-2.62	108.08	110.52
22	8	306	CLA	CHD-C1D-ND	-2.62	122.04	124.45
24	J	104	BCR	C20-C19-C18	-2.62	119.04	126.42
22	7	311	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	6	301	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	5	319	CLA	CMA-C3A-C4A	2.62	118.83	111.77
22	B	801	CLA	C1-C2-C3	-2.62	121.50	126.04
39	3	317	CHL	CMA-C3A-C4A	2.62	118.83	111.77
22	1	306	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
38	1	302	LUT	C19-C9-C10	-2.62	119.25	122.92
22	5	309	CLA	C4B-CHC-C1C	2.62	132.56	126.34
22	3	319	CLA	CMA-C3A-C4A	2.62	118.82	111.77
22	B	817	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
41	7	319	3PH	O31-C31-C32	2.62	120.13	111.91
22	1	310	CLA	C1D-ND-C4D	-2.62	104.47	106.33
22	9	313	CLA	C4B-CHC-C1C	2.62	132.55	126.34
22	7	314	CLA	C3B-C4B-NB	-2.62	108.08	110.52
22	8	310	CLA	C3B-C4B-NB	-2.62	108.09	110.52
22	B	828	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	9	306	CLA	C4B-CHC-C1C	2.62	132.55	126.34
25	B	850	LHG	C5-O7-C7	-2.62	111.35	117.79
22	3	315	CLA	C2C-C1C-NC	2.62	112.42	109.97
22	B	813	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
22	5	311	CLA	C1D-ND-C4D	-2.62	104.48	106.33
39	2	303	CHL	CMA-C3A-C4A	2.62	118.81	111.77
22	A	828	CLA	C3B-C4B-NB	-2.62	108.09	110.52
22	A	836	CLA	C3B-C4B-NB	-2.62	108.09	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	304	CLA	CMA-C3A-C4A	2.62	118.80	111.77
22	F	305	CLA	C3B-C4B-NB	-2.62	108.09	110.52
22	7	322	CLA	C3B-C4B-NB	-2.62	108.09	110.52
22	9	310	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
22	K	205	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
36	5	306	C7Z	C28-C27-C26	-2.61	119.86	127.20
22	B	835	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	9	307	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	4	805	CLA	O2A-CGA-CBA	2.61	120.11	111.91
22	Z	303	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	A	825	CLA	C3B-C4B-NB	-2.61	108.09	110.52
38	5	302	LUT	C30-C31-C32	-2.61	115.07	123.22
22	G	201	CLA	CMA-C3A-C4A	2.61	118.79	111.77
22	4	805	CLA	C4B-CHC-C1C	2.61	132.53	126.34
22	A	821	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	A	837	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	A	841	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	B	806	CLA	C1D-ND-C4D	-2.61	104.48	106.33
22	B	837	CLA	C3B-C4B-NB	-2.61	108.09	110.52
22	A	834	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	1	310	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	3	309	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	8	309	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
22	6	317	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
32	F	306	RRX	C23-C24-C25	-2.61	119.88	127.20
22	B	828	CLA	C4B-CHC-C1C	2.61	132.52	126.34
22	B	820	CLA	C1D-ND-C4D	-2.61	104.48	106.33
22	B	837	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
22	3	312	CLA	C4B-CHC-C1C	2.61	132.52	126.34
22	5	320	CLA	C2A-C1A-CHA	2.61	128.42	123.86
22	1	307	CLA	C4B-CHC-C1C	2.61	132.52	126.34
22	4	811	CLA	C4B-CHC-C1C	2.61	132.52	126.34
22	5	312	CLA	CMA-C3A-C4A	2.61	118.78	111.77
22	B	834	CLA	C1D-ND-C4D	-2.61	104.48	106.33
22	8	305	CLA	C4B-CHC-C1C	2.61	132.52	126.34
22	Z	316	CLA	CMA-C3A-C4A	2.61	118.78	111.77
22	7	323	CLA	C3B-C4B-NB	-2.61	108.10	110.52
24	B	853	BCR	C30-C25-C24	2.60	123.15	115.78
24	L	204	BCR	C38-C26-C27	2.60	118.62	113.62
22	4	806	CLA	C1D-ND-C4D	-2.60	104.48	106.33
22	A	841	CLA	C4B-CHC-C1C	2.60	132.51	126.34
22	B	817	CLA	C3B-C4B-NB	-2.60	108.10	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	313	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	A	814	CLA	C1D-ND-C4D	-2.60	104.49	106.33
22	4	807	CLA	C1D-ND-C4D	-2.60	104.49	106.33
24	6	306	BCR	C38-C26-C27	2.60	118.62	113.62
22	4	811	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
38	Z	301	LUT	C19-C9-C10	-2.60	119.28	122.92
22	B	829	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	7	304	CLA	C3B-C4B-NB	-2.60	108.10	110.52
34	F	308	LMG	O8-C28-C29	2.60	120.07	111.91
22	B	820	CLA	C1-C2-C3	-2.60	121.55	126.04
24	A	856	BCR	C20-C19-C18	-2.60	119.11	126.42
24	3	305	BCR	C7-C8-C9	-2.60	122.31	126.23
22	B	818	CLA	C4B-CHC-C1C	2.60	132.50	126.34
22	A	819	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
32	F	306	RRX	C33-C5-C4	2.60	118.61	113.62
25	8	317	LHG	O8-C23-C24	2.60	120.06	111.91
38	1	303	LUT	C22-C23-C24	2.60	114.70	111.74
22	A	822	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	B	808	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	Z	306	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
39	9	314	CHL	C2B-C1B-NB	-2.60	108.49	110.23
22	L	201	CLA	C4B-CHC-C1C	2.60	132.50	126.34
22	5	326	CLA	C4B-CHC-C1C	2.60	132.50	126.34
22	A	820	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
22	A	827	CLA	C3B-C4B-NB	-2.60	108.11	110.52
22	6	310	CLA	C4B-CHC-C1C	2.60	132.50	126.34
22	B	815	CLA	C1D-ND-C4D	-2.60	104.49	106.33
22	9	309	CLA	C1D-ND-C4D	-2.60	104.49	106.33
22	F	301	CLA	C4B-CHC-C1C	2.60	132.50	126.34
22	A	815	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	A	817	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	A	818	CLA	C3B-C4B-NB	-2.60	108.11	110.52
22	8	316	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	A	840	CLA	C3B-C4B-NB	-2.60	108.11	110.52
22	G	202	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
22	9	307	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	Z	317	LHG	O8-C23-C24	2.59	120.05	111.91
22	A	804	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
22	7	316	CLA	CMA-C3A-C4A	2.59	118.74	111.77
22	3	310	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	7	306	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	4	815	CLA	C1C-C2C-C3C	-2.59	104.23	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	205	CLA	C2A-C1A-CHA	2.59	128.39	123.86
22	A	804	CLA	C1D-ND-C4D	-2.59	104.49	106.33
22	8	311	CLA	C4B-CHC-C1C	2.59	132.49	126.34
22	F	305	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
39	4	814	CHL	CMA-C3A-C4A	2.59	118.74	111.77
22	Z	303	CLA	C4B-CHC-C1C	2.59	132.49	126.34
21	A	801	CL0	CMB-C2B-C1B	2.59	129.31	125.37
22	3	319	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	2	301	CLA	C4B-CHC-C1C	2.59	132.48	126.34
22	6	322	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	A	810	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
22	B	825	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	B	826	CLA	C3B-C4B-NB	-2.59	108.11	110.52
38	3	302	LUT	C8-C7-C6	-2.59	119.93	127.20
22	A	813	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
22	Z	308	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	3	318	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	B	814	CLA	CMA-C3A-C4A	2.59	118.73	111.77
25	9	315	LHG	O8-C23-C24	2.59	120.03	111.91
22	B	809	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	6	321	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	5	326	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
24	3	305	BCR	C8-C7-C6	-2.59	119.94	127.20
24	4	804	BCR	C15-C16-C17	-2.59	118.18	123.47
22	A	855	CLA	C4B-CHC-C1C	2.59	132.47	126.34
22	A	803	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
22	A	831	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
22	2	302	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
22	5	315	CLA	C4B-CHC-C1C	2.58	132.46	126.34
25	A	850	LHG	O8-C23-C24	2.58	120.01	111.91
22	1	308	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	7	307	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	5	318	CLA	C1-C2-C3	-2.58	121.58	126.04
22	8	316	CLA	C4B-CHC-C1C	2.58	132.46	126.34
22	B	814	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	B	830	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
24	7	303	BCR	C29-C30-C25	2.58	114.45	110.48
22	1	309	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	G	201	CLA	CHA-C4D-ND	2.58	137.90	132.50
22	B	831	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	Z	305	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	1	316	CLA	CHA-C4D-ND	2.58	137.89	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	310	CLA	C4B-CHC-C1C	2.58	132.45	126.34
22	B	840	CLA	C3B-C4B-NB	-2.58	108.12	110.52
38	5	302	LUT	C8-C7-C6	-2.58	119.96	127.20
36	5	306	C7Z	C38-C25-C24	2.58	119.13	114.36
22	5	314	CLA	C4B-CHC-C1C	2.58	132.45	126.34
22	5	312	CLA	C1D-ND-C4D	-2.58	104.50	106.33
22	A	829	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	B	852	DGD	O1G-C1A-C2A	2.58	119.99	111.91
22	A	825	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
22	9	304	CLA	CHA-C4D-ND	2.57	137.88	132.50
22	4	808	CLA	C4B-CHC-C1C	2.57	132.44	126.34
22	B	842	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	A	854	CLA	CMA-C3A-C4A	2.57	118.69	111.77
22	7	306	CLA	C1D-ND-C4D	-2.57	104.51	106.33
22	6	307	CLA	C1-C2-C3	-2.57	121.59	126.04
22	9	313	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	5	307	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	A	809	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
24	B	853	BCR	C2-C1-C6	2.57	114.44	110.48
22	3	314	CLA	C4B-CHC-C1C	2.57	132.44	126.34
22	Z	307	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	B	837	CLA	C1D-ND-C4D	-2.57	104.51	106.33
22	B	825	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	B	826	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
24	B	848	BCR	C1-C6-C5	-2.57	118.99	122.61
22	A	824	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	1	316	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	7	314	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
22	4	806	CLA	CHA-C4D-ND	2.57	137.87	132.50
24	5	304	BCR	C7-C8-C9	-2.57	122.36	126.23
24	3	304	BCR	C4-C5-C6	-2.57	119.00	122.73
22	B	816	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
22	4	818	CLA	C4B-CHC-C1C	2.57	132.43	126.34
22	5	319	CLA	C1D-ND-C4D	-2.57	104.51	106.33
24	3	305	BCR	C33-C5-C4	2.57	118.54	113.62
32	F	306	RRX	C36-C18-C17	-2.56	119.33	122.92
22	A	813	CLA	C1D-ND-C4D	-2.56	104.51	106.33
24	J	104	BCR	C23-C24-C25	-2.56	120.00	127.20
24	I	4001	BCR	C36-C18-C17	-2.56	119.33	122.92
22	A	854	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
22	A	839	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	B	803	LHG	O8-C23-C24	2.56	119.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	310	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
22	B	839	CLA	CMA-C3A-C4A	2.56	118.66	111.77
22	B	835	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	5	310	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	7	315	CLA	C1D-ND-C4D	-2.56	104.52	106.33
22	3	308	CLA	C4B-CHC-C1C	2.56	132.41	126.34
22	3	308	CLA	O2A-CGA-CBA	2.56	119.94	111.91
22	B	836	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
24	B	848	BCR	C23-C24-C25	-2.56	120.01	127.20
22	A	829	CLA	C4B-CHC-C1C	2.56	132.41	126.34
22	A	804	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	3	314	CLA	C1-C2-C3	-2.56	121.62	126.04
22	1	304	CLA	C4B-CHC-C1C	2.56	132.40	126.34
24	B	844	BCR	C15-C14-C13	-2.56	123.66	127.31
22	9	310	CLA	C4B-CHC-C1C	2.56	132.40	126.34
24	5	305	BCR	C8-C7-C6	-2.56	120.02	127.20
24	B	847	BCR	C33-C5-C4	2.56	118.53	113.62
22	6	308	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
22	3	322	CLA	C4B-CHC-C1C	2.55	132.40	126.34
22	8	308	CLA	C4B-CHC-C1C	2.55	132.40	126.34
22	7	324	CLA	O2A-CGA-CBA	2.55	119.92	111.91
22	7	322	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
22	B	839	CLA	C3B-C4B-NB	-2.55	108.15	110.52
38	Z	302	LUT	C18-C5-C4	2.55	119.08	114.36
39	8	315	CHL	C2C-C3C-C4C	2.55	108.31	106.49
22	A	810	CLA	C3B-C4B-NB	-2.55	108.15	110.52
39	8	315	CHL	C1-O2A-CGA	2.55	123.14	116.44
22	A	812	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
39	6	315	CHL	CMA-C3A-C4A	2.55	118.63	111.77
39	6	320	CHL	C2C-C3C-C4C	2.55	108.31	106.49
22	A	805	CLA	C3B-C4B-NB	-2.55	108.15	110.52
24	A	846	BCR	C2-C1-C6	2.55	114.41	110.48
24	G	203	BCR	C20-C19-C18	-2.55	119.25	126.42
22	3	310	CLA	C1D-ND-C4D	-2.55	104.52	106.33
22	3	308	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	6	322	CLA	CMA-C3A-C4A	2.55	118.62	111.77
22	A	807	CLA	C4B-CHC-C1C	2.55	132.38	126.34
22	5	318	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
22	6	302	CLA	C4B-CHC-C1C	2.55	132.38	126.34
38	1	303	LUT	C11-C12-C13	-2.55	119.26	126.42
38	3	302	LUT	C35-C15-C14	-2.55	118.26	123.47
22	9	303	CLA	O2D-CGD-O1D	-2.55	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Z	309	CLA	C4B-CHC-C1C	2.55	132.38	126.34
22	B	810	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	K	202	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
22	B	831	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	5	313	CLA	CHA-C4D-ND	2.54	137.82	132.50
22	A	809	CLA	C6-C5-C3	-2.54	106.78	113.45
22	L	203	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	6	311	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	A	835	CLA	O2A-CGA-CBA	2.54	119.89	111.91
39	6	320	CHL	CMA-C3A-C4A	2.54	118.61	111.77
22	A	855	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
22	6	314	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	9	311	CLA	C4B-CHC-C1C	2.54	132.37	126.34
38	5	303	LUT	C18-C5-C4	2.54	119.06	114.36
22	9	307	CLA	C1D-ND-C4D	-2.54	104.53	106.33
22	6	301	CLA	C4B-CHC-C1C	2.54	132.36	126.34
22	B	842	CLA	C1D-ND-C4D	-2.54	104.53	106.33
22	6	309	CLA	CHA-C4D-ND	2.54	137.81	132.50
22	B	807	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
22	5	308	CLA	CHA-C4D-ND	2.54	137.81	132.50
38	1	302	LUT	C21-C26-C27	-2.54	109.49	112.70
39	4	819	CHL	CHC-C1C-NC	2.54	128.05	124.20
22	1	316	CLA	CHA-C1A-NA	-2.54	120.59	126.40
24	G	203	BCR	C30-C25-C26	-2.54	119.04	122.61
22	7	317	CLA	C4B-CHC-C1C	2.54	132.35	126.34
22	A	811	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
22	A	841	CLA	O2A-CGA-CBA	2.54	119.87	111.91
22	A	828	CLA	O2A-CGA-CBA	2.54	119.86	111.91
22	B	815	CLA	C4B-CHC-C1C	2.54	132.35	126.34
22	1	309	CLA	CMA-C3A-C4A	2.53	118.59	111.77
36	5	306	C7Z	C8-C7-C6	-2.53	120.08	127.20
22	7	309	CLA	C3B-C4B-NB	-2.53	108.16	110.52
22	4	809	CLA	CHA-C4D-ND	2.53	137.80	132.50
22	B	832	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
22	7	305	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
38	6	303	LUT	C38-C25-C24	-2.53	118.14	123.56
22	6	311	CLA	C1D-ND-C4D	-2.53	104.54	106.33
22	B	812	CLA	C1D-ND-C4D	-2.53	104.54	106.33
22	Z	314	CLA	C4B-CHC-C1C	2.53	132.34	126.34
24	K	206	BCR	C15-C16-C17	-2.53	118.29	123.47
38	3	303	LUT	C21-C26-C27	-2.53	109.50	112.70
22	Z	310	CLA	C4B-CHC-C1C	2.53	132.34	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	304	CLA	CHA-C4D-ND	2.53	137.79	132.50
22	9	304	CLA	C4B-CHC-C1C	2.53	132.34	126.34
22	8	313	CLA	C3B-C4B-NB	-2.53	108.17	110.52
22	6	317	CLA	C4B-CHC-C1C	2.53	132.33	126.34
24	B	849	BCR	C2-C1-C6	2.53	114.37	110.48
22	5	326	CLA	CHA-C4D-ND	2.53	137.79	132.50
22	9	304	CLA	CHA-C1A-NA	-2.53	120.61	126.40
22	6	322	CLA	CHA-C4D-ND	2.53	137.78	132.50
22	3	320	CLA	C1D-ND-C4D	-2.53	104.54	106.33
22	A	834	CLA	C3B-C4B-NB	-2.53	108.17	110.52
22	B	808	CLA	C3B-C4B-NB	-2.53	108.17	110.52
38	5	303	LUT	C21-C26-C27	-2.53	109.51	112.70
22	8	306	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
22	B	836	CLA	C3B-C4B-NB	-2.53	108.17	110.52
22	G	202	CLA	C3B-C4B-NB	-2.53	108.17	110.52
22	9	309	CLA	CHA-C4D-ND	2.53	137.78	132.50
22	5	308	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	A	842	CLA	C3B-C4B-NB	-2.52	108.17	110.52
22	Z	315	CLA	C1D-ND-C4D	-2.52	104.54	106.33
22	A	828	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
22	4	805	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
22	5	301	CLA	C4B-CHC-C1C	2.52	132.32	126.34
22	1	305	CLA	CHA-C4D-ND	2.52	137.78	132.50
39	4	819	CHL	CMA-C3A-C4A	2.52	118.55	111.77
22	6	307	CLA	C4B-CHC-C1C	2.52	132.32	126.34
22	8	308	CLA	C3B-C4B-NB	-2.52	108.17	110.52
39	2	303	CHL	C2C-C3C-C4C	2.52	108.29	106.49
22	4	810	CLA	CMA-C3A-C4A	2.52	118.55	111.77
22	1	307	CLA	O2A-CGA-CBA	2.52	119.82	111.91
22	Z	303	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
22	B	819	CLA	C4B-CHC-C1C	2.52	132.32	126.34
39	6	316	CHL	CHC-C1C-NC	2.52	128.03	124.20
22	K	205	CLA	CMA-C3A-C2A	2.52	124.00	113.83
24	8	304	BCR	C8-C7-C6	-2.52	120.12	127.20
22	3	315	CLA	C4B-CHC-C1C	2.52	132.32	126.34
22	9	306	CLA	O2A-CGA-CBA	2.52	119.82	111.91
22	7	308	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	5	313	CLA	C4B-CHC-C1C	2.52	132.31	126.34
39	4	814	CHL	C2C-C3C-C4C	2.52	108.28	106.49
22	B	826	CLA	CHA-C4D-ND	2.52	137.77	132.50
22	5	322	CLA	C3B-C4B-NB	-2.52	108.18	110.52
22	A	809	CLA	O2A-CGA-CBA	2.52	119.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	319	CLA	C4B-CHC-C1C	2.52	132.31	126.34
39	7	313	CHL	C2C-C3C-C4C	2.52	108.28	106.49
22	A	834	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	9	306	CLA	C3B-C4B-NB	-2.52	108.18	110.52
22	A	830	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	3	315	CLA	CHA-C4D-ND	2.52	137.76	132.50
22	3	311	CLA	C4B-CHC-C1C	2.52	132.30	126.34
22	2	302	CLA	C4B-CHC-C1C	2.51	132.30	126.34
24	6	305	BCR	C23-C24-C25	-2.51	120.14	127.20
22	1	315	CLA	C3B-C4B-NB	-2.51	108.18	110.52
24	3	307	BCR	C8-C7-C6	-2.51	120.14	127.20
22	B	838	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	7	317	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
22	B	831	CLA	C4B-CHC-C1C	2.51	132.29	126.34
38	Z	302	LUT	C11-C12-C13	-2.51	119.36	126.42
22	3	311	CLA	C3B-C4B-NB	-2.51	108.19	110.52
38	9	301	LUT	C21-C26-C25	2.51	115.91	111.42
22	L	202	CLA	C4B-CHC-C1C	2.51	132.29	126.34
22	7	312	CLA	O2A-CGA-CBA	2.51	119.78	111.91
22	B	835	CLA	C4B-CHC-C1C	2.51	132.29	126.34
22	A	812	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
38	3	302	LUT	C1-C6-C5	-2.51	119.08	122.61
22	B	822	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
22	4	810	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	6	308	CLA	C3B-C4B-NB	-2.51	108.19	110.52
24	A	845	BCR	C8-C7-C6	-2.51	120.16	127.20
39	9	314	CHL	CMA-C3A-C4A	2.51	118.51	111.77
22	7	307	CLA	CMD-C2D-C3D	-2.51	121.85	127.61
22	1	311	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	5	311	CLA	CHA-C4D-ND	2.51	137.74	132.50
22	8	305	CLA	C1C-C2C-C3C	-2.50	104.32	106.96
22	B	821	CLA	C4B-CHC-C1C	2.50	132.28	126.34
22	A	833	CLA	C4B-CHC-C1C	2.50	132.28	126.34
22	2	301	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
22	B	813	CLA	CHA-C4D-ND	2.50	137.74	132.50
39	8	315	CHL	C3B-C4B-NB	-2.50	108.19	110.52
22	9	309	CLA	CMA-C3A-C4A	2.50	118.50	111.77
22	Z	309	CLA	O2A-CGA-CBA	2.50	119.76	111.91
24	J	104	BCR	C8-C7-C6	-2.50	120.17	127.20
22	9	310	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	A	813	CLA	C4B-CHC-C1C	2.50	132.27	126.34
24	A	847	BCR	C8-C7-C6	-2.50	120.18	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	306	CLA	CHA-C4D-ND	2.50	137.73	132.50
24	3	304	BCR	C10-C11-C12	2.50	131.02	123.22
22	A	817	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	7	315	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	B	834	CLA	CHA-C4D-ND	2.50	137.73	132.50
22	B	824	CLA	C4B-CHC-C1C	2.50	132.27	126.34
24	B	847	BCR	C35-C13-C14	-2.50	119.42	122.92
22	9	304	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	3	307	BCR	C34-C9-C10	-2.50	119.42	122.92
39	7	313	CHL	CMA-C3A-C4A	2.50	118.49	111.77
22	1	310	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	5	320	CLA	CHA-C1A-NA	-2.50	120.68	126.40
22	5	320	CLA	C4B-CHC-C1C	2.50	132.26	126.34
22	7	322	CLA	C4B-CHC-C1C	2.50	132.26	126.34
22	A	807	CLA	CHA-C4D-ND	2.50	137.72	132.50
22	A	816	CLA	CHA-C4D-ND	2.49	137.72	132.50
22	A	835	CLA	C4B-CHC-C1C	2.49	132.25	126.34
22	J	103	CLA	C4B-CHC-C1C	2.49	132.25	126.34
22	3	320	CLA	CHA-C4D-ND	2.49	137.72	132.50
22	B	835	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
22	9	307	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	8	309	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	6	312	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	1	307	CLA	C3B-C4B-NB	-2.49	108.20	110.52
22	A	805	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	7	311	CLA	C4B-CHC-C1C	2.49	132.24	126.34
22	4	811	CLA	CHA-C4D-ND	2.49	137.71	132.50
22	Z	303	CLA	C3B-C4B-NB	-2.49	108.21	110.52
24	L	204	BCR	C23-C24-C25	-2.49	120.21	127.20
22	9	304	CLA	C3D-C2D-C1D	-2.49	102.44	105.83
22	6	307	CLA	O2A-CGA-CBA	2.49	119.72	111.91
22	A	823	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	6	319	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	6	322	CLA	C1D-ND-C4D	-2.49	104.57	106.33
22	B	823	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
22	A	811	CLA	O2A-CGA-CBA	2.49	119.71	111.91
22	B	832	CLA	C4B-CHC-C1C	2.49	132.24	126.34
24	F	303	BCR	C23-C24-C25	-2.49	120.22	127.20
22	B	828	CLA	CHA-C4D-ND	2.49	137.70	132.50
24	B	848	BCR	C4-C5-C6	-2.49	119.12	122.73
22	3	313	CLA	CMA-C3A-C4A	2.49	118.45	111.77
22	A	812	CLA	CHA-C4D-ND	2.48	137.69	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	202	CLA	CHA-C4D-ND	2.48	137.69	132.50
24	A	856	BCR	C15-C16-C17	-2.48	118.39	123.47
22	2	302	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
22	Z	306	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	A	830	CLA	C4B-CHC-C1C	2.48	132.23	126.34
22	6	307	CLA	CHA-C4D-ND	2.48	137.69	132.50
32	F	306	RRX	C2-C1-C6	2.48	114.30	110.48
22	A	819	CLA	C4B-CHC-C1C	2.48	132.22	126.34
22	7	304	CLA	C4B-CHC-C1C	2.48	132.22	126.34
22	A	804	CLA	CMA-C3A-C4A	2.48	118.44	111.77
22	7	323	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	B	810	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	1	309	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	1	313	CLA	C4B-CHC-C1C	2.48	132.22	126.34
22	K	205	CLA	CHA-C4D-ND	2.48	137.69	132.50
22	A	816	CLA	C3B-C4B-NB	-2.48	108.21	110.52
22	A	826	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	K	202	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	K	203	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	3	313	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	6	312	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	A	834	CLA	C4B-CHC-C1C	2.48	132.22	126.34
22	1	313	CLA	CHA-C4D-ND	2.48	137.68	132.50
22	B	838	CLA	CMD-C2D-C3D	-2.48	121.91	127.61
39	4	819	CHL	C2C-C3C-C4C	2.48	108.25	106.49
22	A	826	CLA	C4B-CHC-C1C	2.48	132.21	126.34
22	F	304	CLA	C4B-CHC-C1C	2.48	132.21	126.34
22	B	835	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	A	804	CLA	CHA-C4D-ND	2.48	137.68	132.50
24	7	303	BCR	C30-C25-C26	-2.48	119.13	122.61
22	1	315	CLA	CHA-C4D-ND	2.48	137.68	132.50
22	Z	313	CLA	CHA-C4D-ND	2.48	137.68	132.50
22	K	203	CLA	CHA-C4D-ND	2.48	137.68	132.50
22	7	324	CLA	CHA-C4D-ND	2.48	137.68	132.50
22	B	814	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
24	3	306	BCR	C35-C13-C14	-2.48	119.46	122.92
22	B	807	CLA	C4B-CHC-C1C	2.47	132.21	126.34
22	B	831	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	Z	307	CLA	C4B-CHC-C1C	2.47	132.21	126.34
22	1	315	CLA	C4B-CHC-C1C	2.47	132.21	126.34
22	5	312	CLA	CHA-C4D-ND	2.47	137.67	132.50
22	A	804	CLA	C4B-CHC-C1C	2.47	132.20	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	810	CLA	C4B-CHC-C1C	2.47	132.20	126.34
22	B	840	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	B	805	CLA	CHA-C4D-ND	2.47	137.67	132.50
22	B	815	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
38	9	301	LUT	C35-C15-C14	-2.47	118.41	123.47
24	4	804	BCR	C8-C7-C6	-2.47	120.26	127.20
22	5	311	CLA	C4B-CHC-C1C	2.47	132.20	126.34
22	6	313	CLA	C4B-CHC-C1C	2.47	132.20	126.34
22	8	310	CLA	C4B-CHC-C1C	2.47	132.20	126.34
22	A	816	CLA	O2A-CGA-CBA	2.47	119.66	111.91
22	5	309	CLA	CHA-C4D-ND	2.47	137.66	132.50
21	A	801	CL0	O2D-CGD-O1D	-2.47	119.01	123.84
39	8	312	CHL	CHC-C1C-NC	2.47	127.95	124.20
24	F	303	BCR	C20-C19-C18	-2.47	119.48	126.42
22	F	305	CLA	C4B-CHC-C1C	2.47	132.19	126.34
22	3	309	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	5	312	CLA	C3B-C4B-NB	-2.47	108.23	110.52
24	A	845	BCR	C36-C18-C17	-2.47	119.47	122.92
24	B	853	BCR	C20-C19-C18	-2.47	119.49	126.42
22	B	806	CLA	CHA-C4D-ND	2.47	137.66	132.50
22	9	307	CLA	C4B-CHC-C1C	2.46	132.18	126.34
22	A	805	CLA	C4B-CHC-C1C	2.46	132.18	126.34
22	4	805	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	B	825	CLA	O2A-CGA-CBA	2.46	119.64	111.91
22	B	834	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	4	818	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
22	A	818	CLA	C4B-CHC-C1C	2.46	132.18	126.34
22	G	201	CLA	C1D-ND-C4D	-2.46	104.58	106.33
22	4	805	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
22	9	307	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	A	820	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	K	202	CLA	C4B-CHC-C1C	2.46	132.18	126.34
22	5	311	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	9	305	CLA	CAA-CBA-CGA	-2.46	106.06	113.25
22	A	826	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	5	307	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
22	A	827	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	3	312	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	5	307	CLA	CHA-C4D-ND	2.46	137.65	132.50
22	B	826	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	802	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	A	824	CLA	C1-C2-C3	-2.46	121.79	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	833	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	806	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	B	842	CLA	C4B-CHC-C1C	2.46	132.17	126.34
22	6	309	CLA	CHA-C1A-NA	-2.46	120.77	126.40
22	B	816	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	A	826	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	A	818	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	B	837	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	4	806	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	3	322	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	B	838	CLA	C4B-CHC-C1C	2.46	132.16	126.34
22	8	309	CLA	C4B-CHC-C1C	2.46	132.16	126.34
22	F	302	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	5	310	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	6	312	CLA	O2A-CGA-CBA	2.46	119.61	111.91
22	B	841	CLA	C4B-CHC-C1C	2.46	132.16	126.34
22	A	825	CLA	CHA-C4D-ND	2.46	137.64	132.50
22	3	310	CLA	O2A-CGA-CBA	2.46	119.61	111.91
22	9	305	CLA	CHA-C4D-ND	2.46	137.63	132.50
22	B	837	CLA	C4B-CHC-C1C	2.46	132.16	126.34
22	3	312	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
22	Z	313	CLA	C1-C2-C3	-2.45	121.80	126.04
22	B	813	CLA	C4B-CHC-C1C	2.45	132.16	126.34
22	B	842	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	7	312	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	5	307	CLA	C4B-CHC-C1C	2.45	132.16	126.34
22	A	840	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	Z	303	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	3	316	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	A	840	CLA	C4B-CHC-C1C	2.45	132.16	126.34
22	A	813	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	3	301	DGD	O1G-C1A-C2A	2.45	119.60	111.91
22	A	837	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	6	309	CLA	C1D-ND-C4D	-2.45	104.59	106.33
24	A	847	BCR	C11-C12-C13	-2.45	119.53	126.42
22	A	804	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
24	K	206	BCR	C8-C7-C6	-2.45	120.32	127.20
22	A	833	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	4	810	CLA	CHA-C4D-ND	2.45	137.63	132.50
22	3	320	CLA	CMA-C3A-C4A	2.45	118.36	111.77
21	A	801	CL0	C3D-C4D-ND	2.45	114.20	110.24
22	7	308	CLA	C3B-C4B-NB	-2.45	108.24	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	308	CLA	C4B-CHC-C1C	2.45	132.15	126.34
39	3	317	CHL	C2B-C1B-NB	-2.45	108.59	110.23
22	3	320	CLA	CHA-C1A-NA	-2.45	120.79	126.40
22	K	205	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	4	807	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	7	306	CLA	CHA-C1A-NA	-2.45	120.79	126.40
22	7	324	CLA	C4B-CHC-C1C	2.45	132.15	126.34
22	5	315	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	B	827	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	B	816	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
22	9	306	CLA	CHA-C4D-ND	2.45	137.62	132.50
22	3	309	CLA	C4B-CHC-C1C	2.45	132.14	126.34
22	3	318	CLA	C4B-CHC-C1C	2.45	132.14	126.34
22	4	806	CLA	C4B-CHC-C1C	2.45	132.14	126.34
22	A	822	CLA	C4B-CHC-C1C	2.45	132.14	126.34
22	6	321	CLA	C4B-CHC-C1C	2.45	132.14	126.34
22	A	830	CLA	CHA-C4D-ND	2.45	137.62	132.50
24	A	846	BCR	C23-C24-C25	-2.45	120.33	127.20
41	5	325	3PH	O31-C31-C32	2.45	119.58	111.91
22	4	810	CLA	C4B-CHC-C1C	2.45	132.14	126.34
38	5	303	LUT	C11-C12-C13	-2.45	119.55	126.42
25	5	324	LHG	C5-O7-C7	-2.44	111.77	117.79
22	A	839	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	7	315	CLA	C4B-CHC-C1C	2.44	132.13	126.34
22	L	201	CLA	CHA-C4D-ND	2.44	137.61	132.50
22	A	814	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	5	308	CLA	CMA-C3A-C4A	2.44	118.33	111.77
22	8	307	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	827	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	F	305	CLA	CHA-C4D-ND	2.44	137.60	132.50
24	5	305	BCR	C38-C26-C27	2.44	118.30	113.62
22	B	808	CLA	O2A-CGA-CBA	2.44	119.56	111.91
22	A	836	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	3	308	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	A	830	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	A	803	CLA	O2A-CGA-CBA	2.44	119.56	111.91
22	L	203	CLA	C4B-CHC-C1C	2.44	132.12	126.34
24	I	4001	BCR	C8-C7-C6	-2.44	120.35	127.20
22	5	322	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	1	314	CLA	C4B-CHC-C1C	2.44	132.12	126.34
22	9	311	CLA	CHA-C4D-ND	2.44	137.60	132.50
39	1	312	CHL	C3B-C4B-NB	-2.44	108.25	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	819	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	A	815	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	A	836	CLA	CMA-C3A-C4A	2.44	118.32	111.77
22	1	307	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	3	310	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	822	CLA	C4B-CHC-C1C	2.44	132.12	126.34
22	4	817	CLA	C4B-CHC-C1C	2.44	132.12	126.34
25	A	849	LHG	O8-C23-C24	2.44	119.56	111.91
22	B	819	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	820	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	6	301	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	6	314	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	B	827	CLA	C4B-CHC-C1C	2.44	132.12	126.34
22	4	812	CLA	C4B-CHC-C1C	2.44	132.12	126.34
22	A	854	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
22	7	306	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	A	842	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
22	B	811	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	8	310	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	3	310	CLA	CHA-C1A-NA	-2.44	120.82	126.40
22	B	814	CLA	CHA-C4D-ND	2.44	137.59	132.50
22	F	301	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	1	316	CLA	C4B-CHC-C1C	2.43	132.11	126.34
22	9	309	CLA	O2A-CGA-CBA	2.43	119.55	111.91
22	A	814	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	6	310	CLA	O2A-CGA-CBA	2.43	119.55	111.91
22	B	808	CLA	C4B-CHC-C1C	2.43	132.11	126.34
24	A	847	BCR	C2-C1-C6	2.43	114.23	110.48
22	3	309	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	8	307	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	A	821	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	B	817	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	7	323	CLA	C1-C2-C3	-2.43	121.84	126.04
22	5	318	CLA	C4B-CHC-C1C	2.43	132.11	126.34
22	B	836	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	3	314	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	2	301	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	A	855	CLA	CHA-C4D-ND	2.43	137.59	132.50
22	6	311	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	5	318	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	A	819	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	G	202	CLA	CHA-C4D-ND	2.43	137.58	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	833	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	B	840	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	B	816	CLA	C4B-CHC-C1C	2.43	132.10	126.34
22	5	322	CLA	C4B-CHC-C1C	2.43	132.10	126.34
22	7	311	CLA	CHA-C4D-ND	2.43	137.58	132.50
24	8	304	BCR	C23-C24-C25	-2.43	120.38	127.20
22	B	815	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	2	302	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	L	203	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	1	308	CLA	CHA-C4D-ND	2.43	137.58	132.50
22	8	314	CLA	C4B-CHC-C1C	2.43	132.10	126.34
24	K	206	BCR	C23-C24-C25	-2.43	120.39	127.20
22	A	854	CLA	CHA-C4D-ND	2.43	137.57	132.50
22	4	815	CLA	CHA-C4D-ND	2.43	137.57	132.50
22	6	319	CLA	CHA-C4D-ND	2.43	137.57	132.50
22	A	811	CLA	CHA-C4D-ND	2.43	137.57	132.50
22	A	827	CLA	C4B-CHC-C1C	2.43	132.09	126.34
22	A	831	CLA	C4B-CHC-C1C	2.43	132.09	126.34
22	Z	315	CLA	C4B-CHC-C1C	2.43	132.09	126.34
22	8	313	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
38	6	304	LUT	C15-C35-C34	-2.43	118.51	123.47
22	B	836	CLA	C4B-CHC-C1C	2.43	132.09	126.34
22	4	815	CLA	C4B-CHC-C1C	2.43	132.09	126.34
22	5	320	CLA	CHA-C4D-ND	2.43	137.57	132.50
22	B	834	CLA	O2A-CGA-CBA	2.43	119.52	111.91
22	A	803	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
22	B	825	CLA	C4B-CHC-C1C	2.42	132.09	126.34
22	3	320	CLA	C4B-CHC-C1C	2.42	132.09	126.34
22	6	309	CLA	C4B-CHC-C1C	2.42	132.09	126.34
22	A	832	CLA	C3B-C4B-NB	-2.42	108.27	110.52
38	5	302	LUT	C18-C5-C4	2.42	118.84	114.36
22	B	838	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	Z	315	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	5	312	CLA	C4B-CHC-C1C	2.42	132.08	126.34
24	6	306	BCR	C37-C22-C23	2.42	121.89	118.08
22	6	302	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
22	A	822	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	A	831	CLA	CHA-C4D-ND	2.42	137.57	132.50
22	1	304	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	6	322	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	A	828	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	A	832	CLA	CHA-C4D-ND	2.42	137.56	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	319	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	7	314	CLA	O2A-CGA-CBA	2.42	119.51	111.91
22	A	838	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	B	818	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
22	A	842	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	6	312	CLA	C4B-CHC-C1C	2.42	132.08	126.34
22	1	309	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
22	B	841	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
38	7	302	LUT	C19-C9-C10	-2.42	119.53	122.92
22	A	808	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	7	307	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	B	841	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	8	316	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	A	838	CLA	C4B-CHC-C1C	2.42	132.07	126.34
22	6	319	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	7	316	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	B	801	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	A	822	CLA	O2A-CGA-CBA	2.42	119.49	111.91
39	5	317	CHL	CMA-C3A-C4A	2.42	118.27	111.77
22	7	305	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	1	309	CLA	C4B-CHC-C1C	2.42	132.07	126.34
22	Z	308	CLA	C4B-CHC-C1C	2.42	132.07	126.34
22	8	311	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	8	313	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	B	809	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	Z	307	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	1	306	CLA	C4B-CHC-C1C	2.42	132.07	126.34
22	1	311	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	6	302	CLA	CHA-C4D-ND	2.42	137.55	132.50
36	5	306	C7Z	C24-C25-C26	-2.42	115.47	120.85
22	B	820	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
24	6	306	BCR	C34-C9-C10	-2.42	119.54	122.92
22	A	829	CLA	CHA-C4D-ND	2.42	137.55	132.50
22	4	817	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	B	810	CLA	C4B-CHC-C1C	2.41	132.06	126.34
22	4	817	CLA	CHA-C4D-ND	2.41	137.55	132.50
24	A	856	BCR	C29-C30-C25	2.41	114.20	110.48
22	B	826	CLA	C4B-CHC-C1C	2.41	132.06	126.34
22	B	818	CLA	CHA-C4D-ND	2.41	137.55	132.50
22	B	821	CLA	CHA-C4D-ND	2.41	137.55	132.50
22	B	835	CLA	CHA-C4D-ND	2.41	137.55	132.50
22	4	809	CLA	O2A-CGA-CBA	2.41	119.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	835	CLA	CMA-C3A-C4A	2.41	118.26	111.77
22	B	812	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	A	821	CLA	C4B-CHC-C1C	2.41	132.06	126.34
22	4	805	CLA	C1-C2-C3	-2.41	121.87	126.04
22	Z	308	CLA	CHA-C4D-ND	2.41	137.54	132.50
24	6	306	BCR	C8-C7-C6	-2.41	120.43	127.20
22	B	820	CLA	C4B-CHC-C1C	2.41	132.06	126.34
22	B	829	CLA	C4B-CHC-C1C	2.41	132.06	126.34
38	1	302	LUT	C38-C25-C24	-2.41	118.40	123.56
32	F	306	RRX	C30-C25-C26	-2.41	119.22	122.61
22	8	305	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
22	A	816	CLA	C1D-ND-C4D	-2.41	104.62	106.33
22	1	306	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	3	313	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	9	313	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	6	317	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	6	321	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	6	307	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	1	306	CLA	O2A-CGA-CBA	2.41	119.47	111.91
22	1	304	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	5	323	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	3	316	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	A	836	CLA	C4B-CHC-C1C	2.41	132.05	126.34
22	B	839	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	B	809	CLA	C4B-CHC-C1C	2.41	132.05	126.34
22	6	317	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	B	826	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
22	4	812	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	G	202	CLA	C4B-CHC-C1C	2.41	132.05	126.34
22	6	307	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	A	838	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	B	808	CLA	CHA-C4D-ND	2.41	137.54	132.50
22	A	828	CLA	C4B-CHC-C1C	2.41	132.05	126.34
22	6	308	CLA	C4B-CHC-C1C	2.41	132.05	126.34
22	9	308	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	3	312	CLA	O2A-CGA-CBA	2.41	119.46	111.91
22	Z	309	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	A	810	CLA	CHA-C4D-ND	2.41	137.53	132.50
22	3	311	CLA	O2A-CGA-CBA	2.41	119.46	111.91
33	4	801	LMT	C1B-O1B-C4'	-2.41	112.01	117.96
22	A	822	CLA	C3B-C4B-NB	-2.41	108.28	110.52
24	A	847	BCR	C27-C26-C25	-2.41	119.24	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	311	CLA	CHA-C4D-ND	2.41	137.53	132.50
24	7	303	BCR	C1-C6-C7	2.41	122.58	115.78
22	B	827	CLA	C3B-C4B-NB	-2.40	108.28	110.52
22	3	314	CLA	C1-O2A-CGA	2.40	122.75	116.44
22	B	822	CLA	CHA-C4D-ND	2.40	137.53	132.50
39	5	317	CHL	C2C-C3C-C4C	2.40	108.20	106.49
22	Z	305	CLA	C4B-CHC-C1C	2.40	132.04	126.34
22	A	820	CLA	C6-C5-C3	-2.40	107.15	113.45
22	1	304	CLA	O2A-CGA-CBA	2.40	119.45	111.91
22	4	818	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	7	324	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	A	849	LHG	C5-O7-C7	-2.40	111.87	117.79
22	A	815	CLA	C3B-C4B-NB	-2.40	108.28	110.52
22	8	308	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	4	812	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	6	311	CLA	C4B-CHC-C1C	2.40	132.04	126.34
38	6	303	LUT	C11-C12-C13	-2.40	119.67	126.42
22	5	318	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	B	833	CLA	C3B-C4B-NB	-2.40	108.29	110.52
22	B	812	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	7	322	CLA	CHA-C4D-ND	2.40	137.53	132.50
22	5	311	CLA	O2A-CGA-CBA	2.40	119.45	111.91
24	B	848	BCR	C1-C6-C7	2.40	122.57	115.78
38	4	803	LUT	C11-C12-C13	-2.40	119.67	126.42
39	9	312	CHL	C4D-CHA-C1A	2.40	124.17	121.25
22	6	309	CLA	C3B-C4B-NB	-2.40	108.29	110.52
22	A	816	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	B	837	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	B	840	CLA	C4B-CHC-C1C	2.40	132.03	126.34
22	5	314	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	Z	306	CLA	O2A-CGA-CBA	2.40	119.44	111.91
22	8	314	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	7	309	CLA	C4B-CHC-C1C	2.40	132.03	126.34
24	B	846	BCR	C10-C11-C12	-2.40	115.73	123.22
22	7	317	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	8	311	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	7	304	CLA	C1-O2A-CGA	2.40	122.74	116.44
22	B	801	CLA	CMA-C3A-C4A	2.40	118.22	111.77
22	A	823	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	B	824	CLA	CHA-C4D-ND	2.40	137.52	132.50
22	7	316	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
24	3	306	BCR	C8-C7-C6	-2.40	120.47	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	1	312	CHL	CHC-C1C-NC	2.40	127.84	124.20
22	A	834	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	4	807	CLA	CHA-C1A-NA	-2.40	120.91	126.40
22	B	832	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	A	842	CLA	C4B-CHC-C1C	2.40	132.02	126.34
22	7	305	CLA	C4B-CHC-C1C	2.40	132.02	126.34
22	B	824	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
22	B	828	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	B	812	CLA	C4B-CHC-C1C	2.40	132.02	126.34
22	J	103	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	7	314	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	6	310	CLA	CHA-C4D-ND	2.40	137.51	132.50
41	6	324	3PH	O31-C31-C32	2.40	119.43	111.91
22	B	834	CLA	C4B-CHC-C1C	2.40	132.02	126.34
22	6	313	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	A	803	CLA	CHA-C4D-ND	2.40	137.51	132.50
22	B	827	CLA	O2A-CGA-CBA	2.40	119.42	111.91
22	B	841	CLA	O2A-CGA-CBA	2.40	119.42	111.91
25	7	318	LHG	C5-O7-C7	-2.39	111.89	117.79
22	B	833	CLA	C4B-CHC-C1C	2.39	132.02	126.34
24	3	304	BCR	C7-C6-C5	-2.39	115.66	121.46
22	Z	306	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
23	B	843	PQN	C2M-C2-C3	-2.39	120.50	124.40
22	8	305	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	3	310	CLA	C4B-CHC-C1C	2.39	132.01	126.34
22	5	308	CLA	C3B-C4B-NB	-2.39	108.30	110.52
22	Z	316	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	B	807	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	5	319	CLA	CHA-C4D-ND	2.39	137.50	132.50
35	J	102	T7X	O18-C11-C31	2.39	119.41	111.91
22	5	323	CLA	C4B-CHC-C1C	2.39	132.01	126.34
22	A	835	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	5	310	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
22	B	823	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	3	318	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	A	818	CLA	O2A-CGA-CBA	2.39	119.41	111.91
22	A	839	CLA	C4B-CHC-C1C	2.39	132.00	126.34
22	Z	307	CLA	O2A-CGA-CBA	2.39	119.41	111.91
24	3	304	BCR	C36-C18-C19	2.39	121.84	118.08
22	A	815	CLA	C4B-CHC-C1C	2.39	132.00	126.34
22	Z	313	CLA	CHD-C1D-ND	-2.39	122.26	124.45
22	K	203	CLA	C4B-CHC-C1C	2.39	132.00	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	825	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	6	308	CLA	CHA-C4D-ND	2.39	137.49	132.50
34	J	101	LMG	C8-O7-C10	-2.39	111.91	117.79
22	K	204	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	1	311	CLA	CMA-C3A-C4A	2.39	118.19	111.77
22	Z	307	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
22	4	811	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	A	841	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	5	301	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	6	301	CLA	O2A-CGA-CBA	2.39	119.40	111.91
22	A	839	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	L	202	CLA	CHA-C4D-ND	2.39	137.49	132.50
22	6	309	CLA	CMD-C2D-C3D	-2.39	122.13	127.61
24	B	846	BCR	C8-C9-C10	2.39	122.60	118.94
22	7	306	CLA	C4B-CHC-C1C	2.39	132.00	126.34
22	8	313	CLA	C4B-CHC-C1C	2.38	131.99	126.34
22	A	832	CLA	C6-C5-C3	-2.38	107.20	113.45
22	8	306	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	8	305	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
24	3	307	BCR	C38-C26-C27	2.38	118.19	113.62
22	B	817	CLA	C4B-CHC-C1C	2.38	131.99	126.34
22	7	310	CLA	C4B-CHC-C1C	2.38	131.99	126.34
39	8	312	CHL	C3B-C4B-NB	-2.38	108.30	110.52
22	A	825	CLA	C4B-CHC-C1C	2.38	131.99	126.34
22	6	308	CLA	O2A-CGA-CBA	2.38	119.39	111.91
38	Z	301	LUT	C21-C26-C27	-2.38	109.69	112.70
22	9	313	CLA	O2A-CGA-CBA	2.38	119.38	111.91
22	1	311	CLA	C4B-CHC-C1C	2.38	131.99	126.34
22	B	830	CLA	CHA-C4D-ND	2.38	137.48	132.50
22	Z	314	CLA	CHA-C4D-ND	2.38	137.48	132.50
22	A	822	CLA	C1D-ND-C4D	-2.38	104.64	106.33
22	A	832	CLA	C4B-CHC-C1C	2.38	131.98	126.34
22	Z	313	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
22	A	820	CLA	C1-C2-C3	-2.38	121.93	126.04
24	7	303	BCR	C23-C24-C25	-2.38	120.52	127.20
22	4	807	CLA	C4B-CHC-C1C	2.38	131.98	126.34
22	A	818	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
24	B	849	BCR	C37-C22-C21	-2.38	119.59	122.92
22	9	303	CLA	C3D-C2D-C1D	-2.38	102.58	105.83
22	K	204	CLA	C4B-CHC-C1C	2.38	131.98	126.34
22	5	319	CLA	C4B-CHC-C1C	2.38	131.98	126.34
22	B	810	CLA	O2D-CGD-O1D	-2.38	119.19	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	808	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	Z	303	CLA	O2A-CGA-CBA	2.38	119.37	111.91
22	3	319	CLA	C4B-CHC-C1C	2.38	131.98	126.34
22	A	802	CLA	C4B-CHC-C1C	2.38	131.97	126.34
22	2	304	CLA	CHA-C4D-ND	2.38	137.47	132.50
24	B	846	BCR	C37-C22-C21	-2.38	119.59	122.92
22	A	821	CLA	C3B-C4B-NB	-2.38	108.31	110.52
22	7	316	CLA	C4B-CHC-C1C	2.38	131.97	126.34
22	A	806	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
22	A	814	CLA	C4B-CHC-C1C	2.37	131.97	126.34
39	9	312	CHL	C3C-C4C-NC	-2.37	107.91	110.57
22	B	818	CLA	O2A-CGA-CBA	2.37	119.36	111.91
22	B	814	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
25	Z	317	LHG	C5-O7-C7	-2.37	111.95	117.79
22	9	308	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	1	316	CLA	C2A-C1A-CHA	2.37	128.00	123.86
39	9	314	CHL	C2C-C3C-C4C	2.37	108.18	106.49
24	5	304	BCR	C23-C24-C25	-2.37	120.54	127.20
22	7	304	CLA	O2A-CGA-CBA	2.37	119.35	111.91
22	A	823	CLA	C11-C12-C13	-2.37	108.26	115.92
38	Z	301	LUT	C31-C30-C29	-2.37	123.93	127.31
22	B	825	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
22	A	838	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	6	322	CLA	C4B-CHC-C1C	2.37	131.96	126.34
22	A	805	CLA	CHA-C4D-ND	2.37	137.45	132.50
22	B	839	CLA	C4B-CHC-C1C	2.37	131.95	126.34
39	8	312	CHL	C1-O2A-CGA	2.37	122.65	116.44
22	A	824	CLA	CHA-C4D-ND	2.37	137.45	132.50
22	3	314	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	7	309	CLA	O2A-CGA-CBA	2.37	119.33	111.91
22	B	806	CLA	C4B-CHC-C1C	2.37	131.95	126.34
22	B	824	CLA	O2A-CGA-CBA	2.37	119.33	111.91
32	F	306	RRX	C37-C22-C21	-2.37	119.61	122.92
22	A	807	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
22	A	821	CLA	O2A-CGA-CBA	2.36	119.33	111.91
22	B	839	CLA	O2A-CGA-CBA	2.36	119.33	111.91
22	A	823	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
25	7	318	LHG	O8-C23-C24	2.36	119.33	111.91
22	F	302	CLA	O2A-CGA-CBA	2.36	119.33	111.91
22	F	304	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	B	829	CLA	CHA-C4D-ND	2.36	137.44	132.50
22	Z	304	CLA	CHA-C4D-ND	2.36	137.44	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	313	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	1	316	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	A	816	CLA	C4B-CHC-C1C	2.36	131.94	126.34
22	B	834	CLA	C3B-C4B-NB	-2.36	108.32	110.52
24	3	307	BCR	C29-C30-C25	2.36	114.12	110.48
22	7	323	CLA	C4B-CHC-C1C	2.36	131.94	126.34
22	5	320	CLA	C1-O2A-CGA	2.36	122.64	116.44
22	9	308	CLA	C3B-C4B-NB	-2.36	108.33	110.52
22	8	307	CLA	C4B-CHC-C1C	2.36	131.94	126.34
22	9	313	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	A	848	BCR	C37-C22-C21	-2.36	119.62	122.92
22	1	315	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
39	5	321	CHL	CHC-C1C-NC	2.36	127.78	124.20
24	B	845	BCR	C30-C25-C24	2.36	122.45	115.78
22	4	805	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
39	4	813	CHL	C1-O2A-CGA	2.36	122.63	116.44
24	B	847	BCR	C2-C1-C6	2.36	114.11	110.48
22	G	202	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	A	839	CLA	O2A-CGA-CBA	2.36	119.31	111.91
22	B	801	CLA	C4B-CHC-C1C	2.36	131.93	126.34
22	A	808	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	5	313	CLA	CHA-C1A-NA	-2.36	121.00	126.40
27	A	852	DGA	OG1-CA1-CA2	2.36	119.30	111.91
22	A	825	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
22	5	319	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	9	308	CLA	C4B-CHC-C1C	2.36	131.93	126.34
22	F	304	CLA	CMD-C2D-C3D	-2.36	122.20	127.61
38	8	303	LUT	C35-C15-C14	-2.35	118.65	123.47
22	A	837	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	Z	310	CLA	CHA-C4D-ND	2.35	137.42	132.50
22	5	326	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	B	809	CLA	O2A-CGA-CBA	2.35	119.29	111.91
22	5	322	CLA	O2A-CGA-CBA	2.35	119.29	111.91
22	A	854	CLA	C4B-CHC-C1C	2.35	131.92	126.34
22	5	308	CLA	C4B-CHC-C1C	2.35	131.92	126.34
22	G	201	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
39	5	321	CHL	C2C-C3C-C4C	2.35	108.17	106.49
39	5	317	CHL	CHC-C1C-NC	2.35	127.77	124.20
22	Z	309	CLA	CHA-C4D-ND	2.35	137.42	132.50
22	7	309	CLA	CHA-C4D-ND	2.35	137.42	132.50
36	J	105	C7Z	C11-C12-C13	-2.35	119.81	126.42
22	B	824	CLA	O2D-CGD-O1D	-2.35	119.24	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	315	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	3	320	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
22	8	309	CLA	O2A-CGA-CBA	2.35	119.28	111.91
39	4	814	CHL	C3B-C4B-NB	-2.35	108.33	110.52
22	9	303	CLA	CHA-C1A-NA	-2.35	121.02	126.40
22	9	309	CLA	C4B-CHC-C1C	2.35	131.91	126.34
22	1	311	CLA	C1D-ND-C4D	-2.35	104.67	106.33
24	B	849	BCR	C23-C24-C25	-2.35	120.60	127.20
22	A	802	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	A	833	CLA	O2A-CGA-CBA	2.35	119.28	111.91
22	B	806	CLA	O2A-CGA-CBA	2.35	119.28	111.91
22	3	313	CLA	C4B-CHC-C1C	2.35	131.91	126.34
22	B	801	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	J	103	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	4	808	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
39	4	814	CHL	CHC-C1C-NC	2.35	127.76	124.20
22	A	809	CLA	CHA-C4D-ND	2.35	137.41	132.50
22	B	811	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
39	5	316	CHL	C1-C2-C3	-2.35	121.99	126.04
24	A	844	BCR	C7-C6-C5	-2.35	115.78	121.46
22	A	841	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	7	311	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	A	846	BCR	C35-C13-C14	-2.35	119.64	122.92
22	B	832	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
22	A	811	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
22	7	307	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
24	F	303	BCR	C30-C25-C26	-2.34	119.31	122.61
22	A	813	CLA	O2A-CGA-CBA	2.34	119.26	111.91
22	1	307	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	1	307	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
22	B	808	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
22	9	305	CLA	CHD-C1D-ND	-2.34	122.30	124.45
22	B	816	CLA	O2A-CGA-CBA	2.34	119.24	111.91
39	5	316	CHL	C2B-C1B-NB	-2.34	108.67	110.23
22	B	806	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
22	Z	305	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
24	A	845	BCR	C11-C12-C13	-2.34	119.85	126.42
22	B	822	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	1	319	DGD	O6D-C5D-C6D	2.34	111.38	106.67
39	6	320	CHL	CHC-C1C-NC	2.34	127.75	124.20
22	B	812	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
38	3	303	LUT	C30-C31-C32	-2.34	115.93	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	315	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
24	A	856	BCR	C29-C28-C27	2.33	116.59	111.38
22	Z	305	CLA	O2A-CGA-CBA	2.33	119.23	111.91
22	7	312	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
22	A	842	CLA	O2A-CGA-CBA	2.33	119.23	111.91
39	8	315	CHL	C1-C2-C3	-2.33	122.01	126.04
22	A	819	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
22	6	322	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
38	9	301	LUT	C21-C26-C27	-2.33	109.75	112.70
39	4	819	CHL	C2B-C1B-NB	-2.33	108.67	110.23
22	7	304	CLA	CHA-C4D-ND	2.33	137.38	132.50
24	A	847	BCR	C38-C26-C27	2.33	118.10	113.62
24	B	853	BCR	C35-C13-C14	-2.33	119.66	122.92
22	B	829	CLA	O2A-CGA-CBA	2.33	119.22	111.91
39	4	816	CHL	CHC-C1C-NC	2.33	127.74	124.20
22	Z	315	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	K	205	CLA	C1D-ND-C4D	-2.33	104.68	106.33
22	A	810	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
22	7	308	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	A	838	CLA	O2A-CGA-CBA	2.33	119.22	111.91
39	Z	311	CHL	C2B-C1B-NB	-2.33	108.67	110.23
22	7	310	CLA	CHA-C4D-ND	2.33	137.37	132.50
22	3	322	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	3	319	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
22	B	819	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
22	5	314	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
22	3	308	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
22	6	317	CLA	O2A-CGA-CBA	2.33	119.21	111.91
22	1	309	CLA	CAA-CBA-CGA	-2.33	106.46	113.25
22	A	820	CLA	O2A-CGA-CBA	2.32	119.20	111.91
22	A	805	CLA	O2A-CGA-CBA	2.32	119.20	111.91
22	5	323	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
22	5	309	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	Z	314	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	B	840	CLA	O2A-CGA-CBA	2.32	119.20	111.91
40	1	318	SQD	O3-C3-C2	-2.32	104.98	110.35
22	A	836	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	9	305	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	1	306	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	5	326	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	8	316	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
22	7	314	CLA	C4B-CHC-C1C	2.32	131.84	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	318	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
38	7	301	LUT	C8-C7-C6	-2.32	120.69	127.20
22	B	801	CLA	O2A-CGA-CBA	2.32	119.19	111.91
22	Z	310	CLA	O2A-CGA-CBA	2.32	119.19	111.91
24	G	203	BCR	C37-C22-C21	-2.32	119.67	122.92
22	4	805	CLA	C3B-C4B-NB	-2.32	108.36	110.52
22	5	313	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
24	6	306	BCR	C29-C30-C25	2.32	114.05	110.48
22	A	821	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	6	301	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
36	5	306	C7Z	C2-C3-C4	2.32	113.48	110.30
22	9	303	CLA	C6-C5-C3	-2.32	107.38	113.45
22	A	807	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	6	317	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	4	810	CLA	O2A-CGA-CBA	2.32	119.17	111.91
22	A	828	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
22	F	305	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
22	B	819	CLA	O2A-CGA-CBA	2.32	119.17	111.91
24	B	844	BCR	C37-C22-C21	-2.32	119.68	122.92
39	6	316	CHL	C2B-C1B-NB	-2.32	108.68	110.23
24	A	847	BCR	C30-C25-C26	-2.31	119.35	122.61
22	1	314	CLA	CHA-C4D-ND	2.31	137.34	132.50
22	A	839	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
22	A	840	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
39	2	303	CHL	CHC-C1C-NC	2.31	127.71	124.20
22	5	315	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
39	5	316	CHL	CMA-C3A-C2A	2.31	123.16	113.83
22	8	307	CLA	CHA-C1A-NA	-2.31	121.10	126.40
22	6	314	CLA	O2A-CGA-CBA	2.31	119.16	111.91
22	5	307	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
22	6	313	CLA	O2A-CGA-CBA	2.31	119.16	111.91
22	K	202	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	A	816	CLA	CHA-C1A-NA	-2.31	121.11	126.40
38	6	303	LUT	C30-C31-C32	-2.31	116.01	123.22
22	6	301	CLA	C6-C5-C3	-2.31	107.40	113.45
39	Z	312	CHL	CHC-C1C-NC	2.31	127.71	124.20
22	B	815	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	F	305	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	6	313	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	6	311	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	A	811	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
22	Z	308	CLA	CMA-C3A-C4A	2.31	117.98	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	309	CLA	O2A-CGA-CBA	2.31	119.15	111.91
22	B	816	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
24	B	845	BCR	C8-C7-C6	-2.31	120.72	127.20
22	8	311	CLA	O2A-CGA-CBA	2.31	119.15	111.91
41	8	320	3PH	O31-C31-C32	2.31	119.15	111.91
22	6	307	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
38	8	302	LUT	C18-C5-C4	2.31	118.63	114.36
24	B	845	BCR	C11-C12-C13	-2.31	119.94	126.42
22	B	815	CLA	O2A-CGA-CBA	2.31	119.14	111.91
24	6	305	BCR	C37-C22-C21	-2.31	119.69	122.92
22	3	322	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
22	7	308	CLA	O2A-CGA-CBA	2.31	119.14	111.91
22	7	323	CLA	O2A-CGA-CBA	2.31	119.14	111.91
24	G	203	BCR	C16-C15-C14	-2.31	118.75	123.47
24	B	847	BCR	C8-C7-C6	-2.31	120.73	127.20
39	8	301	CHL	C2B-C1B-NB	-2.30	108.69	110.23
22	6	302	CLA	O2A-CGA-CBA	2.30	119.14	111.91
22	A	821	CLA	CMA-C3A-C4A	2.30	117.97	111.77
22	K	205	CLA	CHA-C1A-NA	-2.30	121.12	126.40
22	8	310	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	B	840	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
22	9	306	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
24	6	306	BCR	C35-C13-C12	2.30	121.70	118.08
22	A	855	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	B	807	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	3	310	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
24	3	305	BCR	C1-C6-C7	2.30	122.28	115.78
24	7	303	BCR	C11-C12-C13	-2.30	119.96	126.42
22	9	306	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
22	3	319	CLA	O2A-CGA-CBA	2.30	119.11	111.91
22	A	809	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
21	A	801	CL0	CMD-C2D-C3D	-2.30	122.33	127.61
38	4	802	LUT	C15-C35-C34	-2.30	118.77	123.47
22	7	304	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
22	A	823	CLA	O2A-CGA-CBA	2.30	119.11	111.91
22	6	322	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
22	5	301	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
38	3	303	LUT	C11-C12-C13	-2.29	119.97	126.42
22	4	806	CLA	O2A-CGA-CBA	2.29	119.11	111.91
22	L	201	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
39	4	819	CHL	CHD-C4C-C3C	2.29	128.21	124.84
38	4	802	LUT	C11-C12-C13	-2.29	119.97	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	813	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
24	B	853	BCR	C37-C22-C21	-2.29	119.71	122.92
22	A	817	CLA	C4B-CHC-C1C	2.29	131.77	126.34
22	A	817	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	A	834	CLA	O2A-CGA-CBA	2.29	119.09	111.91
22	6	312	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
22	4	807	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	1	311	CLA	CHA-C1A-NA	-2.29	121.16	126.40
22	B	824	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
39	2	303	CHL	C1-O2A-CGA	2.29	122.44	116.44
22	1	305	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	3	310	CLA	C6-C7-C8	-2.29	108.53	115.92
24	B	853	BCR	C15-C14-C13	-2.29	124.05	127.31
22	A	820	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
22	7	315	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
22	A	814	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	A	831	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
36	5	306	C7Z	C31-C32-C33	-2.28	120.00	126.42
22	3	309	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	A	837	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
22	9	305	CLA	C4B-CHC-C1C	2.28	131.75	126.34
22	7	324	CLA	C1-O2A-CGA	2.28	122.44	116.44
22	A	832	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	A	814	CLA	O2A-CGA-CBA	2.28	119.07	111.91
38	Z	302	LUT	C19-C9-C10	-2.28	119.73	122.92
38	7	301	LUT	C11-C12-C13	-2.28	120.01	126.42
22	B	842	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
22	4	810	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
39	7	313	CHL	CHC-C1C-NC	2.28	127.66	124.20
22	B	828	CLA	CHA-C1A-NA	-2.28	121.17	126.40
22	1	316	CLA	C1-C2-C3	-2.28	122.10	126.04
22	6	321	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	4	805	CLA	CHA-C1A-NA	-2.28	121.18	126.40
38	Z	301	LUT	C40-C33-C34	-2.28	119.73	122.92
39	2	303	CHL	C2B-C1B-NB	-2.28	108.70	110.23
24	5	305	BCR	C19-C18-C17	-2.28	115.45	118.94
22	A	825	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	B	823	CLA	O2A-CGA-CBA	2.28	119.05	111.91
32	F	306	RRX	C34-C9-C10	-2.28	119.73	122.92
22	B	815	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
22	A	831	CLA	O2A-CGA-CBA	2.28	119.05	111.91
22	L	203	CLA	O2D-CGD-O1D	-2.28	119.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	311	CLA	CHA-C1A-NA	-2.28	121.19	126.40
39	5	317	CHL	C3B-C4B-NB	-2.28	108.40	110.52
22	4	809	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
22	B	818	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
22	8	306	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
22	2	301	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
22	A	840	CLA	O2A-CGA-CBA	2.27	119.04	111.91
22	B	813	CLA	O2A-CGA-CBA	2.27	119.04	111.91
22	1	310	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
22	7	322	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
22	3	316	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
24	A	848	BCR	C8-C9-C10	2.27	122.43	118.94
24	G	203	BCR	C11-C10-C9	-2.27	124.07	127.31
22	A	832	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
22	Z	316	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
22	A	818	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	Z	303	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
22	1	316	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
22	Z	306	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
39	9	312	CHL	C2B-C1B-NB	-2.27	108.71	110.23
24	7	303	BCR	C38-C26-C27	2.27	117.97	113.62
22	Z	308	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
24	A	846	BCR	C36-C18-C19	2.27	121.65	118.08
39	8	315	CHL	C4A-NA-C1A	2.27	107.72	106.71
22	A	810	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
36	J	105	C7Z	C28-C27-C26	-2.27	120.84	127.20
22	A	812	CLA	O2A-CGA-CBA	2.27	119.02	111.91
22	A	814	CLA	CHA-C1A-NA	-2.27	121.21	126.40
22	8	308	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
22	A	823	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
22	Z	305	CLA	CHA-C4D-ND	2.26	137.24	132.50
22	Z	316	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	A	815	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
22	Z	315	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
22	A	826	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	9	310	CLA	CHA-C1A-NA	-2.26	121.21	126.40
22	K	204	CLA	O2A-CGA-CBA	2.26	119.01	111.91
22	6	310	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
22	A	809	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
22	B	809	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
22	9	303	CLA	CHA-C4D-ND	2.26	137.23	132.50
22	8	305	CLA	C3B-C4B-NB	-2.26	108.42	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	6	316	CHL	CMA-C3A-C2A	2.26	122.95	113.83
22	A	824	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	3	308	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
22	B	811	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
24	6	305	BCR	C8-C7-C6	-2.26	120.85	127.20
22	A	817	CLA	O2A-CGA-CBA	2.26	119.00	111.91
22	5	301	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
22	5	310	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
24	A	847	BCR	C23-C24-C25	-2.26	120.86	127.20
39	7	313	CHL	C2B-C1B-NB	-2.26	108.72	110.23
24	3	305	BCR	C11-C10-C9	-2.26	124.08	127.31
22	Z	306	CLA	C6-C5-C3	-2.26	107.53	113.45
22	A	839	CLA	CAA-CBA-CGA	-2.26	106.65	113.25
22	G	201	CLA	CHA-C1A-NA	-2.26	121.22	126.40
22	A	821	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
22	Z	308	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
22	B	818	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	B	801	CLA	CHA-C1A-NA	-2.26	121.23	126.40
38	9	301	LUT	C8-C7-C6	-2.26	120.86	127.20
22	K	205	CLA	C4B-CHC-C1C	2.26	131.69	126.34
22	A	812	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
22	A	806	CLA	O2A-CGA-CBA	2.26	118.99	111.91
22	8	309	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
22	6	310	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
22	B	812	CLA	O2A-CGA-CBA	2.26	118.99	111.91
39	9	312	CHL	C3B-C4B-NB	-2.26	108.42	110.52
22	A	855	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
22	7	323	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
22	6	309	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
39	Z	311	CHL	C1-O2A-CGA	2.25	122.35	116.44
22	A	802	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
22	3	318	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
22	1	305	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
22	A	841	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
22	F	301	CLA	C6-C5-C3	-2.25	107.56	113.45
22	7	306	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
22	1	310	CLA	CHA-C1A-NA	-2.25	121.25	126.40
22	B	836	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
22	B	809	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
25	A	850	LHG	C5-O7-C7	-2.25	112.26	117.79
22	7	324	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
22	B	825	CLA	O2D-CGD-O1D	-2.25	119.44	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	805	CLA	O2A-CGA-CBA	2.25	118.95	111.91
22	A	822	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
36	5	306	C7Z	C19-C9-C10	-2.25	119.78	122.92
22	5	323	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
22	5	313	CLA	C1D-ND-C4D	-2.24	104.74	106.33
22	B	821	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
22	L	203	CLA	O2A-CGA-CBA	2.24	118.95	111.91
22	F	302	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
22	9	303	CLA	C2C-C1C-NC	2.24	112.07	109.97
22	3	319	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
22	7	314	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
22	B	821	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
22	A	831	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
38	5	302	LUT	C20-C13-C12	2.24	121.61	118.08
22	B	833	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
38	4	802	LUT	C1-C6-C5	-2.24	119.46	122.61
22	5	315	CLA	CHA-C1A-NA	-2.24	121.27	126.40
22	4	805	CLA	C2D-C1D-ND	2.24	111.75	110.10
22	B	814	CLA	O2A-CGA-CBA	2.24	118.94	111.91
25	4	820	LHG	C5-O7-C7	-2.24	112.28	117.79
22	B	806	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
22	A	838	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
22	B	842	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
22	B	808	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
39	6	320	CHL	CHD-C4C-C3C	2.24	128.13	124.84
39	6	315	CHL	CHB-C4A-NA	2.24	127.61	124.51
22	A	805	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
22	7	308	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
22	8	310	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
22	7	315	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
22	1	313	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
22	5	309	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
24	8	304	BCR	C30-C25-C26	-2.24	119.47	122.61
39	5	316	CHL	CHB-C4A-NA	2.24	127.60	124.51
22	G	202	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
36	5	306	C7Z	C4-C5-C6	-2.23	115.87	120.85
22	4	809	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
24	3	307	BCR	C1-C6-C7	2.23	122.10	115.78
22	B	829	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
38	6	303	LUT	C40-C33-C34	-2.23	119.79	122.92
22	A	813	CLA	C3B-C4B-NB	-2.23	108.44	110.52
22	A	805	CLA	O2D-CGD-O1D	-2.23	119.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	308	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	5	301	CLA	O2A-CGA-CBA	2.23	118.91	111.91
22	B	823	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
24	B	848	BCR	C29-C30-C25	2.23	113.92	110.48
39	8	301	CHL	CMA-C3A-C2A	2.23	122.83	113.83
22	B	835	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	B	810	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	4	812	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	B	839	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	7	304	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
22	B	839	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	K	203	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
39	6	320	CHL	C2B-C1B-NB	-2.23	108.74	110.23
22	L	201	CLA	O2A-CGA-CBA	2.23	118.90	111.91
22	B	838	CLA	C1-C2-C3	-2.23	122.19	126.04
31	3	301	DGD	C2G-O2G-C1B	-2.23	112.31	117.79
22	7	305	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	B	848	BCR	C7-C6-C5	-2.23	116.06	121.46
22	3	316	CLA	O2A-CGA-CBA	2.23	118.90	111.91
22	Z	316	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	A	817	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	B	805	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
22	L	203	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	A	815	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	A	833	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	5	309	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	A	813	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	L	201	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
22	B	832	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
24	7	303	BCR	C27-C26-C25	-2.22	119.50	122.73
39	5	317	CHL	CHD-C4C-C3C	2.22	128.11	124.84
22	6	312	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
22	B	827	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
22	3	309	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
36	J	105	C7Z	C2-C3-C4	2.22	113.34	110.30
38	4	803	LUT	C8-C7-C6	-2.22	120.96	127.20
22	B	813	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
22	6	319	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
24	B	849	BCR	C29-C30-C25	2.22	113.90	110.48
22	A	816	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
22	B	825	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
24	3	304	BCR	C19-C18-C17	-2.22	115.53	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	811	CLA	CHA-C1A-NA	-2.22	121.31	126.40
24	F	303	BCR	C27-C26-C25	-2.22	119.51	122.73
22	8	316	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
24	I	4001	BCR	C23-C24-C25	-2.22	120.97	127.20
36	5	306	C7Z	C40-C33-C34	-2.22	119.81	122.92
22	B	828	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
22	K	203	CLA	CHA-C1A-NA	-2.22	121.32	126.40
22	4	806	CLA	CHA-C1A-NA	-2.22	121.32	126.40
24	B	846	BCR	C35-C13-C14	-2.22	119.82	122.92
24	B	846	BCR	C23-C24-C25	-2.22	120.97	127.20
22	6	311	CLA	O2A-CGA-CBA	2.22	118.86	111.91
22	3	322	CLA	O2A-CGA-CBA	2.22	118.86	111.91
22	A	835	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
22	9	310	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
22	4	818	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
22	A	836	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
22	8	307	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
22	5	308	CLA	O2A-CGA-CBA	2.21	118.85	111.91
22	3	313	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
39	Z	311	CHL	CHC-C1C-NC	2.21	127.56	124.20
24	B	845	BCR	C15-C16-C17	-2.21	118.94	123.47
22	9	305	CLA	C3A-C2A-C1A	2.21	104.65	101.34
22	B	820	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
22	A	817	CLA	C1D-ND-C4D	-2.21	104.76	106.33
22	4	818	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	A	812	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	9	311	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	B	833	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	6	311	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	2	302	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	6	308	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
39	8	315	CHL	CHC-C1C-NC	2.21	127.56	124.20
22	3	311	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
22	A	828	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	6	301	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	A	830	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	3	312	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	8	306	CLA	O2A-CGA-CBA	2.21	118.84	111.91
38	5	302	LUT	C39-C29-C28	2.21	121.56	118.08
22	L	202	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
22	7	312	CLA	CHA-C1A-NA	-2.21	121.34	126.40
24	K	206	BCR	C34-C9-C10	-2.21	119.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	842	CLA	CHA-C1A-NA	-2.21	121.35	126.40
24	5	304	BCR	C36-C18-C17	-2.21	119.83	122.92
22	8	314	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
22	B	819	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
22	B	836	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
22	9	308	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
24	4	804	BCR	C23-C24-C25	-2.20	121.01	127.20
22	F	304	CLA	CHA-C1A-NA	-2.20	121.35	126.40
39	6	318	CHL	CHC-C1C-NC	2.20	127.55	124.20
22	A	834	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
22	L	202	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
22	B	833	CLA	O2A-CGA-CBA	2.20	118.82	111.91
33	4	822	LMT	C1B-O5B-C5B	2.20	118.01	113.69
24	B	849	BCR	C36-C18-C17	-2.20	119.84	122.92
22	F	301	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
22	4	810	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
22	5	312	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
24	5	305	BCR	C1-C6-C7	2.20	122.00	115.78
22	4	805	CLA	C1D-ND-C4D	-2.20	104.77	106.33
31	1	319	DGD	O2G-C1B-O1B	-2.20	118.39	123.70
22	A	802	CLA	C1-O2A-CGA	2.20	122.22	116.44
32	F	306	RRX	C35-C13-C12	-2.20	114.61	118.08
22	4	817	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
24	7	303	BCR	C37-C22-C21	-2.20	119.84	122.92
39	4	816	CHL	C2C-C3C-C4C	2.20	108.06	106.49
22	Z	310	CLA	CHA-C1A-NA	-2.20	121.37	126.40
22	A	827	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	B	834	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	A	824	CLA	C6-C5-C3	-2.20	107.70	113.45
22	K	204	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	B	831	CLA	O2A-CGA-CBA	2.19	118.79	111.91
22	A	820	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	7	317	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	A	842	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
38	5	303	LUT	C22-C23-C24	2.19	114.24	111.74
38	6	304	LUT	C8-C7-C6	-2.19	121.05	127.20
22	F	301	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	5	308	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
39	5	316	CHL	C2C-C3C-C4C	2.19	108.05	106.49
22	A	804	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
22	G	201	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
24	K	206	BCR	C37-C22-C21	-2.19	119.85	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	309	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
22	6	319	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
24	B	846	BCR	C8-C7-C6	-2.19	121.05	127.20
39	9	314	CHL	CHB-C4A-NA	2.19	127.54	124.51
24	A	846	BCR	C34-C9-C10	-2.19	119.86	122.92
22	A	809	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
31	3	301	DGD	O2G-C1B-O1B	-2.19	118.41	123.70
22	7	322	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	1	308	CLA	O2A-CGA-CBA	2.19	118.77	111.91
22	5	326	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
22	B	821	CLA	O2A-CGA-CBA	2.19	118.77	111.91
22	3	318	CLA	O2A-CGA-CBA	2.19	118.77	111.91
22	A	840	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
22	K	205	CLA	CMA-C3A-C4A	2.19	117.65	111.77
22	A	820	CLA	CHA-C1A-NA	-2.19	121.39	126.40
22	6	321	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
22	A	816	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
22	2	302	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
39	5	316	CHL	CHC-C1C-NC	2.19	127.52	124.20
22	7	314	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	5	319	CLA	O2A-CGA-CBA	2.18	118.76	111.91
22	6	322	CLA	O2A-CGA-CBA	2.18	118.76	111.91
22	6	314	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
22	J	103	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
22	2	304	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	A	803	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
22	K	203	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	6	311	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	7	312	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
25	9	315	LHG	C9-C8-C7	-2.18	105.69	113.62
22	Z	304	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	K	202	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
22	B	830	CLA	O2A-CGA-CBA	2.18	118.74	111.91
22	A	826	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
22	A	804	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	A	811	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	1	304	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
22	4	809	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	7	304	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	7	316	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
22	9	307	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
21	A	801	CL0	C4D-C3D-CAD	2.17	110.66	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	838	CLA	O2A-CGA-CBA	2.17	118.73	111.91
22	1	306	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
22	3	320	CLA	C2A-C1A-CHA	2.17	127.66	123.86
22	4	808	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
22	8	308	CLA	O2A-CGA-CBA	2.17	118.72	111.91
22	7	309	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
22	6	308	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
22	3	310	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
22	A	827	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
22	9	304	CLA	C2A-C1A-CHA	2.17	127.65	123.86
22	Z	313	CLA	CHA-C1A-NA	-2.17	121.43	126.40
39	1	312	CHL	CHD-C4C-C3C	2.17	128.03	124.84
22	1	310	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
22	2	302	CLA	CHA-C1A-NA	-2.17	121.43	126.40
22	B	826	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
24	G	203	BCR	C4-C5-C6	-2.17	119.58	122.73
22	B	829	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
39	2	303	CHL	CMA-C3A-C2A	2.17	122.57	113.83
22	A	827	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
22	7	305	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
22	1	304	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
39	5	317	CHL	C1-O2A-CGA	2.17	122.13	116.44
22	B	832	CLA	O2A-CGA-CBA	2.17	118.70	111.91
22	5	310	CLA	O2A-CGA-CBA	2.17	118.70	111.91
39	8	301	CHL	CHB-C4A-NA	2.17	127.51	124.51
22	F	302	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
22	A	802	CLA	O2A-CGA-CBA	2.17	118.70	111.91
22	A	831	CLA	CHA-C1A-NA	-2.17	121.44	126.40
22	B	829	CLA	CHA-C1A-NA	-2.17	121.44	126.40
22	7	316	CLA	CAA-C2A-C3A	-2.17	108.85	114.26
22	4	808	CLA	O2A-CGA-CBA	2.17	118.70	111.91
22	8	309	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
22	5	318	CLA	O2A-CGA-CBA	2.16	118.70	111.91
22	Z	308	CLA	CHA-C1A-NA	-2.16	121.44	126.40
22	B	838	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
22	9	311	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
22	A	805	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
22	4	812	CLA	O2A-CGA-CBA	2.16	118.70	111.91
22	J	103	CLA	CHA-C1A-NA	-2.16	121.44	126.40
38	3	302	LUT	C11-C12-C13	-2.16	120.34	126.42
22	5	326	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
22	B	812	CLA	CMD-C2D-C3D	-2.16	122.64	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	320	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
22	A	808	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
39	7	313	CHL	C1-C2-C3	-2.16	122.31	126.04
22	F	301	CLA	O2A-CGA-CBA	2.16	118.69	111.91
22	K	204	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	9	307	CLA	O2A-CGA-CBA	2.16	118.69	111.91
22	1	314	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
22	5	311	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
22	4	818	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
39	5	321	CHL	C4A-NA-C1A	2.16	107.68	106.71
22	7	323	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
22	8	313	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
22	A	830	CLA	O2A-CGA-CBA	2.16	118.68	111.91
39	6	316	CHL	CHD-C4C-C3C	2.16	128.01	124.84
22	A	809	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	7	316	CLA	CHA-C1A-NA	-2.16	121.45	126.40
39	4	813	CHL	C2C-C3C-C4C	2.16	108.03	106.49
22	2	301	CLA	O2A-CGA-CBA	2.16	118.68	111.91
22	7	310	CLA	CHA-C1A-NA	-2.16	121.46	126.40
25	1	317	LHG	O7-C7-O9	-2.16	118.49	123.70
22	B	823	CLA	CAA-CBA-CGA	-2.16	106.95	113.25
38	9	302	LUT	C11-C12-C13	-2.15	120.36	126.42
22	4	818	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	A	813	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	9	303	CLA	C1-O2A-CGA	2.15	122.09	116.44
22	B	810	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	A	854	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	B	835	CLA	O2A-CGA-CBA	2.15	118.66	111.91
22	A	814	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	B	837	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
24	3	307	BCR	C21-C20-C19	2.15	129.93	123.22
22	B	820	CLA	O2A-CGA-CBA	2.15	118.66	111.91
22	3	322	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	5	322	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	5	318	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
22	B	828	CLA	O2A-CGA-CBA	2.15	118.66	111.91
22	Z	315	CLA	CHA-C1A-NA	-2.15	121.47	126.40
22	7	305	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
22	1	310	CLA	O2A-CGA-CBA	2.15	118.66	111.91
22	B	839	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
34	F	308	LMG	O6-C1-C2	-2.15	105.80	110.35
22	7	317	CLA	O2A-CGA-CBA	2.15	118.65	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	4	813	CHL	CHC-C1C-NC	2.15	127.46	124.20
22	B	834	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	5	322	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
22	6	312	CLA	CHA-C1A-NA	-2.15	121.48	126.40
38	5	303	LUT	C19-C9-C10	-2.15	119.91	122.92
22	A	827	CLA	O2A-CGA-CBA	2.15	118.64	111.91
22	9	311	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
24	6	305	BCR	C34-C9-C10	-2.15	119.92	122.92
24	B	847	BCR	C21-C20-C19	-2.15	116.52	123.22
22	A	836	CLA	CHA-C1A-NA	-2.15	121.48	126.40
38	7	301	LUT	C40-C33-C34	-2.15	119.92	122.92
22	A	825	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	3	312	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	9	305	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
24	K	206	BCR	C35-C13-C14	-2.15	119.92	122.92
22	A	806	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
22	7	311	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
22	3	319	CLA	CHA-C1A-NA	-2.14	121.49	126.40
24	B	845	BCR	C33-C5-C6	-2.14	122.12	124.53
22	5	313	CLA	OBD-CAD-C3D	-2.14	123.36	128.52
22	F	301	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
22	B	824	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	823	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
39	4	814	CHL	CHD-C4C-C3C	2.14	127.99	124.84
22	4	812	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	B	806	CLA	CHA-C1A-NA	-2.14	121.49	126.40
22	8	314	CLA	CHA-C1A-NA	-2.14	121.49	126.40
39	9	314	CHL	C4A-NA-C1A	2.14	107.67	106.71
22	A	824	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
39	8	301	CHL	CHD-C4C-C3C	2.14	127.99	124.84
22	B	824	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	5	308	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
22	B	839	CLA	CHA-C1A-NA	-2.14	121.50	126.40
34	J	101	LMG	O8-C28-C29	2.14	118.62	111.91
39	2	303	CHL	CHB-C4A-NA	2.14	127.47	124.51
22	A	827	CLA	CHA-C1A-NA	-2.14	121.50	126.40
39	6	318	CHL	CMA-C3A-C2A	2.14	122.45	113.83
22	4	806	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
22	Z	307	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
22	A	810	CLA	O2A-CGA-CBA	2.14	118.61	111.91
38	1	303	LUT	C19-C9-C10	-2.14	119.93	122.92
22	A	840	CLA	CHA-C1A-NA	-2.14	121.51	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	326	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
24	K	206	BCR	C36-C18-C17	-2.13	119.93	122.92
22	5	319	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
22	7	306	CLA	O2A-CGA-CBA	2.13	118.61	111.91
22	B	840	CLA	CHA-C1A-NA	-2.13	121.51	126.40
39	9	314	CHL	CHC-C1C-NC	2.13	127.44	124.20
38	1	303	LUT	C8-C7-C6	-2.13	121.21	127.20
22	A	835	CLA	CHA-C1A-NA	-2.13	121.51	126.40
22	A	833	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	1	305	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
39	2	303	CHL	CHD-C4C-C3C	2.13	127.97	124.84
22	7	317	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	3	311	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	7	315	CLA	O2A-CGA-CBA	2.13	118.59	111.91
38	3	302	LUT	C21-C26-C27	-2.13	110.01	112.70
22	A	803	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
22	B	815	CLA	C3B-C4B-NB	-2.13	108.54	110.52
22	A	821	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	B	836	CLA	CHA-C1A-NA	-2.13	121.53	126.40
39	9	312	CHL	CMA-C3A-C2A	2.13	122.41	113.83
22	B	828	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
22	B	807	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
22	7	322	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
24	4	804	BCR	C1-C6-C5	-2.12	119.62	122.61
22	3	311	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
22	A	829	CLA	CHA-C1A-NA	-2.12	121.53	126.40
22	A	854	CLA	CHA-C1A-NA	-2.12	121.53	126.40
22	B	820	CLA	CHA-C1A-NA	-2.12	121.53	126.40
22	9	304	CLA	CHD-C1D-ND	-2.12	122.50	124.45
24	5	304	BCR	C21-C20-C19	-2.12	116.59	123.22
24	A	845	BCR	C34-C9-C10	-2.12	119.95	122.92
22	A	825	CLA	O2A-CGA-CBA	2.12	118.57	111.91
39	Z	312	CHL	CMA-C3A-C2A	2.12	122.39	113.83
36	5	306	C7Z	C20-C13-C14	-2.12	119.95	122.92
38	Z	301	LUT	C8-C7-C6	-2.12	121.24	127.20
22	F	302	CLA	CHA-C1A-NA	-2.12	121.54	126.40
22	3	309	CLA	CHA-C1A-NA	-2.12	121.54	126.40
24	J	104	BCR	C30-C25-C24	2.12	121.78	115.78
39	8	312	CHL	CHB-C4A-NA	2.12	127.45	124.51
22	6	319	CLA	CHA-C1A-NA	-2.12	121.54	126.40
24	3	305	BCR	C23-C24-C25	-2.12	121.24	127.20
38	3	302	LUT	C22-C23-C24	2.12	114.16	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	308	CLA	CHA-C1A-NA	-2.12	121.54	126.40
22	3	308	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
22	9	310	CLA	CHD-C1D-ND	-2.12	122.51	124.45
38	7	302	LUT	C15-C35-C34	-2.12	119.13	123.47
22	3	316	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	1	315	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	A	855	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	J	103	CLA	CAA-C2A-C3A	-2.12	108.97	114.26
22	3	310	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
25	B	803	LHG	O7-C7-O9	-2.12	118.58	123.70
22	4	807	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
22	G	201	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
39	7	313	CHL	CHB-C4A-NA	2.12	127.44	124.51
22	6	301	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	B	816	CLA	CHA-C1A-NA	-2.12	121.55	126.40
22	A	815	CLA	O2A-CGA-CBA	2.11	118.54	111.91
22	7	304	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
39	Z	312	CHL	C2C-C3C-C4C	2.11	108.00	106.49
22	3	313	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	9	305	CLA	C3B-C4B-NB	-2.11	108.55	110.52
22	7	317	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
22	A	842	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	7	322	CLA	O2A-CGA-CBA	2.11	118.54	111.91
22	K	202	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	9	306	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	K	206	BCR	C29-C30-C25	2.11	113.73	110.48
22	8	306	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
39	6	315	CHL	CHD-C4C-C3C	2.11	127.94	124.84
24	G	203	BCR	C36-C18-C17	-2.11	119.97	122.92
39	5	317	CHL	C4A-NA-C1A	2.11	107.66	106.71
22	6	321	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	8	310	CLA	O2A-CGA-CBA	2.11	118.53	111.91
22	7	324	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	1	304	CLA	CHA-C1A-NA	-2.11	121.57	126.40
38	5	303	LUT	C8-C7-C6	-2.11	121.28	127.20
22	5	311	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	B	812	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	4	810	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	A	832	CLA	O2A-CGA-CBA	2.11	118.52	111.91
22	B	810	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
22	7	306	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	F	304	CLA	C1-O2A-CGA	2.11	121.97	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	811	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	9	308	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	5	315	CLA	O2A-CGA-CBA	2.11	118.52	111.91
24	3	304	BCR	C20-C21-C22	-2.11	124.31	127.31
22	4	807	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
22	A	816	CLA	O1D-CGD-CBD	-2.11	120.18	124.48
22	1	313	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
22	K	205	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
22	4	815	CLA	O2A-CGA-CBA	2.10	118.51	111.91
22	6	302	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	Z	310	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
38	5	303	LUT	C15-C35-C34	-2.10	119.16	123.47
22	9	307	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	1	316	CLA	CMA-C3A-C4A	2.10	117.43	111.77
22	1	314	CLA	O2A-CGA-CBA	2.10	118.51	111.91
24	A	856	BCR	C10-C11-C12	-2.10	116.65	123.22
22	B	833	CLA	CHA-C1A-NA	-2.10	121.58	126.40
24	5	304	BCR	C34-C9-C10	-2.10	119.98	122.92
22	7	309	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
22	3	318	CLA	C6-C7-C8	-2.10	109.12	115.92
39	Z	312	CHL	CHD-C4C-C3C	2.10	127.93	124.84
22	B	819	CLA	CHA-C1A-NA	-2.10	121.58	126.40
39	8	301	CHL	CHC-C1C-NC	2.10	127.39	124.20
39	8	315	CHL	C2B-C1B-NB	-2.10	108.82	110.23
22	7	311	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	5	308	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	7	309	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
31	1	319	DGD	O1G-C1A-C2A	2.10	118.50	111.91
22	B	801	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
22	B	822	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
22	B	807	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	9	313	CLA	CHA-C1A-NA	-2.10	121.59	126.40
38	6	303	LUT	C31-C30-C29	-2.10	124.31	127.31
38	Z	301	LUT	C20-C13-C14	-2.10	119.98	122.92
22	7	314	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
22	5	319	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	1	313	CLA	CHA-C1A-NA	-2.10	121.59	126.40
36	J	105	C7Z	C40-C33-C34	-2.10	119.98	122.92
22	A	802	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	3	315	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
22	B	815	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	A	807	CLA	CHA-C1A-NA	-2.10	121.60	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	305	CLA	O2A-CGA-CBA	2.10	118.49	111.91
22	F	302	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
22	5	322	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
22	A	824	CLA	CHA-C1A-NA	-2.10	121.60	126.40
22	Z	303	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
22	7	322	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
24	J	104	BCR	C1-C6-C7	2.09	121.70	115.78
22	4	812	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
22	B	805	CLA	CHA-C1A-NA	-2.09	121.60	126.40
22	B	841	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
22	1	313	CLA	O2A-CGA-CBA	2.09	118.48	111.91
24	5	305	BCR	C12-C13-C14	2.09	122.15	118.94
22	1	305	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
39	8	312	CHL	CMA-C3A-C2A	2.09	122.27	113.83
22	B	813	CLA	CHA-C1A-NA	-2.09	121.61	126.40
38	7	302	LUT	C20-C13-C14	-2.09	119.99	122.92
22	5	312	CLA	O2A-CGA-CBA	2.09	118.47	111.91
22	A	818	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	9	309	CLA	CHA-C1A-NA	-2.09	121.61	126.40
39	1	312	CHL	CMA-C3A-C2A	2.09	122.26	113.83
22	B	822	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	B	821	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	B	832	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
22	A	810	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	A	811	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	A	837	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	9	305	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
23	A	843	PQN	C16-C17-C18	-2.09	109.17	115.92
22	7	315	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	4	809	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	5	309	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	6	307	CLA	CHA-C1A-NA	-2.09	121.62	126.40
39	5	321	CHL	CHD-C4C-C3C	2.09	127.91	124.84
24	8	304	BCR	C2-C1-C6	2.09	113.69	110.48
22	F	301	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	5	310	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
39	8	312	CHL	CHD-C4C-C3C	2.09	127.91	124.84
39	6	318	CHL	CHB-C4A-NA	2.09	127.40	124.51
39	6	315	CHL	CHC-C1C-NC	2.09	127.37	124.20
39	5	321	CHL	C2B-C1B-NB	-2.09	108.83	110.23
22	5	307	CLA	O2A-CGA-CBA	2.09	118.45	111.91
22	9	313	CLA	CMD-C2D-C3D	-2.08	122.82	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	807	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	B	842	CLA	O2A-CGA-CBA	2.08	118.45	111.91
39	4	814	CHL	C4A-NA-C1A	2.08	107.64	106.71
38	8	303	LUT	C30-C31-C32	-2.08	116.71	123.22
22	Z	313	CLA	C6-C5-C3	-2.08	107.99	113.45
22	3	309	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
39	6	315	CHL	CMA-C3A-C2A	2.08	122.23	113.83
22	A	803	CLA	CHA-C1A-NA	-2.08	121.63	126.40
24	8	304	BCR	C34-C9-C10	-2.08	120.01	122.92
22	7	311	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
38	7	302	LUT	C8-C7-C6	-2.08	121.36	127.20
22	A	834	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	B	835	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	A	815	CLA	CHA-C1A-NA	-2.08	121.63	126.40
25	4	820	LHG	O7-C7-O9	-2.08	118.67	123.70
22	6	322	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	B	826	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	B	836	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
22	Z	316	CLA	CHA-C1A-NA	-2.08	121.64	126.40
38	8	302	LUT	C38-C25-C24	-2.08	119.11	123.56
39	4	813	CHL	CMA-C3A-C2A	2.08	122.21	113.83
22	A	841	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	L	201	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	4	817	CLA	CHA-C1A-NA	-2.08	121.64	126.40
22	K	204	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
22	7	307	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
22	Z	314	CLA	O2A-CGA-CBA	2.08	118.43	111.91
22	A	813	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
22	8	313	CLA	O2A-CGA-CBA	2.08	118.42	111.91
38	5	302	LUT	C38-C25-C24	-2.08	119.11	123.56
22	9	308	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
22	A	808	CLA	O2A-CGA-CBA	2.08	118.42	111.91
22	B	815	CLA	CAC-C3C-C4C	2.08	127.50	124.81
24	A	856	BCR	C36-C18-C17	-2.08	120.02	122.92
22	5	307	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	A	855	CLA	O2A-CGA-CBA	2.07	118.42	111.91
22	B	837	CLA	O2A-CGA-CBA	2.07	118.42	111.91
22	Z	313	CLA	O2A-CGA-CBA	2.07	118.41	111.91
22	L	202	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	5	323	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
22	B	810	CLA	C6-C7-C8	-2.07	109.22	115.92
24	5	305	BCR	C7-C8-C9	-2.07	123.10	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	301	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	7	309	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	B	805	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
22	Z	314	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	A	833	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
22	1	305	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	5	312	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
22	B	819	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
22	4	811	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
22	A	830	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	B	841	CLA	CHA-C1A-NA	-2.07	121.66	126.40
39	5	317	CHL	CHB-C4A-NA	2.07	127.37	124.51
22	B	829	CLA	C6-C5-C3	-2.07	108.03	113.45
38	6	303	LUT	C39-C29-C28	2.07	121.34	118.08
22	Z	309	CLA	CHA-C1A-NA	-2.07	121.66	126.40
39	3	317	CHL	CHD-C4C-C3C	2.07	127.88	124.84
22	8	309	CLA	CHA-C1A-NA	-2.07	121.66	126.40
39	4	819	CHL	CHB-C4A-NA	2.07	127.37	124.51
22	4	806	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
22	B	831	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	B	810	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
22	5	310	CLA	CHA-C1A-NA	-2.07	121.67	126.40
24	F	303	BCR	C36-C18-C17	-2.07	120.03	122.92
22	6	310	CLA	CHA-C1A-NA	-2.06	121.67	126.40
22	A	804	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
22	8	310	CLA	CHA-C1A-NA	-2.06	121.67	126.40
33	G	204	LMT	C1'-O5'-C5'	-2.06	109.64	113.69
22	7	312	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
22	B	805	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
22	B	811	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
22	9	310	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
22	8	313	CLA	CHA-C1A-NA	-2.06	121.67	126.40
22	9	313	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
22	7	305	CLA	CHA-C1A-NA	-2.06	121.67	126.40
22	7	304	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
23	A	843	PQN	C2M-C2-C1	2.06	119.69	116.27
22	9	305	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
22	B	817	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
22	8	311	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
38	6	304	LUT	C20-C13-C14	-2.06	120.04	122.92
22	1	307	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	B	813	CLA	C3D-C2D-C1D	-2.06	103.02	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	810	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
22	B	830	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
22	F	301	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	K	204	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	8	309	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	A	826	CLA	CHA-C1A-NA	-2.06	121.68	126.40
22	5	319	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
22	A	827	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
22	B	823	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	B	837	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	1	306	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	1	314	CLA	CHA-C1A-NA	-2.06	121.69	126.40
24	A	846	BCR	C11-C12-C13	-2.06	120.64	126.42
22	3	313	CLA	O2A-CGA-CBA	2.06	118.36	111.91
22	Z	313	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
22	5	312	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	5	318	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	3	311	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
22	5	308	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
22	4	808	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	B	810	CLA	C6-C5-C3	-2.06	108.06	113.45
22	G	201	CLA	O2A-CGA-CBA	2.06	118.36	111.91
22	Z	306	CLA	CHA-C1A-NA	-2.05	121.69	126.40
22	1	314	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
22	A	839	CLA	CHA-C1A-NA	-2.05	121.69	126.40
22	A	829	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
22	B	808	CLA	CHA-C1A-NA	-2.05	121.69	126.40
22	A	832	CLA	CHA-C1A-NA	-2.05	121.70	126.40
22	8	306	CLA	CHA-C1A-NA	-2.05	121.70	126.40
22	6	308	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
22	A	812	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
22	K	202	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
22	B	826	CLA	C16-C15-C13	-2.05	109.29	115.92
22	A	838	CLA	CHA-C1A-NA	-2.05	121.70	126.40
22	A	829	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
22	3	318	CLA	C11-C10-C8	-2.05	109.29	115.92
38	3	303	LUT	C40-C33-C32	2.05	121.31	118.08
39	4	813	CHL	CHB-C4A-NA	2.05	127.35	124.51
22	6	301	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
22	7	314	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	8	316	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	A	817	CLA	CHA-C1A-NA	-2.05	121.71	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	827	CLA	CHA-C1A-NA	-2.05	121.71	126.40
33	G	204	LMT	C1B-O1B-C4'	-2.05	112.89	117.96
24	B	845	BCR	C2-C1-C6	2.05	113.63	110.48
22	A	836	CLA	C6-C5-C3	-2.05	108.09	113.45
22	B	834	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	5	322	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	Z	308	CLA	O2A-CGA-CBA	2.05	118.33	111.91
22	A	834	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	L	201	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	9	311	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	6	317	CLA	CHA-C1A-NA	-2.05	121.71	126.40
22	7	323	CLA	C1-O2A-CGA	2.05	121.81	116.44
22	4	817	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
22	K	203	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
22	A	819	CLA	O2A-CGA-CBA	2.04	118.32	111.91
22	A	835	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
22	B	820	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
24	A	844	BCR	C21-C20-C19	-2.04	116.84	123.22
22	B	819	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
22	Z	307	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
22	9	309	CLA	C2A-C1A-CHA	2.04	127.43	123.86
24	A	856	BCR	C30-C25-C24	2.04	121.56	115.78
22	Z	310	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
39	Z	311	CHL	CMA-C3A-C2A	2.04	122.07	113.83
22	3	310	CLA	C11-C10-C8	-2.04	109.32	115.92
22	5	314	CLA	CHA-C1A-NA	-2.04	121.72	126.40
39	6	318	CHL	CHD-C4C-C3C	2.04	127.84	124.84
24	A	848	BCR	C8-C7-C6	-2.04	121.47	127.20
22	Z	310	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
22	8	314	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
22	6	312	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
22	4	808	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	2	302	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	A	824	CLA	O2A-CGA-CBA	2.04	118.31	111.91
22	F	305	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	Z	303	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
22	G	202	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	2	304	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	J	104	BCR	C16-C15-C14	-2.04	119.30	123.47
38	8	303	LUT	C11-C12-C13	-2.04	120.69	126.42
39	Z	312	CHL	CHB-C4A-NA	2.04	127.33	124.51
22	A	823	CLA	C6-C5-C3	-2.04	108.11	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	313	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	6	314	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	3	314	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
22	F	302	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
22	7	310	CLA	O2A-CGA-CBA	2.04	118.30	111.91
39	Z	311	CHL	CHB-C4A-NA	2.04	127.33	124.51
39	6	316	CHL	CHB-C4A-NA	2.04	127.33	124.51
22	A	806	CLA	CHA-C1A-NA	-2.04	121.74	126.40
38	Z	302	LUT	C8-C7-C6	-2.04	121.49	127.20
24	3	304	BCR	C11-C12-C13	2.04	132.13	126.42
22	5	301	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
38	5	302	LUT	C15-C14-C13	-2.03	124.41	127.31
22	B	815	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
22	L	202	CLA	O2A-CGA-CBA	2.03	118.29	111.91
22	5	313	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	A	809	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	G	201	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
22	B	833	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	A	818	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
22	8	308	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	B	823	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
22	4	811	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
39	6	318	CHL	C1-O2A-CGA	2.03	121.78	116.44
22	L	203	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	A	845	BCR	C29-C30-C25	2.03	113.61	110.48
22	G	202	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	A	835	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
22	B	818	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
22	A	827	CLA	C1-O2A-CGA	2.03	121.77	116.44
22	1	316	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	B	849	BCR	C8-C7-C6	-2.03	121.50	127.20
22	Z	303	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	3	312	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	2	304	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
36	J	105	C7Z	C19-C9-C10	-2.03	120.08	122.92
22	A	837	CLA	O2A-CGA-CBA	2.03	118.27	111.91
22	B	810	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
40	1	318	SQD	O8-S-C6	-2.03	102.51	105.74
38	Z	302	LUT	C20-C13-C14	-2.03	120.08	122.92
22	A	832	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
22	B	830	CLA	CHA-C1A-NA	-2.03	121.76	126.40
22	A	808	CLA	C11-C12-C13	-2.03	109.37	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	306	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
22	B	829	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	B	841	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	8	310	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
22	A	841	CLA	C1-O2A-CGA	2.02	121.75	116.44
38	8	303	LUT	C20-C13-C12	2.02	121.27	118.08
38	7	302	LUT	C38-C25-C24	-2.02	119.23	123.56
22	B	805	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	3	318	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	7	316	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
39	5	316	CHL	C1-O2A-CGA	2.02	121.75	116.44
22	1	316	CLA	C6-C7-C8	-2.02	109.38	115.92
22	Z	309	CLA	C6-C5-C3	-2.02	108.15	113.45
22	K	203	CLA	O2A-CGA-CBA	2.02	118.26	111.91
22	Z	305	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
22	Z	304	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	B	811	CLA	O2A-CGA-CBA	2.02	118.25	111.91
22	6	308	CLA	CHA-C1A-NA	-2.02	121.77	126.40
32	F	306	RRX	C19-C18-C17	2.02	122.04	118.94
22	B	822	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
22	K	204	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
22	A	822	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
22	6	310	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
22	9	303	CLA	CMC-C2C-C1C	2.02	128.12	125.04
22	5	326	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
22	7	310	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	3	305	BCR	C29-C30-C25	2.02	113.59	110.48
22	5	318	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
38	4	803	LUT	C40-C33-C34	-2.02	120.09	122.92
22	Z	308	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	7	324	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	B	825	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
39	1	312	CHL	C2C-C3C-C4C	2.02	107.93	106.49
38	9	302	LUT	C35-C15-C14	-2.02	119.34	123.47
22	A	836	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	7	323	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	9	306	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	4	818	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
38	7	301	LUT	C15-C35-C34	-2.02	119.34	123.47
22	A	825	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	6	310	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	1	308	CLA	CMC-C2C-C1C	2.02	128.11	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	814	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
22	A	819	CLA	CHA-C1A-NA	-2.02	121.78	126.40
34	F	308	LMG	O7-C8-C9	2.02	115.70	108.40
22	1	304	CLA	O2D-CGD-O1D	-2.02	119.90	123.84
22	A	831	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
22	A	816	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	5	314	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
24	A	845	BCR	C20-C19-C18	-2.02	120.75	126.42
24	A	848	BCR	C35-C13-C14	-2.02	120.10	122.92
22	B	818	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
22	J	103	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	K	206	BCR	C2-C1-C6	2.02	113.58	110.48
22	K	202	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	6	312	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
39	4	814	CHL	C2B-C1B-NB	-2.01	108.88	110.23
22	8	307	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	A	833	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
22	3	308	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	1	306	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	3	311	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	9	308	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
22	3	313	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
24	A	845	BCR	C16-C15-C14	-2.01	119.35	123.47
22	7	306	CLA	C6-C5-C3	-2.01	108.18	113.45
22	1	316	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	B	830	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
22	A	838	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
22	8	305	CLA	C6-C5-C3	-2.01	108.18	113.45
38	4	803	LUT	C15-C35-C34	-2.01	119.36	123.47
22	3	314	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	A	814	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	Z	314	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
24	8	304	BCR	C15-C16-C17	-2.01	119.36	123.47
22	B	807	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	Z	313	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	8	308	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
38	8	302	LUT	C30-C31-C32	-2.01	116.94	123.22
22	6	319	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	L	202	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
38	4	802	LUT	C38-C25-C24	-2.01	119.26	123.56
24	A	845	BCR	C35-C13-C14	-2.01	120.11	122.92
24	A	845	BCR	C15-C16-C17	-2.01	119.36	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	822	LMT	O5B-C5B-C4B	-2.01	106.05	109.69
22	5	313	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
22	6	309	CLA	C2A-C1A-CHA	2.01	127.37	123.86
22	B	837	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
24	4	804	BCR	C36-C18-C17	-2.01	120.11	122.92
22	6	313	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
39	7	313	CHL	CHD-C4C-C3C	2.01	127.79	124.84
24	3	307	BCR	C30-C25-C24	2.01	121.45	115.78
22	4	810	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
22	A	805	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
22	B	808	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
22	5	315	CLA	C6-C5-C3	-2.01	108.20	113.45
22	B	817	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
22	5	315	CLA	C3D-C2D-C1D	-2.00	103.09	105.83
22	1	305	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
24	L	204	BCR	C29-C30-C25	2.00	113.57	110.48
22	B	827	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
22	6	302	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
39	4	814	CHL	CHB-C4A-NA	2.00	127.28	124.51
22	A	813	CLA	C6-C5-C3	-2.00	108.20	113.45
22	1	313	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
38	9	302	LUT	C30-C31-C32	-2.00	116.97	123.22
22	B	809	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	5	323	CLA	CHA-C1A-NA	-2.00	121.81	126.40
36	J	105	C7Z	C4-C5-C6	-2.00	116.39	120.85
22	B	836	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
22	9	308	CLA	O2A-CGA-CBA	2.00	118.19	111.91
22	A	836	CLA	O2A-CGA-CBA	2.00	118.19	111.91
22	A	808	CLA	CHA-C1A-NA	-2.00	121.81	126.40
23	A	843	PQN	C21-C22-C23	-2.00	109.45	115.92
39	6	320	CHL	CMA-C3A-C2A	2.00	121.90	113.83
22	B	811	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
24	I	4001	BCR	C16-C15-C14	-2.00	119.38	123.47
24	6	306	BCR	C36-C18-C17	-2.00	120.12	122.92
22	B	819	CLA	C6-C5-C3	-2.00	108.21	113.45
22	7	308	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
24	A	847	BCR	C36-C18-C17	-2.00	120.12	122.92
22	B	832	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
22	B	812	CLA	C13

All (4136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	802	CLA	C1A-C2A-CAA-CBA
22	A	802	CLA	C2-C1-O2A-CGA
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	803	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	O1A-CGA-O2A-C1
22	A	804	CLA	C3A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	806	CLA	O1A-CGA-O2A-C1
22	A	806	CLA	C6-C7-C8-C9
22	A	807	CLA	C1A-C2A-CAA-CBA
22	A	807	CLA	C3A-C2A-CAA-CBA
22	A	807	CLA	CBD-CGD-O2D-CED
22	A	807	CLA	C11-C10-C8-C9
22	A	808	CLA	C3A-C2A-CAA-CBA
22	A	808	CLA	CHA-CBD-CGD-O1D
22	A	808	CLA	CHA-CBD-CGD-O2D
22	A	810	CLA	C2-C1-O2A-CGA
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	812	CLA	C1A-C2A-CAA-CBA
22	A	812	CLA	C3A-C2A-CAA-CBA
22	A	814	CLA	C2-C1-O2A-CGA
22	A	815	CLA	C3A-C2A-CAA-CBA
22	A	815	CLA	C2-C1-O2A-CGA
22	A	816	CLA	C1A-C2A-CAA-CBA
22	A	816	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	C2-C3-C5-C6
22	A	817	CLA	C4-C3-C5-C6
22	A	818	CLA	C1A-C2A-CAA-CBA
22	A	818	CLA	C3A-C2A-CAA-CBA
22	A	818	CLA	C2-C1-O2A-CGA
22	A	818	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	CBD-CGD-O2D-CED
22	A	821	CLA	C6-C7-C8-C9
22	A	822	CLA	C1A-C2A-CAA-CBA
22	A	822	CLA	C3A-C2A-CAA-CBA
22	A	822	CLA	CAD-CBD-CGD-O1D
22	A	822	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CBD-CGD-O2D-CED
22	A	824	CLA	C1A-C2A-CAA-CBA
22	A	825	CLA	C1A-C2A-CAA-CBA
22	A	825	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	O1A-CGA-O2A-C1
22	A	826	CLA	C3A-C2A-CAA-CBA
22	A	826	CLA	CBA-CGA-O2A-C1
22	A	827	CLA	C1A-C2A-CAA-CBA
22	A	827	CLA	C3A-C2A-CAA-CBA
22	A	828	CLA	C1A-C2A-CAA-CBA
22	A	828	CLA	C3A-C2A-CAA-CBA
22	A	828	CLA	C2-C1-O2A-CGA
22	A	828	CLA	CBD-CGD-O2D-CED
22	A	828	CLA	C11-C10-C8-C7
22	A	829	CLA	CBA-CGA-O2A-C1
22	A	829	CLA	O1A-CGA-O2A-C1
22	A	829	CLA	CHA-CBD-CGD-O1D
22	A	830	CLA	CAD-CBD-CGD-O1D
22	A	831	CLA	C2-C1-O2A-CGA
22	A	832	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C3A-C2A-CAA-CBA
22	A	833	CLA	C2-C1-O2A-CGA
22	A	833	CLA	CBD-CGD-O2D-CED
22	A	834	CLA	CHA-CBD-CGD-O1D
22	A	834	CLA	CHA-CBD-CGD-O2D
22	A	835	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	O1A-CGA-O2A-C1
22	A	835	CLA	CBD-CGD-O2D-CED
22	A	836	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	CHA-CBD-CGD-O1D
22	A	836	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	838	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	C3A-C2A-CAA-CBA
22	A	839	CLA	C1A-C2A-CAA-CBA
22	A	839	CLA	C3A-C2A-CAA-CBA
22	A	839	CLA	CHA-CBD-CGD-O1D
22	A	840	CLA	C1A-C2A-CAA-CBA
22	A	840	CLA	C3A-C2A-CAA-CBA
22	A	841	CLA	C1A-C2A-CAA-CBA
22	A	842	CLA	C1A-C2A-CAA-CBA
22	A	842	CLA	C3A-C2A-CAA-CBA
22	A	842	CLA	CHA-CBD-CGD-O1D
22	A	842	CLA	CHA-CBD-CGD-O2D
22	A	842	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	CBD-CGD-O2D-CED
22	A	854	CLA	O1D-CGD-O2D-CED
22	A	855	CLA	C2-C1-O2A-CGA
22	A	855	CLA	CBD-CGD-O2D-CED
22	B	801	CLA	CBD-CGD-O2D-CED
22	B	805	CLA	CHA-CBD-CGD-O1D
22	B	805	CLA	CHA-CBD-CGD-O2D
22	B	805	CLA	CBD-CGD-O2D-CED
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	807	CLA	C1A-C2A-CAA-CBA
22	B	808	CLA	CBD-CGD-O2D-CED
22	B	810	CLA	C1A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	811	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C3A-C2A-CAA-CBA
22	B	811	CLA	CHA-CBD-CGD-O1D
22	B	811	CLA	CHA-CBD-CGD-O2D
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C3A-C2A-CAA-CBA
22	B	812	CLA	O1A-CGA-O2A-C1
22	B	812	CLA	C2-C1-O2A-CGA
22	B	812	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	CAD-CBD-CGD-O1D
22	B	814	CLA	CBD-CGD-O2D-CED
22	B	815	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	CHA-CBD-CGD-O1D
22	B	815	CLA	CHA-CBD-CGD-O2D
22	B	816	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	817	CLA	C3A-C2A-CAA-CBA
22	B	817	CLA	CHA-CBD-CGD-O1D
22	B	817	CLA	CHA-CBD-CGD-O2D
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C2-C1-O2A-CGA
22	B	820	CLA	C3A-C2A-CAA-CBA
22	B	821	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	CBA-CGA-O2A-C1
22	B	822	CLA	O1A-CGA-O2A-C1
22	B	824	CLA	C1A-C2A-CAA-CBA
22	B	824	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	C3A-C2A-CAA-CBA
22	B	826	CLA	CHA-CBD-CGD-O1D
22	B	826	CLA	CHA-CBD-CGD-O2D
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	CBA-CGA-O2A-C1
22	B	827	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	CHA-CBD-CGD-O1D
22	B	829	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	CHA-CBD-CGD-O1D
22	B	829	CLA	CHA-CBD-CGD-O2D
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C3A-C2A-CAA-CBA
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	CBD-CGD-O2D-CED
22	B	832	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	B	834	CLA	C2-C1-O2A-CGA
22	B	834	CLA	CHA-CBD-CGD-O1D
22	B	834	CLA	CHA-CBD-CGD-O2D
22	B	835	CLA	C1A-C2A-CAA-CBA
22	B	835	CLA	C3A-C2A-CAA-CBA
22	B	835	CLA	C2-C1-O2A-CGA
22	B	836	CLA	C1A-C2A-CAA-CBA
22	B	837	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	841	CLA	CBD-CGD-O2D-CED
22	B	841	CLA	C11-C10-C8-C9
22	F	301	CLA	C1A-C2A-CAA-CBA
22	F	301	CLA	C3A-C2A-CAA-CBA
22	F	301	CLA	CHA-CBD-CGD-O1D
22	F	301	CLA	CHA-CBD-CGD-O2D
22	F	302	CLA	C2-C1-O2A-CGA
22	F	302	CLA	CBD-CGD-O2D-CED
22	F	304	CLA	C1A-C2A-CAA-CBA
22	F	304	CLA	CBA-CGA-O2A-C1
22	F	304	CLA	O1A-CGA-O2A-C1
22	F	304	CLA	CHA-CBD-CGD-O1D
22	F	304	CLA	CHA-CBD-CGD-O2D
22	F	304	CLA	CAD-CBD-CGD-O1D
22	F	304	CLA	CAD-CBD-CGD-O2D
22	F	305	CLA	C1A-C2A-CAA-CBA
22	F	305	CLA	C3A-C2A-CAA-CBA
22	G	202	CLA	C1A-C2A-CAA-CBA
22	G	202	CLA	C3A-C2A-CAA-CBA
22	G	202	CLA	CHA-CBD-CGD-O2D
22	J	103	CLA	C1A-C2A-CAA-CBA
22	K	202	CLA	CHA-CBD-CGD-O1D
22	K	204	CLA	C2B-C3B-CAB-CBB
22	K	204	CLA	C4B-C3B-CAB-CBB
22	K	204	CLA	CAD-CBD-CGD-O2D
22	K	205	CLA	C2B-C3B-CAB-CBB
22	K	205	CLA	C4B-C3B-CAB-CBB
22	K	205	CLA	CBD-CGD-O2D-CED
22	K	205	CLA	C2-C3-C5-C6
22	K	205	CLA	C4-C3-C5-C6
22	L	201	CLA	C1A-C2A-CAA-CBA
22	L	202	CLA	C1A-C2A-CAA-CBA
22	L	202	CLA	C3A-C2A-CAA-CBA
22	L	203	CLA	C3A-C2A-CAA-CBA
22	1	304	CLA	C1A-C2A-CAA-CBA
22	1	304	CLA	C3A-C2A-CAA-CBA
22	1	306	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	C1A-C2A-CAA-CBA
22	1	307	CLA	C3A-C2A-CAA-CBA
22	1	308	CLA	C2-C1-O2A-CGA
22	1	308	CLA	CHA-CBD-CGD-O1D
22	1	308	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	1	309	CLA	C1A-C2A-CAA-CBA
22	1	309	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C1A-C2A-CAA-CBA
22	1	311	CLA	C2B-C3B-CAB-CBB
22	1	311	CLA	C4B-C3B-CAB-CBB
22	1	313	CLA	CBD-CGD-O2D-CED
22	1	313	CLA	O2A-C1-C2-C3
22	1	314	CLA	C3A-C2A-CAA-CBA
22	1	315	CLA	C1A-C2A-CAA-CBA
22	1	316	CLA	C2B-C3B-CAB-CBB
22	1	316	CLA	C4B-C3B-CAB-CBB
22	Z	303	CLA	C3A-C2A-CAA-CBA
22	Z	303	CLA	CBA-CGA-O2A-C1
22	Z	303	CLA	O1A-CGA-O2A-C1
22	Z	303	CLA	CHA-CBD-CGD-O1D
22	Z	303	CLA	CHA-CBD-CGD-O2D
22	Z	303	CLA	CBD-CGD-O2D-CED
22	Z	305	CLA	CBD-CGD-O2D-CED
22	Z	306	CLA	C3A-C2A-CAA-CBA
22	Z	307	CLA	CHA-CBD-CGD-O1D
22	Z	307	CLA	CHA-CBD-CGD-O2D
22	Z	308	CLA	C1A-C2A-CAA-CBA
22	Z	308	CLA	CBD-CGD-O2D-CED
22	Z	310	CLA	C1A-C2A-CAA-CBA
22	Z	310	CLA	C2-C1-O2A-CGA
22	Z	313	CLA	O2A-C1-C2-C3
22	Z	314	CLA	C1A-C2A-CAA-CBA
22	Z	314	CLA	C3A-C2A-CAA-CBA
22	Z	314	CLA	CBD-CGD-O2D-CED
22	Z	315	CLA	CBD-CGD-O2D-CED
22	Z	316	CLA	O1A-CGA-O2A-C1
22	Z	316	CLA	CBD-CGD-O2D-CED
22	Z	316	CLA	C11-C10-C8-C9
22	3	308	CLA	C1A-C2A-CAA-CBA
22	3	308	CLA	C3A-C2A-CAA-CBA
22	3	309	CLA	CBD-CGD-O2D-CED
22	3	310	CLA	CHA-CBD-CGD-O1D
22	3	310	CLA	CHA-CBD-CGD-O2D
22	3	310	CLA	CBD-CGD-O2D-CED
22	3	311	CLA	C3A-C2A-CAA-CBA
22	3	311	CLA	C6-C7-C8-C9
22	3	311	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	3	312	CLA	CBD-CGD-O2D-CED
22	3	313	CLA	C3A-C2A-CAA-CBA
22	3	314	CLA	C1A-C2A-CAA-CBA
22	3	314	CLA	C3A-C2A-CAA-CBA
22	3	315	CLA	C1A-C2A-CAA-CBA
22	3	315	CLA	C2B-C3B-CAB-CBB
22	3	315	CLA	C4B-C3B-CAB-CBB
22	3	315	CLA	CBD-CGD-O2D-CED
22	3	316	CLA	C1A-C2A-CAA-CBA
22	3	316	CLA	CBD-CGD-O2D-CED
22	3	318	CLA	C3A-C2A-CAA-CBA
22	3	319	CLA	C4-C3-C5-C6
22	3	320	CLA	C2B-C3B-CAB-CBB
22	3	320	CLA	C4B-C3B-CAB-CBB
22	7	304	CLA	C2-C1-O2A-CGA
22	7	305	CLA	C2B-C3B-CAB-CBB
22	7	305	CLA	C4B-C3B-CAB-CBB
22	7	305	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	C1A-C2A-CAA-CBA
22	7	306	CLA	CBD-CGD-O2D-CED
22	7	307	CLA	C3A-C2A-CAA-CBA
22	7	308	CLA	CBA-CGA-O2A-C1
22	7	308	CLA	O1A-CGA-O2A-C1
22	7	309	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	C1A-C2A-CAA-CBA
22	7	310	CLA	C6-C7-C8-C9
22	7	311	CLA	C1A-C2A-CAA-CBA
22	7	312	CLA	C3A-C2A-CAA-CBA
22	7	312	CLA	CHA-CBD-CGD-O1D
22	7	312	CLA	CBD-CGD-O2D-CED
22	7	314	CLA	C1A-C2A-CAA-CBA
22	7	314	CLA	C3A-C2A-CAA-CBA
22	7	314	CLA	CBA-CGA-O2A-C1
22	7	314	CLA	O1A-CGA-O2A-C1
22	7	315	CLA	CHA-CBD-CGD-O1D
22	7	315	CLA	CHA-CBD-CGD-O2D
22	7	316	CLA	C1A-C2A-CAA-CBA
22	7	316	CLA	CBD-CGD-O2D-CED
22	7	317	CLA	C1A-C2A-CAA-CBA
22	7	317	CLA	C3A-C2A-CAA-CBA
22	7	317	CLA	C2-C1-O2A-CGA
22	7	323	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	7	323	CLA	C3A-C2A-CAA-CBA
22	7	323	CLA	C2-C1-O2A-CGA
22	7	323	CLA	CHA-CBD-CGD-O1D
22	7	323	CLA	CHA-CBD-CGD-O2D
22	7	323	CLA	CAD-CBD-CGD-O1D
22	7	323	CLA	CAD-CBD-CGD-O2D
22	7	324	CLA	C3A-C2A-CAA-CBA
22	7	324	CLA	C2-C1-O2A-CGA
22	8	305	CLA	C1A-C2A-CAA-CBA
22	8	305	CLA	C3A-C2A-CAA-CBA
22	8	305	CLA	CBD-CGD-O2D-CED
22	8	307	CLA	C1A-C2A-CAA-CBA
22	8	308	CLA	C3A-C2A-CAA-CBA
22	8	309	CLA	C1A-C2A-CAA-CBA
22	8	309	CLA	C3A-C2A-CAA-CBA
22	8	310	CLA	CBD-CGD-O2D-CED
22	8	311	CLA	C1A-C2A-CAA-CBA
22	8	311	CLA	C3A-C2A-CAA-CBA
22	8	311	CLA	CHA-CBD-CGD-O1D
22	8	313	CLA	CBD-CGD-O2D-CED
22	8	314	CLA	C1A-C2A-CAA-CBA
22	8	316	CLA	C1A-C2A-CAA-CBA
22	8	316	CLA	C3A-C2A-CAA-CBA
22	4	805	CLA	C1A-C2A-CAA-CBA
22	4	805	CLA	C3A-C2A-CAA-CBA
22	4	806	CLA	C2A-CAA-CBA-CGA
22	4	806	CLA	C2-C1-O2A-CGA
22	4	806	CLA	C2B-C3B-CAB-CBB
22	4	806	CLA	C4B-C3B-CAB-CBB
22	4	807	CLA	C1A-C2A-CAA-CBA
22	4	808	CLA	C3A-C2A-CAA-CBA
22	4	808	CLA	C2-C3-C5-C6
22	4	808	CLA	C4-C3-C5-C6
22	4	809	CLA	CBA-CGA-O2A-C1
22	4	809	CLA	O1A-CGA-O2A-C1
22	4	809	CLA	CBD-CGD-O2D-CED
22	4	811	CLA	CBA-CGA-O2A-C1
22	4	811	CLA	O1A-CGA-O2A-C1
22	4	815	CLA	C3A-C2A-CAA-CBA
22	4	815	CLA	CHA-CBD-CGD-O1D
22	4	815	CLA	CHA-CBD-CGD-O2D
22	4	815	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	4	818	CLA	C1A-C2A-CAA-CBA
22	4	818	CLA	C2-C1-O2A-CGA
22	5	301	CLA	CBD-CGD-O2D-CED
22	5	307	CLA	C1A-C2A-CAA-CBA
22	5	307	CLA	C3A-C2A-CAA-CBA
22	5	308	CLA	C1A-C2A-CAA-CBA
22	5	308	CLA	CBA-CGA-O2A-C1
22	5	308	CLA	O1A-CGA-O2A-C1
22	5	308	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	C2-C1-O2A-CGA
22	5	310	CLA	C3A-C2A-CAA-CBA
22	5	310	CLA	C6-C7-C8-C9
22	5	311	CLA	C3A-C2A-CAA-CBA
22	5	313	CLA	CBA-CGA-O2A-C1
22	5	313	CLA	CHA-CBD-CGD-O1D
22	5	313	CLA	CHA-CBD-CGD-O2D
22	5	314	CLA	C1A-C2A-CAA-CBA
22	5	314	CLA	CHA-CBD-CGD-O1D
22	5	315	CLA	C1A-C2A-CAA-CBA
22	5	315	CLA	C3A-C2A-CAA-CBA
22	5	315	CLA	CHA-CBD-CGD-O1D
22	5	315	CLA	CBD-CGD-O2D-CED
22	5	315	CLA	C6-C7-C8-C9
22	5	318	CLA	C3A-C2A-CAA-CBA
22	5	319	CLA	C1A-C2A-CAA-CBA
22	5	319	CLA	C3A-C2A-CAA-CBA
22	5	319	CLA	C2B-C3B-CAB-CBB
22	5	319	CLA	C4B-C3B-CAB-CBB
22	5	320	CLA	C1A-C2A-CAA-CBA
22	5	320	CLA	C3A-C2A-CAA-CBA
22	5	320	CLA	C2B-C3B-CAB-CBB
22	5	320	CLA	C4B-C3B-CAB-CBB
22	5	320	CLA	CBD-CGD-O2D-CED
22	5	322	CLA	C1A-C2A-CAA-CBA
22	5	322	CLA	C3A-C2A-CAA-CBA
22	5	323	CLA	CBD-CGD-O2D-CED
22	5	326	CLA	C1A-C2A-CAA-CBA
22	5	326	CLA	CBD-CGD-O2D-CED
22	6	301	CLA	C1A-C2A-CAA-CBA
22	6	301	CLA	C3A-C2A-CAA-CBA
22	6	302	CLA	C1A-C2A-CAA-CBA
22	6	302	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	6	302	CLA	CHA-CBD-CGD-O1D
22	6	302	CLA	CHA-CBD-CGD-O2D
22	6	302	CLA	CBD-CGD-O2D-CED
22	6	307	CLA	C1A-C2A-CAA-CBA
22	6	307	CLA	CBD-CGD-O2D-CED
22	6	308	CLA	C2-C1-O2A-CGA
22	6	309	CLA	CHA-CBD-CGD-O1D
22	6	311	CLA	C1A-C2A-CAA-CBA
22	6	311	CLA	C3A-C2A-CAA-CBA
22	6	311	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	C2-C1-O2A-CGA
22	6	313	CLA	CHA-CBD-CGD-O1D
22	6	313	CLA	CHA-CBD-CGD-O2D
22	6	314	CLA	CHA-CBD-CGD-O1D
22	6	317	CLA	C3A-C2A-CAA-CBA
22	6	317	CLA	CBA-CGA-O2A-C1
22	6	317	CLA	O1A-CGA-O2A-C1
22	6	317	CLA	CHA-CBD-CGD-O2D
22	6	319	CLA	C3A-C2A-CAA-CBA
22	6	321	CLA	C1A-C2A-CAA-CBA
22	6	321	CLA	C3A-C2A-CAA-CBA
22	6	321	CLA	CBA-CGA-O2A-C1
22	6	322	CLA	C1A-C2A-CAA-CBA
22	6	322	CLA	C3A-C2A-CAA-CBA
22	6	322	CLA	CHA-CBD-CGD-O2D
22	9	303	CLA	C1A-C2A-CAA-CBA
22	9	305	CLA	C2B-C3B-CAB-CBB
22	9	305	CLA	C4B-C3B-CAB-CBB
22	9	308	CLA	C2-C1-O2A-CGA
22	9	308	CLA	CBD-CGD-O2D-CED
22	9	309	CLA	C2B-C3B-CAB-CBB
22	9	309	CLA	C4B-C3B-CAB-CBB
22	9	309	CLA	CHA-CBD-CGD-O1D
22	9	310	CLA	C2B-C3B-CAB-CBB
22	9	310	CLA	C4B-C3B-CAB-CBB
22	9	311	CLA	C1A-C2A-CAA-CBA
22	9	311	CLA	CBD-CGD-O2D-CED
22	9	313	CLA	CBA-CGA-O2A-C1
22	2	301	CLA	CBA-CGA-O2A-C1
22	2	301	CLA	O1A-CGA-O2A-C1
22	2	301	CLA	CHA-CBD-CGD-O1D
22	2	301	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	2	302	CLA	C1A-C2A-CAA-CBA
22	2	302	CLA	CHA-CBD-CGD-O2D
22	2	304	CLA	C1A-C2A-CAA-CBA
22	2	304	CLA	C3A-C2A-CAA-CBA
22	2	304	CLA	CBA-CGA-O2A-C1
24	A	844	BCR	C5-C6-C7-C8
24	A	844	BCR	C21-C22-C23-C24
24	A	844	BCR	C37-C22-C23-C24
24	A	845	BCR	C7-C8-C9-C34
24	A	845	BCR	C21-C22-C23-C24
24	A	845	BCR	C37-C22-C23-C24
24	A	846	BCR	C7-C8-C9-C10
24	A	846	BCR	C7-C8-C9-C34
24	A	847	BCR	C1-C6-C7-C8
24	A	847	BCR	C11-C12-C13-C14
24	A	847	BCR	C11-C12-C13-C35
24	A	847	BCR	C13-C14-C15-C16
24	A	847	BCR	C19-C20-C21-C22
24	A	847	BCR	C23-C24-C25-C26
24	A	848	BCR	C15-C16-C17-C18
24	A	848	BCR	C17-C18-C19-C20
24	A	848	BCR	C36-C18-C19-C20
24	A	848	BCR	C21-C22-C23-C24
24	A	848	BCR	C37-C22-C23-C24
24	A	856	BCR	C1-C6-C7-C8
24	A	856	BCR	C9-C10-C11-C12
24	A	856	BCR	C11-C12-C13-C14
24	A	856	BCR	C11-C12-C13-C35
24	A	856	BCR	C17-C18-C19-C20
24	A	856	BCR	C36-C18-C19-C20
24	A	856	BCR	C23-C24-C25-C30
24	B	844	BCR	C1-C6-C7-C8
24	B	844	BCR	C7-C8-C9-C34
24	B	845	BCR	C7-C8-C9-C10
24	B	845	BCR	C7-C8-C9-C34
24	B	845	BCR	C9-C10-C11-C12
24	B	845	BCR	C11-C12-C13-C14
24	B	846	BCR	C11-C12-C13-C14
24	B	846	BCR	C11-C12-C13-C35
24	B	846	BCR	C15-C16-C17-C18
24	B	846	BCR	C17-C18-C19-C20
24	B	846	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	B	846	BCR	C21-C22-C23-C24
24	B	846	BCR	C37-C22-C23-C24
24	B	847	BCR	C11-C12-C13-C14
24	B	847	BCR	C17-C18-C19-C20
24	B	847	BCR	C36-C18-C19-C20
24	B	848	BCR	C1-C6-C7-C8
24	B	848	BCR	C5-C6-C7-C8
24	B	848	BCR	C11-C12-C13-C14
24	B	848	BCR	C11-C12-C13-C35
24	B	848	BCR	C13-C14-C15-C16
24	B	848	BCR	C21-C22-C23-C24
24	B	848	BCR	C37-C22-C23-C24
24	B	849	BCR	C9-C10-C11-C12
24	B	849	BCR	C11-C12-C13-C14
24	B	849	BCR	C11-C12-C13-C35
24	B	849	BCR	C36-C18-C19-C20
24	B	849	BCR	C21-C22-C23-C24
24	B	849	BCR	C37-C22-C23-C24
24	B	849	BCR	C23-C24-C25-C30
24	B	853	BCR	C7-C8-C9-C10
24	B	853	BCR	C7-C8-C9-C34
24	B	853	BCR	C36-C18-C19-C20
24	B	853	BCR	C19-C20-C21-C22
24	F	303	BCR	C1-C6-C7-C8
24	F	303	BCR	C9-C10-C11-C12
24	F	303	BCR	C11-C12-C13-C14
24	F	303	BCR	C11-C12-C13-C35
24	F	303	BCR	C13-C14-C15-C16
24	F	303	BCR	C17-C18-C19-C20
24	F	303	BCR	C36-C18-C19-C20
24	F	303	BCR	C19-C20-C21-C22
24	G	203	BCR	C7-C8-C9-C10
24	G	203	BCR	C7-C8-C9-C34
24	I	4001	BCR	C5-C6-C7-C8
24	I	4001	BCR	C17-C18-C19-C20
24	I	4001	BCR	C36-C18-C19-C20
24	I	4001	BCR	C19-C20-C21-C22
24	I	4001	BCR	C21-C22-C23-C24
24	I	4001	BCR	C37-C22-C23-C24
24	J	104	BCR	C11-C12-C13-C14
24	J	104	BCR	C11-C12-C13-C35
24	J	104	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	J	104	BCR	C36-C18-C19-C20
24	K	206	BCR	C7-C8-C9-C10
24	K	206	BCR	C7-C8-C9-C34
24	K	206	BCR	C19-C20-C21-C22
24	K	206	BCR	C23-C24-C25-C26
24	K	206	BCR	C23-C24-C25-C30
24	L	204	BCR	C7-C8-C9-C10
24	L	204	BCR	C13-C14-C15-C16
24	L	204	BCR	C15-C16-C17-C18
24	L	204	BCR	C36-C18-C19-C20
24	L	204	BCR	C19-C20-C21-C22
24	L	204	BCR	C21-C22-C23-C24
24	L	204	BCR	C37-C22-C23-C24
24	3	304	BCR	C7-C8-C9-C10
24	3	304	BCR	C7-C8-C9-C34
24	3	304	BCR	C13-C14-C15-C16
24	3	304	BCR	C17-C18-C19-C20
24	3	304	BCR	C36-C18-C19-C20
24	3	305	BCR	C1-C6-C7-C8
24	3	305	BCR	C5-C6-C7-C8
24	3	305	BCR	C9-C10-C11-C12
24	3	305	BCR	C11-C12-C13-C14
24	3	305	BCR	C11-C12-C13-C35
24	3	305	BCR	C19-C20-C21-C22
24	3	305	BCR	C21-C22-C23-C24
24	3	305	BCR	C37-C22-C23-C24
24	3	306	BCR	C11-C12-C13-C14
24	3	306	BCR	C11-C12-C13-C35
24	3	306	BCR	C17-C18-C19-C20
24	3	306	BCR	C19-C20-C21-C22
24	3	306	BCR	C21-C22-C23-C24
24	3	306	BCR	C37-C22-C23-C24
24	3	307	BCR	C11-C12-C13-C14
24	3	307	BCR	C11-C12-C13-C35
24	3	307	BCR	C17-C18-C19-C20
24	3	307	BCR	C36-C18-C19-C20
24	3	307	BCR	C23-C24-C25-C26
24	7	303	BCR	C7-C8-C9-C10
24	7	303	BCR	C7-C8-C9-C34
24	7	303	BCR	C11-C12-C13-C14
24	7	303	BCR	C11-C12-C13-C35
24	7	303	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	7	303	BCR	C23-C24-C25-C26
24	8	304	BCR	C11-C12-C13-C14
24	8	304	BCR	C11-C12-C13-C35
24	8	304	BCR	C13-C14-C15-C16
24	4	804	BCR	C7-C8-C9-C10
24	4	804	BCR	C7-C8-C9-C34
24	4	804	BCR	C9-C10-C11-C12
24	4	804	BCR	C23-C24-C25-C26
24	5	304	BCR	C7-C8-C9-C10
24	5	304	BCR	C7-C8-C9-C34
24	5	304	BCR	C11-C12-C13-C14
24	5	304	BCR	C11-C12-C13-C35
24	5	304	BCR	C13-C14-C15-C16
24	5	304	BCR	C23-C24-C25-C26
24	5	305	BCR	C5-C6-C7-C8
24	5	305	BCR	C9-C10-C11-C12
24	5	305	BCR	C17-C18-C19-C20
24	5	305	BCR	C36-C18-C19-C20
24	6	305	BCR	C1-C6-C7-C8
24	6	305	BCR	C11-C12-C13-C14
24	6	305	BCR	C11-C12-C13-C35
24	6	306	BCR	C1-C6-C7-C8
24	6	306	BCR	C5-C6-C7-C8
24	6	306	BCR	C7-C8-C9-C34
24	6	306	BCR	C23-C24-C25-C26
25	A	849	LHG	C4-O6-P-O4
25	A	849	LHG	C4-O6-P-O5
25	A	850	LHG	O1-C1-C2-C3
25	A	850	LHG	C1-C2-C3-O3
25	A	850	LHG	C4-O6-P-O5
25	B	803	LHG	O9-C7-O7-C5
25	B	803	LHG	C8-C7-O7-C5
25	B	850	LHG	C3-O3-P-O6
25	B	850	LHG	O9-C7-O7-C5
25	B	851	LHG	O1-C1-C2-O2
25	B	851	LHG	C3-O3-P-O5
25	B	851	LHG	O9-C7-O7-C5
25	1	317	LHG	C8-C7-O7-C5
25	Z	317	LHG	O1-C1-C2-O2
25	3	321	LHG	O9-C7-O7-C5
25	7	318	LHG	C1-C2-C3-O3
25	7	318	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
25	8	317	LHG	O1-C1-C2-C3
25	8	317	LHG	C4-O6-P-O4
25	4	820	LHG	C3-O3-P-O4
25	4	820	LHG	C8-C7-O7-C5
25	5	324	LHG	O1-C1-C2-O2
25	6	323	LHG	O1-C1-C2-O2
25	6	323	LHG	C3-O3-P-O5
25	6	323	LHG	C4-O6-P-O4
25	6	323	LHG	C4-O6-P-O5
25	6	323	LHG	C24-C23-O8-C6
25	9	315	LHG	C3-O3-P-O4
27	A	852	DGA	CA2-CA1-OG1-CG1
27	A	852	DGA	OA1-CA1-OG1-CG1
31	B	852	DGD	O1B-C1B-O2G-C2G
31	1	319	DGD	C2A-C1A-O1G-C1G
31	1	319	DGD	O1A-C1A-O1G-C1G
31	1	319	DGD	C2B-C1B-O2G-C2G
31	1	319	DGD	O1B-C1B-O2G-C2G
31	1	319	DGD	O6E-C1E-O5D-C6D
31	3	301	DGD	C2B-C1B-O2G-C2G
31	3	301	DGD	O1B-C1B-O2G-C2G
32	F	306	RRX	C7-C8-C9-C10
32	F	306	RRX	C7-C8-C9-C34
32	F	306	RRX	C1-C6-C7-C8
32	F	306	RRX	C5-C6-C7-C8
33	F	307	LMT	C2'-C1'-O1'-C1
33	F	307	LMT	O5'-C1'-O1'-C1
33	G	204	LMT	C2'-C1'-O1'-C1
33	G	204	LMT	O5'-C1'-O1'-C1
33	1	301	LMT	C2'-C1'-O1'-C1
33	1	301	LMT	O5'-C1'-O1'-C1
33	1	301	LMT	C2-C1-O1'-C1'
34	F	308	LMG	C11-C10-O7-C8
36	J	105	C7Z	C1-C6-C7-C8
36	J	105	C7Z	C5-C6-C7-C8
36	J	105	C7Z	C7-C8-C9-C10
36	J	105	C7Z	C31-C32-C33-C34
36	J	105	C7Z	C31-C32-C33-C40
36	5	306	C7Z	C11-C12-C13-C20
36	5	306	C7Z	C11-C12-C13-C14
36	5	306	C7Z	C31-C32-C33-C40
38	1	302	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
38	1	302	LUT	C11-C12-C13-C20
38	1	302	LUT	C27-C28-C29-C30
38	1	302	LUT	C27-C28-C29-C39
38	1	302	LUT	C31-C32-C33-C34
38	1	302	LUT	C31-C32-C33-C40
38	1	303	LUT	C11-C12-C13-C14
38	1	303	LUT	C11-C12-C13-C20
38	1	303	LUT	C31-C32-C33-C34
38	1	303	LUT	C31-C32-C33-C40
38	Z	301	LUT	C11-C12-C13-C14
38	Z	301	LUT	C11-C12-C13-C20
38	Z	302	LUT	C7-C8-C9-C10
38	Z	302	LUT	C11-C12-C13-C14
38	Z	302	LUT	C11-C12-C13-C20
38	3	302	LUT	C11-C12-C13-C14
38	3	302	LUT	C11-C12-C13-C20
38	3	302	LUT	C31-C32-C33-C34
38	3	302	LUT	C31-C32-C33-C40
38	3	303	LUT	C11-C12-C13-C14
38	3	303	LUT	C11-C12-C13-C20
38	7	301	LUT	C11-C12-C13-C14
38	7	301	LUT	C11-C12-C13-C20
38	7	301	LUT	C31-C32-C33-C34
38	7	301	LUT	C31-C32-C33-C40
38	7	302	LUT	C7-C8-C9-C10
38	8	302	LUT	C11-C12-C13-C14
38	8	302	LUT	C11-C12-C13-C20
38	8	302	LUT	C27-C28-C29-C30
38	8	302	LUT	C27-C28-C29-C39
38	8	303	LUT	C11-C12-C13-C14
38	8	303	LUT	C11-C12-C13-C20
38	4	802	LUT	C5-C6-C7-C8
38	4	802	LUT	C7-C8-C9-C10
38	4	802	LUT	C7-C8-C9-C19
38	4	802	LUT	C31-C32-C33-C34
38	4	802	LUT	C31-C32-C33-C40
38	4	803	LUT	C1-C6-C7-C8
38	4	803	LUT	C11-C12-C13-C14
38	4	803	LUT	C11-C12-C13-C20
38	5	302	LUT	C7-C8-C9-C19
38	5	302	LUT	C11-C12-C13-C14
38	5	302	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
38	5	302	LUT	C31-C32-C33-C34
38	5	302	LUT	C31-C32-C33-C40
38	5	303	LUT	C1-C6-C7-C8
38	5	303	LUT	C11-C12-C13-C14
38	5	303	LUT	C11-C12-C13-C20
38	6	303	LUT	C7-C8-C9-C10
38	6	303	LUT	C7-C8-C9-C19
38	6	303	LUT	C11-C12-C13-C14
38	6	303	LUT	C11-C12-C13-C20
38	6	303	LUT	C31-C32-C33-C40
38	6	304	LUT	C11-C12-C13-C14
38	6	304	LUT	C11-C12-C13-C20
38	9	301	LUT	C11-C12-C13-C14
38	9	301	LUT	C11-C12-C13-C20
38	9	301	LUT	C31-C32-C33-C34
38	9	301	LUT	C31-C32-C33-C40
38	9	302	LUT	C7-C8-C9-C10
38	9	302	LUT	C7-C8-C9-C19
38	9	302	LUT	C11-C12-C13-C20
39	Z	312	CHL	CBD-CGD-O2D-CED
39	7	313	CHL	CHA-CBD-CGD-O1D
39	7	313	CHL	CHA-CBD-CGD-O2D
39	8	312	CHL	CHA-CBD-CGD-O1D
39	8	312	CHL	CHA-CBD-CGD-O2D
39	8	312	CHL	CBD-CGD-O2D-CED
39	4	814	CHL	CHA-CBD-CGD-O1D
39	4	814	CHL	CHA-CBD-CGD-O2D
39	4	814	CHL	CBD-CGD-O2D-CED
39	4	816	CHL	CHA-CBD-CGD-O1D
39	4	816	CHL	CHA-CBD-CGD-O2D
39	5	317	CHL	C1A-C2A-CAA-CBA
39	5	317	CHL	C3A-C2A-CAA-CBA
39	5	321	CHL	C3A-C2A-CAA-CBA
39	6	315	CHL	CHA-CBD-CGD-O1D
39	6	315	CHL	CHA-CBD-CGD-O2D
39	6	316	CHL	C1A-C2A-CAA-CBA
39	6	316	CHL	C3A-C2A-CAA-CBA
39	6	316	CHL	CBA-CGA-O2A-C1
39	6	316	CHL	O1A-CGA-O2A-C1
39	6	318	CHL	CBD-CGD-O2D-CED
39	9	312	CHL	CBD-CGD-O2D-CED
39	2	303	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
40	1	318	SQD	O5-C5-C6-S
41	7	319	3PH	C22-C21-O21-C2
41	8	320	3PH	C1-O11-P-O13
41	8	320	3PH	C1-O11-P-O14
41	8	320	3PH	C2-C1-O11-P
41	5	325	3PH	O22-C21-O21-C2
41	5	325	3PH	C22-C21-O21-C2
41	6	324	3PH	C22-C21-O21-C2
42	7	320	SPH	O1-C1-C2-N2
42	7	321	SPH	C1-C2-C3-O3
42	7	321	SPH	C1-C2-C3-C4
42	7	321	SPH	N2-C2-C3-O3
42	7	321	SPH	N2-C2-C3-C4
43	8	319	LPX	C4-C3-O1-P1
43	8	319	LPX	C2-C1-O2-P1
22	B	809	CLA	O1D-CGD-O2D-CED
22	F	302	CLA	O1D-CGD-O2D-CED
22	1	315	CLA	O1D-CGD-O2D-CED
22	Z	315	CLA	O1D-CGD-O2D-CED
22	3	308	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	7	309	CLA	O1D-CGD-O2D-CED
22	8	316	CLA	O1D-CGD-O2D-CED
22	4	818	CLA	O1D-CGD-O2D-CED
22	5	319	CLA	O1D-CGD-O2D-CED
22	6	302	CLA	O1D-CGD-O2D-CED
22	6	308	CLA	O1D-CGD-O2D-CED
22	6	311	CLA	O1D-CGD-O2D-CED
22	9	310	CLA	O1D-CGD-O2D-CED
33	F	307	LMT	O5B-C1B-O1B-C4'
22	A	811	CLA	O1D-CGD-O2D-CED
22	A	823	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1D-CGD-O2D-CED
22	B	805	CLA	O1D-CGD-O2D-CED
22	B	829	CLA	O1D-CGD-O2D-CED
22	J	103	CLA	O1D-CGD-O2D-CED
22	K	204	CLA	O1D-CGD-O2D-CED
22	L	203	CLA	O1D-CGD-O2D-CED
22	3	309	CLA	O1D-CGD-O2D-CED
22	3	314	CLA	O1D-CGD-O2D-CED
22	7	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	7	312	CLA	O1D-CGD-O2D-CED
22	8	310	CLA	O1D-CGD-O2D-CED
22	4	809	CLA	O1D-CGD-O2D-CED
22	4	817	CLA	O1D-CGD-O2D-CED
22	5	309	CLA	O1D-CGD-O2D-CED
22	5	315	CLA	O1D-CGD-O2D-CED
22	9	303	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	CBD-CGD-O2D-CED
22	A	804	CLA	CBD-CGD-O2D-CED
22	A	808	CLA	CBD-CGD-O2D-CED
22	A	809	CLA	CBD-CGD-O2D-CED
22	A	812	CLA	CBD-CGD-O2D-CED
22	A	814	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	CBD-CGD-O2D-CED
22	A	821	CLA	CBD-CGD-O2D-CED
22	A	825	CLA	CBD-CGD-O2D-CED
22	A	832	CLA	CBD-CGD-O2D-CED
22	A	834	CLA	CBD-CGD-O2D-CED
22	A	836	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	CBD-CGD-O2D-CED
22	B	807	CLA	CBD-CGD-O2D-CED
22	B	809	CLA	CBD-CGD-O2D-CED
22	B	811	CLA	CBD-CGD-O2D-CED
22	B	818	CLA	CBD-CGD-O2D-CED
22	B	819	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	CBD-CGD-O2D-CED
22	B	827	CLA	CBD-CGD-O2D-CED
22	B	828	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	CBD-CGD-O2D-CED
22	B	840	CLA	CBD-CGD-O2D-CED
22	F	301	CLA	CBD-CGD-O2D-CED
22	F	304	CLA	CBD-CGD-O2D-CED
22	F	305	CLA	CBD-CGD-O2D-CED
22	G	201	CLA	CBD-CGD-O2D-CED
22	G	202	CLA	CBD-CGD-O2D-CED
22	J	103	CLA	CBD-CGD-O2D-CED
22	K	204	CLA	CBD-CGD-O2D-CED
22	L	203	CLA	CBD-CGD-O2D-CED
22	1	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	307	CLA	CBD-CGD-O2D-CED
22	1	309	CLA	CBD-CGD-O2D-CED
22	1	311	CLA	CBD-CGD-O2D-CED
22	1	315	CLA	CBD-CGD-O2D-CED
22	1	316	CLA	CBD-CGD-O2D-CED
22	Z	304	CLA	CBD-CGD-O2D-CED
22	Z	306	CLA	CBD-CGD-O2D-CED
22	Z	307	CLA	CBD-CGD-O2D-CED
22	Z	313	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	3	314	CLA	CBD-CGD-O2D-CED
22	3	318	CLA	CBD-CGD-O2D-CED
22	3	319	CLA	CBD-CGD-O2D-CED
22	3	320	CLA	CBD-CGD-O2D-CED
22	7	304	CLA	CBD-CGD-O2D-CED
22	7	308	CLA	CBD-CGD-O2D-CED
22	7	315	CLA	CBD-CGD-O2D-CED
22	7	324	CLA	CBD-CGD-O2D-CED
22	8	306	CLA	CBD-CGD-O2D-CED
22	8	307	CLA	CBD-CGD-O2D-CED
22	8	309	CLA	CBD-CGD-O2D-CED
22	8	316	CLA	CBD-CGD-O2D-CED
22	4	806	CLA	CBD-CGD-O2D-CED
22	4	811	CLA	CBD-CGD-O2D-CED
22	4	812	CLA	CBD-CGD-O2D-CED
22	4	817	CLA	CBD-CGD-O2D-CED
22	4	818	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CBD-CGD-O2D-CED
22	5	319	CLA	CBD-CGD-O2D-CED
22	5	322	CLA	CBD-CGD-O2D-CED
22	6	301	CLA	CBD-CGD-O2D-CED
22	6	308	CLA	CBD-CGD-O2D-CED
22	6	309	CLA	CBD-CGD-O2D-CED
22	6	317	CLA	CBD-CGD-O2D-CED
22	6	322	CLA	CBD-CGD-O2D-CED
22	9	303	CLA	CBD-CGD-O2D-CED
22	9	304	CLA	CBD-CGD-O2D-CED
22	9	305	CLA	CBD-CGD-O2D-CED
22	9	306	CLA	CBD-CGD-O2D-CED
22	9	307	CLA	CBD-CGD-O2D-CED
22	9	310	CLA	CBD-CGD-O2D-CED
22	9	313	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	2	301	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CBD-CGD-O2D-CED
39	7	313	CHL	CBD-CGD-O2D-CED
39	4	813	CHL	CBD-CGD-O2D-CED
22	A	816	CLA	O1A-CGA-O2A-C1
22	A	826	CLA	O1A-CGA-O2A-C1
22	A	831	CLA	O1A-CGA-O2A-C1
22	A	841	CLA	O1A-CGA-O2A-C1
22	A	855	CLA	O1A-CGA-O2A-C1
22	B	805	CLA	O1A-CGA-O2A-C1
22	B	808	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	B	823	CLA	O1A-CGA-O2A-C1
22	B	832	CLA	O1A-CGA-O2A-C1
22	B	839	CLA	O1A-CGA-O2A-C1
22	K	204	CLA	O1A-CGA-O2A-C1
22	Z	308	CLA	O1A-CGA-O2A-C1
22	Z	309	CLA	O1A-CGA-O2A-C1
22	7	315	CLA	O1A-CGA-O2A-C1
22	7	322	CLA	O1A-CGA-O2A-C1
22	8	309	CLA	O1A-CGA-O2A-C1
22	5	307	CLA	O1A-CGA-O2A-C1
22	5	313	CLA	O1A-CGA-O2A-C1
22	6	314	CLA	O1A-CGA-O2A-C1
22	9	313	CLA	O1A-CGA-O2A-C1
25	6	323	LHG	O10-C23-O8-C6
34	J	101	LMG	O10-C28-O8-C9
39	5	316	CHL	O1A-CGA-O2A-C1
39	9	312	CHL	O1A-CGA-O2A-C1
22	K	202	CLA	O1A-CGA-O2A-C1
22	8	316	CLA	O1A-CGA-O2A-C1
22	2	304	CLA	O1A-CGA-O2A-C1
33	F	307	LMT	C2B-C1B-O1B-C4'
22	A	802	CLA	O1D-CGD-O2D-CED
22	A	821	CLA	O1D-CGD-O2D-CED
22	A	832	CLA	O1D-CGD-O2D-CED
22	B	827	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	O1D-CGD-O2D-CED
22	B	836	CLA	O1D-CGD-O2D-CED
22	F	301	CLA	O1D-CGD-O2D-CED
22	Z	305	CLA	O1D-CGD-O2D-CED
22	Z	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	Z	316	CLA	O1D-CGD-O2D-CED
22	3	310	CLA	O1D-CGD-O2D-CED
22	3	319	CLA	O1D-CGD-O2D-CED
22	5	320	CLA	O1D-CGD-O2D-CED
22	2	301	CLA	O1D-CGD-O2D-CED
22	7	308	CLA	C8-C10-C11-C12
22	K	202	CLA	CBA-CGA-O2A-C1
22	1	311	CLA	CBA-CGA-O2A-C1
22	1	315	CLA	CBA-CGA-O2A-C1
22	Z	315	CLA	CBA-CGA-O2A-C1
22	3	309	CLA	CBA-CGA-O2A-C1
22	8	316	CLA	CBA-CGA-O2A-C1
39	9	312	CHL	C4C-C3C-CAC-CBC
22	A	818	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	O1D-CGD-O2D-CED
22	B	801	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	B	808	CLA	O1D-CGD-O2D-CED
22	B	831	CLA	O1D-CGD-O2D-CED
22	B	841	CLA	O1D-CGD-O2D-CED
22	F	304	CLA	O1D-CGD-O2D-CED
22	K	205	CLA	O1D-CGD-O2D-CED
22	1	306	CLA	O1D-CGD-O2D-CED
22	1	313	CLA	O1D-CGD-O2D-CED
22	1	316	CLA	O1D-CGD-O2D-CED
22	Z	303	CLA	O1D-CGD-O2D-CED
22	3	312	CLA	O1D-CGD-O2D-CED
22	3	315	CLA	O1D-CGD-O2D-CED
22	3	316	CLA	O1D-CGD-O2D-CED
22	7	324	CLA	O1D-CGD-O2D-CED
22	4	815	CLA	O1D-CGD-O2D-CED
22	5	301	CLA	O1D-CGD-O2D-CED
22	5	323	CLA	O1D-CGD-O2D-CED
22	6	317	CLA	O1D-CGD-O2D-CED
22	9	313	CLA	O1D-CGD-O2D-CED
39	Z	312	CHL	O1D-CGD-O2D-CED
39	6	318	CHL	O1D-CGD-O2D-CED
22	A	816	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	CBA-CGA-O2A-C1
22	B	805	CLA	CBA-CGA-O2A-C1
22	B	812	CLA	CBA-CGA-O2A-C1
22	B	839	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	K	204	CLA	CBA-CGA-O2A-C1
22	Z	308	CLA	CBA-CGA-O2A-C1
22	Z	309	CLA	CBA-CGA-O2A-C1
22	7	315	CLA	CBA-CGA-O2A-C1
22	7	322	CLA	CBA-CGA-O2A-C1
22	4	812	CLA	CBA-CGA-O2A-C1
22	6	314	CLA	CBA-CGA-O2A-C1
34	J	101	LMG	C29-C28-O8-C9
39	9	312	CHL	CBA-CGA-O2A-C1
25	3	321	LHG	C24-C23-O8-C6
22	A	803	CLA	CBD-CGD-O2D-CED
22	A	830	CLA	CBD-CGD-O2D-CED
22	A	831	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	CBD-CGD-O2D-CED
22	B	834	CLA	CBD-CGD-O2D-CED
22	B	837	CLA	CBD-CGD-O2D-CED
22	B	842	CLA	CBD-CGD-O2D-CED
22	K	202	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	CBD-CGD-O2D-CED
22	7	311	CLA	CBD-CGD-O2D-CED
22	8	311	CLA	CBD-CGD-O2D-CED
22	4	805	CLA	CBD-CGD-O2D-CED
22	4	808	CLA	CBD-CGD-O2D-CED
22	5	307	CLA	CBD-CGD-O2D-CED
22	5	311	CLA	CBD-CGD-O2D-CED
39	5	316	CHL	CBD-CGD-O2D-CED
39	6	315	CHL	CBD-CGD-O2D-CED
39	Z	311	CHL	C2C-C3C-CAC-CBC
39	9	312	CHL	C2C-C3C-CAC-CBC
22	A	807	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	O1A-CGA-O2A-C1
22	A	814	CLA	O1A-CGA-O2A-C1
22	A	815	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1A-CGA-O2A-C1
22	A	821	CLA	O1A-CGA-O2A-C1
22	A	822	CLA	O1A-CGA-O2A-C1
22	A	823	CLA	O1A-CGA-O2A-C1
22	A	827	CLA	O1A-CGA-O2A-C1
22	A	837	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	819	CLA	O1A-CGA-O2A-C1
22	B	821	CLA	O1A-CGA-O2A-C1
22	B	834	CLA	O1A-CGA-O2A-C1
22	1	307	CLA	O1A-CGA-O2A-C1
22	1	309	CLA	O1A-CGA-O2A-C1
22	Z	307	CLA	O1A-CGA-O2A-C1
22	3	308	CLA	O1A-CGA-O2A-C1
22	7	310	CLA	O1A-CGA-O2A-C1
22	7	324	CLA	O1A-CGA-O2A-C1
22	8	305	CLA	O1A-CGA-O2A-C1
22	4	805	CLA	O1A-CGA-O2A-C1
22	4	810	CLA	O1A-CGA-O2A-C1
22	4	812	CLA	O1A-CGA-O2A-C1
22	4	818	CLA	O1A-CGA-O2A-C1
22	5	301	CLA	O1A-CGA-O2A-C1
22	6	312	CLA	O1A-CGA-O2A-C1
22	6	313	CLA	O1A-CGA-O2A-C1
22	9	309	CLA	O1A-CGA-O2A-C1
40	1	318	SQD	O10-C23-O48-C46
41	7	319	3PH	O32-C31-O31-C3
22	1	311	CLA	O1A-CGA-O2A-C1
22	1	315	CLA	O1A-CGA-O2A-C1
22	Z	315	CLA	O1A-CGA-O2A-C1
22	3	309	CLA	O1A-CGA-O2A-C1
22	6	321	CLA	O1A-CGA-O2A-C1
22	9	311	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	O1D-CGD-O2D-CED
22	A	828	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	O1D-CGD-O2D-CED
22	B	824	CLA	O1D-CGD-O2D-CED
22	7	305	CLA	O1D-CGD-O2D-CED
22	7	316	CLA	O1D-CGD-O2D-CED
22	8	305	CLA	O1D-CGD-O2D-CED
22	8	313	CLA	O1D-CGD-O2D-CED
22	5	326	CLA	O1D-CGD-O2D-CED
22	6	307	CLA	O1D-CGD-O2D-CED
22	9	308	CLA	O1D-CGD-O2D-CED
22	9	311	CLA	O1D-CGD-O2D-CED
39	8	312	CHL	O1D-CGD-O2D-CED
39	9	312	CHL	O1D-CGD-O2D-CED
22	B	811	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	812	CLA	C5-C6-C7-C8
22	7	306	CLA	C5-C6-C7-C8
22	A	807	CLA	O1D-CGD-O2D-CED
22	A	833	CLA	O1D-CGD-O2D-CED
22	A	855	CLA	O1D-CGD-O2D-CED
22	B	816	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	O1D-CGD-O2D-CED
22	Z	308	CLA	O1D-CGD-O2D-CED
22	8	309	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	B	826	CLA	CBD-CGD-O2D-CED
22	A	810	CLA	C8-C10-C11-C12
22	B	838	CLA	C8-C10-C11-C12
23	A	843	PQN	C18-C20-C21-C22
22	A	816	CLA	O1D-CGD-O2D-CED
22	A	835	CLA	O1D-CGD-O2D-CED
22	B	821	CLA	O1D-CGD-O2D-CED
22	F	305	CLA	O1D-CGD-O2D-CED
22	G	201	CLA	O1D-CGD-O2D-CED
22	Z	313	CLA	O1D-CGD-O2D-CED
22	9	304	CLA	O1D-CGD-O2D-CED
39	4	814	CHL	O1D-CGD-O2D-CED
39	2	303	CHL	O1D-CGD-O2D-CED
25	1	317	LHG	O9-C7-O7-C5
34	F	308	LMG	O9-C10-O7-C8
34	J	101	LMG	O9-C10-O7-C8
41	7	319	3PH	O22-C21-O21-C2
41	6	324	3PH	O22-C21-O21-C2
22	1	306	CLA	O1A-CGA-O2A-C1
22	8	314	CLA	CBA-CGA-O2A-C1
22	9	311	CLA	CBA-CGA-O2A-C1
39	Z	311	CHL	C4C-C3C-CAC-CBC
31	3	301	DGD	C2G-C1G-O1G-C1A
22	A	802	CLA	C3-C5-C6-C7
22	A	805	CLA	C3-C5-C6-C7
22	A	818	CLA	C3-C5-C6-C7
22	A	820	CLA	C3-C5-C6-C7
22	A	855	CLA	C3-C5-C6-C7
22	B	801	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	827	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	828	CLA	C3-C5-C6-C7
22	B	829	CLA	C3-C5-C6-C7
22	F	302	CLA	C3-C5-C6-C7
22	L	202	CLA	C3-C5-C6-C7
22	1	314	CLA	C3-C5-C6-C7
22	Z	306	CLA	C3-C5-C6-C7
22	Z	307	CLA	C3-C5-C6-C7
22	3	314	CLA	C3-C5-C6-C7
22	8	307	CLA	C3-C5-C6-C7
22	8	310	CLA	C3-C5-C6-C7
22	5	315	CLA	C3-C5-C6-C7
22	5	322	CLA	C3-C5-C6-C7
22	6	311	CLA	C3-C5-C6-C7
22	6	313	CLA	C3-C5-C6-C7
22	9	305	CLA	C3-C5-C6-C7
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	CBA-CGA-O2A-C1
22	A	814	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBA-CGA-O2A-C1
22	A	823	CLA	CBA-CGA-O2A-C1
22	A	831	CLA	CBA-CGA-O2A-C1
22	A	837	CLA	CBA-CGA-O2A-C1
22	A	855	CLA	CBA-CGA-O2A-C1
22	B	808	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	B	814	CLA	CBA-CGA-O2A-C1
22	B	823	CLA	CBA-CGA-O2A-C1
22	B	831	CLA	CBA-CGA-O2A-C1
22	B	832	CLA	CBA-CGA-O2A-C1
22	1	307	CLA	CBA-CGA-O2A-C1
22	1	309	CLA	CBA-CGA-O2A-C1
22	Z	316	CLA	CBA-CGA-O2A-C1
22	3	316	CLA	CBA-CGA-O2A-C1
22	7	324	CLA	CBA-CGA-O2A-C1
22	8	305	CLA	CBA-CGA-O2A-C1
22	8	309	CLA	CBA-CGA-O2A-C1
22	4	810	CLA	CBA-CGA-O2A-C1
22	4	818	CLA	CBA-CGA-O2A-C1
22	5	301	CLA	CBA-CGA-O2A-C1
22	5	307	CLA	CBA-CGA-O2A-C1
22	5	326	CLA	CBA-CGA-O2A-C1
22	6	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	A	851	NKP	CAL-CAK-OAJ-CAI
39	5	316	CHL	CBA-CGA-O2A-C1
40	1	318	SQD	C24-C23-O48-C46
41	7	319	3PH	C32-C31-O31-C3
25	B	850	LHG	C24-C23-O8-C6
25	B	851	LHG	C24-C23-O8-C6
22	A	814	CLA	C8-C10-C11-C12
22	B	831	CLA	C5-C6-C7-C8
25	B	850	LHG	C8-C7-O7-C5
31	B	852	DGD	C2B-C1B-O2G-C2G
34	J	101	LMG	C11-C10-O7-C8
22	B	840	CLA	O1D-CGD-O2D-CED
22	3	318	CLA	O1D-CGD-O2D-CED
22	5	322	CLA	O1D-CGD-O2D-CED
22	6	309	CLA	O1D-CGD-O2D-CED
22	6	322	CLA	O1D-CGD-O2D-CED
22	A	815	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CBD-CGD-O2D-CED
22	1	304	CLA	CBD-CGD-O2D-CED
22	Z	310	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	5	314	CLA	CBD-CGD-O2D-CED
39	6	316	CHL	CBD-CGD-O2D-CED
22	8	314	CLA	O1A-CGA-O2A-C1
39	4	813	CHL	O1D-CGD-O2D-CED
22	3	320	CLA	CBA-CGA-O2A-C1
22	6	308	CLA	C3-C5-C6-C7
22	3	319	CLA	C2-C3-C5-C6
22	L	201	CLA	CBD-CGD-O2D-CED
22	3	313	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	CBD-CGD-O2D-CED
22	B	839	CLA	C2A-CAA-CBA-CGA
22	K	204	CLA	C2A-CAA-CBA-CGA
22	K	205	CLA	C2A-CAA-CBA-CGA
22	3	310	CLA	C2A-CAA-CBA-CGA
22	3	315	CLA	C2A-CAA-CBA-CGA
22	3	320	CLA	C2A-CAA-CBA-CGA
22	8	309	CLA	C2A-CAA-CBA-CGA
22	4	810	CLA	C2A-CAA-CBA-CGA
22	5	313	CLA	C2A-CAA-CBA-CGA
22	5	318	CLA	C2A-CAA-CBA-CGA
22	9	305	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	836	CLA	O1A-CGA-O2A-C1
22	B	840	CLA	O1A-CGA-O2A-C1
22	5	312	CLA	O1A-CGA-O2A-C1
22	G	202	CLA	O1D-CGD-O2D-CED
22	Z	306	CLA	O1D-CGD-O2D-CED
22	3	320	CLA	O1D-CGD-O2D-CED
25	Z	317	LHG	C11-C12-C13-C14
31	B	852	DGD	C8A-C9A-CAA-CBA
31	3	301	DGD	C8A-C9A-CAA-CBA
22	A	803	CLA	C3-C5-C6-C7
22	A	812	CLA	C3-C5-C6-C7
22	A	828	CLA	C3-C5-C6-C7
22	A	836	CLA	C3-C5-C6-C7
22	A	841	CLA	C3-C5-C6-C7
22	B	815	CLA	C3-C5-C6-C7
22	1	313	CLA	C3-C5-C6-C7
22	Z	313	CLA	C3-C5-C6-C7
22	3	308	CLA	C3-C5-C6-C7
22	3	310	CLA	C3-C5-C6-C7
22	3	312	CLA	C3-C5-C6-C7
22	7	312	CLA	C3-C5-C6-C7
22	7	324	CLA	C3-C5-C6-C7
22	8	308	CLA	C3-C5-C6-C7
22	9	307	CLA	C3-C5-C6-C7
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	815	CLA	CBA-CGA-O2A-C1
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	CBA-CGA-O2A-C1
22	A	827	CLA	CBA-CGA-O2A-C1
22	A	828	CLA	CBA-CGA-O2A-C1
22	A	832	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	B	820	CLA	CBA-CGA-O2A-C1
22	B	821	CLA	CBA-CGA-O2A-C1
22	B	834	CLA	CBA-CGA-O2A-C1
22	B	840	CLA	CBA-CGA-O2A-C1
22	1	304	CLA	CBA-CGA-O2A-C1
22	1	306	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	CBA-CGA-O2A-C1
22	Z	307	CLA	CBA-CGA-O2A-C1
22	Z	310	CLA	CBA-CGA-O2A-C1
22	3	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	7	310	CLA	CBA-CGA-O2A-C1
22	7	312	CLA	CBA-CGA-O2A-C1
22	8	311	CLA	CBA-CGA-O2A-C1
22	4	805	CLA	CBA-CGA-O2A-C1
22	4	806	CLA	CBA-CGA-O2A-C1
22	6	301	CLA	CBA-CGA-O2A-C1
22	6	311	CLA	CBA-CGA-O2A-C1
22	6	313	CLA	CBA-CGA-O2A-C1
22	9	306	CLA	CBA-CGA-O2A-C1
22	9	309	CLA	CBA-CGA-O2A-C1
39	2	303	CHL	CBA-CGA-O2A-C1
22	A	804	CLA	O1D-CGD-O2D-CED
22	A	809	CLA	O1D-CGD-O2D-CED
22	4	812	CLA	O1D-CGD-O2D-CED
22	4	807	CLA	CBD-CGD-O2D-CED
22	A	814	CLA	O1D-CGD-O2D-CED
22	A	838	CLA	O1D-CGD-O2D-CED
22	B	818	CLA	O1D-CGD-O2D-CED
22	1	311	CLA	O1D-CGD-O2D-CED
22	Z	307	CLA	O1D-CGD-O2D-CED
22	7	304	CLA	O1D-CGD-O2D-CED
22	7	315	CLA	O1D-CGD-O2D-CED
22	4	806	CLA	O1D-CGD-O2D-CED
22	9	307	CLA	O1D-CGD-O2D-CED
25	4	820	LHG	O9-C7-O7-C5
33	G	204	LMT	C4'-C5'-C6'-O6'
22	A	828	CLA	O1A-CGA-O2A-C1
22	A	832	CLA	O1A-CGA-O2A-C1
22	A	842	CLA	O1A-CGA-O2A-C1
22	B	820	CLA	O1A-CGA-O2A-C1
22	B	831	CLA	O1A-CGA-O2A-C1
22	1	304	CLA	O1A-CGA-O2A-C1
22	1	310	CLA	O1A-CGA-O2A-C1
22	Z	306	CLA	O1A-CGA-O2A-C1
22	Z	310	CLA	O1A-CGA-O2A-C1
22	3	316	CLA	O1A-CGA-O2A-C1
22	7	312	CLA	O1A-CGA-O2A-C1
22	4	806	CLA	O1A-CGA-O2A-C1
22	5	322	CLA	O1A-CGA-O2A-C1
22	6	301	CLA	O1A-CGA-O2A-C1
22	9	306	CLA	O1A-CGA-O2A-C1
26	A	851	NKP	OAE-CAK-OAJ-CAI

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Mol	Chain	Res	Type	Atoms
39	7	313	CHL	O1A-CGA-O2A-C1
39	2	303	CHL	O1A-CGA-O2A-C1
22	3	320	CLA	O1A-CGA-O2A-C1
24	A	845	BCR	C9-C10-C11-C12
24	A	845	BCR	C19-C20-C21-C22
24	A	846	BCR	C9-C10-C11-C12
24	A	846	BCR	C15-C16-C17-C18
24	B	848	BCR	C15-C16-C17-C18
24	B	849	BCR	C19-C20-C21-C22
24	B	853	BCR	C15-C16-C17-C18
24	G	203	BCR	C19-C20-C21-C22
24	I	4001	BCR	C13-C14-C15-C16
24	J	104	BCR	C19-C20-C21-C22
24	K	206	BCR	C15-C16-C17-C18
24	L	204	BCR	C9-C10-C11-C12
24	7	303	BCR	C9-C10-C11-C12
24	7	303	BCR	C19-C20-C21-C22
24	4	804	BCR	C13-C14-C15-C16
24	5	304	BCR	C9-C10-C11-C12
24	6	305	BCR	C9-C10-C11-C12
24	6	305	BCR	C13-C14-C15-C16
24	6	306	BCR	C13-C14-C15-C16
24	6	306	BCR	C19-C20-C21-C22
36	5	306	C7Z	C29-C30-C31-C32
22	B	822	CLA	CBD-CGD-O2D-CED
22	B	838	CLA	CBD-CGD-O2D-CED
22	3	322	CLA	CBD-CGD-O2D-CED
22	6	310	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	O1D-CGD-O2D-CED
22	1	309	CLA	O1D-CGD-O2D-CED
39	7	313	CHL	O1D-CGD-O2D-CED
25	A	849	LHG	O2-C2-C3-O3
25	A	850	LHG	O2-C2-C3-O3
25	B	803	LHG	O2-C2-C3-O3
25	B	850	LHG	O2-C2-C3-O3
25	3	321	LHG	O2-C2-C3-O3
25	9	315	LHG	O2-C2-C3-O3
21	A	801	CL0	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	A	816	CLA	C3-C5-C6-C7
22	A	821	CLA	C3-C5-C6-C7
22	B	810	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	822	CLA	C3-C5-C6-C7
22	B	823	CLA	C3-C5-C6-C7
22	B	825	CLA	C3-C5-C6-C7
22	1	308	CLA	C3-C5-C6-C7
22	3	319	CLA	C3-C5-C6-C7
22	5	318	CLA	C3-C5-C6-C7
22	6	302	CLA	C3-C5-C6-C7
22	6	309	CLA	C3-C5-C6-C7
22	6	319	CLA	C3-C5-C6-C7
22	6	322	CLA	C3-C5-C6-C7
22	2	301	CLA	C3-C5-C6-C7
22	A	833	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBA-CGA-O2A-C1
22	A	839	CLA	CBA-CGA-O2A-C1
22	B	816	CLA	CBA-CGA-O2A-C1
22	F	302	CLA	CBA-CGA-O2A-C1
22	Z	306	CLA	CBA-CGA-O2A-C1
22	3	311	CLA	CBA-CGA-O2A-C1
22	4	808	CLA	CBA-CGA-O2A-C1
22	5	312	CLA	CBA-CGA-O2A-C1
39	7	313	CHL	CBA-CGA-O2A-C1
22	A	808	CLA	O1A-CGA-O2A-C1
22	B	833	CLA	O1A-CGA-O2A-C1
22	3	311	CLA	O1A-CGA-O2A-C1
22	5	326	CLA	O1A-CGA-O2A-C1
22	6	311	CLA	O1A-CGA-O2A-C1
22	A	808	CLA	O1D-CGD-O2D-CED
22	A	834	CLA	O1D-CGD-O2D-CED
22	A	836	CLA	O1D-CGD-O2D-CED
22	B	807	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	O1D-CGD-O2D-CED
22	Z	304	CLA	O1D-CGD-O2D-CED
22	8	307	CLA	O1D-CGD-O2D-CED
22	9	305	CLA	O1D-CGD-O2D-CED
22	2	302	CLA	O1D-CGD-O2D-CED
22	A	825	CLA	C8-C10-C11-C12
25	7	318	LHG	C8-C7-O7-C5
35	J	102	T7X	C12-C10-O16-C8
25	Z	317	LHG	C23-C24-C25-C26
22	A	819	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	CBD-CGD-O2D-CED
22	1	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	7	323	CLA	CBD-CGD-O2D-CED
22	8	314	CLA	CBD-CGD-O2D-CED
22	5	313	CLA	CBD-CGD-O2D-CED
22	B	816	CLA	O1A-CGA-O2A-C1
22	1	307	CLA	O1D-CGD-O2D-CED
22	A	837	CLA	CBD-CGD-O2D-CED
22	A	807	CLA	C3-C5-C6-C7
22	A	814	CLA	C3-C5-C6-C7
22	B	821	CLA	C3-C5-C6-C7
22	B	838	CLA	C3-C5-C6-C7
22	F	301	CLA	C3-C5-C6-C7
22	7	322	CLA	C3-C5-C6-C7
22	4	812	CLA	C3-C5-C6-C7
22	5	301	CLA	C3-C5-C6-C7
22	5	310	CLA	C3-C5-C6-C7
22	A	842	CLA	CBA-CGA-O2A-C1
22	B	833	CLA	CBA-CGA-O2A-C1
22	5	322	CLA	CBA-CGA-O2A-C1
41	6	324	3PH	C22-C23-C24-C25
26	A	851	NKP	CAH-CAG-OAF-PAC
22	A	839	CLA	O1A-CGA-O2A-C1
22	F	302	CLA	O1A-CGA-O2A-C1
22	8	311	CLA	O1A-CGA-O2A-C1
22	4	808	CLA	O1A-CGA-O2A-C1
22	A	842	CLA	C3-C5-C6-C7
22	A	817	CLA	C8-C10-C11-C12
22	3	314	CLA	C4-C3-C5-C6
22	3	314	CLA	C2-C3-C5-C6
25	3	321	LHG	O10-C23-O8-C6
22	A	824	CLA	C2A-CAA-CBA-CGA
22	F	304	CLA	C2A-CAA-CBA-CGA
22	1	306	CLA	C2A-CAA-CBA-CGA
22	Z	303	CLA	C2A-CAA-CBA-CGA
22	9	308	CLA	C2A-CAA-CBA-CGA
22	B	811	CLA	O1D-CGD-O2D-CED
22	1	305	CLA	O1D-CGD-O2D-CED
22	8	306	CLA	O1D-CGD-O2D-CED
22	6	301	CLA	O1D-CGD-O2D-CED
22	9	306	CLA	O1D-CGD-O2D-CED
22	A	833	CLA	O1A-CGA-O2A-C1
22	L	203	CLA	O1A-CGA-O2A-C1
22	8	310	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	840	CLA	CBA-CGA-O2A-C1
22	L	203	CLA	CBA-CGA-O2A-C1
22	7	317	CLA	CBA-CGA-O2A-C1
22	8	310	CLA	CBA-CGA-O2A-C1
22	9	308	CLA	CBA-CGA-O2A-C1
39	6	315	CHL	CBA-CGA-O2A-C1
22	A	840	CLA	CBD-CGD-O2D-CED
22	G	202	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	O1D-CGD-O2D-CED
22	B	834	CLA	O1D-CGD-O2D-CED
22	4	805	CLA	O1D-CGD-O2D-CED
22	4	808	CLA	O1D-CGD-O2D-CED
22	4	811	CLA	O1D-CGD-O2D-CED
25	8	317	LHG	C25-C26-C27-C28
22	B	817	CLA	O1D-CGD-O2D-CED
22	B	833	CLA	O1D-CGD-O2D-CED
22	B	842	CLA	O1D-CGD-O2D-CED
22	7	311	CLA	O1D-CGD-O2D-CED
39	6	315	CHL	O1D-CGD-O2D-CED
22	A	806	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	O1D-CGD-O2D-CED
22	5	311	CLA	O1D-CGD-O2D-CED
25	B	803	LHG	C1-C2-C3-O3
25	4	820	LHG	C1-C2-C3-O3
25	5	324	LHG	C1-C2-C3-O3
25	6	323	LHG	C1-C2-C3-O3
35	J	102	T7X	O17-C10-O16-C8
22	9	308	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	C3-C5-C6-C7
22	A	830	CLA	C3-C5-C6-C7
22	B	811	CLA	C3-C5-C6-C7
22	7	310	CLA	C3-C5-C6-C7
22	9	306	CLA	C3-C5-C6-C7
22	B	837	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	CBA-CGA-O2A-C1
22	A	824	CLA	CBA-CGA-O2A-C1
22	A	834	CLA	CBA-CGA-O2A-C1
22	B	809	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	K	205	CLA	CBA-CGA-O2A-C1
22	1	308	CLA	CBA-CGA-O2A-C1
22	7	309	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	8	308	CLA	CBA-CGA-O2A-C1
22	5	319	CLA	CBA-CGA-O2A-C1
22	6	308	CLA	CBA-CGA-O2A-C1
22	9	307	CLA	CBA-CGA-O2A-C1
25	5	324	LHG	C24-C23-O8-C6
39	8	315	CHL	CBA-CGA-O2A-C1
22	B	839	CLA	CBD-CGD-O2D-CED
24	A	847	BCR	C15-C16-C17-C18
24	A	856	BCR	C13-C14-C15-C16
24	A	856	BCR	C19-C20-C21-C22
24	B	845	BCR	C15-C16-C17-C18
24	B	845	BCR	C19-C20-C21-C22
24	I	4001	BCR	C15-C16-C17-C18
24	7	303	BCR	C15-C16-C17-C18
24	8	304	BCR	C15-C16-C17-C18
24	8	304	BCR	C19-C20-C21-C22
24	4	804	BCR	C15-C16-C17-C18
24	4	804	BCR	C19-C20-C21-C22
24	6	306	BCR	C15-C16-C17-C18
22	9	307	CLA	O1A-CGA-O2A-C1
22	1	306	CLA	C5-C6-C7-C8
22	6	314	CLA	C8-C10-C11-C12
25	4	820	LHG	O2-C2-C3-O3
43	8	319	LPX	O1-C3-C4-O5
39	9	312	CHL	C3-C5-C6-C7
25	6	323	LHG	C7-C8-C9-C10
22	B	839	CLA	C3-C5-C6-C7
22	3	316	CLA	C3-C5-C6-C7
25	B	850	LHG	O10-C23-O8-C6
25	B	851	LHG	O10-C23-O8-C6
22	A	834	CLA	O1A-CGA-O2A-C1
22	A	840	CLA	O1A-CGA-O2A-C1
22	B	817	CLA	O1A-CGA-O2A-C1
22	K	205	CLA	O1A-CGA-O2A-C1
22	1	308	CLA	O1A-CGA-O2A-C1
33	G	204	LMT	O5'-C5'-C6'-O6'
22	A	802	CLA	C6-C7-C8-C9
22	A	803	CLA	C6-C7-C8-C9
22	A	807	CLA	C6-C7-C8-C9
22	A	808	CLA	C6-C7-C8-C9
22	A	812	CLA	C6-C7-C8-C9
22	A	812	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	814	CLA	C6-C7-C8-C9
22	A	815	CLA	C6-C7-C8-C9
22	A	816	CLA	C6-C7-C8-C9
22	A	818	CLA	C6-C7-C8-C9
22	A	818	CLA	C11-C10-C8-C9
22	A	820	CLA	C6-C7-C8-C9
22	A	823	CLA	C6-C7-C8-C9
22	A	823	CLA	C11-C10-C8-C9
22	A	830	CLA	C6-C7-C8-C9
22	A	832	CLA	C6-C7-C8-C9
22	A	834	CLA	C6-C7-C8-C9
22	A	835	CLA	C6-C7-C8-C9
22	A	838	CLA	C11-C10-C8-C9
22	A	854	CLA	C6-C7-C8-C9
22	A	855	CLA	C11-C12-C13-C14
22	B	801	CLA	C6-C7-C8-C9
22	B	809	CLA	C6-C7-C8-C9
22	B	813	CLA	C6-C7-C8-C9
22	B	815	CLA	C6-C7-C8-C9
22	B	818	CLA	C11-C12-C13-C14
22	B	819	CLA	C6-C7-C8-C9
22	B	820	CLA	C6-C7-C8-C9
22	B	824	CLA	C11-C10-C8-C9
22	B	825	CLA	C6-C7-C8-C9
22	B	828	CLA	C11-C10-C8-C9
22	B	829	CLA	C6-C7-C8-C9
22	B	830	CLA	C6-C7-C8-C9
22	B	833	CLA	C6-C7-C8-C9
22	B	842	CLA	C11-C10-C8-C9
22	F	304	CLA	C6-C7-C8-C9
22	L	202	CLA	C11-C12-C13-C14
22	1	304	CLA	C6-C7-C8-C9
22	1	306	CLA	C11-C12-C13-C14
22	1	307	CLA	C6-C7-C8-C9
22	1	309	CLA	C6-C7-C8-C9
22	1	310	CLA	C11-C10-C8-C9
22	1	313	CLA	C6-C7-C8-C9
22	1	316	CLA	C11-C10-C8-C9
22	Z	303	CLA	C6-C7-C8-C9
22	Z	313	CLA	C6-C7-C8-C9
22	3	312	CLA	C11-C10-C8-C9
22	3	314	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	3	318	CLA	C6-C7-C8-C9
22	3	322	CLA	C6-C7-C8-C9
22	3	322	CLA	C11-C10-C8-C9
22	3	322	CLA	C11-C12-C13-C14
22	7	304	CLA	C6-C7-C8-C9
22	7	307	CLA	C11-C10-C8-C9
22	7	312	CLA	C11-C10-C8-C9
22	7	324	CLA	C6-C7-C8-C9
22	7	324	CLA	C11-C10-C8-C9
22	8	308	CLA	C6-C7-C8-C9
22	4	807	CLA	C6-C7-C8-C9
22	5	313	CLA	C11-C10-C8-C9
22	5	318	CLA	C6-C7-C8-C9
22	5	322	CLA	C11-C10-C8-C9
22	6	307	CLA	C6-C7-C8-C9
22	6	312	CLA	C6-C7-C8-C9
22	9	305	CLA	C6-C7-C8-C9
39	3	317	CHL	C11-C10-C8-C9
39	5	316	CHL	C14-C13-C15-C16
22	A	830	CLA	O1D-CGD-O2D-CED
22	A	831	CLA	O1D-CGD-O2D-CED
22	7	307	CLA	CBD-CGD-O2D-CED
24	A	844	BCR	C11-C12-C13-C35
24	A	844	BCR	C36-C18-C19-C20
24	A	846	BCR	C11-C12-C13-C35
24	A	847	BCR	C7-C8-C9-C34
24	A	847	BCR	C36-C18-C19-C20
24	A	848	BCR	C11-C12-C13-C35
24	A	856	BCR	C7-C8-C9-C34
24	A	856	BCR	C37-C22-C23-C24
24	B	845	BCR	C11-C12-C13-C35
24	B	845	BCR	C36-C18-C19-C20
24	B	846	BCR	C7-C8-C9-C34
24	B	847	BCR	C11-C12-C13-C35
24	B	848	BCR	C7-C8-C9-C34
24	B	853	BCR	C11-C12-C13-C35
24	B	853	BCR	C37-C22-C23-C24
24	F	303	BCR	C37-C22-C23-C24
24	G	203	BCR	C37-C22-C23-C24
24	I	4001	BCR	C7-C8-C9-C34
24	I	4001	BCR	C11-C12-C13-C35
24	J	104	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	K	206	BCR	C11-C12-C13-C35
24	K	206	BCR	C37-C22-C23-C24
24	L	204	BCR	C7-C8-C9-C34
24	3	304	BCR	C37-C22-C23-C24
24	3	305	BCR	C7-C8-C9-C34
24	3	306	BCR	C36-C18-C19-C20
24	3	307	BCR	C7-C8-C9-C34
24	3	307	BCR	C37-C22-C23-C24
24	7	303	BCR	C36-C18-C19-C20
24	4	804	BCR	C36-C18-C19-C20
24	5	304	BCR	C36-C18-C19-C20
24	5	305	BCR	C37-C22-C23-C24
24	6	305	BCR	C7-C8-C9-C34
24	6	305	BCR	C36-C18-C19-C20
24	6	306	BCR	C11-C12-C13-C35
24	6	306	BCR	C36-C18-C19-C20
36	J	105	C7Z	C7-C8-C9-C19
36	J	105	C7Z	C11-C12-C13-C20
36	5	306	C7Z	C7-C8-C9-C19
36	5	306	C7Z	C27-C28-C29-C39
38	3	303	LUT	C7-C8-C9-C19
38	7	302	LUT	C11-C12-C13-C20
38	5	302	LUT	C27-C28-C29-C39
38	5	303	LUT	C7-C8-C9-C19
38	6	304	LUT	C7-C8-C9-C19
24	A	844	BCR	C11-C12-C13-C14
24	A	844	BCR	C17-C18-C19-C20
24	A	845	BCR	C7-C8-C9-C10
24	A	846	BCR	C11-C12-C13-C14
24	A	847	BCR	C17-C18-C19-C20
24	A	856	BCR	C7-C8-C9-C10
24	A	856	BCR	C21-C22-C23-C24
24	B	844	BCR	C7-C8-C9-C10
24	B	845	BCR	C21-C22-C23-C24
24	B	848	BCR	C7-C8-C9-C10
24	B	849	BCR	C17-C18-C19-C20
24	B	853	BCR	C11-C12-C13-C14
24	B	853	BCR	C21-C22-C23-C24
24	F	303	BCR	C21-C22-C23-C24
24	G	203	BCR	C21-C22-C23-C24
24	I	4001	BCR	C7-C8-C9-C10
24	I	4001	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	J	104	BCR	C7-C8-C9-C10
24	K	206	BCR	C21-C22-C23-C24
24	L	204	BCR	C11-C12-C13-C14
24	L	204	BCR	C17-C18-C19-C20
24	3	304	BCR	C21-C22-C23-C24
24	3	305	BCR	C7-C8-C9-C10
24	3	305	BCR	C17-C18-C19-C20
24	3	307	BCR	C7-C8-C9-C10
24	3	307	BCR	C21-C22-C23-C24
24	7	303	BCR	C17-C18-C19-C20
24	4	804	BCR	C11-C12-C13-C14
24	4	804	BCR	C17-C18-C19-C20
24	5	304	BCR	C17-C18-C19-C20
24	6	305	BCR	C7-C8-C9-C10
24	6	305	BCR	C17-C18-C19-C20
24	6	306	BCR	C7-C8-C9-C10
24	6	306	BCR	C11-C12-C13-C14
24	6	306	BCR	C17-C18-C19-C20
36	J	105	C7Z	C11-C12-C13-C14
36	5	306	C7Z	C7-C8-C9-C10
36	5	306	C7Z	C31-C32-C33-C34
36	5	306	C7Z	C27-C28-C29-C30
38	1	302	LUT	C7-C8-C9-C10
38	3	303	LUT	C7-C8-C9-C10
38	5	302	LUT	C7-C8-C9-C10
38	5	303	LUT	C7-C8-C9-C10
38	6	304	LUT	C7-C8-C9-C10
38	9	302	LUT	C11-C12-C13-C14
25	7	318	LHG	O9-C7-O7-C5
22	B	809	CLA	O1A-CGA-O2A-C1
22	7	309	CLA	O1A-CGA-O2A-C1
22	6	308	CLA	O1A-CGA-O2A-C1
39	8	315	CHL	O1A-CGA-O2A-C1
22	B	805	CLA	C5-C6-C7-C8
22	B	818	CLA	C10-C11-C12-C13
22	5	310	CLA	C5-C6-C7-C8
27	A	852	DGA	CA7-CA8-CA9-CAA
22	A	834	CLA	C3-C5-C6-C7
22	K	203	CLA	C3-C5-C6-C7
22	7	307	CLA	C3-C5-C6-C7
22	6	310	CLA	C3-C5-C6-C7
22	3	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	9	303	CLA	CBA-CGA-O2A-C1
22	A	818	CLA	C5-C6-C7-C8
22	B	829	CLA	C5-C6-C7-C8
22	9	303	CLA	C10-C11-C12-C13
22	5	307	CLA	O1D-CGD-O2D-CED
39	5	316	CHL	O1D-CGD-O2D-CED
22	A	839	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	C5-C6-C7-C8
22	B	825	CLA	C5-C6-C7-C8
22	B	828	CLA	C10-C11-C12-C13
22	F	304	CLA	C5-C6-C7-C8
22	1	316	CLA	C10-C11-C12-C13
22	3	313	CLA	C10-C11-C12-C13
22	7	306	CLA	C8-C10-C11-C12
22	7	306	CLA	C10-C11-C12-C13
22	6	312	CLA	C5-C6-C7-C8
22	9	303	CLA	C5-C6-C7-C8
22	9	305	CLA	C5-C6-C7-C8
41	8	320	3PH	C3A-C3B-C3C-C3D
22	B	813	CLA	O1D-CGD-O2D-CED
22	K	202	CLA	O1D-CGD-O2D-CED
25	7	318	LHG	O1-C1-C2-O2
22	A	810	CLA	O1A-CGA-O2A-C1
25	A	849	LHG	C23-C24-C25-C26
25	A	850	LHG	C7-C8-C9-C10
25	A	850	LHG	C23-C24-C25-C26
25	B	803	LHG	C7-C8-C9-C10
25	Z	317	LHG	C7-C8-C9-C10
25	8	317	LHG	C23-C24-C25-C26
25	4	820	LHG	C23-C24-C25-C26
25	6	323	LHG	C23-C24-C25-C26
34	F	308	LMG	C10-C11-C12-C13
25	5	324	LHG	C11-C10-C9-C8
22	A	819	CLA	C8-C10-C11-C12
22	5	309	CLA	CBA-CGA-O2A-C1
25	7	318	LHG	C11-C10-C9-C8
22	A	803	CLA	O1D-CGD-O2D-CED
22	1	308	CLA	O1D-CGD-O2D-CED
22	A	832	CLA	C2-C1-O2A-CGA
22	A	838	CLA	C2-C1-O2A-CGA
22	A	839	CLA	C2-C1-O2A-CGA
22	B	806	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	B	825	CLA	C2-C1-O2A-CGA
22	B	831	CLA	C2-C1-O2A-CGA
22	1	314	CLA	C2-C1-O2A-CGA
22	3	310	CLA	C2-C1-O2A-CGA
22	3	316	CLA	C2-C1-O2A-CGA
22	8	310	CLA	C2-C1-O2A-CGA
22	8	311	CLA	C2-C1-O2A-CGA
22	4	810	CLA	C2-C1-O2A-CGA
22	6	302	CLA	C2-C1-O2A-CGA
22	6	307	CLA	C2-C1-O2A-CGA
22	3	312	CLA	C8-C10-C11-C12
25	B	803	LHG	C23-C24-C25-C26
22	4	806	CLA	C3-C5-C6-C7
22	A	806	CLA	C11-C10-C8-C7
22	A	810	CLA	C6-C7-C8-C10
22	A	820	CLA	C11-C10-C8-C7
22	A	824	CLA	C6-C7-C8-C10
22	A	827	CLA	C11-C12-C13-C15
22	A	841	CLA	C6-C7-C8-C10
22	B	810	CLA	C6-C7-C8-C10
22	B	815	CLA	C11-C10-C8-C7
22	B	819	CLA	C6-C7-C8-C10
22	B	819	CLA	C11-C10-C8-C7
22	B	828	CLA	C11-C10-C8-C7
22	B	834	CLA	C6-C7-C8-C10
22	B	838	CLA	C6-C7-C8-C10
22	L	201	CLA	C6-C7-C8-C10
22	Z	309	CLA	C6-C7-C8-C10
22	3	314	CLA	C6-C7-C8-C10
22	7	312	CLA	C6-C7-C8-C10
22	7	317	CLA	C6-C7-C8-C10
22	8	310	CLA	C11-C10-C8-C7
22	6	302	CLA	C6-C7-C8-C10
22	6	319	CLA	C6-C7-C8-C10
22	6	322	CLA	C6-C7-C8-C10
22	9	306	CLA	C11-C10-C8-C7
39	8	315	CHL	C11-C10-C8-C7
39	9	312	CHL	C12-C13-C15-C16
22	A	815	CLA	C3-C5-C6-C7
22	A	854	CLA	C3-C5-C6-C7
22	B	808	CLA	C3-C5-C6-C7
22	B	814	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	1	309	CLA	C3-C5-C6-C7
22	7	309	CLA	C3-C5-C6-C7
22	5	319	CLA	O1A-CGA-O2A-C1
25	5	324	LHG	O10-C23-O8-C6
24	A	844	BCR	C15-C16-C17-C18
24	A	848	BCR	C13-C14-C15-C16
24	B	845	BCR	C13-C14-C15-C16
24	B	847	BCR	C9-C10-C11-C12
24	B	849	BCR	C13-C14-C15-C16
24	B	853	BCR	C13-C14-C15-C16
24	I	4001	BCR	C9-C10-C11-C12
24	J	104	BCR	C13-C14-C15-C16
24	J	104	BCR	C15-C16-C17-C18
24	3	306	BCR	C13-C14-C15-C16
24	5	304	BCR	C15-C16-C17-C18
24	6	305	BCR	C15-C16-C17-C18
38	6	303	LUT	C9-C10-C11-C12
38	6	304	LUT	C9-C10-C11-C12
22	A	840	CLA	C2A-CAA-CBA-CGA
22	A	855	CLA	C2A-CAA-CBA-CGA
22	9	306	CLA	C2A-CAA-CBA-CGA
22	A	815	CLA	O1D-CGD-O2D-CED
22	B	826	CLA	O1D-CGD-O2D-CED
22	7	310	CLA	O1D-CGD-O2D-CED
22	8	311	CLA	O1D-CGD-O2D-CED
22	1	306	CLA	C8-C10-C11-C12
22	9	305	CLA	C8-C10-C11-C12
33	4	822	LMT	O1'-C1-C2-C3
22	A	824	CLA	O1A-CGA-O2A-C1
22	L	202	CLA	C8-C10-C11-C12
25	1	317	LHG	C23-C24-C25-C26
25	B	851	LHG	O2-C2-C3-O3
25	Z	317	LHG	O2-C2-C3-O3
25	7	318	LHG	O2-C2-C3-O3
25	8	317	LHG	O2-C2-C3-O3
25	5	324	LHG	O2-C2-C3-O3
25	6	323	LHG	O2-C2-C3-O3
22	A	808	CLA	C3-C5-C6-C7
22	1	307	CLA	C3-C5-C6-C7
22	A	825	CLA	C5-C6-C7-C8
22	Z	309	CLA	C5-C6-C7-C8
22	A	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	6	310	CLA	CBA-CGA-O2A-C1
22	7	317	CLA	O1A-CGA-O2A-C1
22	8	308	CLA	O1A-CGA-O2A-C1
22	5	309	CLA	O1A-CGA-O2A-C1
39	6	315	CHL	O1A-CGA-O2A-C1
25	5	324	LHG	C7-C8-C9-C10
25	9	315	LHG	C23-C24-C25-C26
25	4	820	LHG	C9-C10-C11-C12
42	7	320	SPH	C12-C13-C14-C15
22	A	827	CLA	C8-C10-C11-C12
22	A	840	CLA	C8-C10-C11-C12
22	A	855	CLA	C8-C10-C11-C12
22	B	801	CLA	C13-C15-C16-C17
22	B	806	CLA	C8-C10-C11-C12
22	Z	303	CLA	C5-C6-C7-C8
22	3	313	CLA	C8-C10-C11-C12
22	1	304	CLA	O1D-CGD-O2D-CED
22	5	314	CLA	O1D-CGD-O2D-CED
22	3	310	CLA	O1A-CGA-O2A-C1
22	9	303	CLA	O1A-CGA-O2A-C1
25	4	821	LHG	C8-C7-O7-C5
22	A	806	CLA	C13-C15-C16-C17
22	A	820	CLA	C5-C6-C7-C8
22	A	825	CLA	C15-C16-C17-C18
22	A	828	CLA	C8-C10-C11-C12
22	B	817	CLA	C5-C6-C7-C8
22	B	830	CLA	C8-C10-C11-C12
22	B	841	CLA	C5-C6-C7-C8
22	7	323	CLA	C13-C15-C16-C17
22	8	307	CLA	C8-C10-C11-C12
22	5	315	CLA	C8-C10-C11-C12
22	6	307	CLA	C5-C6-C7-C8
22	6	322	CLA	C8-C10-C11-C12
25	A	849	LHG	C3-O3-P-O6
25	A	849	LHG	C4-O6-P-O3
25	A	850	LHG	C4-O6-P-O3
25	B	803	LHG	C3-O3-P-O6
25	7	318	LHG	C4-O6-P-O3
25	4	820	LHG	C4-O6-P-O3
25	5	324	LHG	C3-O3-P-O6
25	6	323	LHG	C4-O6-P-O3
25	9	315	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
25	9	315	LHG	C4-O6-P-O3
25	5	324	LHG	C23-C24-C25-C26
22	8	309	CLA	C3-C5-C6-C7
22	5	309	CLA	C3-C5-C6-C7
27	A	852	DGA	CCA-CDA-CEA-CFA
22	B	824	CLA	CBA-CGA-O2A-C1
22	B	841	CLA	CBA-CGA-O2A-C1
31	3	301	DGD	C2A-C1A-O1G-C1G
22	2	304	CLA	O1D-CGD-O2D-CED
22	L	201	CLA	O1D-CGD-O2D-CED
22	Z	310	CLA	O1D-CGD-O2D-CED
25	7	318	LHG	C7-C8-C9-C10
22	B	825	CLA	O1D-CGD-O2D-CED
39	6	316	CHL	O1D-CGD-O2D-CED
25	A	849	LHG	C1-C2-C3-O3
25	B	850	LHG	C1-C2-C3-O3
25	B	851	LHG	C1-C2-C3-O3
25	Z	317	LHG	C1-C2-C3-O3
25	8	317	LHG	C1-C2-C3-O3
25	4	821	LHG	O9-C7-O7-C5
22	B	813	CLA	C2A-CAA-CBA-CGA
22	Z	306	CLA	C2A-CAA-CBA-CGA
22	3	313	CLA	C2A-CAA-CBA-CGA
22	5	320	CLA	C2A-CAA-CBA-CGA
39	1	312	CHL	C2A-CAA-CBA-CGA
39	Z	312	CHL	C2A-CAA-CBA-CGA
39	4	813	CHL	C2A-CAA-CBA-CGA
39	4	814	CHL	C2A-CAA-CBA-CGA
39	5	317	CHL	C2A-CAA-CBA-CGA
22	B	823	CLA	C6-C7-C8-C9
22	5	311	CLA	C6-C7-C8-C9
22	6	313	CLA	C6-C7-C8-C10
22	2	301	CLA	C6-C7-C8-C9
22	K	205	CLA	C3-C5-C6-C7
22	5	323	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CBA-CGA-O2A-C1
22	G	201	CLA	CBA-CGA-O2A-C1
25	4	820	LHG	C24-C23-O8-C6
25	4	821	LHG	C24-C23-O8-C6
22	G	202	CLA	O1A-CGA-O2A-C1
23	A	843	PQN	C25-C26-C27-C28
41	7	319	3PH	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
24	A	844	BCR	C19-C20-C21-C22
24	A	847	BCR	C9-C10-C11-C12
24	A	848	BCR	C19-C20-C21-C22
24	A	856	BCR	C15-C16-C17-C18
24	B	848	BCR	C9-C10-C11-C12
24	B	849	BCR	C15-C16-C17-C18
24	F	303	BCR	C15-C16-C17-C18
24	5	304	BCR	C19-C20-C21-C22
24	6	305	BCR	C19-C20-C21-C22
38	4	802	LUT	C9-C10-C11-C12
27	A	852	DGA	CB1-CB2-CB3-CB4
33	4	822	LMT	C6-C7-C8-C9
22	1	316	CLA	C8-C10-C11-C12
22	7	323	CLA	C3-C5-C6-C7
25	A	849	LHG	C11-C12-C13-C14
25	4	820	LHG	C11-C12-C13-C14
27	A	852	DGA	CB9-CAB-CBB-CCB
40	1	318	SQD	C11-C10-C9-C8
22	3	313	CLA	O1D-CGD-O2D-CED
22	3	319	CLA	C6-C7-C8-C9
25	A	850	LHG	C13-C14-C15-C16
25	1	317	LHG	C11-C12-C13-C14
25	8	317	LHG	C11-C12-C13-C14
25	4	821	LHG	C11-C12-C13-C14
22	4	807	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	C8-C10-C11-C12
22	3	322	CLA	C13-C15-C16-C17
25	A	849	LHG	C13-C14-C15-C16
25	1	317	LHG	C27-C28-C29-C30
41	8	320	3PH	C36-C37-C38-C39
25	3	321	LHG	C2-C3-O3-P
22	A	830	CLA	O1A-CGA-O2A-C1
22	6	310	CLA	O1A-CGA-O2A-C1
25	1	317	LHG	C12-C13-C14-C15
22	B	822	CLA	O1D-CGD-O2D-CED
25	1	317	LHG	O2-C2-C3-O3
25	1	317	LHG	C10-C11-C12-C13
25	1	317	LHG	C16-C17-C18-C19
22	7	317	CLA	C3-C5-C6-C7
22	8	305	CLA	C3-C5-C6-C7
22	A	811	CLA	CBA-CGA-O2A-C1
25	B	803	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
25	9	315	LHG	C24-C23-O8-C6
25	Z	317	LHG	C13-C14-C15-C16
25	8	317	LHG	C11-C10-C9-C8
27	A	852	DGA	CA6-CA7-CA8-CA9
22	A	832	CLA	C8-C10-C11-C12
22	B	830	CLA	C5-C6-C7-C8
22	B	812	CLA	C6-C7-C8-C9
22	K	205	CLA	C6-C7-C8-C10
22	7	322	CLA	C6-C7-C8-C9
22	4	812	CLA	C6-C7-C8-C10
22	6	311	CLA	C6-C7-C8-C10
22	B	838	CLA	O1D-CGD-O2D-CED
22	6	310	CLA	O1D-CGD-O2D-CED
25	A	850	LHG	C11-C12-C13-C14
22	A	827	CLA	C11-C12-C13-C14
22	A	828	CLA	C11-C10-C8-C9
22	A	840	CLA	C6-C7-C8-C9
22	B	814	CLA	C6-C7-C8-C9
22	B	817	CLA	C6-C7-C8-C9
22	B	818	CLA	C6-C7-C8-C9
22	1	314	CLA	C14-C13-C15-C16
22	1	316	CLA	C14-C13-C15-C16
22	3	311	CLA	C11-C10-C8-C9
22	4	805	CLA	C6-C7-C8-C9
22	8	308	CLA	C13-C15-C16-C17
25	9	315	LHG	C7-C8-C9-C10
25	4	820	LHG	C28-C29-C30-C31
25	9	315	LHG	C11-C10-C9-C8
22	A	809	CLA	C2A-CAA-CBA-CGA
22	3	311	CLA	C2A-CAA-CBA-CGA
22	7	323	CLA	C2A-CAA-CBA-CGA
22	8	311	CLA	C2A-CAA-CBA-CGA
22	5	308	CLA	C2A-CAA-CBA-CGA
22	6	319	CLA	C2A-CAA-CBA-CGA
39	6	316	CHL	C2A-CAA-CBA-CGA
24	A	845	BCR	C36-C18-C19-C20
24	A	846	BCR	C36-C18-C19-C20
24	A	846	BCR	C37-C22-C23-C24
24	B	845	BCR	C37-C22-C23-C24
24	B	848	BCR	C36-C18-C19-C20
24	B	849	BCR	C7-C8-C9-C34
24	F	303	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	G	203	BCR	C36-C18-C19-C20
24	J	104	BCR	C37-C22-C23-C24
24	K	206	BCR	C36-C18-C19-C20
24	L	204	BCR	C11-C12-C13-C35
24	3	305	BCR	C36-C18-C19-C20
24	8	304	BCR	C7-C8-C9-C34
24	8	304	BCR	C36-C18-C19-C20
24	8	304	BCR	C37-C22-C23-C24
24	4	804	BCR	C11-C12-C13-C35
24	5	305	BCR	C11-C12-C13-C35
24	6	306	BCR	C37-C22-C23-C24
32	F	306	RRX	C37-C22-C23-C24
32	F	306	RRX	C36-C18-C19-C20
38	1	302	LUT	C7-C8-C9-C19
38	1	303	LUT	C7-C8-C9-C19
38	Z	302	LUT	C7-C8-C9-C19
38	7	301	LUT	C7-C8-C9-C19
38	7	302	LUT	C7-C8-C9-C19
38	8	302	LUT	C31-C32-C33-C40
38	4	803	LUT	C7-C8-C9-C19
25	A	849	LHG	O1-C1-C2-C3
25	B	803	LHG	O1-C1-C2-C3
25	B	850	LHG	O1-C1-C2-C3
25	B	851	LHG	O1-C1-C2-C3
25	Z	317	LHG	O1-C1-C2-C3
25	7	318	LHG	O1-C1-C2-C3
25	4	820	LHG	O1-C1-C2-C3
25	4	821	LHG	O1-C1-C2-C3
25	5	324	LHG	O1-C1-C2-C3
25	6	323	LHG	O1-C1-C2-C3
24	A	845	BCR	C17-C18-C19-C20
24	A	846	BCR	C17-C18-C19-C20
24	A	846	BCR	C21-C22-C23-C24
24	A	847	BCR	C7-C8-C9-C10
24	A	848	BCR	C11-C12-C13-C14
24	B	845	BCR	C17-C18-C19-C20
24	B	846	BCR	C7-C8-C9-C10
24	B	848	BCR	C17-C18-C19-C20
24	B	849	BCR	C7-C8-C9-C10
24	F	303	BCR	C7-C8-C9-C10
24	G	203	BCR	C17-C18-C19-C20
24	J	104	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	K	206	BCR	C11-C12-C13-C14
24	K	206	BCR	C17-C18-C19-C20
24	8	304	BCR	C7-C8-C9-C10
24	8	304	BCR	C17-C18-C19-C20
24	8	304	BCR	C21-C22-C23-C24
24	5	305	BCR	C11-C12-C13-C14
24	5	305	BCR	C21-C22-C23-C24
24	6	306	BCR	C21-C22-C23-C24
32	F	306	RRX	C21-C22-C23-C24
32	F	306	RRX	C17-C18-C19-C20
36	J	105	C7Z	C27-C28-C29-C30
38	1	303	LUT	C7-C8-C9-C10
38	7	301	LUT	C7-C8-C9-C10
38	4	803	LUT	C7-C8-C9-C10
22	A	827	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	3	318	CLA	C5-C6-C7-C8
25	4	821	LHG	C9-C10-C11-C12
22	3	322	CLA	O1D-CGD-O2D-CED
25	5	324	LHG	C28-C29-C30-C31
22	B	824	CLA	O1A-CGA-O2A-C1
22	5	323	CLA	C4B-C3B-CAB-CBB
22	6	310	CLA	C4B-C3B-CAB-CBB
22	A	836	CLA	C6-C7-C8-C9
22	A	836	CLA	C6-C7-C8-C10
22	6	311	CLA	C6-C7-C8-C9
22	9	307	CLA	C6-C7-C8-C9
22	9	307	CLA	C6-C7-C8-C10
22	B	809	CLA	C5-C6-C7-C8
39	8	315	CHL	C10-C11-C12-C13
25	Z	317	LHG	C26-C27-C28-C29
25	4	820	LHG	C29-C30-C31-C32
34	F	308	LMG	C29-C30-C31-C32
22	6	319	CLA	CBD-CGD-O2D-CED
25	B	803	LHG	C11-C10-C9-C8
25	8	317	LHG	C28-C29-C30-C31
25	4	820	LHG	C33-C34-C35-C36
27	A	852	DGA	CB7-CB8-CB9-CAB
25	8	317	LHG	C7-C8-C9-C10
22	A	805	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	1	304	CLA	C5-C6-C7-C8
23	B	843	PQN	C23-C25-C26-C27
31	3	301	DGD	O1A-C1A-O1G-C1G
25	9	315	LHG	C26-C27-C28-C29
27	A	852	DGA	CA4-CA5-CA6-CA7
22	A	818	CLA	CBA-CGA-O2A-C1
22	L	201	CLA	CBA-CGA-O2A-C1
22	L	202	CLA	CBA-CGA-O2A-C1
25	A	850	LHG	C24-C23-O8-C6
25	4	820	LHG	C34-C35-C36-C37
41	7	319	3PH	C22-C23-C24-C25
22	A	810	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	C3A-C2A-CAA-CBA
22	A	803	CLA	C3A-C2A-CAA-CBA
22	A	811	CLA	C3A-C2A-CAA-CBA
22	A	813	CLA	C3A-C2A-CAA-CBA
22	A	816	CLA	C3A-C2A-CAA-CBA
22	A	825	CLA	C3A-C2A-CAA-CBA
22	A	837	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	815	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	836	CLA	C3A-C2A-CAA-CBA
22	K	202	CLA	C3A-C2A-CAA-CBA
22	K	205	CLA	C3A-C2A-CAA-CBA
22	L	201	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C3A-C2A-CAA-CBA
22	1	315	CLA	C3A-C2A-CAA-CBA
22	Z	315	CLA	C3A-C2A-CAA-CBA
22	3	315	CLA	C3A-C2A-CAA-CBA
22	7	306	CLA	C3A-C2A-CAA-CBA
22	8	306	CLA	C3A-C2A-CAA-CBA
22	8	307	CLA	C3A-C2A-CAA-CBA
22	8	314	CLA	C3A-C2A-CAA-CBA
22	4	807	CLA	C3A-C2A-CAA-CBA
22	5	308	CLA	C3A-C2A-CAA-CBA
22	5	314	CLA	C3A-C2A-CAA-CBA
22	5	326	CLA	C3A-C2A-CAA-CBA
22	6	307	CLA	C3A-C2A-CAA-CBA
22	9	303	CLA	C3A-C2A-CAA-CBA
39	4	816	CHL	C3A-C2A-CAA-CBA
22	A	838	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	1	307	CLA	C5-C6-C7-C8
22	4	808	CLA	C5-C6-C7-C8
22	6	311	CLA	C5-C6-C7-C8
24	G	203	BCR	C9-C10-C11-C12
25	7	318	LHG	C11-C12-C13-C14
25	7	318	LHG	C28-C29-C30-C31
25	6	323	LHG	C9-C10-C11-C12
22	A	822	CLA	C6-C7-C8-C9
22	8	314	CLA	O1D-CGD-O2D-CED
25	4	821	LHG	C4-C5-C6-O8
22	6	313	CLA	O2A-C1-C2-C3
22	A	811	CLA	C3-C5-C6-C7
22	A	828	CLA	C4-C3-C5-C6
22	F	304	CLA	C4-C3-C5-C6
39	8	315	CHL	C4-C3-C5-C6
22	5	318	CLA	CBA-CGA-O2A-C1
22	A	828	CLA	C2-C3-C5-C6
22	F	304	CLA	C2-C3-C5-C6
25	B	803	LHG	O1-C1-C2-O2
25	B	850	LHG	O1-C1-C2-O2
25	8	317	LHG	O1-C1-C2-O2
25	4	821	LHG	O1-C1-C2-O2
25	6	323	LHG	C25-C26-C27-C28
25	6	323	LHG	C28-C29-C30-C31
28	A	853	OCA	C4-C5-C6-C7
25	B	850	LHG	C7-C8-C9-C10
26	A	851	NKP	CAP-CAQ-CAR-CAS
22	A	805	CLA	O1A-CGA-O2A-C1
22	Z	307	CLA	C6-C7-C8-C9
22	3	319	CLA	C6-C7-C8-C10
22	5	326	CLA	C6-C7-C8-C9
25	4	821	LHG	C11-C10-C9-C8
22	5	323	CLA	C2B-C3B-CAB-CBB
22	6	310	CLA	C2B-C3B-CAB-CBB
22	9	303	CLA	C2B-C3B-CAB-CBB
22	A	802	CLA	C5-C6-C7-C8
22	B	826	CLA	C5-C6-C7-C8
41	7	319	3PH	C27-C28-C29-C2A
22	A	813	CLA	C3-C5-C6-C7
22	A	840	CLA	C3-C5-C6-C7
22	5	307	CLA	C3-C5-C6-C7
25	5	324	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	A	852	DGA	CB5-CB6-CB7-CB8
33	4	822	LMT	C7-C8-C9-C10
22	B	841	CLA	O1A-CGA-O2A-C1
22	G	201	CLA	O1A-CGA-O2A-C1
25	4	820	LHG	O10-C23-O8-C6
25	4	821	LHG	O10-C23-O8-C6
22	B	801	CLA	C8-C10-C11-C12
22	B	814	CLA	C8-C10-C11-C12
22	B	827	CLA	C5-C6-C7-C8
22	6	302	CLA	C5-C6-C7-C8
22	A	805	CLA	C2-C1-O2A-CGA
22	A	820	CLA	C2-C1-O2A-CGA
22	A	822	CLA	C2-C1-O2A-CGA
22	B	808	CLA	C2-C1-O2A-CGA
22	B	820	CLA	C2-C1-O2A-CGA
22	B	823	CLA	C2-C1-O2A-CGA
22	B	829	CLA	C2-C1-O2A-CGA
22	F	301	CLA	C2-C1-O2A-CGA
22	F	304	CLA	C2-C1-O2A-CGA
22	G	201	CLA	C2-C1-O2A-CGA
22	K	205	CLA	C2-C1-O2A-CGA
22	1	313	CLA	C2-C1-O2A-CGA
22	Z	313	CLA	C2-C1-O2A-CGA
22	Z	314	CLA	C2-C1-O2A-CGA
22	3	314	CLA	C2-C1-O2A-CGA
22	7	307	CLA	C2-C1-O2A-CGA
22	6	319	CLA	C2-C1-O2A-CGA
22	6	322	CLA	C2-C1-O2A-CGA
22	9	303	CLA	C2-C1-O2A-CGA
22	A	815	CLA	C5-C6-C7-C8
22	A	820	CLA	C8-C10-C11-C12
22	5	301	CLA	C5-C6-C7-C8
22	A	818	CLA	O1A-CGA-O2A-C1
25	B	803	LHG	O10-C23-O8-C6
25	9	315	LHG	O10-C23-O8-C6
25	1	317	LHG	C9-C10-C11-C12
25	Z	317	LHG	C28-C29-C30-C31
22	B	831	CLA	C3-C5-C6-C7
22	3	311	CLA	C3-C5-C6-C7
24	A	844	BCR	C1-C6-C7-C8
24	A	844	BCR	C23-C24-C25-C26
24	A	845	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	845	BCR	C23-C24-C25-C26
24	A	846	BCR	C5-C6-C7-C8
24	A	846	BCR	C23-C24-C25-C26
24	A	847	BCR	C5-C6-C7-C8
24	A	847	BCR	C23-C24-C25-C30
24	A	848	BCR	C23-C24-C25-C30
24	A	856	BCR	C5-C6-C7-C8
24	A	856	BCR	C23-C24-C25-C26
24	B	845	BCR	C1-C6-C7-C8
24	B	845	BCR	C5-C6-C7-C8
24	B	845	BCR	C23-C24-C25-C30
24	B	846	BCR	C1-C6-C7-C8
24	B	846	BCR	C23-C24-C25-C26
24	B	847	BCR	C23-C24-C25-C26
24	B	848	BCR	C23-C24-C25-C26
24	B	853	BCR	C23-C24-C25-C26
24	B	853	BCR	C23-C24-C25-C30
24	F	303	BCR	C5-C6-C7-C8
24	F	303	BCR	C23-C24-C25-C26
24	G	203	BCR	C1-C6-C7-C8
24	G	203	BCR	C23-C24-C25-C30
24	J	104	BCR	C1-C6-C7-C8
24	J	104	BCR	C23-C24-C25-C26
24	J	104	BCR	C23-C24-C25-C30
24	L	204	BCR	C5-C6-C7-C8
24	3	304	BCR	C5-C6-C7-C8
24	3	305	BCR	C23-C24-C25-C26
24	3	306	BCR	C1-C6-C7-C8
24	7	303	BCR	C1-C6-C7-C8
24	7	303	BCR	C23-C24-C25-C30
24	4	804	BCR	C23-C24-C25-C30
24	5	304	BCR	C23-C24-C25-C30
24	5	305	BCR	C1-C6-C7-C8
24	6	306	BCR	C23-C24-C25-C30
36	5	306	C7Z	C1-C6-C7-C8
36	5	306	C7Z	C21-C26-C27-C28
38	7	301	LUT	C5-C6-C7-C8
38	8	303	LUT	C5-C6-C7-C8
38	4	802	LUT	C1-C6-C7-C8
22	B	829	CLA	C8-C10-C11-C12
31	B	852	DGD	C3A-C4A-C5A-C6A
41	7	319	3PH	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
41	7	319	3PH	C25-C26-C27-C28
22	B	825	CLA	CBA-CGA-O2A-C1
22	B	835	CLA	CBA-CGA-O2A-C1
22	7	305	CLA	CBA-CGA-O2A-C1
39	3	317	CHL	CBA-CGA-O2A-C1
33	4	822	LMT	C1-C2-C3-C4
22	L	202	CLA	O1A-CGA-O2A-C1
41	6	324	3PH	C27-C28-C29-C2A
22	1	313	CLA	C8-C10-C11-C12
22	7	317	CLA	C5-C6-C7-C8
22	5	307	CLA	C8-C10-C11-C12
33	4	822	LMT	C3-C4-C5-C6
22	9	305	CLA	C4-C3-C5-C6
39	9	312	CHL	C4-C3-C5-C6
22	A	805	CLA	C11-C12-C13-C15
22	A	810	CLA	C11-C12-C13-C15
22	A	811	CLA	C11-C10-C8-C7
22	A	819	CLA	C6-C7-C8-C10
22	A	823	CLA	C11-C10-C8-C7
22	A	823	CLA	C11-C12-C13-C15
22	A	829	CLA	C11-C12-C13-C15
22	A	833	CLA	C6-C7-C8-C10
22	A	838	CLA	C6-C7-C8-C10
22	A	838	CLA	C11-C10-C8-C7
22	A	840	CLA	C6-C7-C8-C10
22	B	801	CLA	C12-C13-C15-C16
22	B	809	CLA	C11-C10-C8-C7
22	B	811	CLA	C6-C7-C8-C10
22	B	814	CLA	C6-C7-C8-C10
22	B	815	CLA	C2-C3-C5-C6
22	B	817	CLA	C6-C7-C8-C10
22	B	818	CLA	C6-C7-C8-C10
22	B	818	CLA	C11-C12-C13-C15
22	B	822	CLA	C6-C7-C8-C10
22	B	827	CLA	C6-C7-C8-C10
22	B	831	CLA	C6-C7-C8-C10
22	L	202	CLA	C11-C12-C13-C15
22	L	202	CLA	C12-C13-C15-C16
22	1	306	CLA	C11-C12-C13-C15
22	1	316	CLA	C12-C13-C15-C16
22	Z	305	CLA	C6-C7-C8-C10
22	Z	316	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	3	312	CLA	C11-C10-C8-C7
22	3	322	CLA	C11-C10-C8-C7
22	3	322	CLA	C11-C12-C13-C15
22	7	307	CLA	C11-C10-C8-C7
22	7	312	CLA	C11-C10-C8-C7
22	7	323	CLA	C6-C7-C8-C10
22	8	307	CLA	C11-C12-C13-C15
22	5	308	CLA	C6-C7-C8-C10
22	5	313	CLA	C11-C10-C8-C7
22	6	314	CLA	C6-C7-C8-C10
22	6	322	CLA	C11-C10-C8-C7
23	B	843	PQN	C17-C18-C20-C21
39	3	317	CHL	C2-C3-C5-C6
39	8	315	CHL	C2-C3-C5-C6
39	9	312	CHL	C11-C12-C13-C15
42	7	320	SPH	C4-C5-C6-C7
22	B	809	CLA	C3-C5-C6-C7
22	B	820	CLA	C3-C5-C6-C7
22	A	811	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1A-CGA-O2A-C1
22	L	201	CLA	O1A-CGA-O2A-C1
22	5	318	CLA	O1A-CGA-O2A-C1
25	A	850	LHG	O10-C23-O8-C6
22	Z	313	CLA	C8-C10-C11-C12
24	B	847	BCR	C15-C16-C17-C18
24	G	203	BCR	C15-C16-C17-C18
24	3	306	BCR	C15-C16-C17-C18
24	5	305	BCR	C15-C16-C17-C18
32	F	306	RRX	C19-C20-C21-C22
22	B	842	CLA	C16-C17-C18-C20
22	K	205	CLA	C6-C7-C8-C9
22	7	322	CLA	C6-C7-C8-C10
22	5	319	CLA	C6-C7-C8-C9
42	7	320	SPH	C5-C6-C7-C8
31	1	319	DGD	C1B-C2B-C3B-C4B
22	8	306	CLA	CBA-CGA-O2A-C1
25	Z	317	LHG	C24-C23-O8-C6
35	J	102	T7X	C31-C11-O18-C9
22	A	826	CLA	C2A-CAA-CBA-CGA
22	B	815	CLA	C2A-CAA-CBA-CGA
22	B	831	CLA	C2A-CAA-CBA-CGA
22	Z	307	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	3	318	CLA	C2A-CAA-CBA-CGA
22	4	815	CLA	C2A-CAA-CBA-CGA
22	1	310	CLA	O1D-CGD-O2D-CED
22	7	323	CLA	O1D-CGD-O2D-CED
25	7	318	LHG	C9-C10-C11-C12
22	5	313	CLA	O1D-CGD-O2D-CED
25	A	850	LHG	C34-C35-C36-C37
25	Z	317	LHG	C9-C10-C11-C12
34	F	308	LMG	C12-C13-C14-C15
22	A	840	CLA	O1D-CGD-O2D-CED
22	1	307	CLA	C8-C10-C11-C12
22	Z	305	CLA	C3-C5-C6-C7
22	A	806	CLA	O1D-CGD-O2D-CED
22	B	826	CLA	CBA-CGA-O2A-C1
22	6	302	CLA	CBA-CGA-O2A-C1
22	Z	309	CLA	C11-C12-C13-C15
22	A	834	CLA	C5-C6-C7-C8
22	6	309	CLA	C5-C6-C7-C8
25	A	850	LHG	C28-C29-C30-C31
27	A	852	DGA	CB3-CB4-CB5-CB6
33	F	307	LMT	C2-C3-C4-C5
42	7	321	SPH	C10-C11-C12-C13
25	A	849	LHG	C7-C8-C9-C10
25	6	323	LHG	C8-C7-O7-C5
41	8	320	3PH	C22-C21-O21-C2
25	6	323	LHG	C29-C30-C31-C32
25	4	820	LHG	C30-C31-C32-C33
41	8	320	3PH	O22-C21-O21-C2
22	A	824	CLA	C3-C5-C6-C7
22	Z	309	CLA	C3-C5-C6-C7
22	A	806	CLA	C5-C6-C7-C8
25	A	850	LHG	O7-C5-C6-O8
25	4	821	LHG	O7-C5-C6-O8
25	5	324	LHG	O7-C5-C6-O8
25	6	323	LHG	C12-C13-C14-C15
25	9	315	LHG	C9-C10-C11-C12
22	B	823	CLA	C6-C7-C8-C10
22	5	311	CLA	C6-C7-C8-C10
35	J	102	T7X	C25-C26-C27-C28
22	B	815	CLA	C4-C3-C5-C6
39	3	317	CHL	C4-C3-C5-C6
39	6	318	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	805	CLA	C6-C7-C8-C9
22	A	810	CLA	C6-C7-C8-C9
22	A	819	CLA	C6-C7-C8-C9
22	A	824	CLA	C6-C7-C8-C9
22	A	833	CLA	C6-C7-C8-C9
22	A	855	CLA	C6-C7-C8-C9
22	B	810	CLA	C6-C7-C8-C9
22	B	811	CLA	C6-C7-C8-C9
22	B	822	CLA	C6-C7-C8-C9
22	B	824	CLA	C6-C7-C8-C9
22	B	827	CLA	C6-C7-C8-C9
22	B	831	CLA	C6-C7-C8-C9
22	B	834	CLA	C6-C7-C8-C9
22	B	838	CLA	C6-C7-C8-C9
22	F	302	CLA	C6-C7-C8-C9
22	L	202	CLA	C14-C13-C15-C16
22	1	314	CLA	C6-C7-C8-C9
22	Z	305	CLA	C6-C7-C8-C9
22	Z	306	CLA	C6-C7-C8-C9
22	7	323	CLA	C11-C12-C13-C14
22	8	309	CLA	C6-C7-C8-C9
22	6	314	CLA	C6-C7-C8-C9
22	6	314	CLA	C11-C12-C13-C14
22	6	322	CLA	C6-C7-C8-C9
22	9	306	CLA	C11-C10-C8-C9
23	B	843	PQN	C21-C22-C23-C24
39	9	312	CHL	C14-C13-C15-C16
41	6	324	3PH	C24-C25-C26-C27
22	A	819	CLA	C3-C5-C6-C7
22	B	817	CLA	C3-C5-C6-C7
22	F	304	CLA	C3-C5-C6-C7
22	Z	308	CLA	C3-C5-C6-C7
22	4	807	CLA	C3-C5-C6-C7
22	A	808	CLA	C2A-CAA-CBA-CGA
22	A	842	CLA	C2A-CAA-CBA-CGA
22	B	830	CLA	C2A-CAA-CBA-CGA
22	B	840	CLA	C2A-CAA-CBA-CGA
22	7	312	CLA	C2A-CAA-CBA-CGA
22	6	314	CLA	C2A-CAA-CBA-CGA
33	G	204	LMT	O5B-C5B-C6B-O6B
24	B	844	BCR	C37-C22-C23-C24
24	B	847	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
36	J	105	C7Z	C27-C28-C29-C39
38	Z	301	LUT	C7-C8-C9-C19
22	A	837	CLA	O1D-CGD-O2D-CED
22	A	808	CLA	C8-C10-C11-C12
22	F	301	CLA	C8-C10-C11-C12
22	5	307	CLA	C5-C6-C7-C8
25	7	318	LHG	C29-C30-C31-C32
24	B	853	BCR	C17-C18-C19-C20
38	Z	301	LUT	C7-C8-C9-C10
38	6	303	LUT	C31-C32-C33-C34
22	B	835	CLA	O1A-CGA-O2A-C1
22	7	305	CLA	O1A-CGA-O2A-C1
35	J	102	T7X	O19-C11-O18-C9
39	3	317	CHL	O1A-CGA-O2A-C1
22	B	839	CLA	O1D-CGD-O2D-CED
21	A	801	CL0	C1A-C2A-CAA-CBA
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	808	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	814	CLA	C1A-C2A-CAA-CBA
22	A	815	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C1A-C2A-CAA-CBA
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	837	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	813	CLA	C1A-C2A-CAA-CBA
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	817	CLA	C1A-C2A-CAA-CBA
22	B	820	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	825	CLA	C1A-C2A-CAA-CBA
22	B	826	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	C1A-C2A-CAA-CBA
22	B	832	CLA	C1A-C2A-CAA-CBA
22	B	834	CLA	C1A-C2A-CAA-CBA
22	B	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	839	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C1A-C2A-CAA-CBA
22	B	841	CLA	C1A-C2A-CAA-CBA
22	B	842	CLA	C1A-C2A-CAA-CBA
22	F	302	CLA	C1A-C2A-CAA-CBA
22	K	202	CLA	C1A-C2A-CAA-CBA
22	K	203	CLA	C1A-C2A-CAA-CBA
22	K	205	CLA	C1A-C2A-CAA-CBA
22	L	203	CLA	C1A-C2A-CAA-CBA
22	1	314	CLA	C1A-C2A-CAA-CBA
22	Z	303	CLA	C1A-C2A-CAA-CBA
22	Z	306	CLA	C1A-C2A-CAA-CBA
22	Z	313	CLA	C1A-C2A-CAA-CBA
22	Z	315	CLA	C1A-C2A-CAA-CBA
22	3	311	CLA	C1A-C2A-CAA-CBA
22	3	313	CLA	C1A-C2A-CAA-CBA
22	3	318	CLA	C1A-C2A-CAA-CBA
22	3	322	CLA	C1A-C2A-CAA-CBA
22	7	304	CLA	C1A-C2A-CAA-CBA
22	7	307	CLA	C1A-C2A-CAA-CBA
22	7	312	CLA	C1A-C2A-CAA-CBA
22	7	322	CLA	C1A-C2A-CAA-CBA
22	7	324	CLA	C1A-C2A-CAA-CBA
22	8	306	CLA	C1A-C2A-CAA-CBA
22	8	308	CLA	C1A-C2A-CAA-CBA
22	8	310	CLA	C1A-C2A-CAA-CBA
22	8	313	CLA	C1A-C2A-CAA-CBA
22	4	808	CLA	C1A-C2A-CAA-CBA
22	4	811	CLA	C1A-C2A-CAA-CBA
22	4	815	CLA	C1A-C2A-CAA-CBA
22	5	310	CLA	C1A-C2A-CAA-CBA
22	5	311	CLA	C1A-C2A-CAA-CBA
22	5	313	CLA	C1A-C2A-CAA-CBA
22	5	318	CLA	C1A-C2A-CAA-CBA
22	6	312	CLA	C1A-C2A-CAA-CBA
22	6	314	CLA	C1A-C2A-CAA-CBA
22	6	317	CLA	C1A-C2A-CAA-CBA
22	6	319	CLA	C1A-C2A-CAA-CBA
22	9	308	CLA	C1A-C2A-CAA-CBA
22	9	313	CLA	C1A-C2A-CAA-CBA
22	2	301	CLA	C1A-C2A-CAA-CBA
39	8	315	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
39	4	816	CHL	C1A-C2A-CAA-CBA
22	A	822	CLA	C6-C7-C8-C10
22	B	812	CLA	C6-C7-C8-C10
22	5	319	CLA	C6-C7-C8-C10
22	5	326	CLA	C6-C7-C8-C10
22	2	301	CLA	C6-C7-C8-C10
25	6	323	LHG	O9-C7-O7-C5
25	A	850	LHG	C33-C34-C35-C36
25	4	821	LHG	C10-C11-C12-C13
24	A	846	BCR	C19-C20-C21-C22
24	B	846	BCR	C13-C14-C15-C16
36	5	306	C7Z	C13-C14-C15-C35
38	7	301	LUT	C9-C10-C11-C12
22	3	310	CLA	C5-C6-C7-C8
22	8	310	CLA	C8-C10-C11-C12
25	Z	317	LHG	C4-O6-P-O3
22	3	318	CLA	C3-C5-C6-C7
25	B	851	LHG	C2-C3-O3-P
22	A	835	CLA	C5-C6-C7-C8
22	1	316	CLA	C15-C16-C17-C18
22	B	811	CLA	CBA-CGA-O2A-C1
25	A	850	LHG	O6-C4-C5-C6
25	8	317	LHG	O6-C4-C5-C6
25	5	324	LHG	O6-C4-C5-C6
31	1	319	DGD	O6E-C5E-C6E-O5E
22	A	805	CLA	C15-C16-C17-C18
22	1	308	CLA	C6-C7-C8-C9
22	Z	309	CLA	C11-C12-C13-C14
22	5	308	CLA	C3-C5-C6-C7
22	B	828	CLA	C13-C15-C16-C17
22	B	834	CLA	C8-C10-C11-C12
41	8	320	3PH	C35-C36-C37-C38
22	6	307	CLA	CBA-CGA-O2A-C1
25	1	317	LHG	C1-C2-C3-O3
33	F	307	LMT	O5'-C5'-C6'-O6'
22	A	814	CLA	C4-C3-C5-C6
39	6	315	CHL	C4-C3-C5-C6
22	7	316	CLA	C3A-C2A-CAA-CBA
22	A	812	CLA	C8-C10-C11-C12
22	A	829	CLA	C8-C10-C11-C12
22	B	842	CLA	C5-C6-C7-C8
22	Z	309	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	8	306	CLA	O1A-CGA-O2A-C1
22	1	316	CLA	C3-C5-C6-C7
22	5	311	CLA	C3-C5-C6-C7
25	3	321	LHG	C4-C5-C6-O8
25	7	318	LHG	C4-C5-C6-O8
25	5	324	LHG	C13-C14-C15-C16
25	6	323	LHG	C4-C5-C6-O8
31	B	852	DGD	O1G-C1G-C2G-C3G
41	7	319	3PH	C3C-C3D-C3E-C3F
41	7	319	3PH	C3A-C3B-C3C-C3D
22	B	811	CLA	O1A-CGA-O2A-C1
31	B	852	DGD	C5D-C6D-O5D-C1E
31	3	301	DGD	C2G-C3G-O3G-C1D
22	B	817	CLA	C8-C10-C11-C12
22	Z	306	CLA	C8-C10-C11-C12
39	3	317	CHL	C8-C10-C11-C12
34	F	308	LMG	C15-C16-C17-C18
41	6	324	3PH	C21-C22-C23-C24
25	Z	317	LHG	O10-C23-O8-C6
25	7	318	LHG	C26-C27-C28-C29
21	A	801	CL0	CBA-CGA-O2A-C1
25	8	317	LHG	C24-C23-O8-C6
33	1	301	LMT	O5'-C5'-C6'-O6'
33	4	801	LMT	O5'-C5'-C6'-O6'
25	A	850	LHG	O1-C1-C2-O2
25	4	821	LHG	C23-C24-C25-C26
33	F	307	LMT	O5B-C5B-C6B-O6B
22	B	822	CLA	C5-C6-C7-C8
22	7	310	CLA	C8-C10-C11-C12
22	8	309	CLA	C10-C11-C12-C13
22	A	822	CLA	C4-C3-C5-C6
22	B	842	CLA	C4-C3-C5-C6
25	B	803	LHG	C9-C10-C11-C12
41	7	319	3PH	C39-C3A-C3B-C3C
22	6	302	CLA	O1A-CGA-O2A-C1
22	B	842	CLA	C16-C17-C18-C19
22	A	820	CLA	CBA-CGA-O2A-C1
22	9	305	CLA	CBA-CGA-O2A-C1
41	5	325	3PH	C22-C23-C24-C25
22	B	805	CLA	C8-C10-C11-C12
22	B	823	CLA	C5-C6-C7-C8
22	7	310	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
42	7	321	SPH	C2-C3-C4-C5
25	4	820	LHG	C31-C32-C33-C34
22	A	821	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C2A-CAA-CBA-CGA
22	B	824	CLA	C2A-CAA-CBA-CGA
22	3	314	CLA	C2A-CAA-CBA-CGA
22	A	838	CLA	C5-C6-C7-C8
22	Z	303	CLA	C8-C10-C11-C12
22	A	811	CLA	C2-C1-O2A-CGA
22	Z	316	CLA	C2-C1-O2A-CGA
22	7	315	CLA	C2-C1-O2A-CGA
22	4	808	CLA	C2-C1-O2A-CGA
22	5	301	CLA	C2-C1-O2A-CGA
22	9	307	CLA	C2-C1-O2A-CGA
22	9	313	CLA	C2-C1-O2A-CGA
33	4	822	LMT	O5B-C5B-C6B-O6B
22	7	307	CLA	O1D-CGD-O2D-CED
42	7	321	SPH	C4-C5-C6-C7
22	5	323	CLA	O1A-CGA-O2A-C1
22	A	854	CLA	C5-C6-C7-C8
22	Z	316	CLA	C5-C6-C7-C8
22	4	805	CLA	C5-C6-C7-C8
22	5	313	CLA	C10-C11-C12-C13
25	B	803	LHG	C10-C11-C12-C13
25	8	317	LHG	C13-C14-C15-C16
28	A	853	OCA	C5-C6-C7-C8
22	A	817	CLA	CBA-CGA-O2A-C1
22	1	313	CLA	CBA-CGA-O2A-C1
22	3	313	CLA	CBA-CGA-O2A-C1
35	J	102	T7X	O13-C7-C8-O16
27	A	852	DGA	CA1-CA2-CA3-CA4
25	B	803	LHG	C11-C12-C13-C14
22	B	813	CLA	C5-C6-C7-C8
22	B	818	CLA	C8-C10-C11-C12
22	K	205	CLA	C5-C6-C7-C8
22	7	317	CLA	C8-C10-C11-C12
22	A	839	CLA	O1D-CGD-O2D-CED
22	B	826	CLA	O1A-CGA-O2A-C1
34	J	101	LMG	C2-C1-O1-C7
25	4	820	LHG	O8-C23-C24-C25
25	7	318	LHG	O7-C5-C6-O8
25	8	317	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	1	317	LHG	C31-C32-C33-C34
22	A	823	CLA	C8-C10-C11-C12
21	A	801	CL0	O1A-CGA-O2A-C1
22	1	313	CLA	O1A-CGA-O2A-C1
21	A	801	CL0	C6-C7-C8-C10
22	A	805	CLA	C6-C7-C8-C10
22	A	807	CLA	C11-C10-C8-C7
22	A	813	CLA	C6-C7-C8-C10
22	A	815	CLA	C11-C12-C13-C15
22	A	817	CLA	C11-C10-C8-C7
22	A	818	CLA	C11-C10-C8-C7
22	A	821	CLA	C6-C7-C8-C10
22	A	828	CLA	C11-C12-C13-C15
22	A	830	CLA	C11-C12-C13-C15
22	A	832	CLA	C11-C10-C8-C7
22	A	855	CLA	C6-C7-C8-C10
22	A	855	CLA	C11-C12-C13-C15
22	B	801	CLA	C11-C10-C8-C7
22	B	805	CLA	C6-C7-C8-C10
22	B	808	CLA	C6-C7-C8-C10
22	B	811	CLA	C11-C10-C8-C7
22	B	820	CLA	C11-C10-C8-C7
22	B	821	CLA	C6-C7-C8-C10
22	B	821	CLA	C11-C12-C13-C15
22	B	824	CLA	C6-C7-C8-C10
22	B	824	CLA	C11-C10-C8-C7
22	B	825	CLA	C6-C7-C8-C10
22	B	838	CLA	C12-C13-C15-C16
22	B	842	CLA	C6-C7-C8-C10
22	F	301	CLA	C6-C7-C8-C10
22	F	302	CLA	C6-C7-C8-C10
22	F	304	CLA	C11-C12-C13-C15
22	L	201	CLA	C11-C10-C8-C7
22	1	306	CLA	C6-C7-C8-C10
22	1	310	CLA	C11-C10-C8-C7
22	1	314	CLA	C6-C7-C8-C10
22	1	314	CLA	C11-C10-C8-C7
22	1	314	CLA	C12-C13-C15-C16
22	1	316	CLA	C11-C10-C8-C7
22	Z	306	CLA	C6-C7-C8-C10
22	Z	308	CLA	C6-C7-C8-C10
22	Z	316	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	Z	316	CLA	C11-C12-C13-C15
22	3	308	CLA	C6-C7-C8-C10
22	3	313	CLA	C11-C12-C13-C15
22	3	314	CLA	C11-C10-C8-C7
22	7	304	CLA	C11-C10-C8-C7
22	7	307	CLA	C6-C7-C8-C10
22	7	307	CLA	C11-C12-C13-C15
22	7	324	CLA	C11-C10-C8-C7
22	8	305	CLA	C6-C7-C8-C10
22	8	307	CLA	C6-C7-C8-C10
22	8	309	CLA	C6-C7-C8-C10
22	8	309	CLA	C11-C12-C13-C15
22	4	805	CLA	C11-C10-C8-C7
22	4	807	CLA	C11-C10-C8-C7
22	5	301	CLA	C6-C7-C8-C10
22	5	309	CLA	C6-C7-C8-C10
22	5	310	CLA	C11-C10-C8-C7
22	5	315	CLA	C6-C7-C8-C10
22	5	318	CLA	C6-C7-C8-C10
22	5	322	CLA	C11-C10-C8-C7
22	6	314	CLA	C11-C12-C13-C15
22	9	306	CLA	C6-C7-C8-C10
23	A	843	PQN	C17-C18-C20-C21
23	B	843	PQN	C21-C22-C23-C25
39	3	317	CHL	C11-C10-C8-C7
22	A	806	CLA	C3-C5-C6-C7
21	A	801	CL0	C6-C7-C8-C9
22	A	805	CLA	C11-C10-C8-C9
22	A	811	CLA	C6-C7-C8-C9
22	A	813	CLA	C6-C7-C8-C9
22	A	820	CLA	C11-C10-C8-C9
22	A	827	CLA	C6-C7-C8-C9
22	A	828	CLA	C6-C7-C8-C9
22	A	832	CLA	C11-C10-C8-C9
22	A	838	CLA	C6-C7-C8-C9
22	A	841	CLA	C6-C7-C8-C9
22	A	855	CLA	C11-C10-C8-C9
22	B	801	CLA	C11-C10-C8-C9
22	B	805	CLA	C6-C7-C8-C9
22	B	808	CLA	C6-C7-C8-C9
22	B	821	CLA	C6-C7-C8-C9
22	B	828	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	828	CLA	C11-C12-C13-C14
22	B	838	CLA	C14-C13-C15-C16
22	B	841	CLA	C6-C7-C8-C9
22	B	842	CLA	C6-C7-C8-C9
22	F	301	CLA	C6-C7-C8-C9
22	F	302	CLA	C11-C12-C13-C14
22	L	201	CLA	C11-C10-C8-C9
22	1	314	CLA	C11-C10-C8-C9
22	Z	308	CLA	C6-C7-C8-C9
22	Z	316	CLA	C6-C7-C8-C9
22	3	308	CLA	C6-C7-C8-C9
22	3	314	CLA	C6-C7-C8-C9
22	7	306	CLA	C6-C7-C8-C9
22	7	307	CLA	C6-C7-C8-C9
22	7	308	CLA	C6-C7-C8-C9
22	7	312	CLA	C6-C7-C8-C9
22	7	323	CLA	C6-C7-C8-C9
22	8	305	CLA	C6-C7-C8-C9
22	8	307	CLA	C6-C7-C8-C9
22	8	309	CLA	C11-C12-C13-C14
22	8	310	CLA	C11-C10-C8-C9
22	4	805	CLA	C11-C10-C8-C9
22	4	807	CLA	C11-C10-C8-C9
22	5	301	CLA	C6-C7-C8-C9
22	5	307	CLA	C6-C7-C8-C9
22	5	308	CLA	C6-C7-C8-C9
22	5	309	CLA	C6-C7-C8-C9
22	6	301	CLA	C6-C7-C8-C9
22	6	302	CLA	C6-C7-C8-C9
22	6	310	CLA	C6-C7-C8-C9
22	6	319	CLA	C6-C7-C8-C9
22	9	306	CLA	C6-C7-C8-C9
23	A	843	PQN	C19-C18-C20-C21
39	8	315	CHL	C11-C10-C8-C9
39	9	312	CHL	C11-C12-C13-C14
22	1	314	CLA	C2A-CAA-CBA-CGA
22	3	308	CLA	C2A-CAA-CBA-CGA
22	7	324	CLA	C2A-CAA-CBA-CGA
39	8	312	CHL	C2A-CAA-CBA-CGA
27	A	852	DGA	CA8-CA9-CAA-CBA
25	8	317	LHG	O10-C23-O8-C6
24	G	203	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
24	7	303	BCR	C37-C22-C23-C24
24	4	804	BCR	C37-C22-C23-C24
24	5	304	BCR	C37-C22-C23-C24
24	5	305	BCR	C7-C8-C9-C34
38	Z	301	LUT	C27-C28-C29-C39
22	L	202	CLA	C5-C6-C7-C8
22	K	203	CLA	C6-C7-C8-C9
24	B	847	BCR	C7-C8-C9-C10
24	7	303	BCR	C21-C22-C23-C24
24	4	804	BCR	C21-C22-C23-C24
24	5	305	BCR	C7-C8-C9-C10
22	B	826	CLA	C8-C10-C11-C12
22	9	305	CLA	O1A-CGA-O2A-C1
22	A	813	CLA	CBA-CGA-O2A-C1
22	3	314	CLA	CBA-CGA-O2A-C1
22	7	310	CLA	C15-C16-C17-C18
25	6	323	LHG	C19-C20-C21-C22
22	A	817	CLA	O1A-CGA-O2A-C1
22	6	307	CLA	O1A-CGA-O2A-C1
22	L	202	CLA	CBD-CGD-O2D-CED
25	4	820	LHG	C15-C16-C17-C18
22	Z	315	CLA	C4B-C3B-CAB-CBB
22	4	805	CLA	C4B-C3B-CAB-CBB
22	4	812	CLA	C4B-C3B-CAB-CBB
22	4	818	CLA	C4B-C3B-CAB-CBB
22	9	303	CLA	C4B-C3B-CAB-CBB
25	Z	317	LHG	O6-C4-C5-C6
25	7	318	LHG	O6-C4-C5-C6
41	6	324	3PH	O11-C1-C2-C3
22	7	308	CLA	C3-C5-C6-C7
22	B	842	CLA	CBA-CGA-O2A-C1
21	A	801	CL0	C5-C6-C7-C8
22	A	830	CLA	C5-C6-C7-C8
22	5	308	CLA	C8-C10-C11-C12
22	5	301	CLA	C11-C10-C8-C9
25	6	323	LHG	C35-C36-C37-C38
22	L	201	CLA	C3-C5-C6-C7
41	6	324	3PH	C25-C26-C27-C28
25	1	317	LHG	C24-C23-O8-C6
25	8	317	LHG	C9-C10-C11-C12
26	8	318	NKP	CAH-CAG-OAF-PAC
21	A	801	CL0	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	809	CLA	C3A-C2A-CAA-CBA
22	B	824	CLA	C3A-C2A-CAA-CBA
22	B	826	CLA	C3A-C2A-CAA-CBA
22	Z	310	CLA	C3A-C2A-CAA-CBA
39	Z	311	CHL	C3A-C2A-CAA-CBA
39	8	315	CHL	C3A-C2A-CAA-CBA
31	3	301	DGD	C3A-C4A-C5A-C6A
24	K	206	BCR	C13-C14-C15-C16
24	8	304	BCR	C9-C10-C11-C12
22	4	807	CLA	C5-C6-C7-C8
22	1	308	CLA	C6-C7-C8-C10
22	A	854	CLA	C8-C10-C11-C12
25	A	850	LHG	C4-C5-C6-O8
25	B	851	LHG	C4-C5-C6-O8
25	1	317	LHG	C4-C5-C6-O8
25	Z	317	LHG	C4-C5-C6-O8
25	5	324	LHG	C4-C5-C6-O8
31	3	301	DGD	O1G-C1G-C2G-C3G
34	F	308	LMG	C7-C8-C9-O8
40	1	318	SQD	C44-C45-C46-O48
22	A	820	CLA	O1A-CGA-O2A-C1
25	A	849	LHG	C16-C17-C18-C19
25	Z	317	LHG	C31-C32-C33-C34
22	A	829	CLA	O2A-C1-C2-C3
22	L	202	CLA	O2A-C1-C2-C3
23	A	843	PQN	C13-C15-C16-C17
25	4	821	LHG	C7-C8-C9-C10
22	3	308	CLA	C8-C10-C11-C12
22	8	308	CLA	C8-C10-C11-C12
26	A	851	NKP	OBC-CAH-CAI-OAJ
22	K	203	CLA	C6-C7-C8-C10
22	4	812	CLA	C6-C7-C8-C9
22	9	305	CLA	C2-C3-C5-C6
22	B	824	CLA	C11-C12-C13-C14
39	3	317	CHL	CBD-CGD-O2D-CED
35	J	102	T7X	C7-O13-P1-O1
35	J	102	T7X	C18-C19-C20-C21
35	J	102	T7X	C22-C23-C24-C25
22	6	309	CLA	CAA-CBA-CGA-O2A
22	A	816	CLA	C2A-CAA-CBA-CGA
22	B	835	CLA	C2A-CAA-CBA-CGA
39	7	313	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	830	CLA	C8-C10-C11-C12
22	2	301	CLA	C5-C6-C7-C8
39	8	315	CHL	C8-C10-C11-C12
25	A	850	LHG	O6-C4-C5-O7
25	B	850	LHG	O6-C4-C5-O7
25	Z	317	LHG	O6-C4-C5-O7
25	8	317	LHG	O6-C4-C5-O7
39	Z	312	CHL	CBA-CGA-O2A-C1
25	6	323	LHG	C11-C12-C13-C14
31	1	319	DGD	C1A-C2A-C3A-C4A
22	4	811	CLA	C6-C7-C8-C9
23	A	843	PQN	C26-C27-C28-C30
22	1	314	CLA	C8-C10-C11-C12
22	3	314	CLA	O1A-CGA-O2A-C1
22	A	822	CLA	C3-C5-C6-C7
25	A	849	LHG	O7-C5-C6-O8
25	6	323	LHG	O7-C5-C6-O8
31	1	319	DGD	O2G-C2G-C3G-O3G
40	1	318	SQD	O6-C44-C45-O47
40	1	318	SQD	O47-C45-C46-O48
24	3	306	BCR	C9-C10-C11-C12
22	A	809	CLA	C6-C7-C8-C9
22	1	310	CLA	C11-C12-C13-C15
22	Z	308	CLA	C8-C10-C11-C12
25	3	321	LHG	C1-C2-C3-O3
25	9	315	LHG	C1-C2-C3-O3
25	9	315	LHG	C24-C25-C26-C27
22	B	801	CLA	C2-C1-O2A-CGA
22	5	315	CLA	C2-C1-O2A-CGA
22	6	301	CLA	C2-C1-O2A-CGA
22	A	813	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	C8-C10-C11-C12
22	B	821	CLA	C8-C10-C11-C12
22	B	805	CLA	C11-C12-C13-C14
22	B	816	CLA	C6-C7-C8-C9
22	B	840	CLA	C6-C7-C8-C9
22	L	201	CLA	C6-C7-C8-C9
22	L	202	CLA	C11-C10-C8-C9
22	1	316	CLA	C11-C12-C13-C14
22	Z	309	CLA	C6-C7-C8-C9
22	4	808	CLA	C6-C7-C8-C9
22	6	312	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	Z	317	LHG	C25-C26-C27-C28
25	7	318	LHG	C5-C4-O6-P
25	5	324	LHG	C5-C4-O6-P
35	J	102	T7X	C8-C7-O13-P1
22	3	313	CLA	O1A-CGA-O2A-C1
25	4	820	LHG	C13-C14-C15-C16
22	A	820	CLA	C11-C12-C13-C15
22	Z	307	CLA	C6-C7-C8-C10
22	6	313	CLA	C6-C7-C8-C9
22	K	204	CLA	O2A-C1-C2-C3
39	5	321	CHL	CBD-CGD-O2D-CED
24	G	203	BCR	C23-C24-C25-C26
36	5	306	C7Z	C25-C26-C27-C28
38	3	303	LUT	C1-C6-C7-C8
38	8	302	LUT	C5-C6-C7-C8
22	3	318	CLA	C8-C10-C11-C12
38	3	303	LUT	C31-C32-C33-C40
38	4	802	LUT	C11-C12-C13-C20
24	A	847	BCR	C21-C22-C23-C24
24	5	304	BCR	C21-C22-C23-C24
38	7	302	LUT	C11-C12-C13-C14
38	8	302	LUT	C31-C32-C33-C34
38	5	302	LUT	C27-C28-C29-C30
22	B	824	CLA	C5-C6-C7-C8
22	K	203	CLA	C5-C6-C7-C8
22	7	310	CLA	C5-C6-C7-C8
25	B	803	LHG	C25-C26-C27-C28
27	A	852	DGA	CA2-CA3-CA4-CA5
22	B	810	CLA	C11-C10-C8-C9
22	5	309	CLA	C5-C6-C7-C8
22	6	319	CLA	O1D-CGD-O2D-CED
25	B	803	LHG	O6-C4-C5-C6
25	B	850	LHG	O6-C4-C5-C6
25	6	323	LHG	O6-C4-C5-C6
25	6	323	LHG	C31-C32-C33-C34
22	A	802	CLA	C6-C7-C8-C10
22	A	803	CLA	C6-C7-C8-C10
22	A	806	CLA	C6-C7-C8-C10
22	A	808	CLA	C6-C7-C8-C10
22	A	808	CLA	C12-C13-C15-C16
22	A	811	CLA	C6-C7-C8-C10
22	A	812	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	A	812	CLA	C11-C10-C8-C7
22	A	815	CLA	C6-C7-C8-C10
22	A	816	CLA	C6-C7-C8-C10
22	A	820	CLA	C6-C7-C8-C10
22	A	823	CLA	C6-C7-C8-C10
22	A	827	CLA	C6-C7-C8-C10
22	A	828	CLA	C6-C7-C8-C10
22	A	830	CLA	C11-C10-C8-C7
22	A	833	CLA	C11-C10-C8-C7
22	A	834	CLA	C6-C7-C8-C10
22	A	854	CLA	C6-C7-C8-C10
22	A	855	CLA	C11-C10-C8-C7
22	B	806	CLA	C11-C12-C13-C15
22	B	814	CLA	C11-C10-C8-C7
22	B	815	CLA	C6-C7-C8-C10
22	B	816	CLA	C6-C7-C8-C10
22	B	826	CLA	C11-C12-C13-C15
22	B	827	CLA	C11-C12-C13-C15
22	B	828	CLA	C6-C7-C8-C10
22	B	833	CLA	C11-C10-C8-C7
22	B	840	CLA	C6-C7-C8-C10
22	B	841	CLA	C6-C7-C8-C10
22	B	841	CLA	C11-C10-C8-C7
22	B	842	CLA	C11-C10-C8-C7
22	L	202	CLA	C11-C10-C8-C7
22	1	306	CLA	C11-C10-C8-C7
22	1	309	CLA	C6-C7-C8-C10
22	1	313	CLA	C6-C7-C8-C10
22	1	316	CLA	C11-C12-C13-C15
22	3	311	CLA	C6-C7-C8-C10
22	7	304	CLA	C6-C7-C8-C10
22	7	306	CLA	C6-C7-C8-C10
22	7	308	CLA	C11-C12-C13-C15
22	7	310	CLA	C6-C7-C8-C10
22	7	317	CLA	C11-C10-C8-C7
22	7	324	CLA	C6-C7-C8-C10
22	8	308	CLA	C11-C10-C8-C7
22	4	807	CLA	C6-C7-C8-C10
22	5	307	CLA	C6-C7-C8-C10
22	5	322	CLA	C6-C7-C8-C10
22	6	301	CLA	C6-C7-C8-C10
22	6	310	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	6	312	CLA	C6-C7-C8-C10
39	5	316	CHL	C12-C13-C15-C16
35	J	102	T7X	C1-O1-P1-O13
35	J	102	T7X	C24-C25-C26-C27
25	6	323	LHG	C30-C31-C32-C33
22	A	812	CLA	C13-C15-C16-C17
22	1	316	CLA	C5-C6-C7-C8
24	3	304	BCR	C19-C20-C21-C22
24	6	306	BCR	C9-C10-C11-C12
38	Z	301	LUT	C9-C10-C11-C12
22	A	842	CLA	CAA-CBA-CGA-O2A
22	K	202	CLA	C2A-CAA-CBA-CGA
39	Z	311	CHL	C2A-CAA-CBA-CGA
39	8	301	CHL	C2A-CAA-CBA-CGA
39	5	316	CHL	C2A-CAA-CBA-CGA
39	6	318	CHL	C2A-CAA-CBA-CGA
39	2	303	CHL	C2A-CAA-CBA-CGA
25	1	317	LHG	C15-C16-C17-C18
22	5	319	CLA	C5-C6-C7-C8
22	6	314	CLA	C10-C11-C12-C13
22	B	812	CLA	C3-C5-C6-C7
22	4	811	CLA	C6-C7-C8-C10
22	A	805	CLA	C8-C10-C11-C12
22	A	824	CLA	C8-C10-C11-C12
21	A	801	CL0	CAA-CBA-CGA-O2A
42	7	321	SPH	C12-C13-C14-C15
22	B	810	CLA	C11-C10-C8-C7
22	7	309	CLA	C11-C10-C8-C7
22	5	301	CLA	C11-C10-C8-C7
22	A	806	CLA	C8-C10-C11-C12
22	A	828	CLA	C5-C6-C7-C8
22	B	809	CLA	C8-C10-C11-C12
22	4	808	CLA	C8-C10-C11-C12
26	8	318	NKP	CAS-CAT-CAU-CAV
25	6	323	LHG	C10-C11-C12-C13
22	B	823	CLA	CAD-CBD-CGD-O2D
22	1	311	CLA	CAD-CBD-CGD-O2D
22	3	322	CLA	CAD-CBD-CGD-O2D
22	8	309	CLA	CAD-CBD-CGD-O2D
22	Z	316	CLA	C3-C5-C6-C7
22	A	825	CLA	C13-C15-C16-C17
22	B	824	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	825	CLA	C8-C10-C11-C12
25	7	318	LHG	C12-C13-C14-C15
22	1	316	CLA	CBA-CGA-O2A-C1
22	8	313	CLA	CBA-CGA-O2A-C1
26	8	318	NKP	CAL-CAK-OAJ-CAI
39	8	312	CHL	CBA-CGA-O2A-C1
22	B	820	CLA	C11-C12-C13-C14
25	Z	317	LHG	C30-C31-C32-C33
25	6	323	LHG	C2-C3-O3-P
25	9	315	LHG	C4-C5-C6-O8
40	1	318	SQD	O6-C44-C45-C46
22	4	810	CLA	CBD-CGD-O2D-CED
22	B	842	CLA	O1A-CGA-O2A-C1
25	7	318	LHG	O6-C4-C5-O7
25	5	324	LHG	O6-C4-C5-O7
22	B	801	CLA	C5-C6-C7-C8
22	1	306	CLA	C3-C5-C6-C7
22	5	309	CLA	CAA-CBA-CGA-O2A
25	A	849	LHG	C24-C23-O8-C6
22	L	202	CLA	C2A-CAA-CBA-CGA
39	Z	312	CHL	O1A-CGA-O2A-C1
22	A	820	CLA	C11-C12-C13-C14
22	1	310	CLA	C11-C12-C13-C14
22	7	304	CLA	C11-C12-C13-C15
22	A	806	CLA	CHA-CBD-CGD-O1D
22	A	806	CLA	CHA-CBD-CGD-O2D
22	A	814	CLA	CHA-CBD-CGD-O1D
22	A	814	CLA	CHA-CBD-CGD-O2D
22	A	815	CLA	CHA-CBD-CGD-O1D
22	A	815	CLA	CHA-CBD-CGD-O2D
22	A	829	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	839	CLA	CHA-CBD-CGD-O2D
22	B	828	CLA	CHA-CBD-CGD-O2D
22	B	837	CLA	CHA-CBD-CGD-O1D
22	B	837	CLA	CHA-CBD-CGD-O2D
22	G	202	CLA	CHA-CBD-CGD-O1D
22	K	202	CLA	CHA-CBD-CGD-O2D
22	L	201	CLA	CHA-CBD-CGD-O1D
22	L	201	CLA	CHA-CBD-CGD-O2D
22	1	305	CLA	CHA-CBD-CGD-O1D
22	1	305	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	Z	304	CLA	CHA-CBD-CGD-O1D
22	Z	305	CLA	CHA-CBD-CGD-O1D
22	Z	305	CLA	CHA-CBD-CGD-O2D
22	7	312	CLA	CHA-CBD-CGD-O2D
22	8	311	CLA	CHA-CBD-CGD-O2D
22	5	314	CLA	CHA-CBD-CGD-O2D
22	5	315	CLA	CHA-CBD-CGD-O2D
22	6	309	CLA	CHA-CBD-CGD-O2D
22	6	312	CLA	CHA-CBD-CGD-O1D
22	6	312	CLA	CHA-CBD-CGD-O2D
22	6	314	CLA	CHA-CBD-CGD-O2D
22	6	317	CLA	CHA-CBD-CGD-O1D
22	6	319	CLA	CHA-CBD-CGD-O1D
22	6	319	CLA	CHA-CBD-CGD-O2D
22	6	322	CLA	CHA-CBD-CGD-O1D
22	9	305	CLA	CHA-CBD-CGD-O1D
22	9	307	CLA	CHA-CBD-CGD-O1D
22	9	309	CLA	CHA-CBD-CGD-O2D
22	2	302	CLA	CHA-CBD-CGD-O1D
39	Z	311	CHL	CHA-CBD-CGD-O1D
39	8	301	CHL	CHA-CBD-CGD-O1D
41	8	320	3PH	C3B-C3C-C3D-C3E
22	1	316	CLA	O1A-CGA-O2A-C1
33	F	307	LMT	C1-C2-C3-C4
22	A	813	CLA	C13-C15-C16-C17
25	B	850	LHG	O7-C5-C6-O8
25	B	851	LHG	O7-C5-C6-O8
25	Z	317	LHG	O7-C5-C6-O8
25	3	321	LHG	O7-C5-C6-O8
31	B	852	DGD	O1G-C1G-C2G-O2G
31	3	301	DGD	O1G-C1G-C2G-O2G
34	F	308	LMG	O1-C7-C8-O7
34	F	308	LMG	O7-C8-C9-O8
22	1	316	CLA	C13-C15-C16-C17
25	A	849	LHG	O1-C1-C2-O2
27	A	852	DGA	CA9-CAA-CBA-CCA
40	1	318	SQD	C10-C11-C12-C13
25	1	317	LHG	O10-C23-O8-C6
22	B	842	CLA	C2-C3-C5-C6
22	B	826	CLA	C6-C7-C8-C9
22	F	302	CLA	C11-C10-C8-C9
22	1	306	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	3	310	CLA	C6-C7-C8-C9
22	7	309	CLA	C6-C7-C8-C9
22	7	310	CLA	C11-C10-C8-C9
22	7	323	CLA	C11-C10-C8-C9
22	6	319	CLA	C11-C12-C13-C14
22	6	301	CLA	C5-C6-C7-C8
40	1	318	SQD	C4-C5-C6-S
22	B	821	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	CBD-CGD-O2D-CED
22	7	309	CLA	C11-C10-C8-C9
22	B	841	CLA	C8-C10-C11-C12
22	Z	313	CLA	CBA-CGA-O2A-C1
24	A	847	BCR	C37-C22-C23-C24
24	6	305	BCR	C37-C22-C23-C24
24	G	203	BCR	C11-C12-C13-C14
24	6	305	BCR	C21-C22-C23-C24
38	4	802	LUT	C11-C12-C13-C14
22	6	301	CLA	C3-C5-C6-C7
22	B	808	CLA	C1A-C2A-CAA-CBA
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	313	CLA	C1A-C2A-CAA-CBA
22	Z	309	CLA	C1A-C2A-CAA-CBA
22	7	315	CLA	C1A-C2A-CAA-CBA
39	4	814	CHL	C1A-C2A-CAA-CBA
22	B	828	CLA	C8-C10-C11-C12
22	Z	309	CLA	C10-C11-C12-C13
22	1	316	CLA	C2-C1-O2A-CGA
22	3	312	CLA	C2-C1-O2A-CGA
22	4	812	CLA	C2-C1-O2A-CGA
22	4	815	CLA	C2-C1-O2A-CGA
24	3	307	BCR	C19-C20-C21-C22
25	8	317	LHG	C4-O6-P-O3
25	6	323	LHG	C34-C35-C36-C37
22	A	838	CLA	C3-C5-C6-C7
22	A	822	CLA	C2-C3-C5-C6
39	6	315	CHL	C2-C3-C5-C6
41	7	319	3PH	C33-C34-C35-C36
22	Z	313	CLA	O1A-CGA-O2A-C1
26	8	318	NKP	OAE-CAK-OAJ-CAI
22	9	304	CLA	C4B-C3B-CAB-CBB
25	A	849	LHG	C3-O3-P-O5
25	A	850	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
25	B	803	LHG	C3-O3-P-O5
25	B	850	LHG	C3-O3-P-O4
25	4	820	LHG	C4-O6-P-O5
25	5	324	LHG	C3-O3-P-O4
25	5	324	LHG	C3-O3-P-O5
25	9	315	LHG	C4-O6-P-O5
25	A	849	LHG	O6-C4-C5-C6
35	J	102	T7X	O13-C7-C8-C9
41	7	319	3PH	O11-C1-C2-C3
22	3	310	CLA	C8-C10-C11-C12
22	1	310	CLA	C3-C5-C6-C7
22	3	313	CLA	C3-C5-C6-C7
25	A	849	LHG	C11-C10-C9-C8
25	6	323	LHG	C11-C10-C9-C8
26	A	851	NKP	CAG-CAH-CAI-OAJ
23	A	843	PQN	C26-C27-C28-C29
22	A	826	CLA	CAD-CBD-CGD-O1D
22	K	205	CLA	CAD-CBD-CGD-O1D
22	1	309	CLA	CAD-CBD-CGD-O1D
22	8	307	CLA	CAD-CBD-CGD-O1D
22	9	305	CLA	CAD-CBD-CGD-O1D
39	Z	311	CHL	CAD-CBD-CGD-O1D
39	8	301	CHL	CAD-CBD-CGD-O1D
22	A	840	CLA	C5-C6-C7-C8
22	F	302	CLA	C13-C15-C16-C17
22	7	308	CLA	C5-C6-C7-C8
22	1	308	CLA	C5-C6-C7-C8
22	A	807	CLA	C11-C12-C13-C15
22	7	324	CLA	C4-C3-C5-C6
22	5	311	CLA	C4-C3-C5-C6
22	A	802	CLA	C11-C12-C13-C15
22	A	807	CLA	C6-C7-C8-C10
22	A	808	CLA	C11-C12-C13-C15
22	A	813	CLA	C11-C12-C13-C15
22	A	814	CLA	C6-C7-C8-C10
22	A	814	CLA	C11-C10-C8-C7
22	A	818	CLA	C6-C7-C8-C10
22	A	835	CLA	C6-C7-C8-C10
22	A	835	CLA	C11-C10-C8-C7
22	A	840	CLA	C11-C10-C8-C7
22	A	854	CLA	C11-C12-C13-C15
22	B	801	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	809	CLA	C6-C7-C8-C10
22	B	813	CLA	C6-C7-C8-C10
22	B	816	CLA	C11-C10-C8-C7
22	B	820	CLA	C6-C7-C8-C10
22	B	825	CLA	C11-C10-C8-C7
22	B	826	CLA	C11-C10-C8-C7
22	B	829	CLA	C6-C7-C8-C10
22	B	830	CLA	C11-C12-C13-C15
22	B	833	CLA	C6-C7-C8-C10
22	B	834	CLA	C11-C10-C8-C7
22	B	838	CLA	C11-C12-C13-C15
22	B	840	CLA	C11-C12-C13-C15
22	F	301	CLA	C11-C10-C8-C7
22	F	302	CLA	C11-C10-C8-C7
22	1	304	CLA	C6-C7-C8-C10
22	1	307	CLA	C6-C7-C8-C10
22	1	307	CLA	C11-C10-C8-C7
22	1	308	CLA	C3A-C2A-CAA-CBA
22	1	309	CLA	C11-C10-C8-C7
22	Z	303	CLA	C6-C7-C8-C10
22	Z	306	CLA	C11-C10-C8-C7
22	Z	309	CLA	C11-C10-C8-C7
22	Z	316	CLA	C12-C13-C15-C16
22	3	308	CLA	C11-C12-C13-C15
22	3	318	CLA	C6-C7-C8-C10
22	3	322	CLA	C6-C7-C8-C10
22	7	306	CLA	C11-C10-C8-C7
22	7	306	CLA	C11-C12-C13-C15
22	7	308	CLA	C11-C10-C8-C7
22	7	309	CLA	C6-C7-C8-C10
22	7	310	CLA	C11-C10-C8-C7
22	8	305	CLA	C11-C10-C8-C7
22	8	310	CLA	C6-C7-C8-C10
22	5	308	CLA	C11-C12-C13-C15
22	5	312	CLA	C3A-C2A-CAA-CBA
22	5	315	CLA	C11-C12-C13-C15
22	6	301	CLA	C11-C10-C8-C7
22	6	302	CLA	C11-C10-C8-C7
22	6	309	CLA	C6-C7-C8-C10
22	6	310	CLA	C11-C10-C8-C7
22	6	310	CLA	C11-C12-C13-C15
22	6	319	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	6	319	CLA	C11-C12-C13-C15
22	9	303	CLA	C11-C10-C8-C7
23	B	843	PQN	C16-C17-C18-C20
25	A	849	LHG	O6-C4-C5-O7
25	B	803	LHG	O6-C4-C5-O7
25	B	851	LHG	O6-C4-C5-O7
25	6	323	LHG	O6-C4-C5-O7
39	Z	312	CHL	C3A-C2A-CAA-CBA
41	7	319	3PH	O11-C1-C2-O21
41	6	324	3PH	O11-C1-C2-O21
22	4	810	CLA	O1D-CGD-O2D-CED
25	5	324	LHG	C26-C27-C28-C29
24	G	203	BCR	C13-C14-C15-C16
22	A	838	CLA	CAA-CBA-CGA-O2A
22	A	827	CLA	C15-C16-C17-C18
22	7	309	CLA	C5-C6-C7-C8
22	8	313	CLA	O1A-CGA-O2A-C1
25	A	849	LHG	O10-C23-O8-C6
39	8	312	CHL	O1A-CGA-O2A-C1
25	A	850	LHG	C30-C31-C32-C33
22	B	835	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	C2A-CAA-CBA-CGA
39	3	317	CHL	C2A-CAA-CBA-CGA
22	Z	306	CLA	C11-C12-C13-C15
25	B	850	LHG	C4-C5-C6-O8
25	4	820	LHG	C4-C5-C6-O8
31	1	319	DGD	C1G-C2G-C3G-O3G
34	F	308	LMG	O1-C7-C8-C9
25	1	317	LHG	O7-C5-C6-O8
25	4	820	LHG	O7-C5-C6-O8
25	7	318	LHG	C30-C31-C32-C33
31	1	319	DGD	C5D-C6D-O5D-C1E
22	3	311	CLA	C8-C10-C11-C12
22	5	313	CLA	C5-C6-C7-C8
22	6	307	CLA	C8-C10-C11-C12
22	L	202	CLA	O1D-CGD-O2D-CED
22	A	816	CLA	C11-C10-C8-C9
22	A	805	CLA	C14-C13-C15-C16
22	A	806	CLA	C11-C10-C8-C9
22	A	817	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C12-C13-C14
22	A	830	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	833	CLA	C11-C10-C8-C9
22	B	806	CLA	C11-C12-C13-C14
22	B	814	CLA	C11-C10-C8-C9
22	B	818	CLA	C11-C10-C8-C9
22	B	819	CLA	C11-C10-C8-C9
22	B	821	CLA	C11-C12-C13-C14
22	B	826	CLA	C11-C12-C13-C14
22	B	827	CLA	C11-C12-C13-C14
22	B	833	CLA	C11-C10-C8-C9
22	Z	316	CLA	C14-C13-C15-C16
22	7	308	CLA	C11-C12-C13-C14
22	7	317	CLA	C6-C7-C8-C9
22	7	317	CLA	C11-C10-C8-C9
22	8	308	CLA	C11-C10-C8-C9
22	5	322	CLA	C6-C7-C8-C9
22	6	302	CLA	C11-C10-C8-C9
39	5	316	CHL	C6-C7-C8-C9
22	B	813	CLA	C3-C5-C6-C7
22	F	304	CLA	C16-C17-C18-C20
22	8	310	CLA	C11-C12-C13-C15
22	1	311	CLA	C2A-CAA-CBA-CGA
39	6	315	CHL	C2A-CAA-CBA-CGA
22	A	805	CLA	CAA-CBA-CGA-O2A
22	B	842	CLA	CAA-CBA-CGA-O2A
22	6	302	CLA	CAA-CBA-CGA-O2A
25	4	820	LHG	O1-C1-C2-O2
24	B	848	BCR	C18-C19-C20-C21
24	3	304	BCR	C10-C11-C12-C13
24	3	307	BCR	C18-C19-C20-C21
24	5	305	BCR	C18-C19-C20-C21
38	6	303	LUT	C27-C28-C29-C39
25	6	323	LHG	C13-C14-C15-C16
22	A	809	CLA	C6-C7-C8-C10
22	B	805	CLA	C16-C17-C18-C20
22	B	820	CLA	C11-C12-C13-C15
22	Z	315	CLA	C2B-C3B-CAB-CBB
22	4	805	CLA	C2B-C3B-CAB-CBB
22	4	812	CLA	C2B-C3B-CAB-CBB
22	4	818	CLA	C2B-C3B-CAB-CBB
27	A	852	DGA	CBB-CCB-CDB-CEB
39	3	317	CHL	O1D-CGD-O2D-CED
22	A	834	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	802	CLA	O1A-CGA-O2A-C1
22	6	312	CLA	C15-C16-C17-C18
26	8	318	NKP	CAQ-CAR-CAS-CAT
22	A	811	CLA	C8-C10-C11-C12
22	7	312	CLA	C8-C10-C11-C12
34	F	308	LMG	C9-C8-O7-C10
25	B	851	LHG	O6-C4-C5-C6
22	A	854	CLA	C2A-CAA-CBA-CGA
22	B	805	CLA	C2A-CAA-CBA-CGA
22	B	810	CLA	C2A-CAA-CBA-CGA
22	B	812	CLA	C2A-CAA-CBA-CGA
22	Z	314	CLA	C2A-CAA-CBA-CGA
22	8	316	CLA	C2A-CAA-CBA-CGA
22	6	312	CLA	O1D-CGD-O2D-CED
21	A	801	CL0	C2-C1-O2A-CGA
22	A	816	CLA	C2-C1-O2A-CGA
22	7	308	CLA	C2-C1-O2A-CGA
25	A	850	LHG	C27-C28-C29-C30
25	8	317	LHG	C29-C30-C31-C32
25	B	803	LHG	C26-C27-C28-C29
25	3	321	LHG	C5-C4-O6-P
41	5	325	3PH	O11-C1-C2-O21
22	6	309	CLA	C16-C17-C18-C19
24	B	847	BCR	C23-C24-C25-C30
24	B	853	BCR	C5-C6-C7-C8
24	7	303	BCR	C5-C6-C7-C8
38	1	302	LUT	C1-C6-C7-C8
38	1	303	LUT	C5-C6-C7-C8
38	Z	302	LUT	C1-C6-C7-C8
38	6	304	LUT	C1-C6-C7-C8
39	9	312	CHL	C2-C3-C5-C6
22	B	835	CLA	O1D-CGD-O2D-CED
39	5	321	CHL	O1D-CGD-O2D-CED
25	7	318	LHG	C10-C11-C12-C13
42	7	321	SPH	C14-C15-C16-C17
22	7	324	CLA	C11-C12-C13-C15
39	4	816	CHL	CBD-CGD-O2D-CED
22	B	825	CLA	C2A-CAA-CBA-CGA
25	9	315	LHG	O7-C5-C6-O8
22	6	312	CLA	CBD-CGD-O2D-CED
25	A	850	LHG	C3-O3-P-O6
25	B	851	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
25	3	321	LHG	C3-O3-P-O6
25	7	318	LHG	C3-O3-P-O6
25	4	820	LHG	C3-O3-P-O6
25	5	324	LHG	C4-O6-P-O3
43	8	319	LPX	C3-O1-P1-O2
31	1	319	DGD	C6A-C7A-C8A-C9A
25	A	849	LHG	C4-C5-C6-O8
25	8	317	LHG	C4-C5-C6-O8
22	A	814	CLA	C2-C3-C5-C6
22	A	824	CLA	C11-C10-C8-C7
22	A	825	CLA	C6-C7-C8-C10
22	B	817	CLA	C11-C10-C8-C7
22	F	302	CLA	C11-C12-C13-C15
22	1	304	CLA	C11-C12-C13-C15
22	Z	308	CLA	C11-C10-C8-C7
22	7	323	CLA	C11-C12-C13-C15
22	A	835	CLA	C11-C10-C8-C9
22	A	840	CLA	C11-C10-C8-C9
22	B	811	CLA	C11-C10-C8-C9
22	B	826	CLA	C11-C10-C8-C9
22	B	830	CLA	C11-C12-C13-C14
22	B	834	CLA	C11-C10-C8-C9
22	F	301	CLA	C11-C10-C8-C9
22	Z	306	CLA	C11-C10-C8-C9
22	Z	309	CLA	C11-C10-C8-C9
22	7	304	CLA	C11-C10-C8-C9
22	7	307	CLA	C11-C12-C13-C14
22	7	308	CLA	C11-C10-C8-C9
22	8	310	CLA	C6-C7-C8-C9
22	5	308	CLA	C11-C12-C13-C14
22	6	301	CLA	C11-C10-C8-C9
22	6	309	CLA	C6-C7-C8-C9
22	6	319	CLA	C11-C10-C8-C9
22	B	821	CLA	C13-C15-C16-C17
24	3	305	BCR	C15-C16-C17-C18
38	4	803	LUT	C9-C10-C11-C12
38	4	803	LUT	C33-C34-C35-C15
22	4	807	CLA	C16-C17-C18-C20
42	7	320	SPH	C11-C10-C9-C8
41	8	320	3PH	O22-C21-C22-C23
22	Z	313	CLA	C5-C6-C7-C8
22	8	307	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	3	306	BCR	C7-C8-C9-C34
22	A	807	CLA	C11-C12-C13-C14
22	A	816	CLA	C11-C10-C8-C7
22	B	813	CLA	C11-C10-C8-C7
22	Z	305	CLA	C11-C10-C8-C7
22	5	309	CLA	C11-C10-C8-C7
26	A	851	NKP	OAF-CAG-CAH-CAI
22	A	816	CLA	C5-C6-C7-C8
22	5	311	CLA	C2-C3-C5-C6
39	6	318	CHL	C2-C3-C5-C6
22	A	802	CLA	CBA-CGA-O2A-C1
22	8	307	CLA	CBA-CGA-O2A-C1
22	F	302	CLA	C8-C10-C11-C12
22	6	302	CLA	C8-C10-C11-C12
42	7	320	SPH	C10-C11-C12-C13
22	A	824	CLA	O1D-CGD-O2D-CED
25	8	317	LHG	C26-C27-C28-C29
22	B	841	CLA	C4B-C3B-CAB-CBB
22	7	310	CLA	C4B-C3B-CAB-CBB
22	B	817	CLA	C2A-CAA-CBA-CGA
22	8	305	CLA	C2A-CAA-CBA-CGA
22	5	310	CLA	C2A-CAA-CBA-CGA
38	8	302	LUT	C9-C10-C11-C12
38	5	302	LUT	C9-C10-C11-C12
25	5	324	LHG	C25-C26-C27-C28
22	B	824	CLA	C3-C5-C6-C7
22	7	304	CLA	C3-C5-C6-C7
22	A	802	CLA	C8-C10-C11-C12
22	B	820	CLA	C8-C10-C11-C12
40	1	318	SQD	C7-C8-C9-C10
22	6	307	CLA	C11-C12-C13-C15
22	L	202	CLA	C4-C3-C5-C6
22	3	312	CLA	C4-C3-C5-C6
22	A	834	CLA	C2-C3-C5-C6
22	L	202	CLA	C2-C3-C5-C6
22	3	312	CLA	C2-C3-C5-C6
41	7	319	3PH	C34-C35-C36-C37
22	5	318	CLA	C5-C6-C7-C8
25	6	323	LHG	C33-C34-C35-C36
22	A	817	CLA	C2-C1-O2A-CGA
22	B	816	CLA	C2-C1-O2A-CGA
22	Z	303	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	4	811	CLA	C2-C1-O2A-CGA
22	9	309	CLA	C2-C1-O2A-CGA
22	Z	306	CLA	C11-C12-C13-C14
22	4	808	CLA	C11-C12-C13-C15
26	8	318	NKP	CAR-CAS-CAT-CAU
22	6	310	CLA	C2A-CAA-CBA-CGA
31	1	319	DGD	O6D-C5D-C6D-O5D
22	Z	316	CLA	C3A-C2A-CAA-CBA
22	5	309	CLA	C3A-C2A-CAA-CBA
22	6	309	CLA	C3A-C2A-CAA-CBA
39	4	814	CHL	C3A-C2A-CAA-CBA
22	B	826	CLA	CAA-CBA-CGA-O2A
36	J	105	C7Z	C29-C30-C31-C32
27	A	852	DGA	CBB-CAB-CB9-CB8
22	B	829	CLA	C4-C3-C5-C6
22	7	309	CLA	C4-C3-C5-C6
42	7	320	SPH	C7-C8-C9-C10
22	B	821	CLA	C11-C10-C8-C9
22	B	838	CLA	C11-C12-C13-C14
22	1	304	CLA	C14-C13-C15-C16
22	1	307	CLA	C11-C10-C8-C9
22	3	313	CLA	C6-C7-C8-C9
22	7	306	CLA	C11-C10-C8-C9
22	7	306	CLA	C11-C12-C13-C14
22	8	309	CLA	C11-C10-C8-C9
22	6	310	CLA	C11-C10-C8-C9
22	6	314	CLA	C11-C10-C8-C9
39	5	316	CHL	C11-C12-C13-C14
22	7	312	CLA	C11-C12-C13-C14
22	A	804	CLA	CAA-CBA-CGA-O1A
22	3	313	CLA	C13-C15-C16-C17
28	A	853	OCA	C3-C4-C5-C6
22	5	315	CLA	C15-C16-C17-C18
24	A	844	BCR	C11-C10-C9-C34
24	A	845	BCR	C35-C13-C14-C15
24	A	848	BCR	C11-C10-C9-C34
24	A	848	BCR	C16-C17-C18-C36
24	B	844	BCR	C35-C13-C14-C15
24	B	844	BCR	C16-C17-C18-C36
24	B	846	BCR	C11-C10-C9-C34
24	B	846	BCR	C20-C21-C22-C37
24	B	848	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
24	B	853	BCR	C11-C10-C9-C34
32	F	306	RRX	C16-C17-C18-C36
32	F	306	RRX	C35-C13-C14-C15
32	F	306	RRX	C11-C10-C9-C34
22	A	802	CLA	C2A-CAA-CBA-CGA
22	7	324	CLA	C11-C12-C13-C14
22	A	810	CLA	O2A-C1-C2-C3
22	A	839	CLA	O2A-C1-C2-C3
22	1	305	CLA	CAA-CBA-CGA-O1A
24	B	844	BCR	C11-C12-C13-C35
38	Z	302	LUT	C31-C32-C33-C40
22	5	308	CLA	C5-C6-C7-C8
25	4	820	LHG	C25-C26-C27-C28
34	J	101	LMG	C9-C8-O7-C10
22	7	322	CLA	C5-C6-C7-C8
22	B	833	CLA	C4-C3-C5-C6
22	A	834	CLA	C1A-C2A-CAA-CBA
22	Z	316	CLA	C1A-C2A-CAA-CBA
22	5	309	CLA	C1A-C2A-CAA-CBA
22	6	310	CLA	C1A-C2A-CAA-CBA
39	Z	311	CHL	C1A-C2A-CAA-CBA
39	Z	312	CHL	C1A-C2A-CAA-CBA
22	A	805	CLA	C11-C10-C8-C7
22	A	821	CLA	C11-C12-C13-C15
22	A	825	CLA	C11-C10-C8-C7
22	A	830	CLA	C6-C7-C8-C10
22	A	832	CLA	C6-C7-C8-C10
22	A	840	CLA	C11-C12-C13-C15
22	B	805	CLA	C11-C10-C8-C7
22	B	809	CLA	C11-C12-C13-C15
22	B	831	CLA	C11-C10-C8-C7
22	1	310	CLA	C6-C7-C8-C10
22	Z	313	CLA	C6-C7-C8-C10
22	5	307	CLA	C11-C10-C8-C7
22	5	308	CLA	C11-C10-C8-C7
22	6	309	CLA	C11-C10-C8-C7
26	A	851	NKP	CAQ-CAR-CAS-CAT
41	8	320	3PH	O21-C21-C22-C23
24	B	847	BCR	C13-C14-C15-C16
38	5	303	LUT	C9-C10-C11-C12
25	1	317	LHG	C17-C18-C19-C20
35	J	102	T7X	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	G	204	LMT	C5-C6-C7-C8
22	8	314	CLA	CAA-CBA-CGA-O2A
31	B	852	DGD	O1A-C1A-O1G-C1G
25	6	323	LHG	C14-C15-C16-C17
39	4	816	CHL	O1D-CGD-O2D-CED
22	A	805	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	822	CLA	C2A-CAA-CBA-CGA
22	A	808	CLA	C5-C6-C7-C8
22	B	811	CLA	C15-C16-C17-C18
22	3	308	CLA	C15-C16-C17-C18
22	3	312	CLA	C5-C6-C7-C8
22	A	835	CLA	C8-C10-C11-C12
22	A	838	CLA	C8-C10-C11-C12
22	B	806	CLA	CBA-CGA-O2A-C1
27	A	852	DGA	CB6-CB7-CB8-CB9
22	A	811	CLA	C10-C11-C12-C13
22	B	831	CLA	C8-C10-C11-C12
22	3	314	CLA	C5-C6-C7-C8
22	6	319	CLA	C8-C10-C11-C12
22	B	807	CLA	CAA-CBA-CGA-O2A
25	A	849	LHG	C10-C11-C12-C13
40	1	318	SQD	C24-C25-C26-C27
22	8	308	CLA	C5-C6-C7-C8
22	B	829	CLA	C2-C3-C5-C6
22	B	841	CLA	C2B-C3B-CAB-CBB
22	7	310	CLA	C2B-C3B-CAB-CBB
22	6	301	CLA	C8-C10-C11-C12
22	7	323	CLA	C16-C17-C18-C20
24	A	844	BCR	C11-C10-C9-C8
24	A	845	BCR	C12-C13-C14-C15
24	A	848	BCR	C11-C10-C9-C8
24	A	848	BCR	C16-C17-C18-C19
24	B	844	BCR	C12-C13-C14-C15
24	B	844	BCR	C16-C17-C18-C19
24	B	846	BCR	C11-C10-C9-C8
24	B	846	BCR	C20-C21-C22-C23
24	B	853	BCR	C11-C10-C9-C8
32	F	306	RRX	C16-C17-C18-C19
32	F	306	RRX	C12-C13-C14-C15
32	F	306	RRX	C11-C10-C9-C8
22	B	833	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	820	CLA	C2A-CAA-CBA-CGA
24	A	845	BCR	C15-C16-C17-C18
24	3	307	BCR	C15-C16-C17-C18
38	7	302	LUT	C9-C10-C11-C12
22	Z	304	CLA	CAA-CBA-CGA-O1A
22	6	309	CLA	C16-C17-C18-C20
22	1	310	CLA	C2C-C3C-CAC-CBC
41	6	324	3PH	C29-C2A-C2B-C2C
22	Z	316	CLA	C13-C15-C16-C17
25	4	820	LHG	O10-C23-C24-C25
22	A	836	CLA	C2-C1-O2A-CGA
22	7	309	CLA	C2-C3-C5-C6
22	B	807	CLA	CAA-CBA-CGA-O1A
22	1	305	CLA	CAA-CBA-CGA-O2A
27	A	852	DGA	CAA-CBA-CCA-CDA
22	A	828	CLA	CAA-CBA-CGA-O2A
22	5	311	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	C11-C10-C8-C9
22	B	815	CLA	C11-C10-C8-C9
22	6	310	CLA	C11-C12-C13-C14
42	7	320	SPH	O1-C1-C2-C3
22	2	304	CLA	CAA-CBA-CGA-O2A
26	A	851	NKP	CAN-CAO-CAP-CAQ
42	7	320	SPH	C13-C14-C15-C16
22	7	308	CLA	C2A-CAA-CBA-CGA
22	4	805	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C11-C12-C13-C15
22	1	307	CLA	C11-C12-C13-C15
22	3	314	CLA	C11-C12-C13-C15
22	A	804	CLA	CAA-CBA-CGA-O2A
22	9	310	CLA	CAA-CBA-CGA-O1A
24	A	845	BCR	C23-C24-C25-C30
24	B	844	BCR	C23-C24-C25-C30
24	3	307	BCR	C23-C24-C25-C30
36	J	105	C7Z	C21-C26-C27-C28
38	1	303	LUT	C1-C6-C7-C8
22	B	834	CLA	CAA-CBA-CGA-O2A
41	6	324	3PH	O21-C21-C22-C23
25	3	321	LHG	O1-C1-C2-C3
25	6	323	LHG	C16-C17-C18-C19
42	7	321	SPH	C13-C14-C15-C16
24	A	848	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	B	844	BCR	C21-C22-C23-C24
38	Z	301	LUT	C27-C28-C29-C30
38	3	303	LUT	C31-C32-C33-C34
22	L	201	CLA	C5-C6-C7-C8
22	B	833	CLA	C2-C3-C5-C6
22	Z	304	CLA	CAA-CBA-CGA-O2A
22	9	310	CLA	CAA-CBA-CGA-O2A
22	6	322	CLA	O1A-CGA-O2A-C1
39	6	318	CHL	O1A-CGA-O2A-C1
22	Z	310	CLA	CAA-CBA-CGA-O2A
22	6	301	CLA	C11-C12-C13-C15
22	Z	305	CLA	C11-C10-C8-C9
42	7	320	SPH	C11-C12-C13-C14
22	B	809	CLA	CAA-CBA-CGA-O2A
22	B	815	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	O1A-CGA-O2A-C1
22	B	820	CLA	C5-C6-C7-C8
25	A	850	LHG	C9-C10-C11-C12
25	8	317	LHG	C24-C25-C26-C27
22	7	306	CLA	C3-C5-C6-C7
22	Z	316	CLA	C15-C16-C17-C18
22	Z	309	CLA	O1D-CGD-O2D-CED
25	A	850	LHG	C25-C26-C27-C28
21	A	801	CL0	C11-C12-C13-C15
22	A	832	CLA	C11-C12-C13-C15
22	B	828	CLA	C11-C12-C13-C15
22	B	830	CLA	C2-C3-C5-C6
22	3	313	CLA	C6-C7-C8-C10
22	7	323	CLA	C12-C13-C15-C16
22	6	309	CLA	C11-C12-C13-C15
39	3	317	CHL	C6-C7-C8-C10
22	9	304	CLA	CAA-CBA-CGA-O2A
22	4	807	CLA	C13-C15-C16-C17
25	B	803	LHG	C2-C3-O3-P
34	F	308	LMG	O10-C28-O8-C9
31	B	852	DGD	C2A-C1A-O1G-C1G
34	F	308	LMG	C29-C28-O8-C9
22	A	823	CLA	C3-C5-C6-C7
22	A	807	CLA	CAA-CBA-CGA-O2A
22	B	810	CLA	CAA-CBA-CGA-O2A
22	L	203	CLA	CAA-CBA-CGA-O2A
22	3	322	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	1	313	CLA	C5-C6-C7-C8
22	6	307	CLA	C11-C12-C13-C14
39	6	318	CHL	CBA-CGA-O2A-C1
22	A	808	CLA	C13-C15-C16-C17
25	A	850	LHG	C11-C10-C9-C8
22	A	841	CLA	C4-C3-C5-C6
22	5	310	CLA	C4-C3-C5-C6
22	B	808	CLA	C8-C10-C11-C12
22	F	304	CLA	C8-C10-C11-C12
22	7	324	CLA	C8-C10-C11-C12
43	8	319	LPX	C1-O2-P1-O1
22	A	825	CLA	C2-C3-C5-C6
22	4	808	CLA	C11-C12-C13-C14
22	6	309	CLA	CAA-CBA-CGA-O1A
22	B	833	CLA	C13-C15-C16-C17
22	B	822	CLA	C11-C10-C8-C7
22	A	802	CLA	C11-C12-C13-C14
22	A	808	CLA	C11-C12-C13-C14
22	A	808	CLA	C14-C13-C15-C16
22	A	811	CLA	C14-C13-C15-C16
22	A	854	CLA	C11-C12-C13-C14
22	B	805	CLA	C11-C10-C8-C9
22	B	809	CLA	C11-C12-C13-C14
22	B	816	CLA	C11-C10-C8-C9
22	B	817	CLA	C11-C10-C8-C9
22	B	825	CLA	C11-C10-C8-C9
22	B	831	CLA	C11-C10-C8-C9
22	1	304	CLA	C11-C12-C13-C14
22	1	309	CLA	C11-C10-C8-C9
22	3	308	CLA	C11-C12-C13-C14
22	3	313	CLA	C11-C10-C8-C9
22	8	305	CLA	C11-C10-C8-C9
22	5	307	CLA	C11-C10-C8-C9
22	5	315	CLA	C11-C12-C13-C14
22	6	322	CLA	C11-C10-C8-C9
22	9	303	CLA	C11-C10-C8-C9
23	B	843	PQN	C16-C17-C18-C19
23	B	843	PQN	C19-C18-C20-C21
39	8	315	CHL	C6-C7-C8-C9
31	B	852	DGD	C9B-CAB-CBB-CCB
25	8	317	LHG	C30-C31-C32-C33
22	B	807	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	838	CLA	C3A-C2A-CAA-CBA
22	F	304	CLA	C3A-C2A-CAA-CBA
22	Z	308	CLA	C3A-C2A-CAA-CBA
22	2	302	CLA	C3A-C2A-CAA-CBA
22	A	812	CLA	CAA-CBA-CGA-O2A
22	3	308	CLA	CAA-CBA-CGA-O2A
25	A	849	LHG	O7-C7-C8-C9
25	1	317	LHG	O8-C23-C24-C25
31	3	301	DGD	O1G-C1A-C2A-C3A
41	8	320	3PH	C38-C39-C3A-C3B
22	2	302	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	CAD-CBD-CGD-O2D
22	3	315	CLA	CAD-CBD-CGD-O2D
22	5	323	CLA	CAD-CBD-CGD-O2D
39	1	312	CHL	CAD-CBD-CGD-O2D
39	Z	312	CHL	CAD-CBD-CGD-O2D
39	4	813	CHL	CAD-CBD-CGD-O2D
39	6	318	CHL	CAD-CBD-CGD-O2D
39	9	312	CHL	CAD-CBD-CGD-O2D
22	7	317	CLA	C2A-CAA-CBA-CGA
25	Z	317	LHG	C24-C25-C26-C27
22	A	821	CLA	C2-C1-O2A-CGA
22	B	838	CLA	C2-C1-O2A-CGA
22	A	837	CLA	CAA-CBA-CGA-O2A
22	4	806	CLA	CAA-CBA-CGA-O2A
22	5	323	CLA	CAA-CBA-CGA-O2A
22	9	306	CLA	CAA-CBA-CGA-O2A
22	9	304	CLA	CAA-CBA-CGA-O1A
22	B	824	CLA	CAA-CBA-CGA-O2A
22	1	306	CLA	CAA-CBA-CGA-O2A
22	3	314	CLA	CAA-CBA-CGA-O2A
24	B	844	BCR	C11-C12-C13-C14
24	3	306	BCR	C7-C8-C9-C10
38	Z	302	LUT	C31-C32-C33-C34
38	6	303	LUT	C27-C28-C29-C30
22	B	813	CLA	C11-C10-C8-C9
22	B	822	CLA	C11-C10-C8-C9
22	5	309	CLA	C11-C10-C8-C9
42	7	321	SPH	C5-C6-C7-C8
25	A	850	LHG	C35-C36-C37-C38
22	7	324	CLA	C10-C11-C12-C13
25	A	850	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
41	8	320	3PH	C1-O11-P-O12
22	1	304	CLA	C8-C10-C11-C12
22	Z	305	CLA	C5-C6-C7-C8
22	A	815	CLA	CAA-CBA-CGA-O2A
22	8	309	CLA	CAA-CBA-CGA-O2A
22	A	831	CLA	O2A-C1-C2-C3
22	1	309	CLA	O2A-C1-C2-C3
22	5	301	CLA	O2A-C1-C2-C3
22	5	320	CLA	O2A-C1-C2-C3
22	9	309	CLA	O2A-C1-C2-C3
39	3	317	CHL	O2A-C1-C2-C3
39	4	814	CHL	O2A-C1-C2-C3
39	5	317	CHL	O2A-C1-C2-C3
39	9	312	CHL	O2A-C1-C2-C3
22	B	812	CLA	CAA-CBA-CGA-O2A
22	7	324	CLA	CAA-CBA-CGA-O2A
22	9	305	CLA	CAA-CBA-CGA-O2A
22	2	302	CLA	CAA-CBA-CGA-O1A
25	1	317	LHG	C28-C29-C30-C31
22	A	802	CLA	CHA-CBD-CGD-O1D
22	A	802	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	CHA-CBD-CGD-O1D
22	A	805	CLA	CHA-CBD-CGD-O2D
22	A	810	CLA	CHA-CBD-CGD-O1D
22	A	810	CLA	CHA-CBD-CGD-O2D
22	A	811	CLA	CHA-CBD-CGD-O2D
22	A	813	CLA	CHA-CBD-CGD-O1D
22	A	813	CLA	CHA-CBD-CGD-O2D
22	A	818	CLA	CHA-CBD-CGD-O1D
22	A	818	CLA	CHA-CBD-CGD-O2D
22	A	819	CLA	CHA-CBD-CGD-O2D
22	A	820	CLA	CHA-CBD-CGD-O1D
22	A	820	CLA	CHA-CBD-CGD-O2D
22	A	821	CLA	CHA-CBD-CGD-O2D
22	A	823	CLA	CHA-CBD-CGD-O1D
22	A	823	CLA	CHA-CBD-CGD-O2D
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D
22	A	827	CLA	CHA-CBD-CGD-O1D
22	A	827	CLA	CHA-CBD-CGD-O2D
22	A	828	CLA	CHA-CBD-CGD-O1D
22	A	828	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	831	CLA	CHA-CBD-CGD-O1D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	A	832	CLA	CHA-CBD-CGD-O2D
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	CHA-CBD-CGD-O1D
22	A	840	CLA	CHA-CBD-CGD-O2D
22	A	854	CLA	CHA-CBD-CGD-O1D
22	A	854	CLA	CHA-CBD-CGD-O2D
22	A	855	CLA	CHA-CBD-CGD-O1D
22	A	855	CLA	CHA-CBD-CGD-O2D
22	B	801	CLA	CHA-CBD-CGD-O1D
22	B	801	CLA	CHA-CBD-CGD-O2D
22	B	806	CLA	CHA-CBD-CGD-O1D
22	B	806	CLA	CHA-CBD-CGD-O2D
22	B	807	CLA	CHA-CBD-CGD-O1D
22	B	807	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	809	CLA	CHA-CBD-CGD-O1D
22	B	809	CLA	CHA-CBD-CGD-O2D
22	B	810	CLA	CHA-CBD-CGD-O1D
22	B	810	CLA	CHA-CBD-CGD-O2D
22	B	812	CLA	CHA-CBD-CGD-O2D
22	B	814	CLA	CHA-CBD-CGD-O1D
22	B	814	CLA	CHA-CBD-CGD-O2D
22	B	816	CLA	CHA-CBD-CGD-O1D
22	B	816	CLA	CHA-CBD-CGD-O2D
22	B	818	CLA	CHA-CBD-CGD-O1D
22	B	818	CLA	CHA-CBD-CGD-O2D
22	B	819	CLA	CHA-CBD-CGD-O1D
22	B	819	CLA	CHA-CBD-CGD-O2D
22	B	820	CLA	CHA-CBD-CGD-O1D
22	B	820	CLA	CHA-CBD-CGD-O2D
22	B	821	CLA	CHA-CBD-CGD-O1D
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	822	CLA	CHA-CBD-CGD-O1D
22	B	822	CLA	CHA-CBD-CGD-O2D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	830	CLA	CHA-CBD-CGD-O1D
22	B	830	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	832	CLA	CHA-CBD-CGD-O1D
22	B	832	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O2D
22	B	836	CLA	CHA-CBD-CGD-O2D
22	B	838	CLA	CHA-CBD-CGD-O1D
22	B	838	CLA	CHA-CBD-CGD-O2D
22	B	839	CLA	CHA-CBD-CGD-O1D
22	B	839	CLA	CHA-CBD-CGD-O2D
22	B	842	CLA	CHA-CBD-CGD-O1D
22	B	842	CLA	CHA-CBD-CGD-O2D
22	F	305	CLA	CHA-CBD-CGD-O1D
22	F	305	CLA	CHA-CBD-CGD-O2D
22	G	201	CLA	CHA-CBD-CGD-O1D
22	G	201	CLA	CHA-CBD-CGD-O2D
22	J	103	CLA	CHA-CBD-CGD-O1D
22	J	103	CLA	CHA-CBD-CGD-O2D
22	K	203	CLA	CHA-CBD-CGD-O1D
22	K	203	CLA	CHA-CBD-CGD-O2D
22	L	202	CLA	CHA-CBD-CGD-O1D
22	L	202	CLA	CHA-CBD-CGD-O2D
22	1	306	CLA	CHA-CBD-CGD-O1D
22	1	306	CLA	CHA-CBD-CGD-O2D
22	1	307	CLA	CHA-CBD-CGD-O1D
22	1	307	CLA	CHA-CBD-CGD-O2D
22	1	310	CLA	CHA-CBD-CGD-O2D
22	1	316	CLA	CHA-CBD-CGD-O2D
22	Z	304	CLA	CHA-CBD-CGD-O2D
22	Z	306	CLA	CHA-CBD-CGD-O1D
22	Z	306	CLA	CHA-CBD-CGD-O2D
22	Z	308	CLA	CHA-CBD-CGD-O1D
22	Z	308	CLA	CHA-CBD-CGD-O2D
22	Z	310	CLA	CHA-CBD-CGD-O1D
22	Z	310	CLA	CHA-CBD-CGD-O2D
22	Z	314	CLA	CHA-CBD-CGD-O1D
22	Z	314	CLA	CHA-CBD-CGD-O2D
22	Z	316	CLA	CHA-CBD-CGD-O1D
22	Z	316	CLA	CHA-CBD-CGD-O2D
22	3	308	CLA	CHA-CBD-CGD-O1D
22	3	308	CLA	CHA-CBD-CGD-O2D
22	3	309	CLA	CHA-CBD-CGD-O2D
22	3	311	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	3	311	CLA	CHA-CBD-CGD-O2D
22	3	312	CLA	CHA-CBD-CGD-O2D
22	3	318	CLA	CHA-CBD-CGD-O2D
22	3	319	CLA	CHA-CBD-CGD-O1D
22	3	319	CLA	CHA-CBD-CGD-O2D
22	7	304	CLA	CHA-CBD-CGD-O2D
22	7	306	CLA	CHA-CBD-CGD-O1D
22	7	306	CLA	CHA-CBD-CGD-O2D
22	7	307	CLA	CHA-CBD-CGD-O1D
22	7	307	CLA	CHA-CBD-CGD-O2D
22	7	308	CLA	CHA-CBD-CGD-O1D
22	7	308	CLA	CHA-CBD-CGD-O2D
22	7	309	CLA	CHA-CBD-CGD-O1D
22	7	309	CLA	CHA-CBD-CGD-O2D
22	7	311	CLA	CHA-CBD-CGD-O1D
22	7	311	CLA	CHA-CBD-CGD-O2D
22	7	314	CLA	CHA-CBD-CGD-O2D
22	7	316	CLA	CHA-CBD-CGD-O2D
22	7	317	CLA	CHA-CBD-CGD-O1D
22	7	317	CLA	CHA-CBD-CGD-O2D
22	7	322	CLA	CHA-CBD-CGD-O1D
22	7	322	CLA	CHA-CBD-CGD-O2D
22	7	324	CLA	CHA-CBD-CGD-O1D
22	7	324	CLA	CHA-CBD-CGD-O2D
22	8	305	CLA	CHA-CBD-CGD-O1D
22	8	305	CLA	CHA-CBD-CGD-O2D
22	8	310	CLA	CHA-CBD-CGD-O1D
22	8	310	CLA	CHA-CBD-CGD-O2D
22	8	313	CLA	CHA-CBD-CGD-O1D
22	8	313	CLA	CHA-CBD-CGD-O2D
22	8	314	CLA	CHA-CBD-CGD-O1D
22	8	314	CLA	CHA-CBD-CGD-O2D
22	8	316	CLA	CHA-CBD-CGD-O1D
22	8	316	CLA	CHA-CBD-CGD-O2D
22	4	808	CLA	CHA-CBD-CGD-O1D
22	4	810	CLA	CHA-CBD-CGD-O1D
22	4	810	CLA	CHA-CBD-CGD-O2D
22	4	818	CLA	CHA-CBD-CGD-O1D
22	4	818	CLA	CHA-CBD-CGD-O2D
22	5	309	CLA	CHA-CBD-CGD-O1D
22	5	309	CLA	CHA-CBD-CGD-O2D
22	5	310	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	5	310	CLA	CHA-CBD-CGD-O2D
22	5	311	CLA	CHA-CBD-CGD-O2D
22	5	312	CLA	CHA-CBD-CGD-O1D
22	5	312	CLA	CHA-CBD-CGD-O2D
22	5	318	CLA	CHA-CBD-CGD-O1D
22	5	318	CLA	CHA-CBD-CGD-O2D
22	5	319	CLA	CHA-CBD-CGD-O1D
22	5	319	CLA	CHA-CBD-CGD-O2D
22	5	320	CLA	CHA-CBD-CGD-O1D
22	5	320	CLA	CHA-CBD-CGD-O2D
22	6	301	CLA	CHA-CBD-CGD-O1D
22	6	301	CLA	CHA-CBD-CGD-O2D
22	6	310	CLA	CHA-CBD-CGD-O1D
22	6	310	CLA	CHA-CBD-CGD-O2D
22	6	311	CLA	CHA-CBD-CGD-O1D
22	6	311	CLA	CHA-CBD-CGD-O2D
22	6	321	CLA	CHA-CBD-CGD-O1D
22	6	321	CLA	CHA-CBD-CGD-O2D
22	9	305	CLA	CHA-CBD-CGD-O2D
22	9	306	CLA	CHA-CBD-CGD-O1D
22	9	306	CLA	CHA-CBD-CGD-O2D
22	9	307	CLA	CHA-CBD-CGD-O2D
22	2	304	CLA	CHA-CBD-CGD-O1D
22	2	304	CLA	CHA-CBD-CGD-O2D
39	Z	311	CHL	CHA-CBD-CGD-O2D
39	8	301	CHL	CHA-CBD-CGD-O2D
22	4	805	CLA	CAA-CBA-CGA-O2A
25	7	318	LHG	C25-C26-C27-C28
22	A	835	CLA	C3-C5-C6-C7
41	5	325	3PH	O11-C1-C2-C3
25	A	850	LHG	C12-C13-C14-C15
22	A	825	CLA	C16-C17-C18-C20
22	5	307	CLA	C11-C12-C13-C15
22	A	833	CLA	C8-C10-C11-C12
22	A	811	CLA	CAA-CBA-CGA-O2A
22	A	820	CLA	CAA-CBA-CGA-O2A
22	B	825	CLA	CAA-CBA-CGA-O2A
22	K	203	CLA	CAA-CBA-CGA-O2A
22	7	312	CLA	CAA-CBA-CGA-O2A
22	8	316	CLA	CAA-CBA-CGA-O2A
22	4	818	CLA	CAA-CBA-CGA-O2A
25	Z	317	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	9	315	LHG	O7-C7-C8-C9
25	9	315	LHG	O8-C23-C24-C25
34	F	308	LMG	O7-C10-C11-C12
35	J	102	T7X	O18-C11-C31-C32
39	4	814	CHL	CAA-CBA-CGA-O2A
35	J	102	T7X	O16-C8-C9-O18
39	8	301	CHL	O1A-CGA-O2A-C1
22	7	304	CLA	C8-C10-C11-C12
22	5	310	CLA	C8-C10-C11-C12
22	A	813	CLA	CAA-CBA-CGA-O2A
22	A	855	CLA	CAA-CBA-CGA-O2A
22	B	814	CLA	CAA-CBA-CGA-O2A
22	B	817	CLA	CAA-CBA-CGA-O2A
22	B	823	CLA	CAA-CBA-CGA-O2A
22	Z	305	CLA	CAA-CBA-CGA-O2A
22	6	317	CLA	CAA-CBA-CGA-O2A
22	7	314	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	C2A-CAA-CBA-CGA
22	A	821	CLA	C16-C17-C18-C20
23	B	843	PQN	C26-C27-C28-C29
22	A	810	CLA	CAA-CBA-CGA-O2A
22	B	818	CLA	CAA-CBA-CGA-O2A
34	F	308	LMG	C13-C14-C15-C16
22	A	803	CLA	C11-C10-C8-C7
22	A	827	CLA	C11-C10-C8-C7
22	B	805	CLA	C11-C12-C13-C15
22	B	827	CLA	C11-C10-C8-C7
22	B	833	CLA	C11-C12-C13-C15
22	3	310	CLA	C11-C10-C8-C7
22	3	313	CLA	C11-C10-C8-C7
22	5	310	CLA	C6-C7-C8-C10
22	5	318	CLA	C11-C12-C13-C15
25	A	849	LHG	O9-C7-O7-C5
39	5	316	CHL	C8-C10-C11-C12
22	6	314	CLA	CAA-CBA-CGA-O2A
22	A	803	CLA	C11-C10-C8-C9
22	A	824	CLA	C11-C10-C8-C9
22	A	825	CLA	C11-C10-C8-C9
22	A	829	CLA	C6-C7-C8-C9
22	A	829	CLA	C11-C12-C13-C14
22	A	840	CLA	C11-C12-C13-C14
22	Z	308	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	6	309	CLA	C11-C10-C8-C9
36	J	105	C7Z	C33-C34-C35-C15
22	6	308	CLA	C2B-C3B-CAB-CBB
39	1	312	CHL	C2B-C3B-CAB-CBB
39	Z	312	CHL	C2B-C3B-CAB-CBB
39	8	312	CHL	C2B-C3B-CAB-CBB
39	8	315	CHL	C2B-C3B-CAB-CBB
39	4	813	CHL	C2B-C3B-CAB-CBB
39	4	814	CHL	C2B-C3B-CAB-CBB
39	4	816	CHL	C2B-C3B-CAB-CBB
39	5	317	CHL	C2B-C3B-CAB-CBB
39	6	315	CHL	C2B-C3B-CAB-CBB
39	6	318	CHL	C2B-C3B-CAB-CBB
42	7	320	SPH	C6-C7-C8-C9
22	6	322	CLA	CBA-CGA-O2A-C1
22	A	827	CLA	CAA-CBA-CGA-O2A
25	8	317	LHG	O7-C7-C8-C9
22	8	308	CLA	O1D-CGD-O2D-CED
22	Z	309	CLA	CBD-CGD-O2D-CED
22	8	308	CLA	CBD-CGD-O2D-CED
22	9	309	CLA	O1D-CGD-O2D-CED
22	1	310	CLA	C4C-C3C-CAC-CBC
22	B	830	CLA	C4-C3-C5-C6
25	1	317	LHG	C24-C25-C26-C27
22	A	807	CLA	CAA-CBA-CGA-O1A
22	A	812	CLA	CAA-CBA-CGA-O1A
38	7	301	LUT	C27-C28-C29-C30
27	A	852	DGA	CDA-CEA-CFA-CGA
22	B	806	CLA	C1A-C2A-CAA-CBA
22	G	201	CLA	C1A-C2A-CAA-CBA
22	4	806	CLA	C1A-C2A-CAA-CBA
22	5	312	CLA	C1A-C2A-CAA-CBA
39	9	312	CHL	C1A-C2A-CAA-CBA
22	A	815	CLA	CAA-CBA-CGA-O1A
22	A	837	CLA	CAA-CBA-CGA-O1A
22	Z	306	CLA	C5-C6-C7-C8
25	Z	317	LHG	C29-C30-C31-C32
22	1	306	CLA	CAA-CBA-CGA-O1A
22	3	322	CLA	CAA-CBA-CGA-O1A
22	9	305	CLA	CAA-CBA-CGA-O1A
27	A	852	DGA	OG1-CG1-CG2-CG3
22	B	828	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	G	201	CLA	CAA-CBA-CGA-O2A
22	5	308	CLA	CAA-CBA-CGA-O2A
39	Z	311	CHL	CAA-CBA-CGA-O2A
27	A	852	DGA	CB4-CB5-CB6-CB7
22	A	834	CLA	C2A-CAA-CBA-CGA
22	6	301	CLA	C2A-CAA-CBA-CGA
25	6	323	LHG	C3-O3-P-O6
22	6	310	CLA	C16-C17-C18-C19
39	6	315	CHL	C6-C7-C8-C10
22	8	309	CLA	CAA-CBA-CGA-O1A
25	A	849	LHG	O9-C7-C8-C9
25	1	317	LHG	O10-C23-C24-C25
25	9	315	LHG	O10-C23-C24-C25
22	A	811	CLA	C13-C15-C16-C17
22	4	808	CLA	C10-C11-C12-C13
22	Z	306	CLA	CAA-CBA-CGA-O2A
39	8	312	CHL	CAA-CBA-CGA-O2A
39	4	813	CHL	CAA-CBA-CGA-O2A
39	5	317	CHL	CAA-CBA-CGA-O2A
39	6	316	CHL	CAA-CBA-CGA-O2A
39	2	303	CHL	CAA-CBA-CGA-O2A
22	Z	303	CLA	C10-C11-C12-C13
25	4	820	LHG	C5-C4-O6-P
22	B	824	CLA	CAA-CBA-CGA-O1A
22	3	308	CLA	CAA-CBA-CGA-O1A
22	7	324	CLA	CAA-CBA-CGA-O1A
22	4	806	CLA	CAA-CBA-CGA-O1A
22	5	323	CLA	CAA-CBA-CGA-O1A
31	1	319	DGD	C2E-C1E-O5D-C6D
22	A	814	CLA	C5-C6-C7-C8
22	A	824	CLA	C5-C6-C7-C8
22	F	304	CLA	C4B-C3B-CAB-CBB
22	7	311	CLA	C4B-C3B-CAB-CBB
22	6	313	CLA	C4B-C3B-CAB-CBB
25	B	850	LHG	C4-O6-P-O5
25	B	851	LHG	C3-O3-P-O4
25	Z	317	LHG	C4-O6-P-O5
25	8	317	LHG	C4-O6-P-O5
25	4	820	LHG	C3-O3-P-O5
25	5	324	LHG	C4-O6-P-O5
39	3	317	CHL	C4B-C3B-CAB-CBB
39	5	321	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
39	6	316	CHL	C4B-C3B-CAB-CBB
39	6	320	CHL	C4B-C3B-CAB-CBB
39	2	303	CHL	C4B-C3B-CAB-CBB
43	8	319	LPX	C1-O2-P1-O4
22	B	814	CLA	C11-C12-C13-C14
22	A	811	CLA	CAA-CBA-CGA-O1A
22	K	203	CLA	CAA-CBA-CGA-O1A
22	8	316	CLA	CAA-CBA-CGA-O1A
22	4	805	CLA	CAA-CBA-CGA-O1A
31	3	301	DGD	O1A-C1A-C2A-C3A
22	B	822	CLA	CAA-CBA-CGA-O2A
22	B	837	CLA	CAA-CBA-CGA-O2A
22	1	310	CLA	C10-C11-C12-C13
24	B	845	BCR	C23-C24-C25-C26
24	I	4001	BCR	C1-C6-C7-C8
22	A	820	CLA	CAA-CBA-CGA-O1A
22	B	812	CLA	CAA-CBA-CGA-O1A
22	B	814	CLA	CAA-CBA-CGA-O1A
22	3	314	CLA	CAA-CBA-CGA-O1A
25	9	315	LHG	O9-C7-C8-C9
39	4	814	CHL	CAA-CBA-CGA-O1A
25	Z	317	LHG	C11-C10-C9-C8
22	Z	303	CLA	CAA-CBA-CGA-O2A
22	9	308	CLA	CAA-CBA-CGA-O2A
26	8	318	NKP	OAJ-CAK-CAL-CAM
22	1	307	CLA	C11-C12-C13-C14
22	7	312	CLA	C11-C12-C13-C15
22	A	810	CLA	CAA-CBA-CGA-O1A
22	A	855	CLA	CAA-CBA-CGA-O1A
25	Z	317	LHG	O10-C23-C24-C25
34	F	308	LMG	O9-C10-C11-C12
35	J	102	T7X	O19-C11-C31-C32
22	A	824	CLA	C15-C16-C17-C18
22	A	834	CLA	C13-C15-C16-C17
21	A	801	CL0	CAA-CBA-CGA-O1A
22	A	842	CLA	CAA-CBA-CGA-O1A
22	Z	305	CLA	CAA-CBA-CGA-O1A
22	5	309	CLA	CAA-CBA-CGA-O1A
24	B	846	BCR	C9-C10-C11-C12
24	B	853	BCR	C9-C10-C11-C12
22	7	324	CLA	C2-C3-C5-C6
23	B	843	PQN	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	A	807	CLA	CAD-CBD-CGD-O1D
22	A	811	CLA	CAD-CBD-CGD-O1D
22	A	817	CLA	CAD-CBD-CGD-O1D
22	A	832	CLA	CAD-CBD-CGD-O1D
22	B	824	CLA	CAD-CBD-CGD-O1D
22	B	836	CLA	CAD-CBD-CGD-O1D
22	B	837	CLA	C2-C3-C5-C6
22	K	204	CLA	CAD-CBD-CGD-O1D
22	1	310	CLA	CAD-CBD-CGD-O1D
22	1	316	CLA	CAD-CBD-CGD-O1D
22	3	309	CLA	CAD-CBD-CGD-O1D
22	3	312	CLA	CAD-CBD-CGD-O1D
22	7	304	CLA	CAD-CBD-CGD-O1D
22	7	314	CLA	CAD-CBD-CGD-O1D
22	7	316	CLA	CAD-CBD-CGD-O1D
22	8	306	CLA	CAD-CBD-CGD-O1D
22	8	308	CLA	CAD-CBD-CGD-O1D
22	4	809	CLA	CAD-CBD-CGD-O1D
22	4	811	CLA	CAD-CBD-CGD-O1D
22	5	301	CLA	CAD-CBD-CGD-O1D
22	5	320	CLA	CAD-CBD-CGD-O1D
41	7	319	3PH	C21-C22-C23-C24
22	A	827	CLA	CAA-CBA-CGA-O1A
22	9	306	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	CAA-CBA-CGA-O2A
22	K	204	CLA	CAA-CBA-CGA-O2A
22	3	316	CLA	CAA-CBA-CGA-O2A
22	A	810	CLA	C11-C12-C13-C14
22	A	811	CLA	C11-C10-C8-C9
22	A	827	CLA	C11-C10-C8-C9
22	B	801	CLA	C14-C13-C15-C16
22	B	808	CLA	C11-C10-C8-C9
22	B	809	CLA	C11-C10-C8-C9
22	B	827	CLA	C11-C10-C8-C9
22	B	833	CLA	C11-C12-C13-C14
22	1	306	CLA	C6-C7-C8-C9
22	3	310	CLA	C11-C10-C8-C9
22	5	318	CLA	C11-C12-C13-C14
23	A	843	PQN	C16-C17-C18-C19
22	A	832	CLA	C15-C16-C17-C18
22	B	814	CLA	C5-C6-C7-C8
22	B	817	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	4	818	CLA	CAA-CBA-CGA-O1A
22	6	317	CLA	CAA-CBA-CGA-O1A
22	A	823	CLA	CAA-CBA-CGA-O2A
22	A	854	CLA	CAA-CBA-CGA-O2A
22	B	831	CLA	CAA-CBA-CGA-O2A
22	F	304	CLA	CAA-CBA-CGA-O2A
22	Z	315	CLA	CAA-CBA-CGA-O2A
22	8	306	CLA	CAA-CBA-CGA-O2A
22	5	310	CLA	CAA-CBA-CGA-O2A
25	6	323	LHG	O7-C7-C8-C9
27	A	852	DGA	OG1-CA1-CA2-CA3
37	K	201	DAO	C7-C8-C9-C10
22	8	314	CLA	C2A-CAA-CBA-CGA
22	A	829	CLA	CAA-CBA-CGA-O2A
22	A	831	CLA	CAA-CBA-CGA-O2A
22	B	808	CLA	CAA-CBA-CGA-O2A
22	B	839	CLA	CAA-CBA-CGA-O2A
22	1	315	CLA	CAA-CBA-CGA-O2A
22	Z	314	CLA	CAA-CBA-CGA-O2A
22	5	318	CLA	CAA-CBA-CGA-O2A
25	4	821	LHG	O7-C7-C8-C9
39	5	316	CHL	CAA-CBA-CGA-O2A
22	L	201	CLA	C8-C10-C11-C12
22	A	813	CLA	CAA-CBA-CGA-O1A
22	6	314	CLA	CAA-CBA-CGA-O1A
22	A	825	CLA	C4-C3-C5-C6
22	3	322	CLA	C4-C3-C5-C6
21	A	801	CL0	C11-C10-C8-C7
22	A	803	CLA	C11-C12-C13-C15
22	A	810	CLA	C11-C10-C8-C7
22	A	812	CLA	C11-C12-C13-C15
22	A	820	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	C3A-C2A-CAA-CBA
22	A	829	CLA	C6-C7-C8-C10
22	A	836	CLA	C3A-C2A-CAA-CBA
22	A	841	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C11-C10-C8-C7
22	B	818	CLA	C11-C10-C8-C7
22	B	825	CLA	C2-C3-C5-C6
22	B	826	CLA	C12-C13-C15-C16
22	B	829	CLA	C11-C10-C8-C7
22	B	830	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	831	CLA	C3A-C2A-CAA-CBA
22	F	304	CLA	C6-C7-C8-C10
22	L	201	CLA	C11-C12-C13-C15
22	7	310	CLA	C3A-C2A-CAA-CBA
22	8	308	CLA	C11-C12-C13-C15
22	6	312	CLA	C11-C12-C13-C15
22	9	305	CLA	C3A-C2A-CAA-CBA
22	9	305	CLA	C6-C7-C8-C10
39	8	315	CHL	C6-C7-C8-C10
22	B	823	CLA	CAA-CBA-CGA-O1A
22	F	304	CLA	CAA-CBA-CGA-O1A
25	8	317	LHG	O9-C7-C8-C9
39	Z	311	CHL	CAA-CBA-CGA-O1A
39	6	316	CHL	CAA-CBA-CGA-O1A
39	2	303	CHL	CAA-CBA-CGA-O1A
22	K	202	CLA	CAA-CBA-CGA-O2A
22	Z	309	CLA	CAA-CBA-CGA-O2A
22	3	313	CLA	CAA-CBA-CGA-O2A
22	6	312	CLA	CAA-CBA-CGA-O2A
22	6	319	CLA	CAA-CBA-CGA-O2A
25	A	849	LHG	O8-C23-C24-C25
39	1	312	CHL	CAA-CBA-CGA-O2A
39	Z	312	CHL	CAA-CBA-CGA-O2A
31	B	852	DGD	C5B-C6B-C7B-C8B
38	4	802	LUT	C27-C28-C29-C30
38	9	301	LUT	C7-C8-C9-C10
22	A	831	CLA	CAA-CBA-CGA-O1A
22	G	201	CLA	CAA-CBA-CGA-O1A
25	A	849	LHG	O10-C23-C24-C25
25	4	821	LHG	O9-C7-C8-C9
39	8	312	CHL	CAA-CBA-CGA-O1A
38	4	803	LUT	C13-C14-C15-C35
39	6	315	CHL	C6-C7-C8-C9
22	A	833	CLA	CAA-CBA-CGA-O2A
22	B	838	CLA	CAA-CBA-CGA-O2A
22	1	307	CLA	CAA-CBA-CGA-O2A
22	Z	313	CLA	CAA-CBA-CGA-O2A
22	Z	316	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	C5-C6-C7-C8
22	B	822	CLA	CAA-CBA-CGA-O1A
22	B	825	CLA	CAA-CBA-CGA-O1A
22	B	831	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	B	837	CLA	CAA-CBA-CGA-O1A
22	B	839	CLA	CAA-CBA-CGA-O1A
22	K	204	CLA	CAA-CBA-CGA-O1A
22	Z	306	CLA	CAA-CBA-CGA-O1A
22	Z	315	CLA	CAA-CBA-CGA-O1A
22	5	308	CLA	CAA-CBA-CGA-O1A
22	A	817	CLA	CAA-CBA-CGA-O2A
22	B	821	CLA	CAA-CBA-CGA-O2A
22	L	201	CLA	CAA-CBA-CGA-O2A
22	6	308	CLA	CAA-CBA-CGA-O2A
25	B	803	LHG	O8-C23-C24-C25
34	J	101	LMG	O7-C10-C11-C12
22	F	302	CLA	C10-C11-C12-C13
22	A	823	CLA	CAA-CBA-CGA-O1A
22	B	828	CLA	CAA-CBA-CGA-O1A
39	4	813	CHL	CAA-CBA-CGA-O1A
39	5	317	CHL	CAA-CBA-CGA-O1A
22	A	832	CLA	C10-C11-C12-C13
22	1	314	CLA	C13-C15-C16-C17
22	6	309	CLA	C15-C16-C17-C18
22	A	814	CLA	CAA-CBA-CGA-O1A
22	8	306	CLA	CAA-CBA-CGA-O1A
39	5	316	CHL	CAA-CBA-CGA-O1A
22	B	825	CLA	C4-C3-C5-C6
22	1	316	CLA	C4C-C3C-CAC-CBC
22	F	302	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

328 monomers are involved in 2926 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	812	CLA	14	0
24	I	4001	BCR	12	0
22	A	855	CLA	14	0
22	7	322	CLA	15	0
25	B	850	LHG	4	0
22	2	301	CLA	17	0
38	7	301	LUT	14	0
39	4	819	CHL	9	0
22	5	311	CLA	13	0
22	7	306	CLA	11	0
38	Z	302	LUT	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	837	CLA	9	0
22	B	817	CLA	17	0
22	B	824	CLA	18	0
22	9	311	CLA	5	0
22	1	307	CLA	17	0
22	9	304	CLA	2	0
22	A	809	CLA	15	0
22	A	811	CLA	15	0
38	6	304	LUT	13	0
22	7	314	CLA	3	0
23	A	843	PQN	10	0
39	Z	311	CHL	11	0
22	A	828	CLA	14	0
22	8	309	CLA	14	0
22	3	318	CLA	18	0
22	4	812	CLA	4	0
38	1	303	LUT	18	0
22	3	310	CLA	7	0
22	3	309	CLA	7	0
22	1	305	CLA	10	0
22	3	320	CLA	10	0
31	1	319	DGD	10	0
41	6	324	3PH	5	0
37	K	201	DAO	8	0
24	6	305	BCR	19	0
22	9	305	CLA	6	0
24	A	844	BCR	30	0
25	5	324	LHG	7	0
22	B	828	CLA	20	0
33	4	801	LMT	7	0
22	6	310	CLA	15	0
22	B	839	CLA	16	0
22	F	304	CLA	27	0
22	B	818	CLA	13	0
38	6	303	LUT	11	0
22	A	831	CLA	5	0
24	L	204	BCR	17	0
22	A	830	CLA	9	0
22	4	818	CLA	9	0
22	5	308	CLA	23	0
22	B	840	CLA	16	0
25	6	323	LHG	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	F	307	LMT	5	0
39	5	317	CHL	8	0
26	A	851	NKP	3	0
22	B	820	CLA	11	0
22	A	816	CLA	23	0
22	5	323	CLA	9	0
22	A	822	CLA	26	0
22	A	825	CLA	18	0
21	A	801	CL0	7	0
22	1	316	CLA	5	0
22	3	311	CLA	14	0
34	F	308	LMG	1	0
39	6	316	CHL	11	0
22	B	825	CLA	21	0
22	B	808	CLA	13	0
22	1	313	CLA	12	0
22	8	310	CLA	12	0
22	1	306	CLA	8	0
22	2	304	CLA	9	0
38	5	303	LUT	16	0
22	9	313	CLA	17	0
22	Z	308	CLA	12	0
38	4	803	LUT	19	0
22	3	314	CLA	12	0
22	B	831	CLA	10	0
25	Z	317	LHG	9	0
24	B	849	BCR	9	0
22	A	832	CLA	13	0
22	A	815	CLA	18	0
22	B	830	CLA	15	0
22	B	837	CLA	1	0
24	3	306	BCR	14	0
22	Z	315	CLA	10	0
22	5	318	CLA	18	0
22	6	317	CLA	11	0
22	1	304	CLA	14	0
22	8	314	CLA	6	0
22	B	838	CLA	14	0
24	A	846	BCR	11	0
22	F	305	CLA	9	0
39	8	312	CHL	14	0
43	8	319	LPX	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	5	325	3PH	3	0
22	6	319	CLA	11	0
22	A	827	CLA	17	0
25	A	850	LHG	8	0
22	L	203	CLA	6	0
24	B	847	BCR	20	0
22	A	833	CLA	18	0
22	1	310	CLA	10	0
25	1	317	LHG	8	0
22	1	309	CLA	4	0
22	5	322	CLA	10	0
22	6	322	CLA	17	0
22	A	803	CLA	7	0
22	4	806	CLA	8	0
38	4	802	LUT	15	0
22	B	819	CLA	15	0
24	A	856	BCR	24	0
39	8	315	CHL	21	0
22	7	317	CLA	4	0
22	1	314	CLA	19	0
22	5	310	CLA	13	0
22	A	839	CLA	8	0
22	8	311	CLA	14	0
22	B	821	CLA	13	0
22	7	312	CLA	4	0
22	3	313	CLA	22	0
33	G	204	LMT	10	0
22	5	319	CLA	13	0
38	Z	301	LUT	23	0
22	A	829	CLA	16	0
22	L	202	CLA	16	0
26	8	318	NKP	7	0
31	3	301	DGD	21	0
22	7	304	CLA	10	0
22	A	813	CLA	18	0
22	6	314	CLA	17	0
24	3	304	BCR	13	0
22	F	301	CLA	8	0
22	A	834	CLA	10	0
41	8	320	3PH	4	0
22	B	809	CLA	13	0
22	B	811	CLA	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	302	CLA	16	0
22	Z	304	CLA	19	0
40	1	318	SQD	12	0
24	6	306	BCR	16	0
29	C	102	SF4	5	0
39	2	303	CHL	8	0
22	B	823	CLA	14	0
42	7	321	SPH	8	0
22	3	315	CLA	8	0
22	A	836	CLA	13	0
22	A	824	CLA	16	0
22	A	842	CLA	6	0
39	9	312	CHL	24	0
22	6	307	CLA	20	0
39	5	321	CHL	6	0
27	A	852	DGA	20	0
39	6	315	CHL	21	0
22	7	315	CLA	10	0
24	3	305	BCR	15	0
22	5	326	CLA	17	0
24	A	848	BCR	7	0
22	4	815	CLA	12	0
22	6	313	CLA	6	0
25	A	849	LHG	5	0
22	6	308	CLA	15	0
22	A	802	CLA	12	0
25	9	315	LHG	2	0
39	6	320	CHL	13	0
22	7	309	CLA	9	0
22	B	827	CLA	23	0
22	3	322	CLA	15	0
22	A	808	CLA	14	0
22	4	810	CLA	17	0
22	6	301	CLA	20	0
39	9	314	CHL	13	0
22	8	307	CLA	15	0
22	4	805	CLA	17	0
22	A	835	CLA	15	0
22	B	815	CLA	23	0
22	2	302	CLA	5	0
38	5	302	LUT	16	0
29	C	101	SF4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	321	CLA	6	0
22	7	305	CLA	6	0
22	A	814	CLA	23	0
22	5	307	CLA	24	0
22	B	835	CLA	10	0
22	A	804	CLA	14	0
22	B	805	CLA	11	0
22	A	810	CLA	20	0
22	5	313	CLA	12	0
24	A	847	BCR	14	0
39	4	814	CHL	5	0
24	3	307	BCR	19	0
22	A	805	CLA	15	0
22	9	310	CLA	1	0
25	B	851	LHG	3	0
38	8	302	LUT	16	0
22	A	826	CLA	7	0
22	A	819	CLA	8	0
22	A	806	CLA	10	0
22	B	822	CLA	11	0
22	B	829	CLA	12	0
22	5	301	CLA	12	0
25	4	820	LHG	15	0
34	J	101	LMG	10	0
25	8	317	LHG	7	0
22	Z	313	CLA	23	0
22	G	201	CLA	12	0
22	6	311	CLA	10	0
22	4	808	CLA	15	0
22	8	306	CLA	14	0
39	5	316	CHL	17	0
22	9	303	CLA	6	0
23	B	843	PQN	5	0
22	Z	307	CLA	10	0
33	4	822	LMT	2	0
22	6	312	CLA	13	0
22	8	305	CLA	24	0
22	Z	310	CLA	2	0
22	B	813	CLA	7	0
22	1	308	CLA	19	0
22	K	203	CLA	9	0
22	1	315	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	812	CLA	24	0
22	A	821	CLA	24	0
22	7	324	CLA	4	0
22	8	313	CLA	9	0
32	F	306	RRX	19	0
22	J	103	CLA	1	0
22	3	308	CLA	18	0
38	3	302	LUT	10	0
39	3	317	CHL	14	0
22	9	308	CLA	9	0
24	B	845	BCR	9	0
38	1	302	LUT	8	0
22	5	312	CLA	8	0
36	5	306	C7Z	1	0
22	B	833	CLA	12	0
22	7	311	CLA	1	0
22	B	816	CLA	12	0
22	A	818	CLA	11	0
33	1	301	LMT	7	0
38	9	302	LUT	17	0
38	8	303	LUT	12	0
24	5	304	BCR	20	0
29	B	802	SF4	6	0
22	9	307	CLA	8	0
24	J	104	BCR	18	0
22	Z	306	CLA	16	0
39	Z	312	CHL	12	0
24	G	203	BCR	12	0
22	A	807	CLA	15	0
24	A	845	BCR	20	0
22	Z	316	CLA	15	0
22	G	202	CLA	14	0
39	1	312	CHL	8	0
22	Z	303	CLA	29	0
38	3	303	LUT	18	0
35	J	102	T7X	2	0
25	B	803	LHG	8	0
24	5	305	BCR	10	0
39	6	318	CHL	12	0
22	B	832	CLA	9	0
25	4	821	LHG	4	0
22	B	841	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	848	BCR	15	0
22	5	315	CLA	19	0
22	L	201	CLA	15	0
38	9	301	LUT	16	0
42	7	320	SPH	4	0
22	K	202	CLA	9	0
22	9	306	CLA	15	0
22	5	314	CLA	7	0
41	7	319	3PH	14	0
39	7	313	CHL	9	0
39	4	813	CHL	12	0
22	4	807	CLA	12	0
22	8	316	CLA	3	0
38	7	302	LUT	15	0
22	3	312	CLA	24	0
22	Z	309	CLA	21	0
24	8	304	BCR	14	0
22	5	309	CLA	13	0
22	7	308	CLA	12	0
22	4	817	CLA	4	0
22	7	310	CLA	13	0
22	A	838	CLA	7	0
22	A	840	CLA	13	0
22	Z	305	CLA	14	0
31	B	852	DGD	17	0
22	B	807	CLA	8	0
22	4	809	CLA	5	0
24	7	303	BCR	14	0
22	4	811	CLA	6	0
22	3	319	CLA	5	0
22	3	316	CLA	12	0
22	A	823	CLA	28	0
39	4	816	CHL	21	0
24	4	804	BCR	26	0
22	Z	314	CLA	6	0
22	K	204	CLA	6	0
24	B	853	BCR	20	0
22	7	307	CLA	18	0
22	B	814	CLA	16	0
22	6	309	CLA	21	0
25	3	321	LHG	1	0
25	7	318	LHG	10	0

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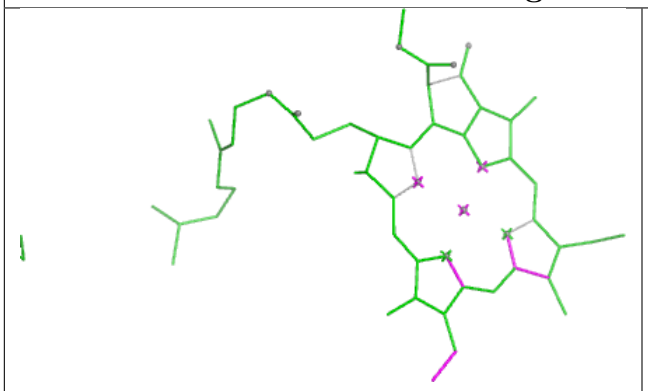
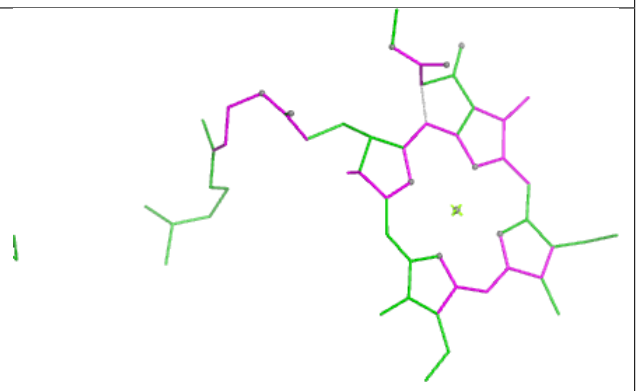
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	846	BCR	12	0
22	A	854	CLA	10	0
22	B	810	CLA	13	0
22	K	205	CLA	4	0
22	A	820	CLA	8	0
24	F	303	BCR	14	0
22	5	320	CLA	11	0
24	K	206	BCR	12	0
22	6	302	CLA	16	0
39	8	301	CHL	11	0
22	A	841	CLA	16	0
22	B	834	CLA	11	0
22	A	817	CLA	14	0
22	B	806	CLA	19	0
22	B	842	CLA	24	0
22	7	323	CLA	16	0
22	B	801	CLA	13	0
22	B	836	CLA	7	0
22	8	308	CLA	11	0
22	B	826	CLA	12	0
36	J	105	C7Z	2	0
24	B	844	BCR	20	0
22	7	316	CLA	8	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.

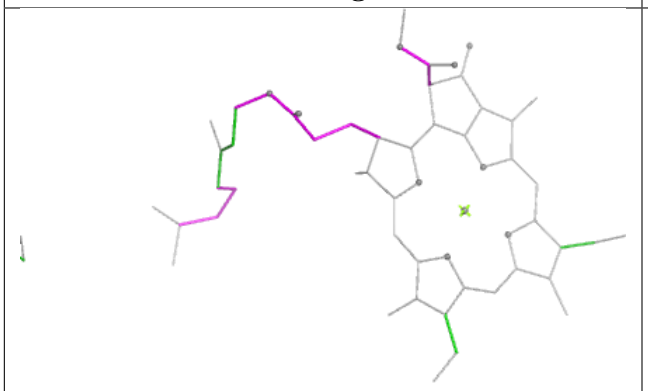
Ligand CLA B 812



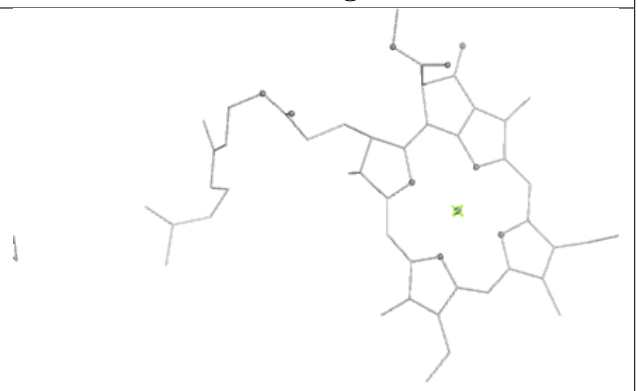
Bond lengths



Bond angles

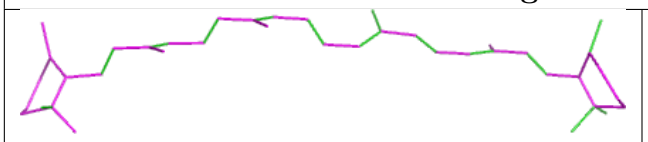


Torsions



Rings

Ligand BCR I 4001



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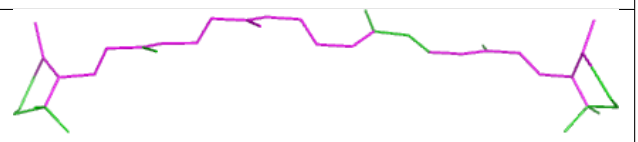

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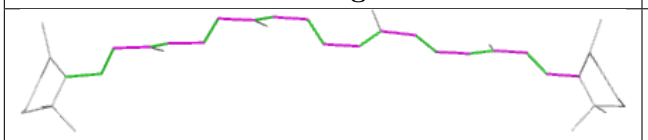
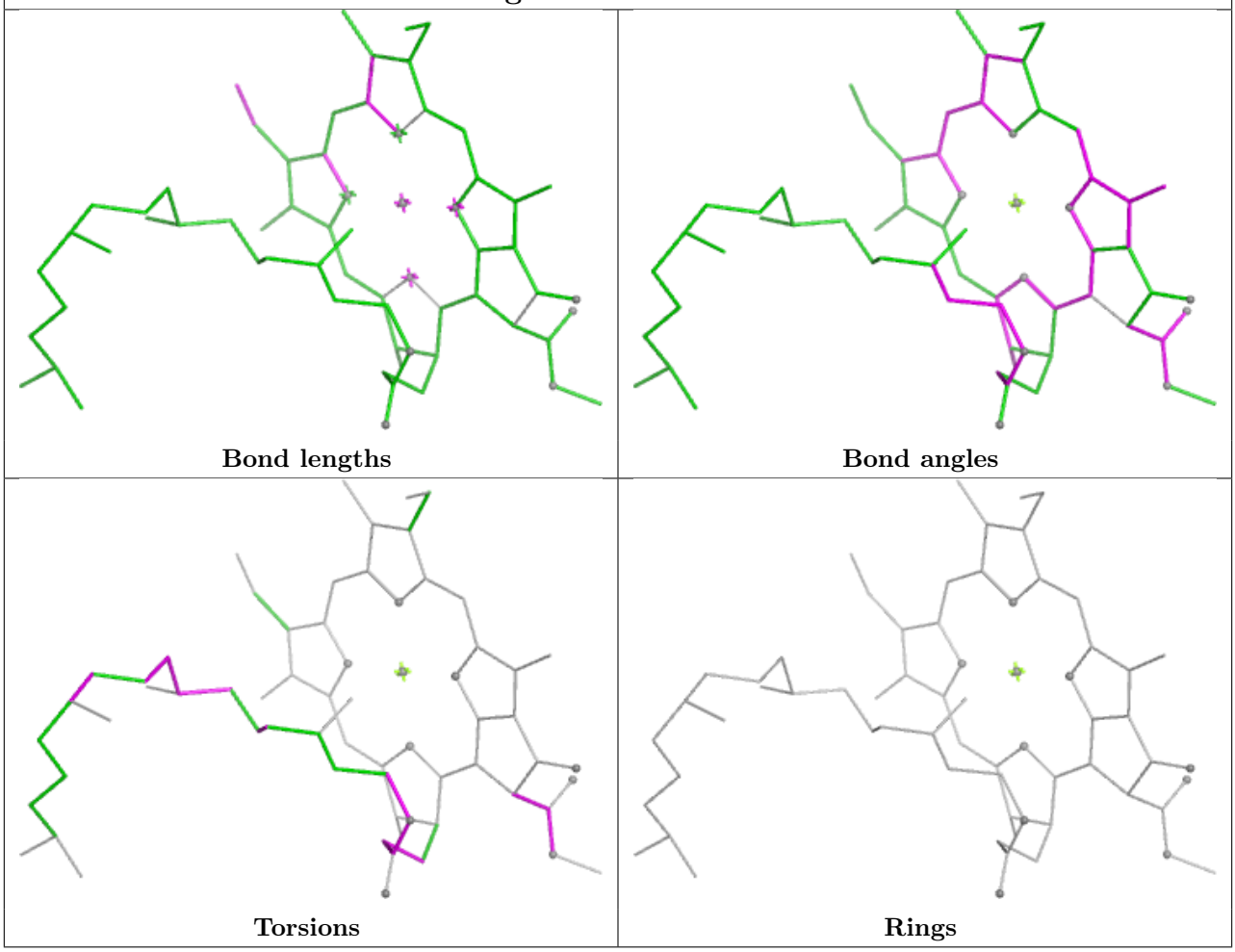


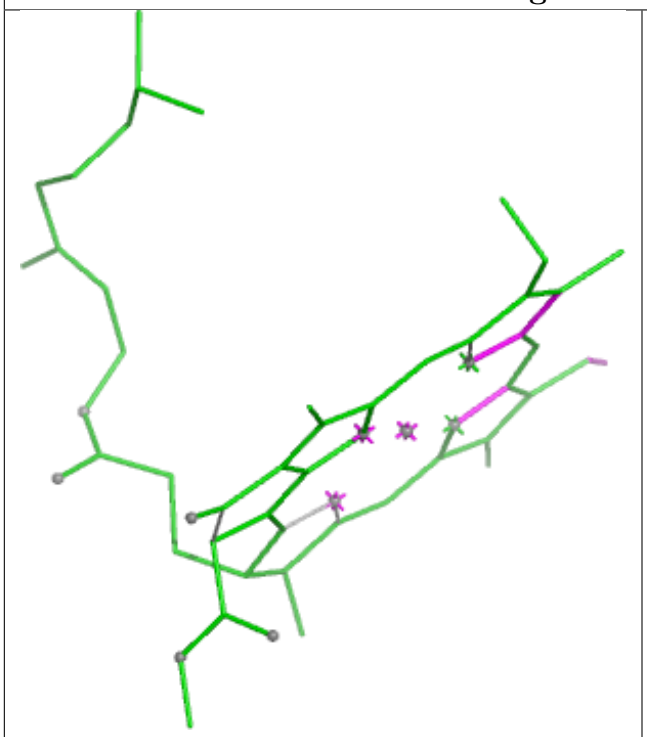
Torsions

Rings

Ligand CLA A 855

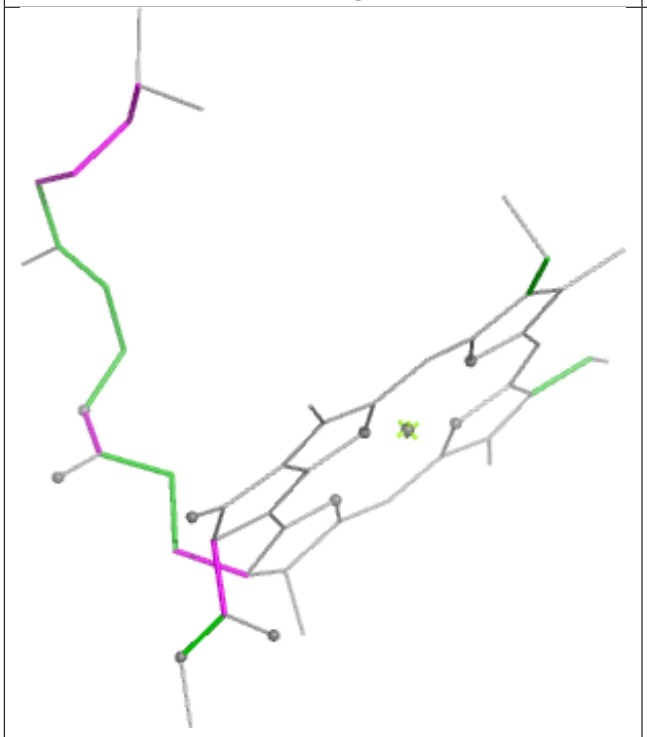


Ligand CLA 7 322



Bond lengths

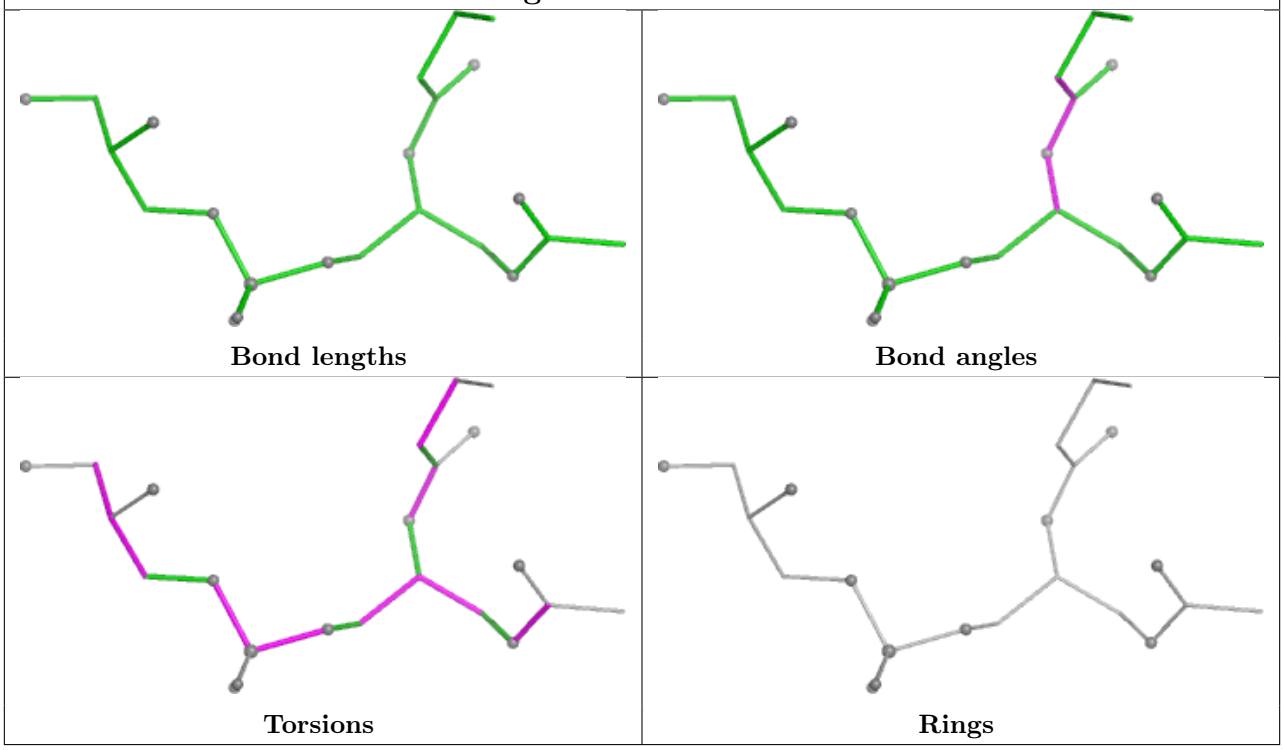
Bond angles



Torsions

Rings

Ligand LHG B 850



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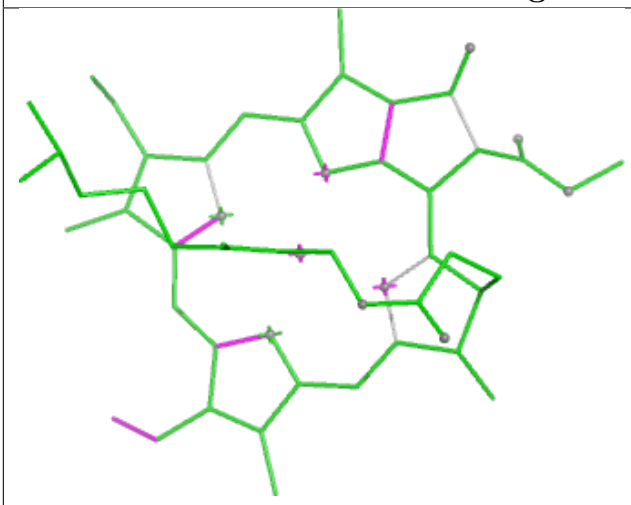

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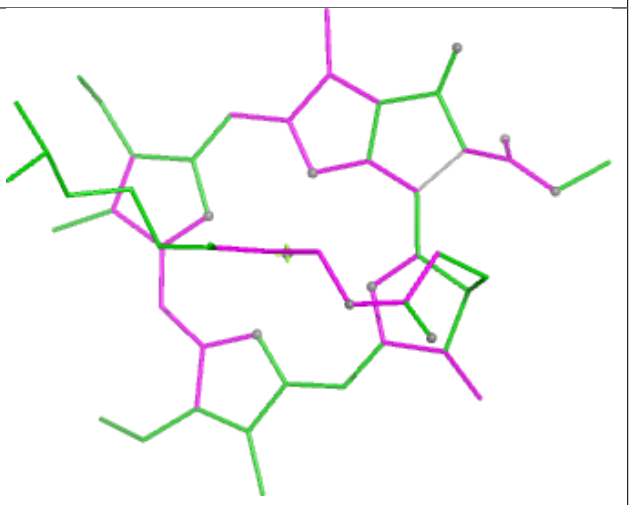

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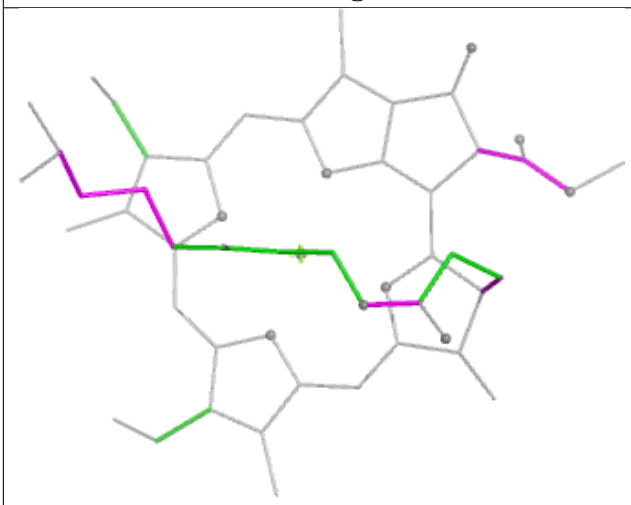

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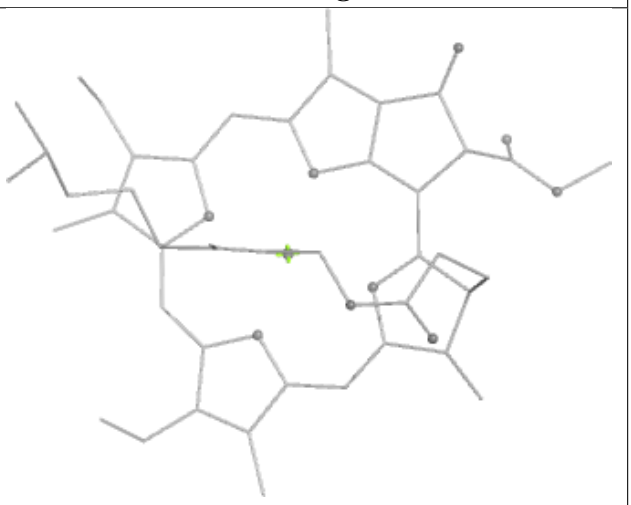
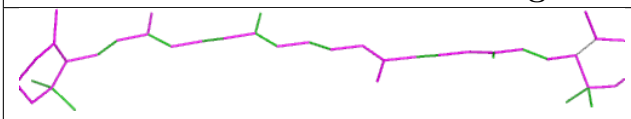


Rings

Ligand LUT 7 301



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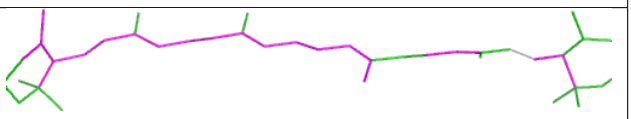
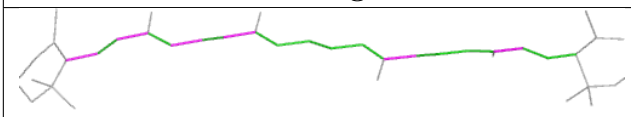


Bond angles



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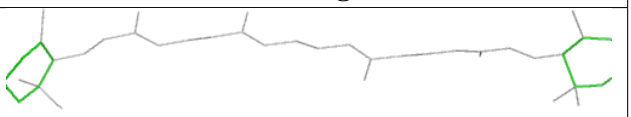
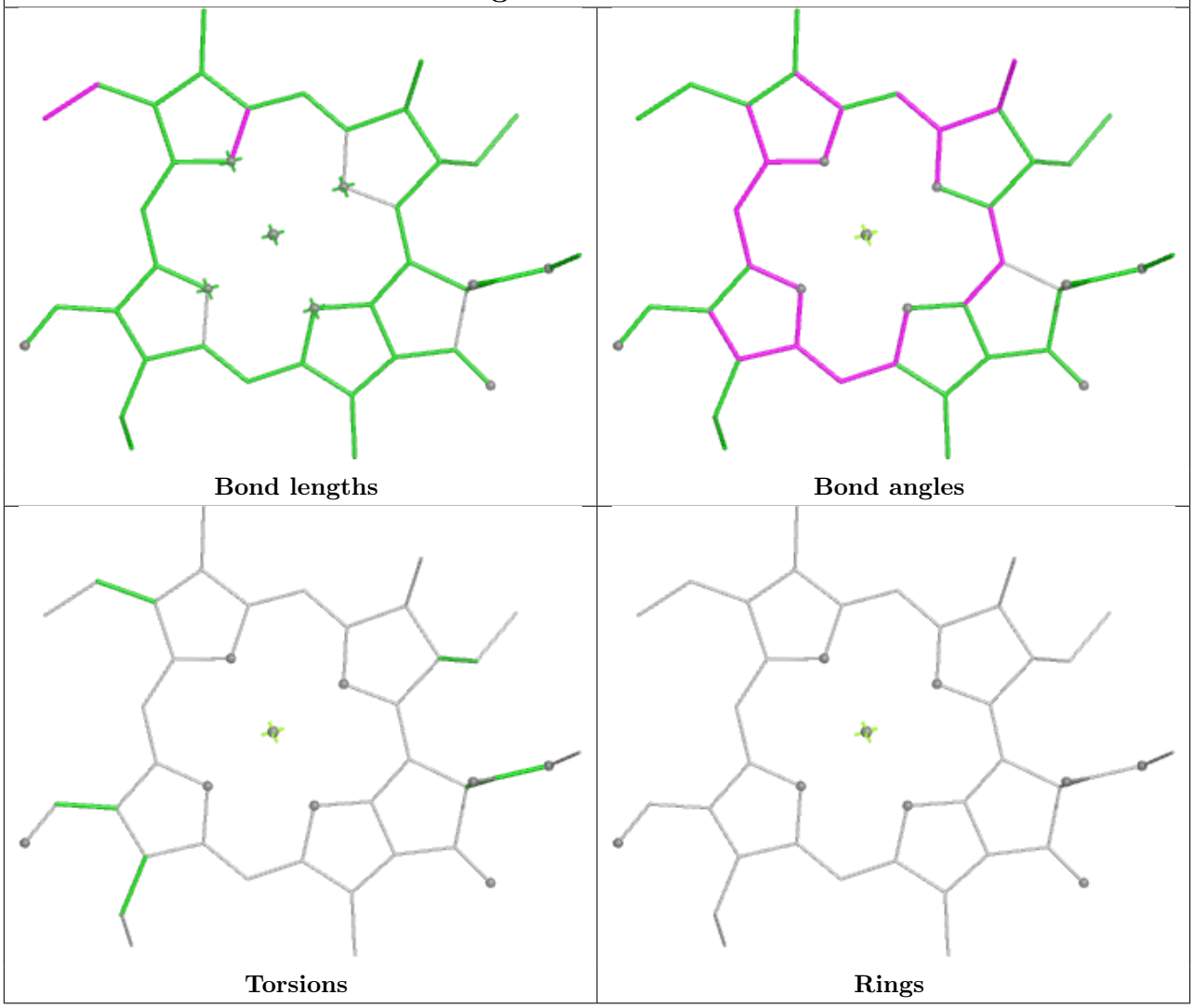
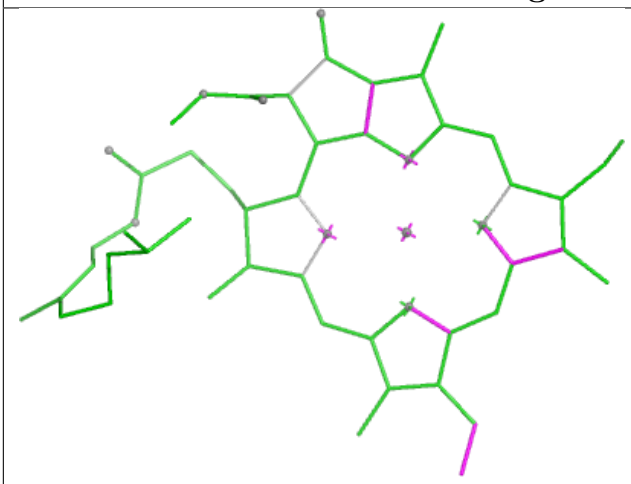


Rings

Ligand CHL 4 819



Ligand CLA 5 311



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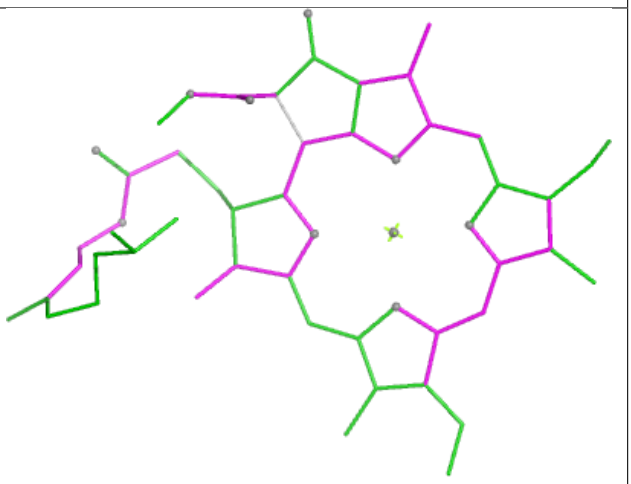

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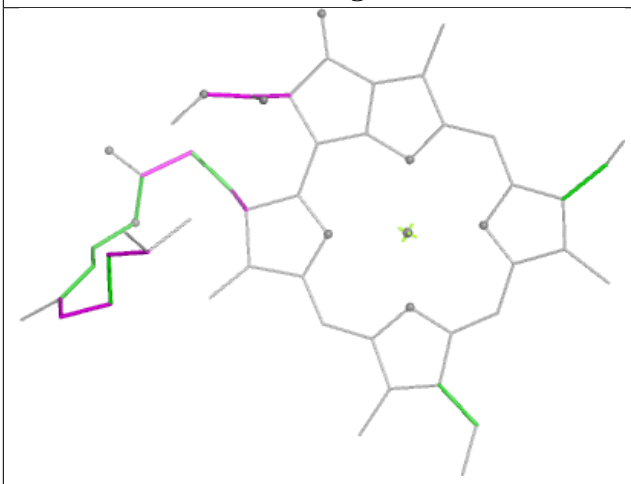

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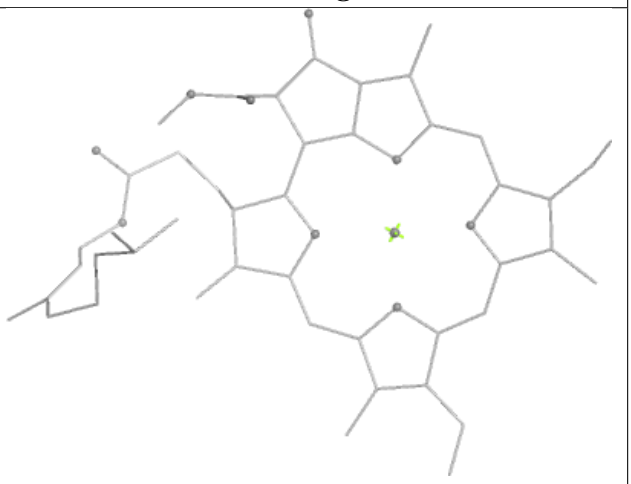

Rings

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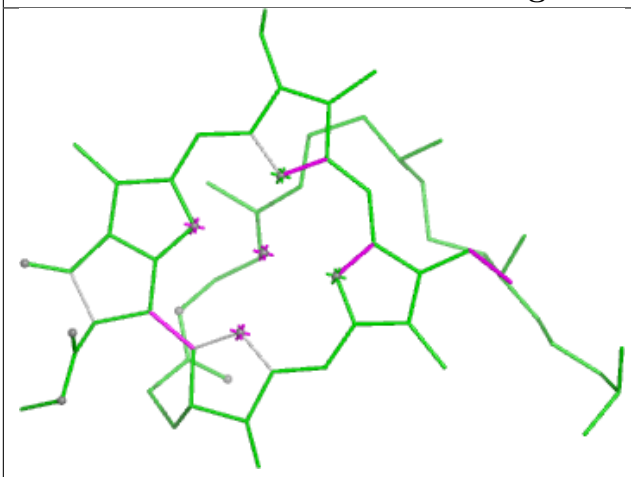

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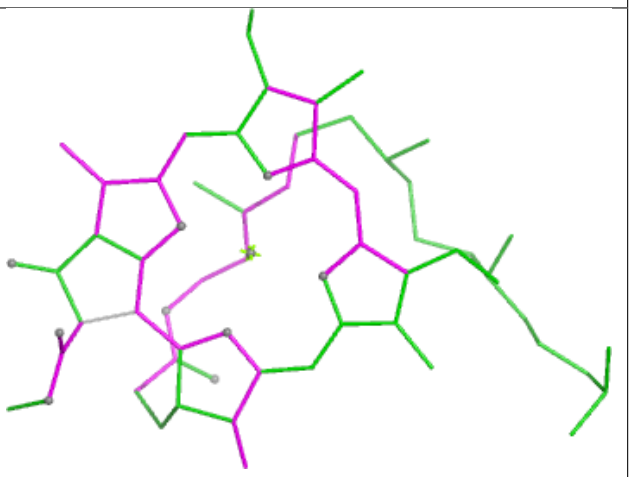
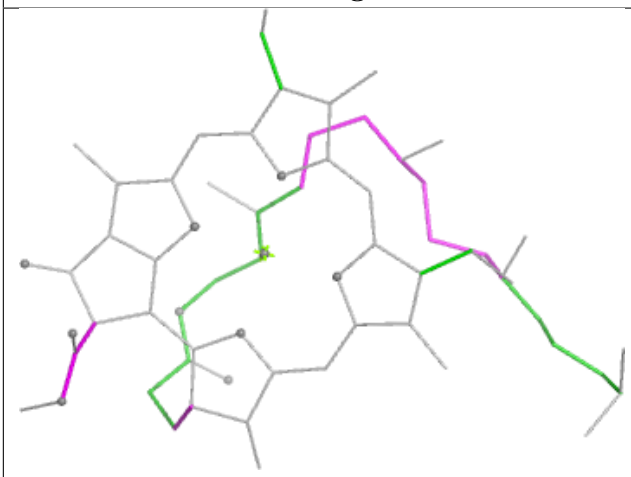


Bond angles



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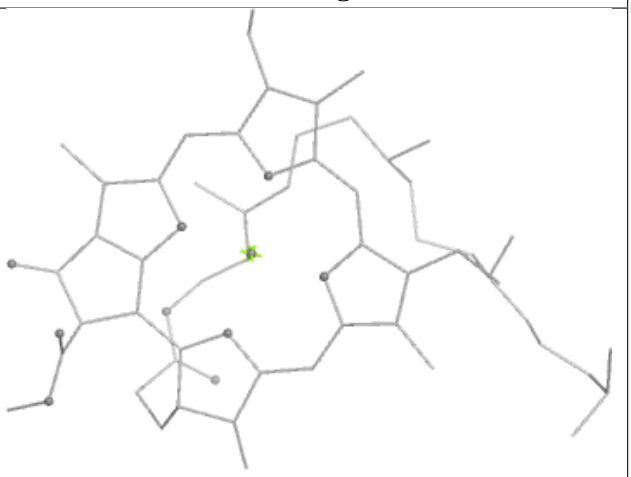
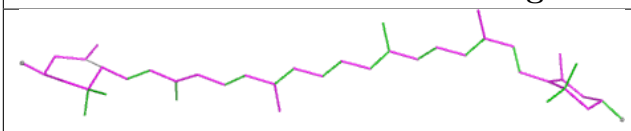


Rings

Ligand LUT Z 302



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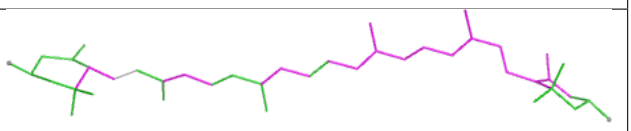
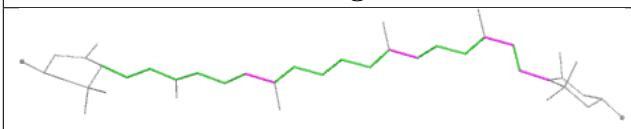


Bond angles



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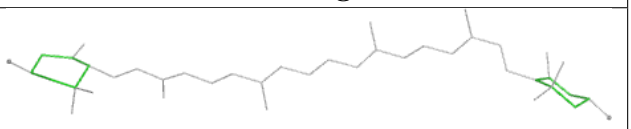
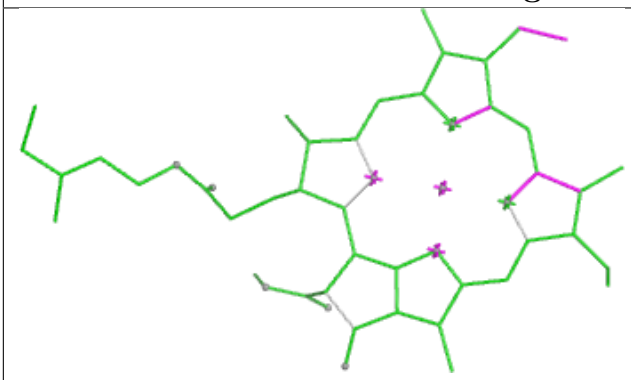
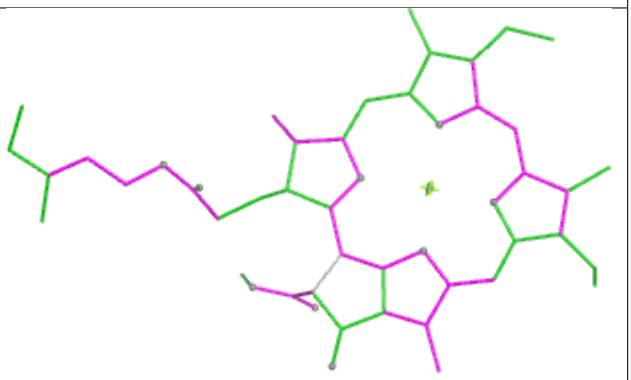
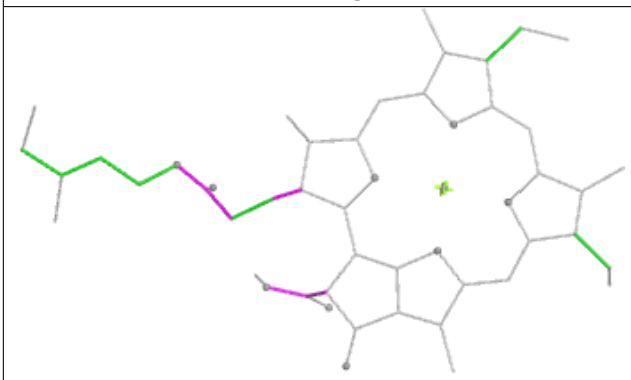
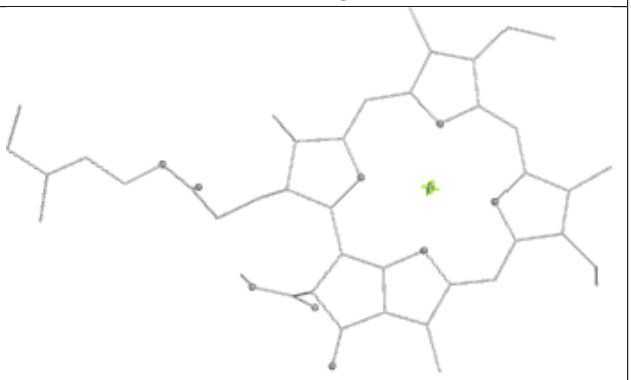
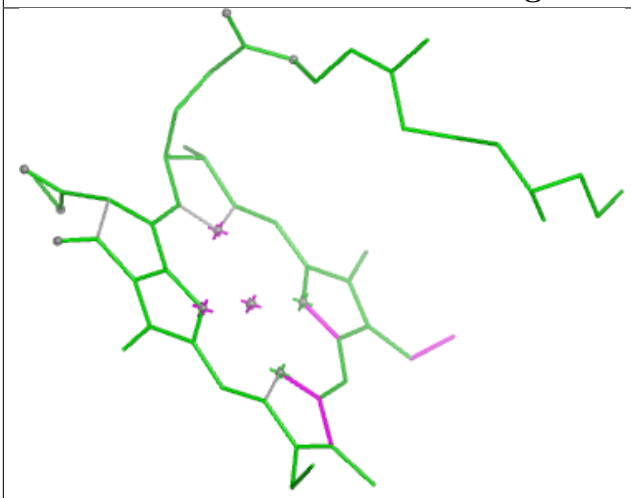


Rings

Ligand CLA A 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 817



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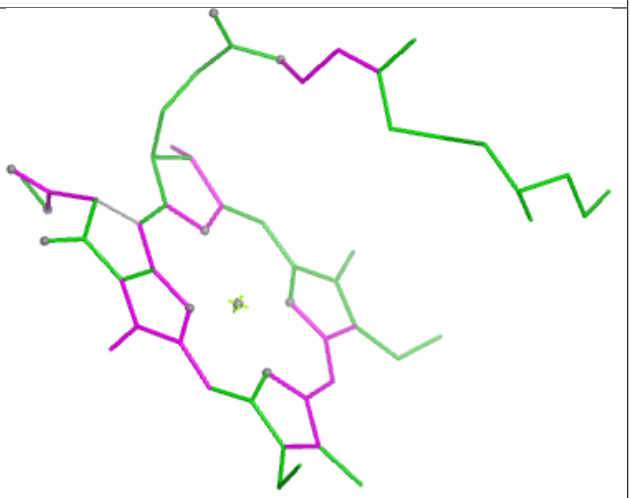
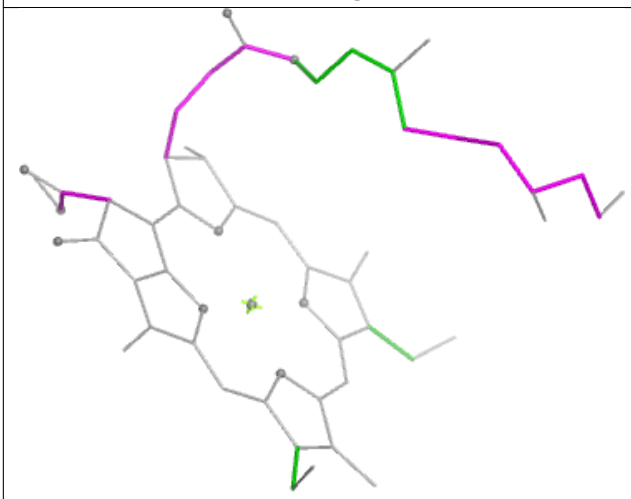
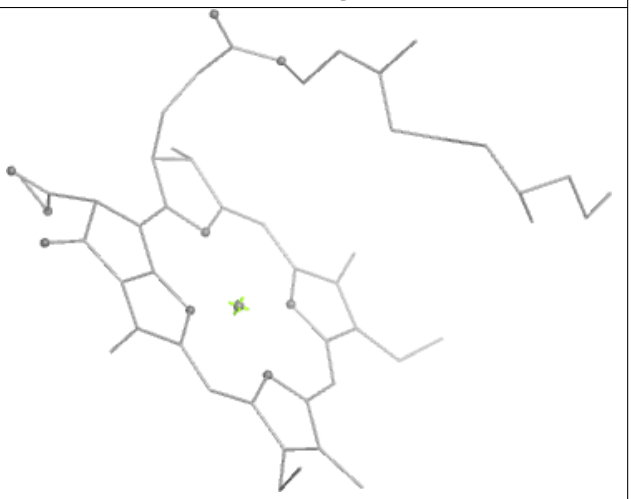


Bond angles

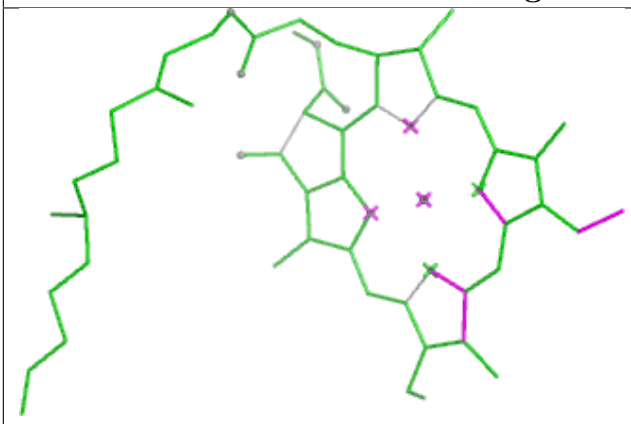


Torsions



Rings

Ligand CLA B 824



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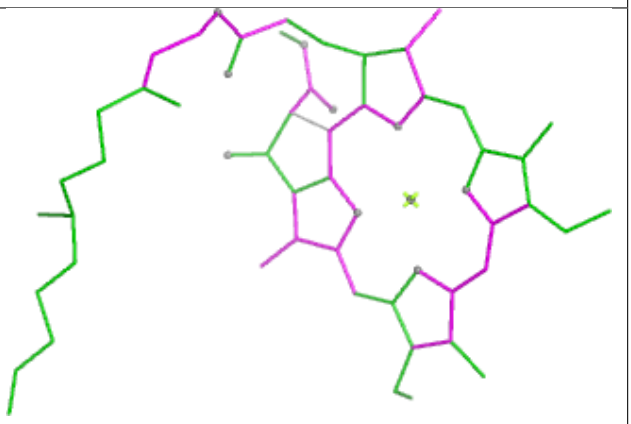
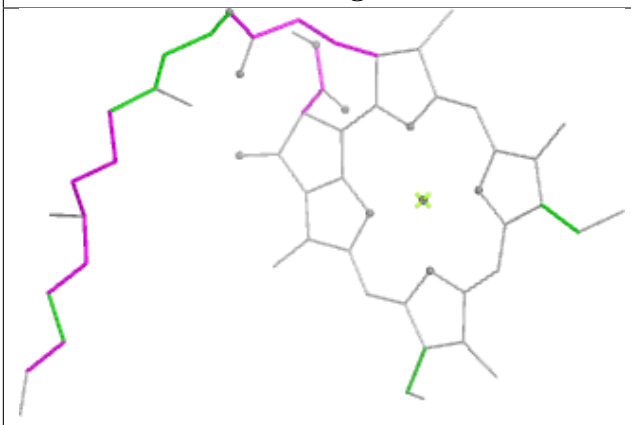


Bond angles



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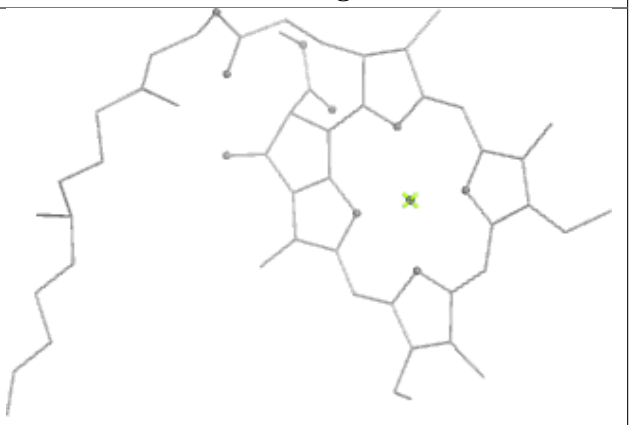
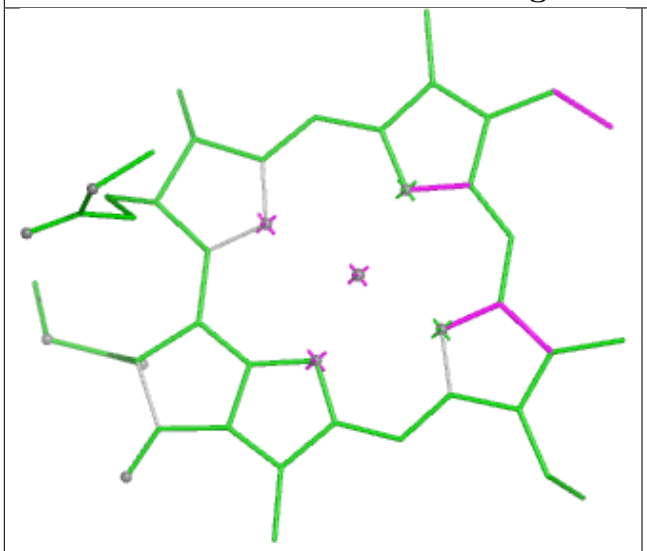


Rings

Ligand CLA 9 311



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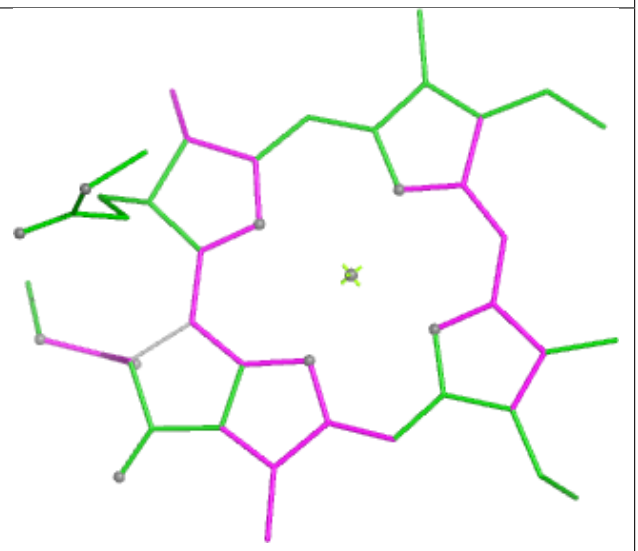

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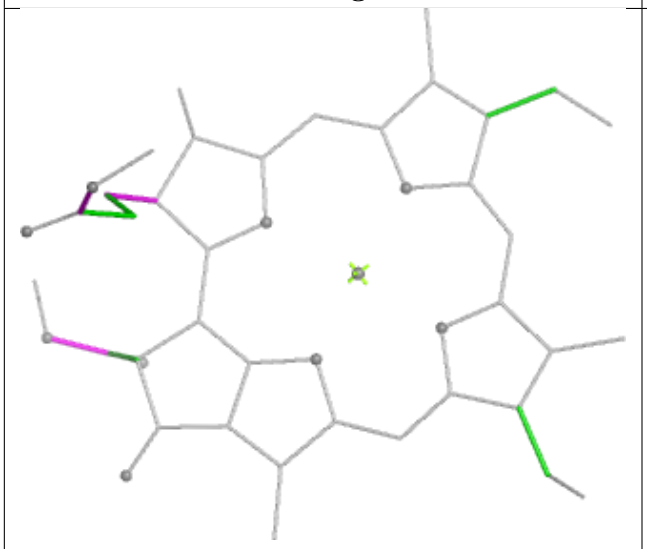

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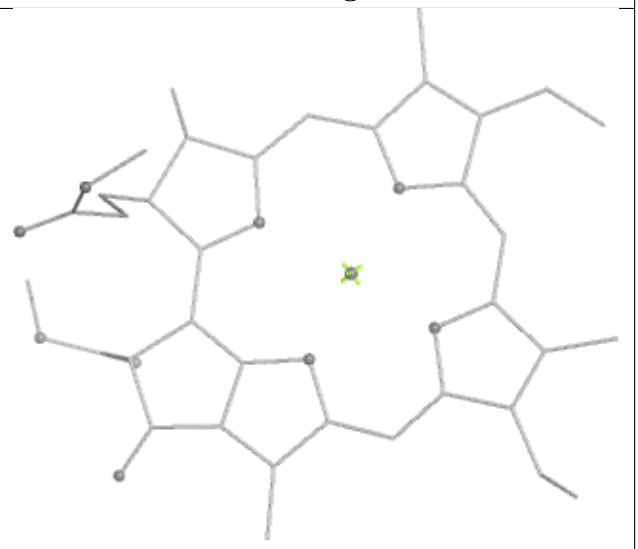
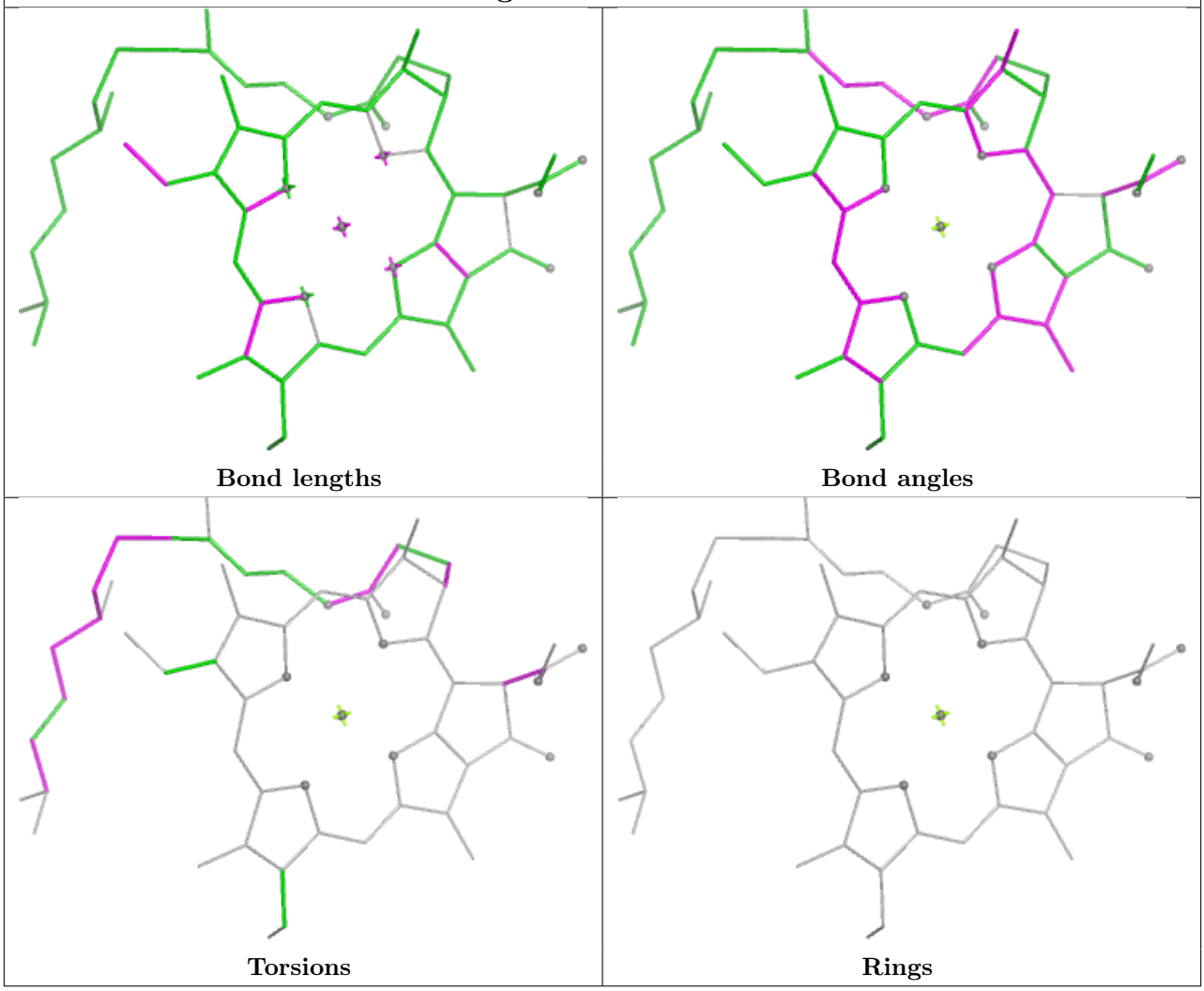


Rings

Ligand CLA 1 307



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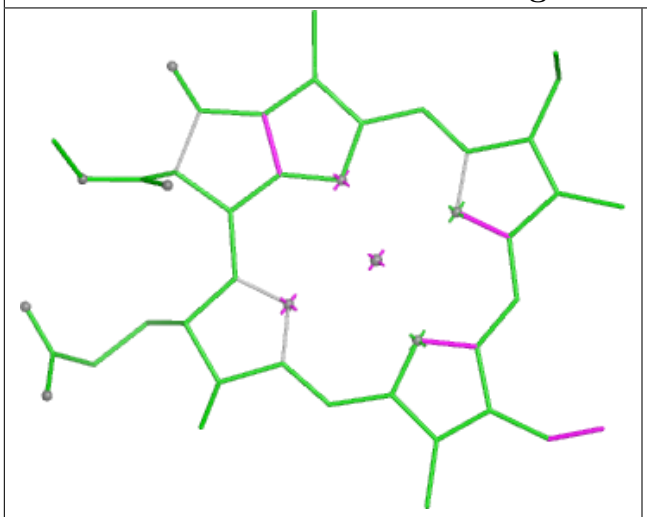
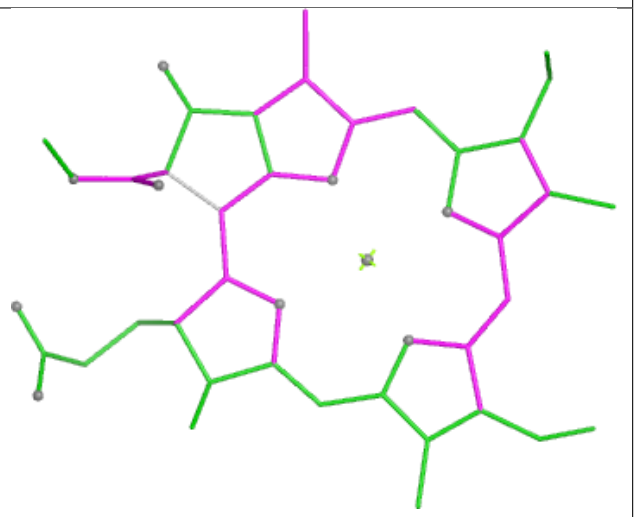
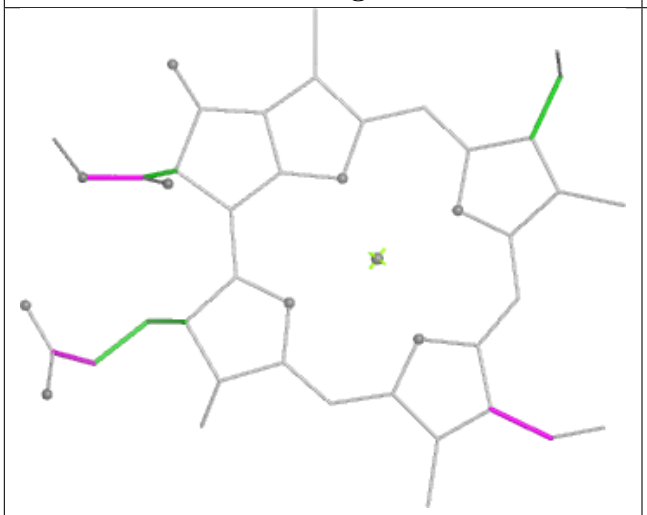


Bond lengths



Bond angles



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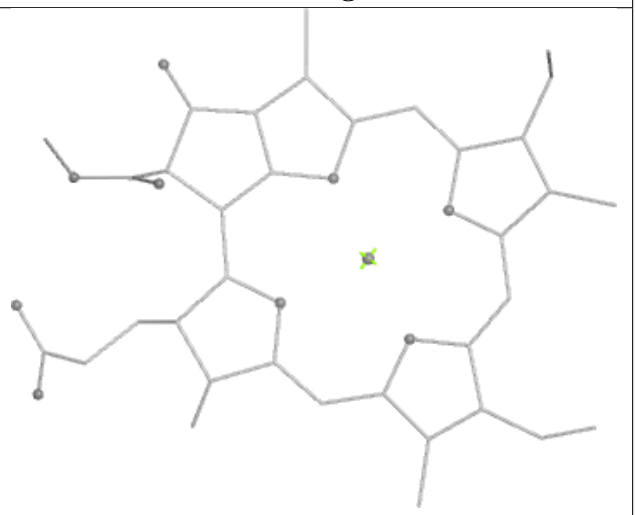
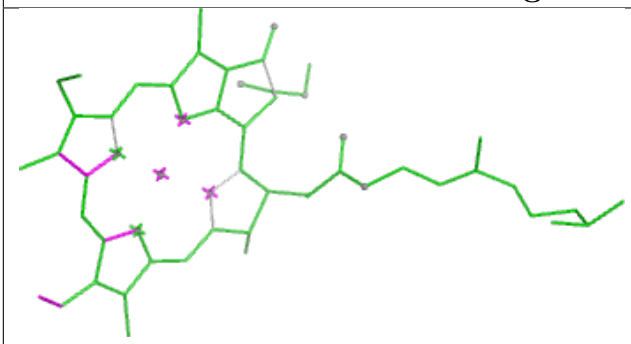
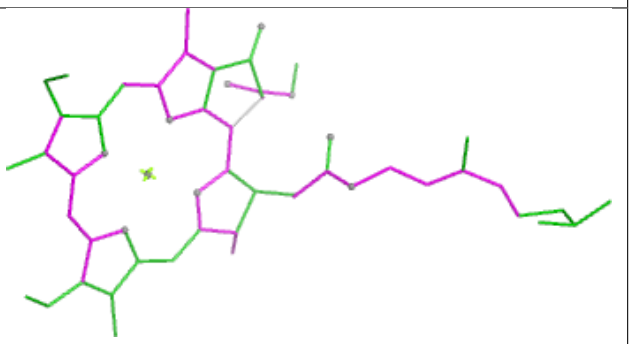


Rings

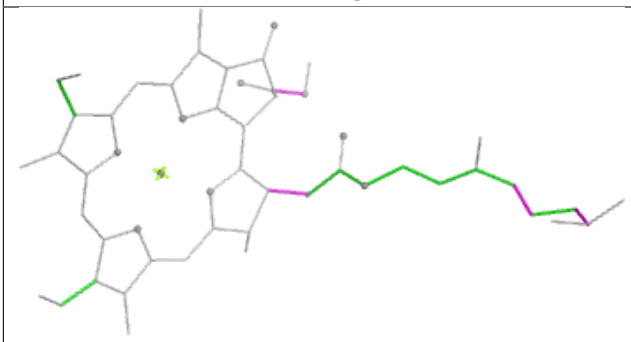
Ligand CLA A 809



Bond lengths



Bond angles



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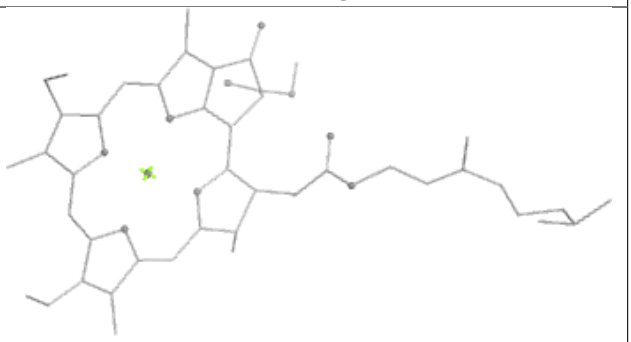
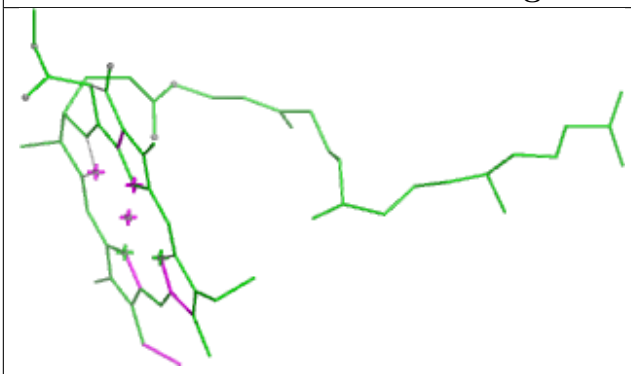
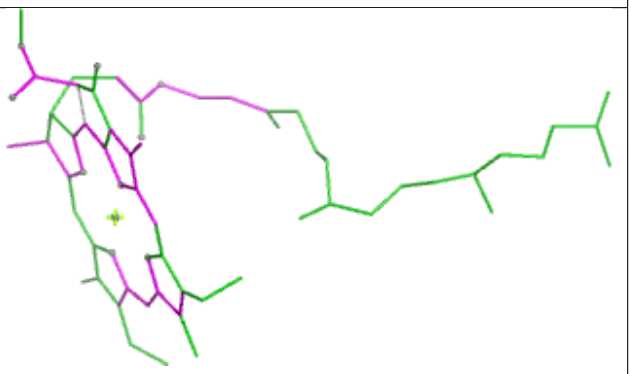


Rings

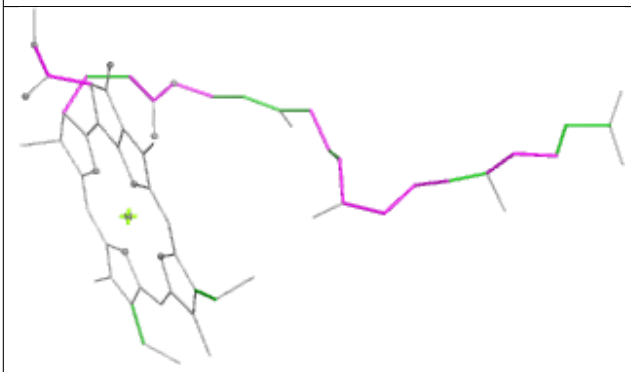
Ligand CLA A 811



Bond lengths



Bond angles



Torsions

Rings

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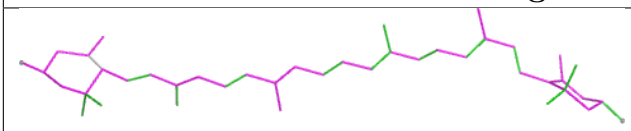
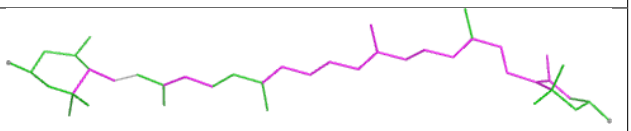
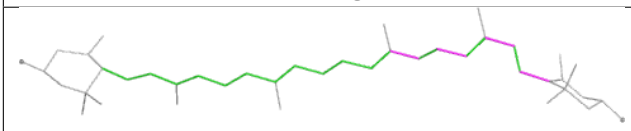
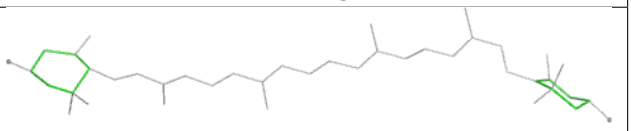
 Bond lengths	 Bond angles
 Torsions	 Rings

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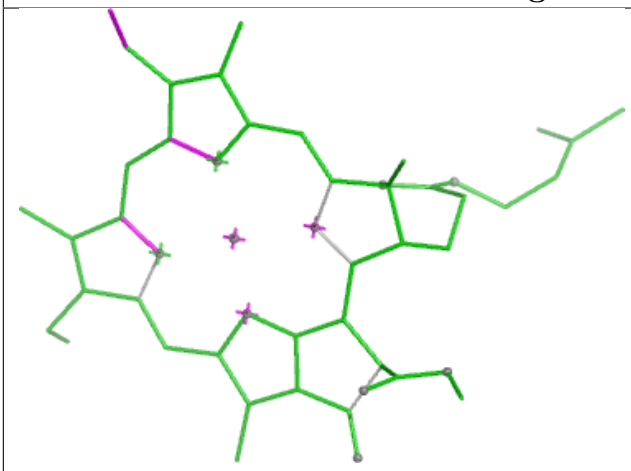
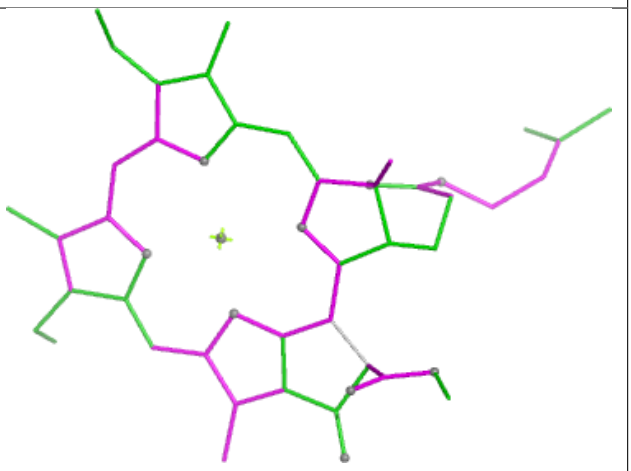
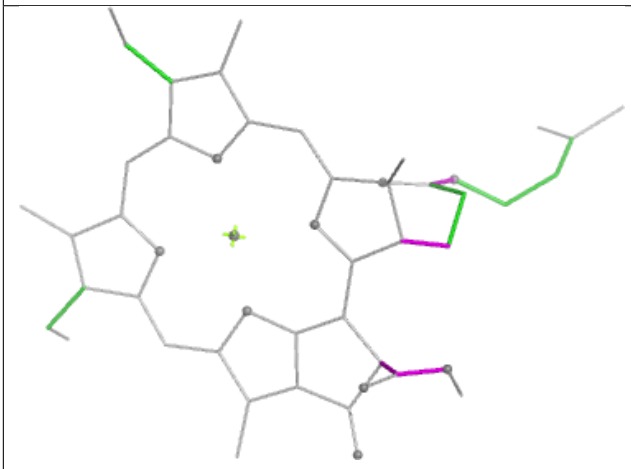
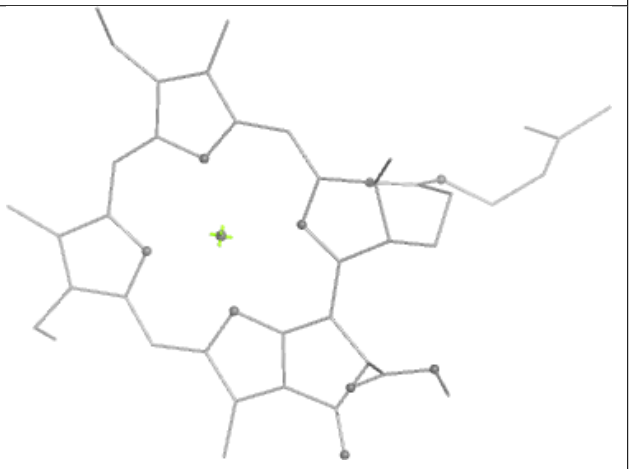
 Bond lengths	 Bond angles
 Torsions	 Rings

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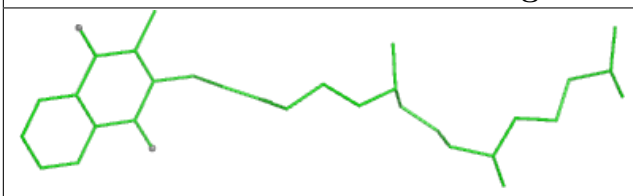

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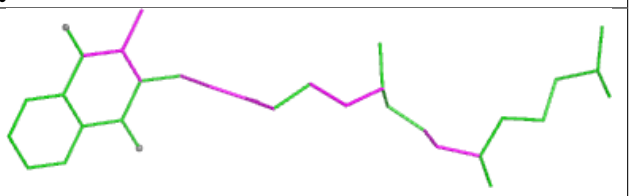

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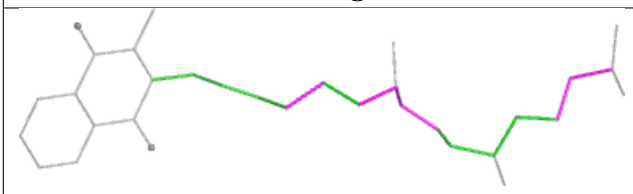

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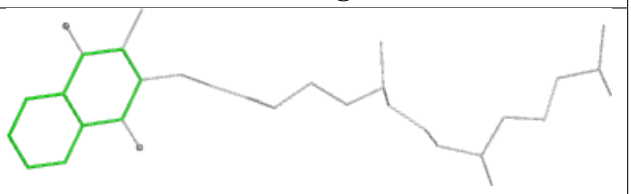

Rings

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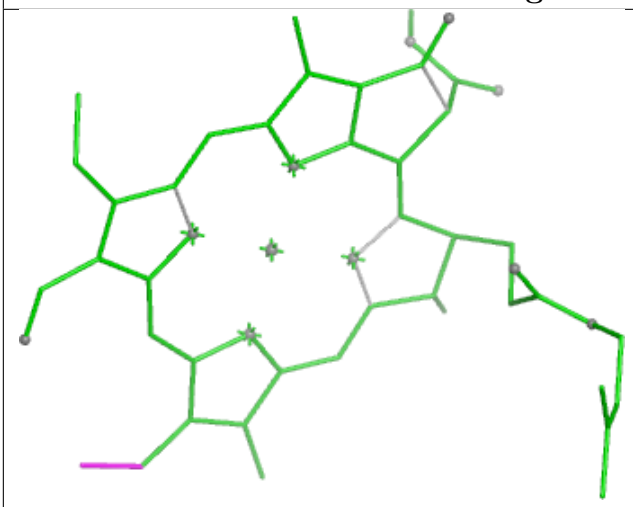

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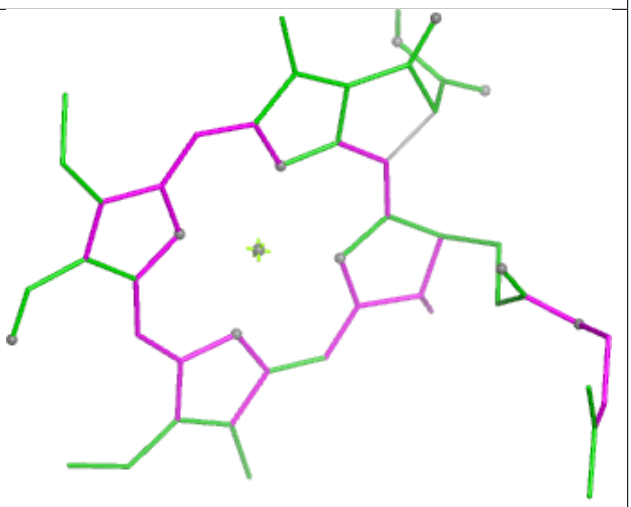

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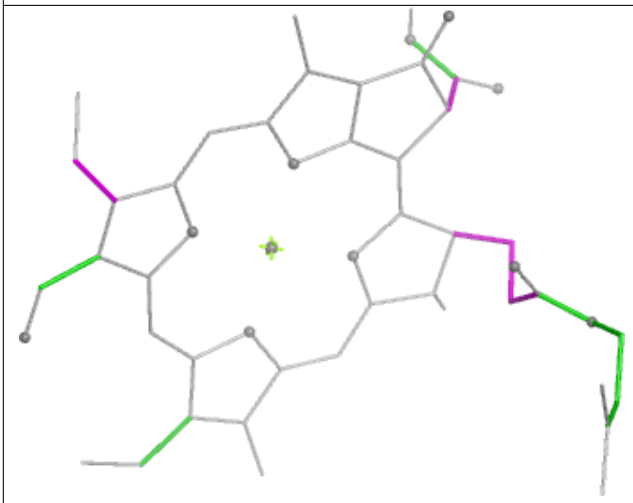
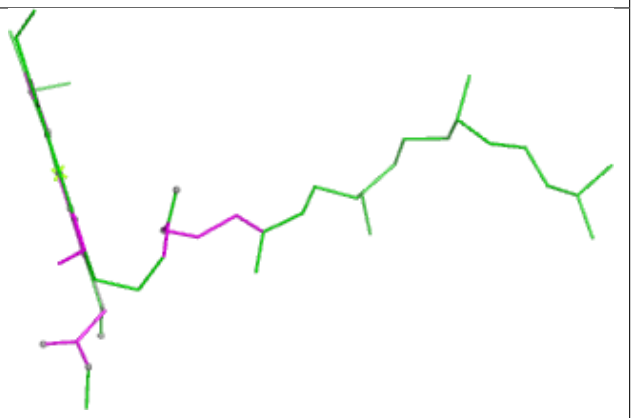
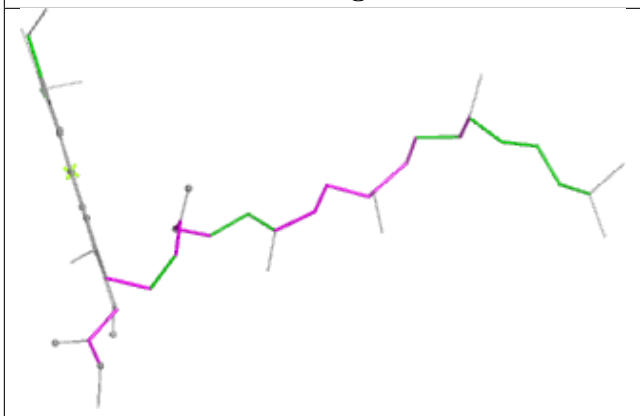
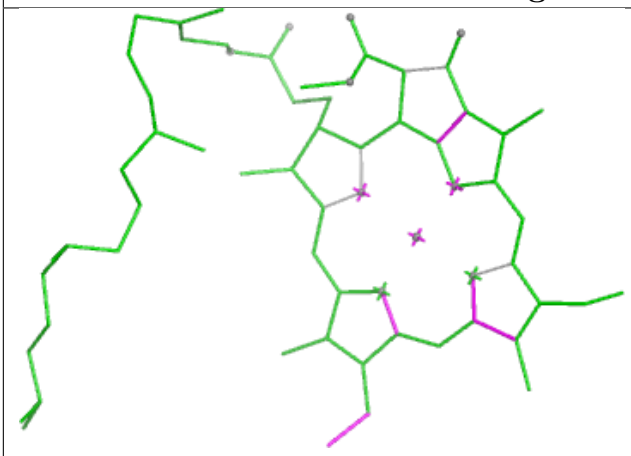


Torsions

Rings

Ligand CLA A 828	
Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 8 309



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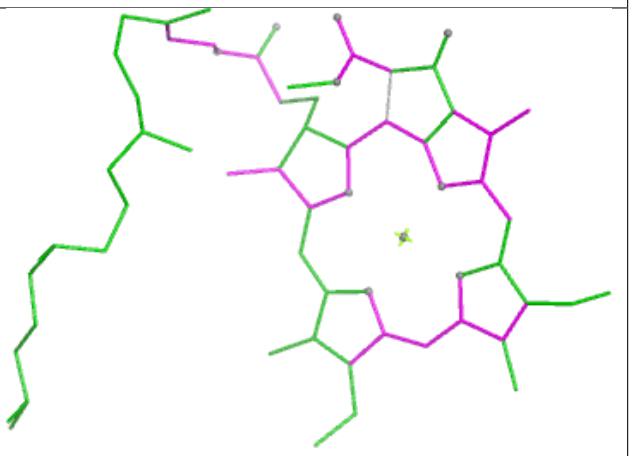

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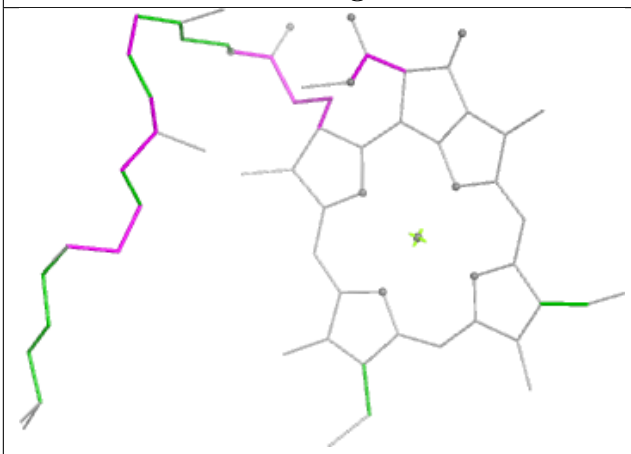

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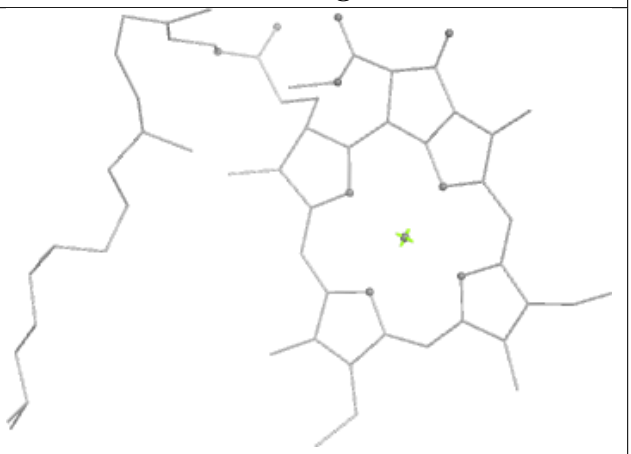

Rings

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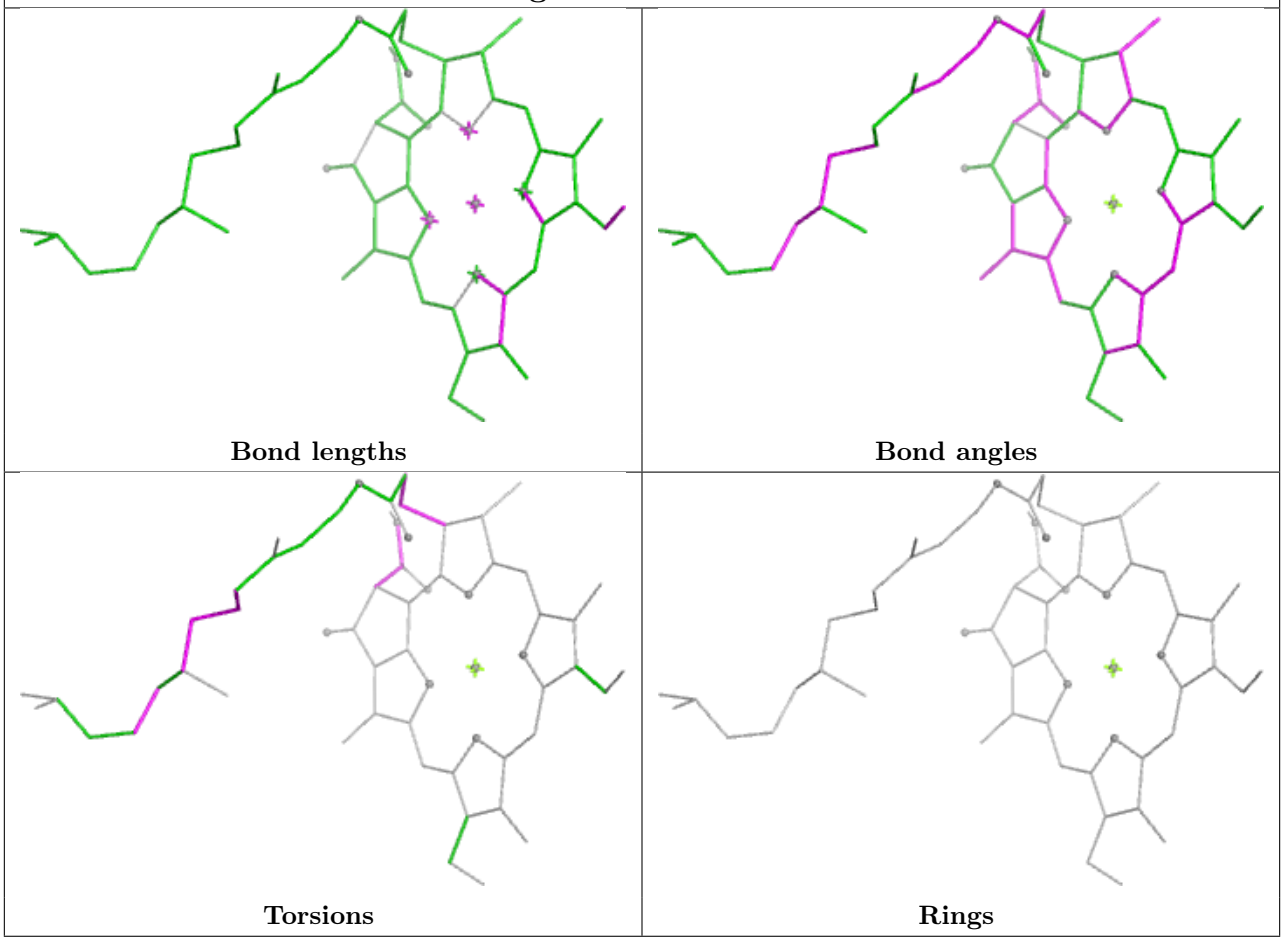

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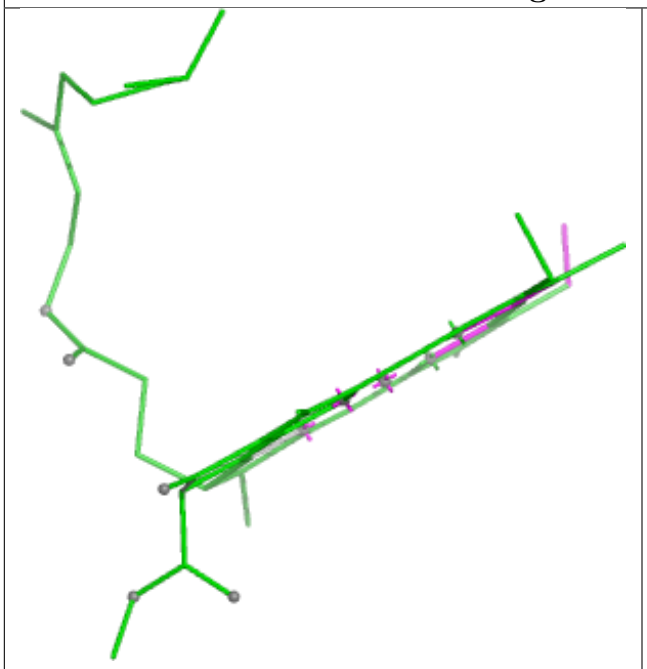

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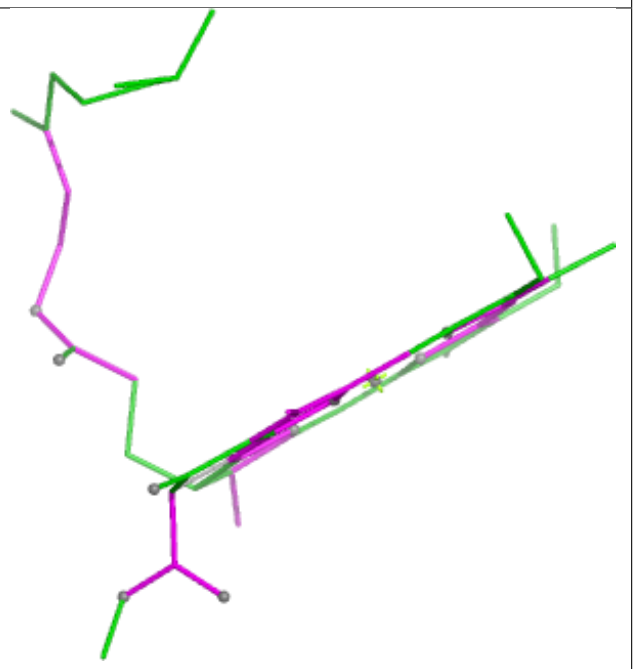

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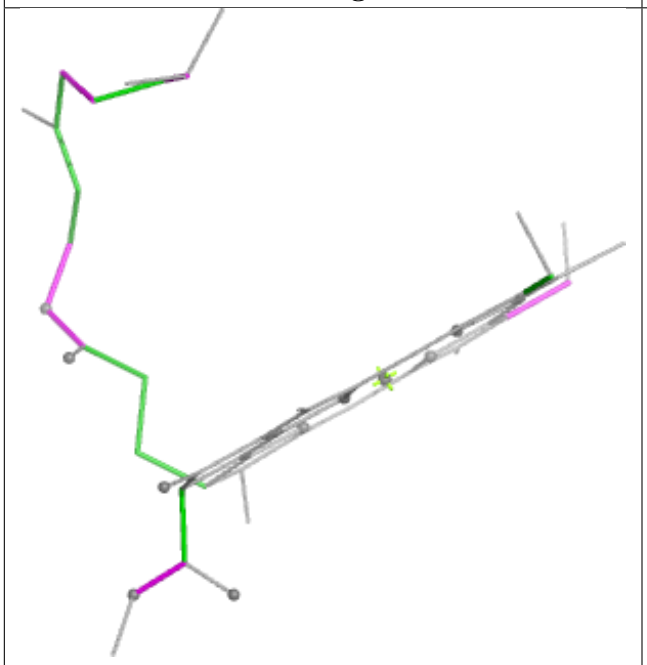

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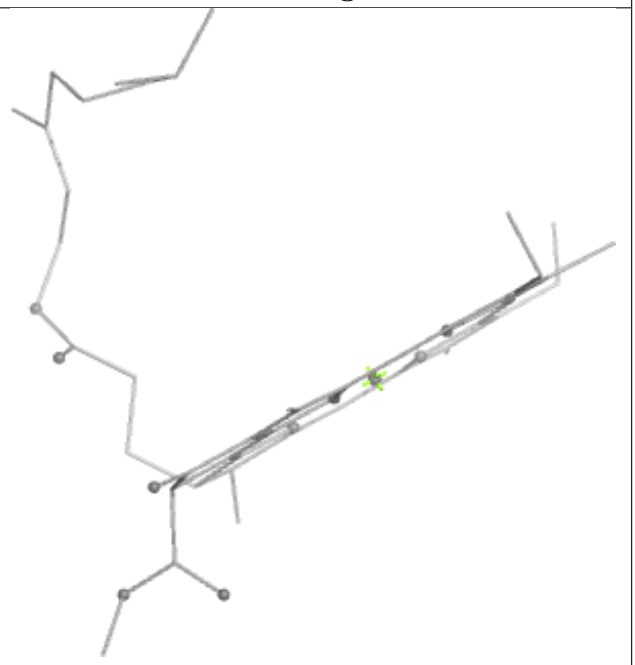
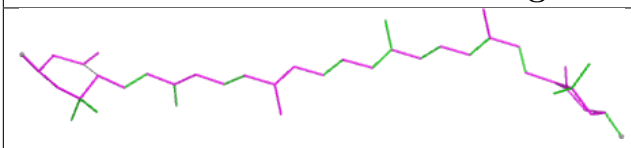
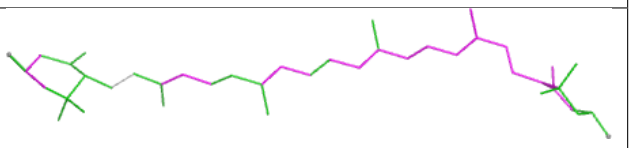
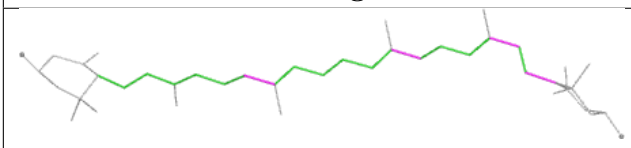
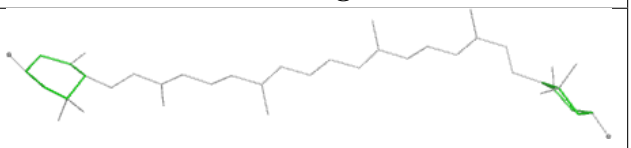


Rings

Ligand LUT 1 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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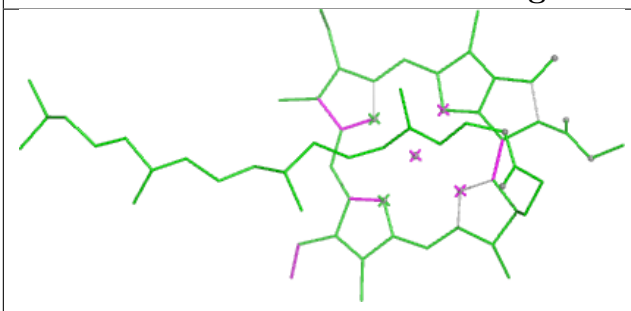
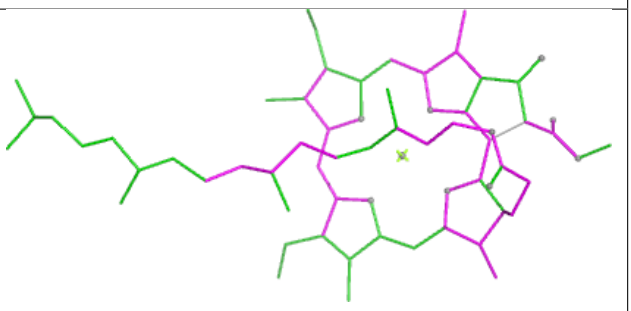
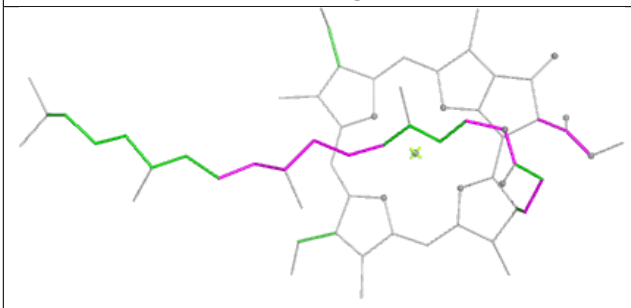
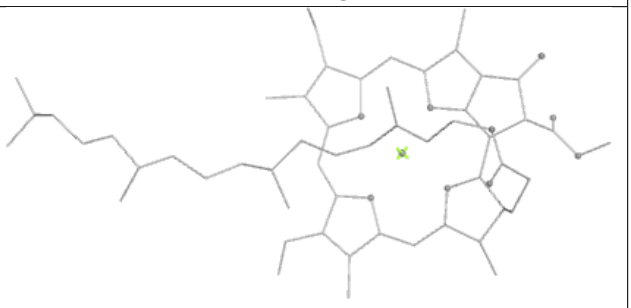
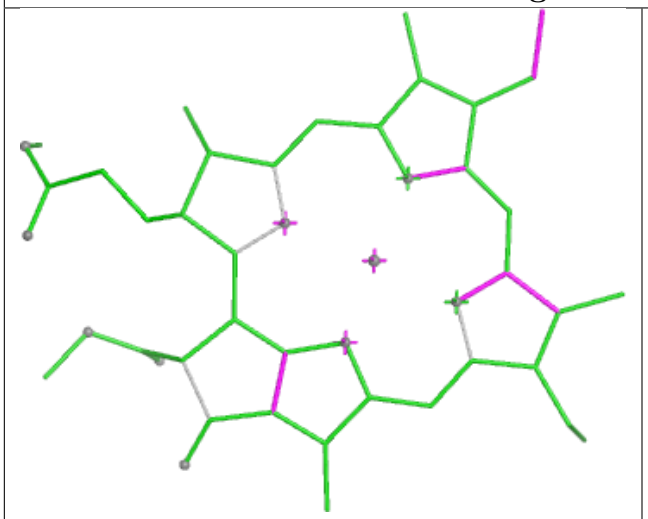
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 309



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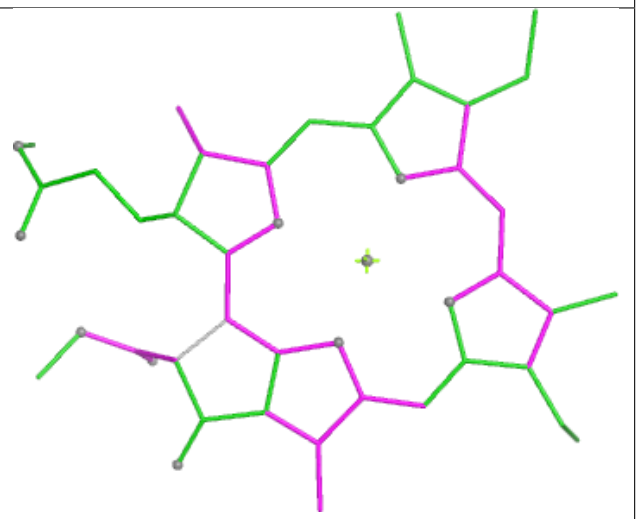

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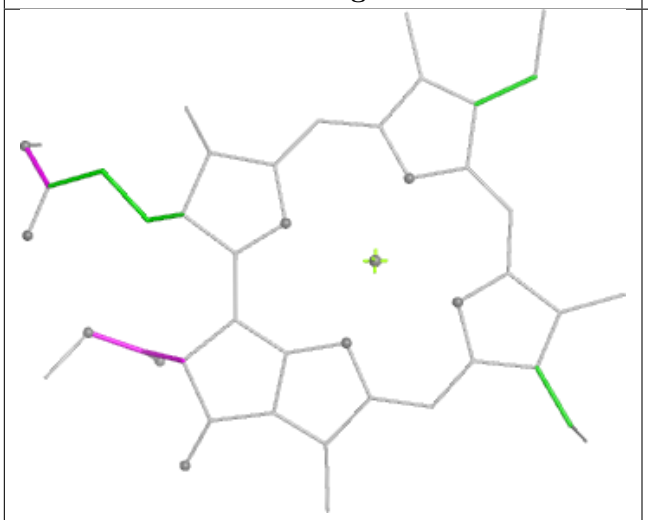

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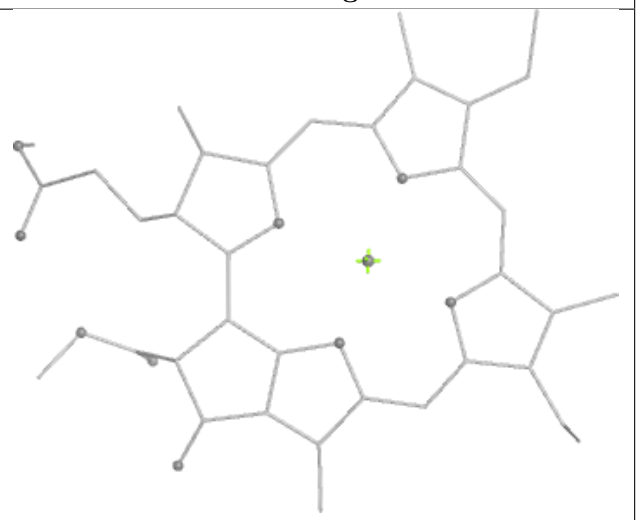
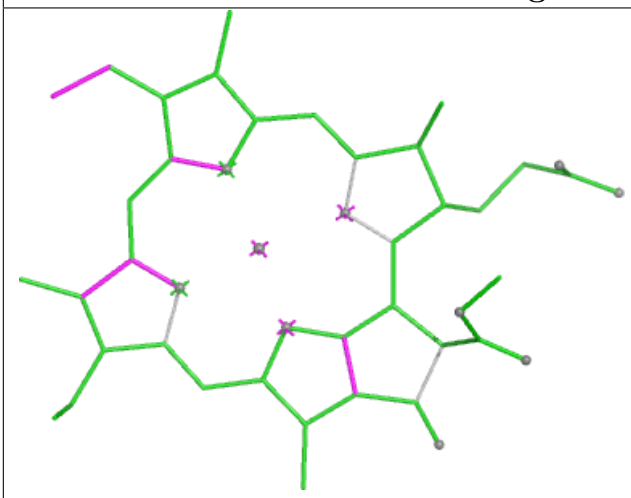


Rings

Ligand CLA 1 305



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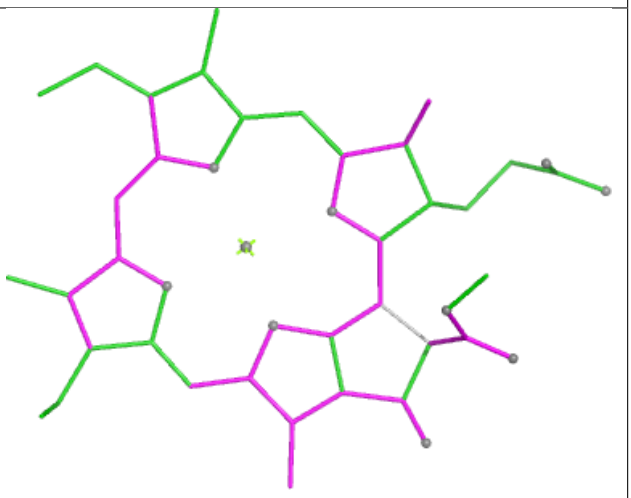
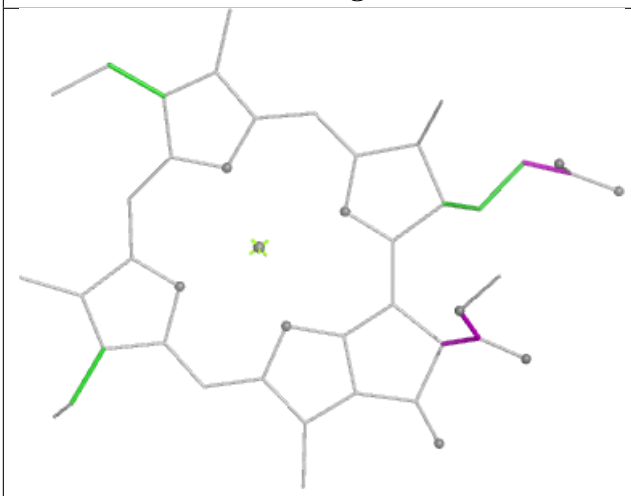


Bond angles



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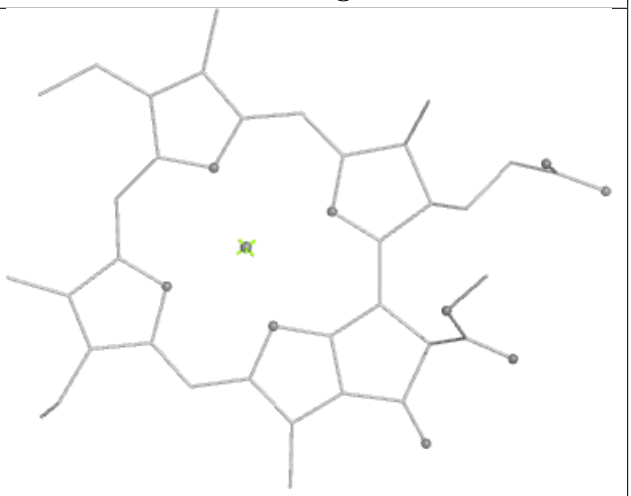
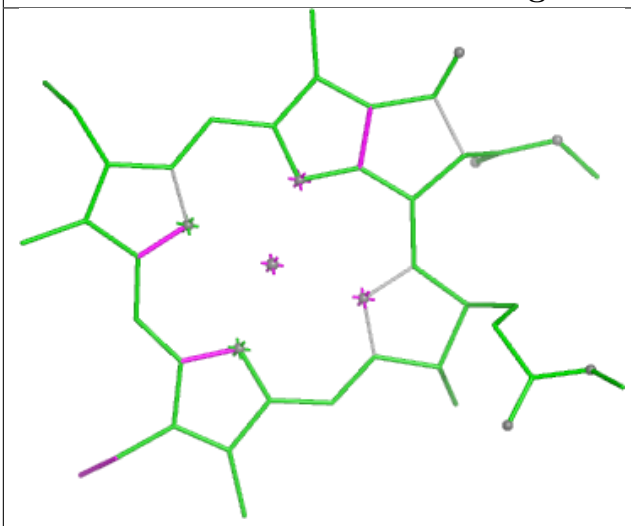


Rings

Ligand CLA 3 320



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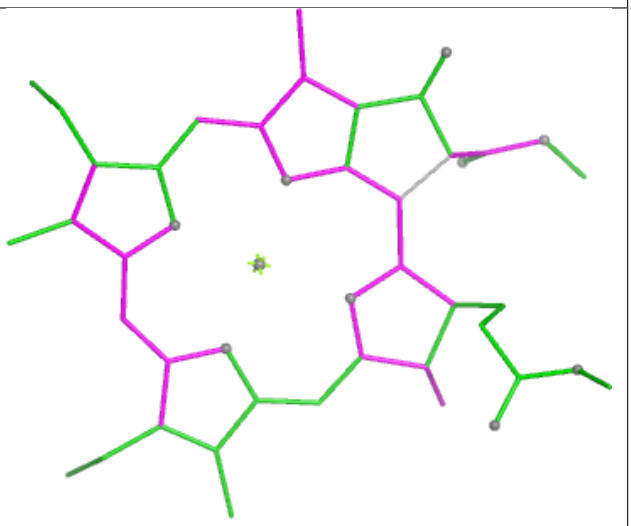

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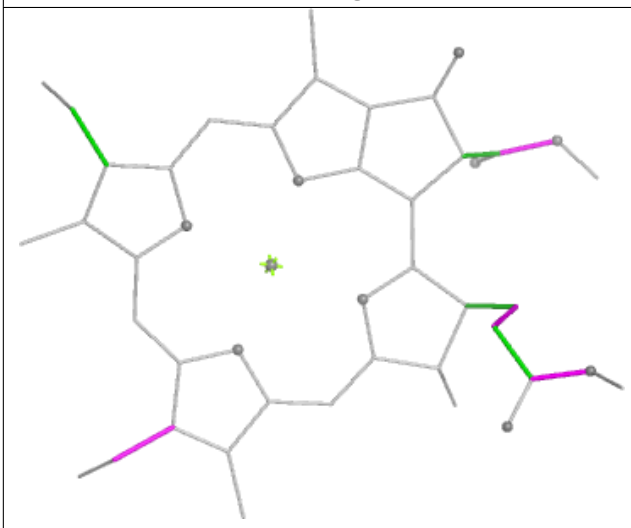

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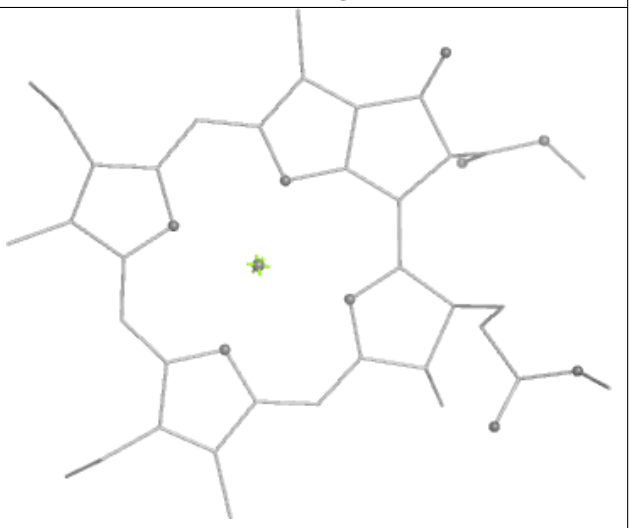
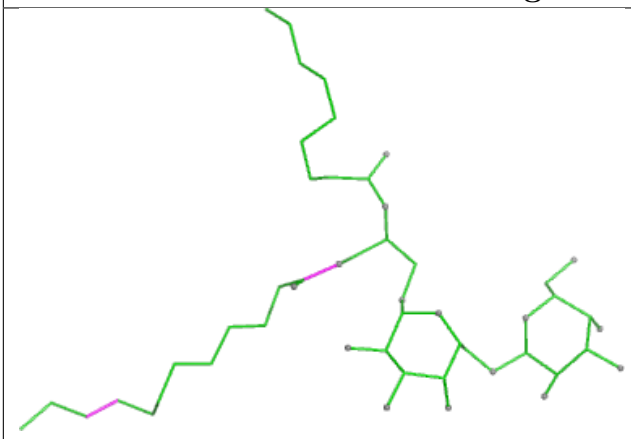


Rings

Ligand DGD 1 319



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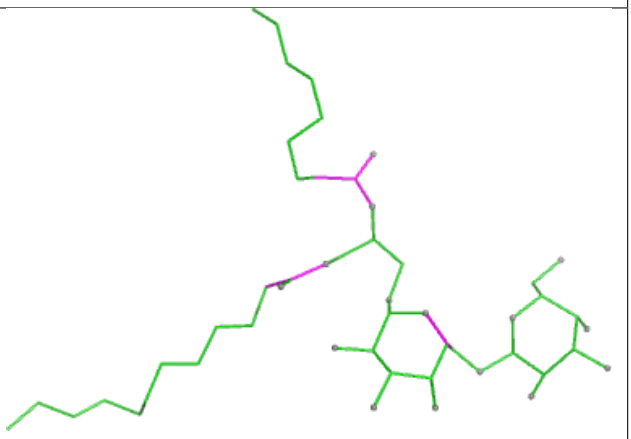
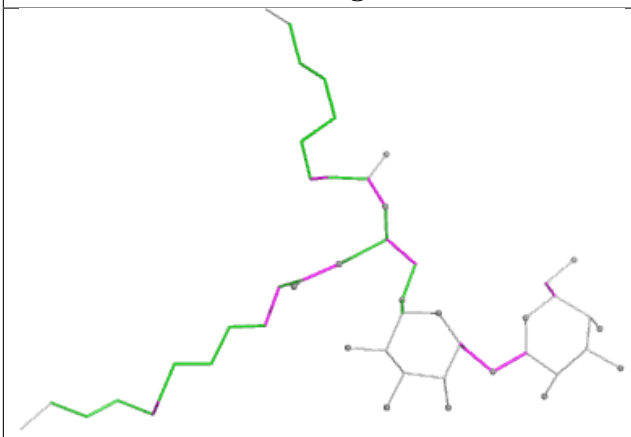


Bond angles



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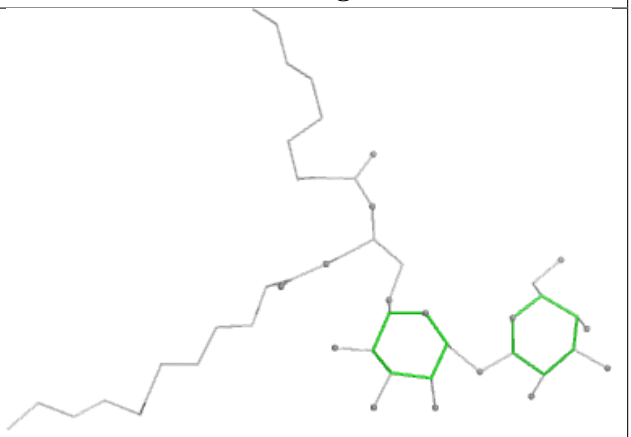
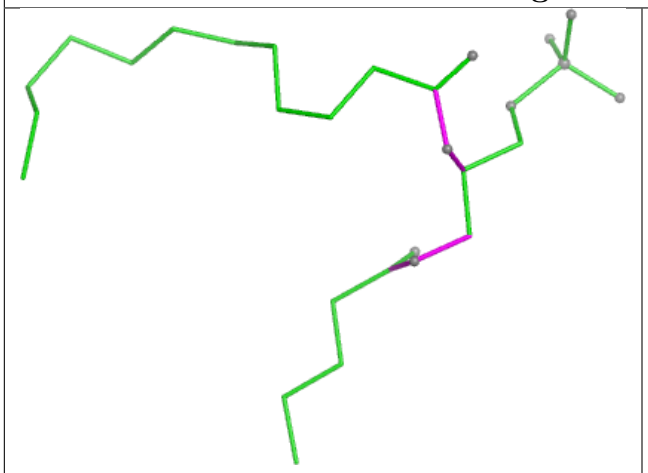


Rings

Ligand 3PH 6 324



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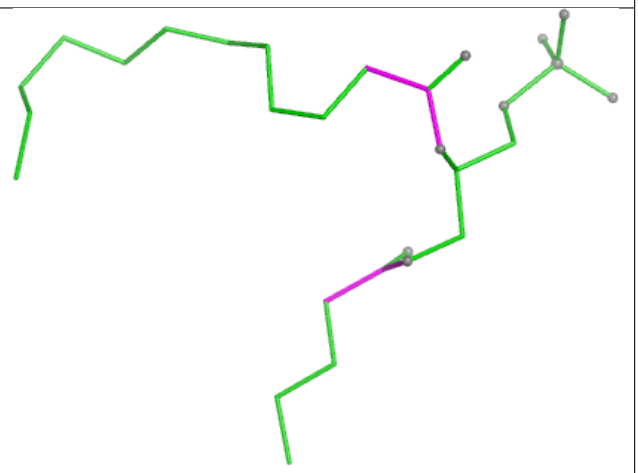
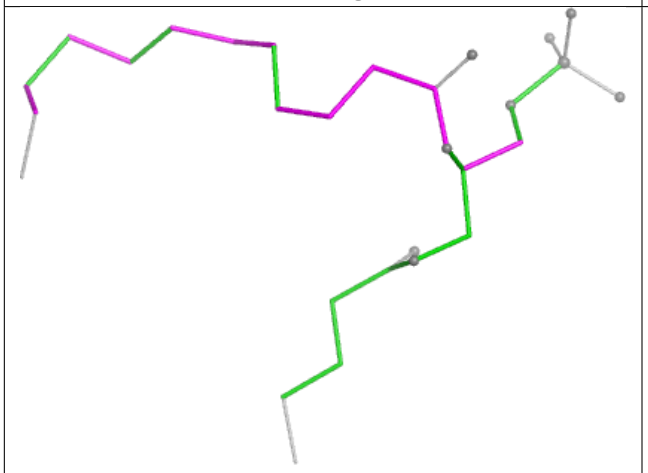
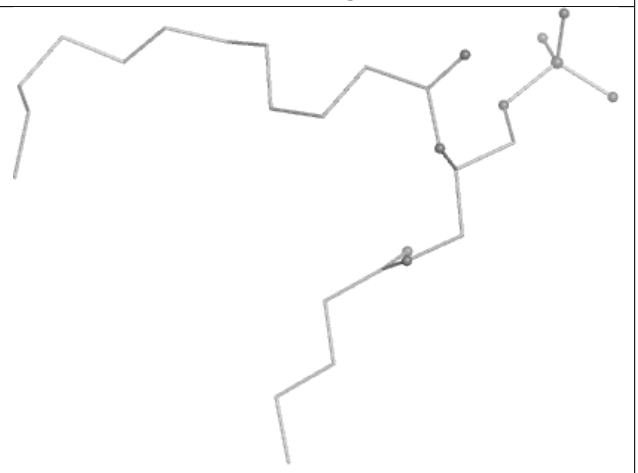


Bond angles



Torsions



Rings

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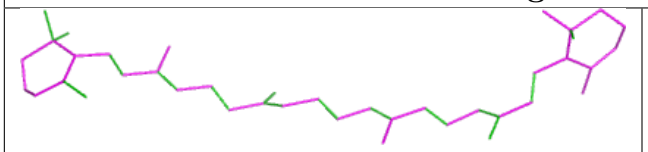
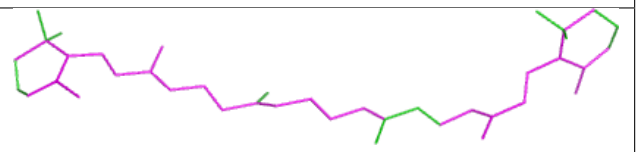
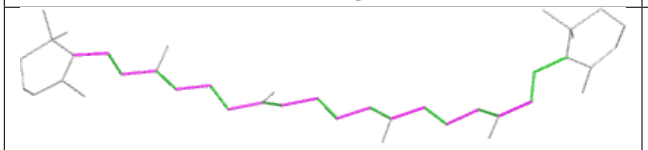


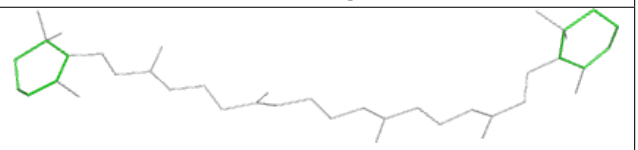
Bond lengths



Bond angles

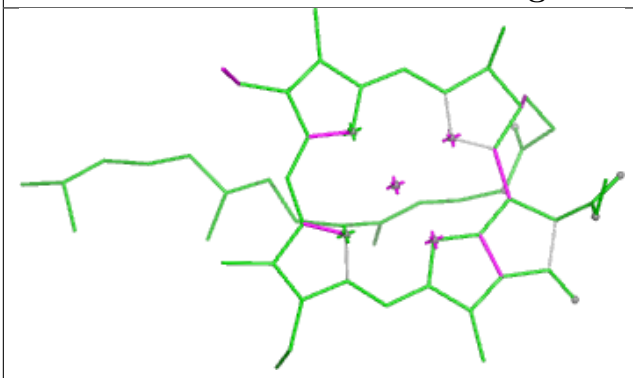


Torsions



Rings

Ligand CLA 9 305



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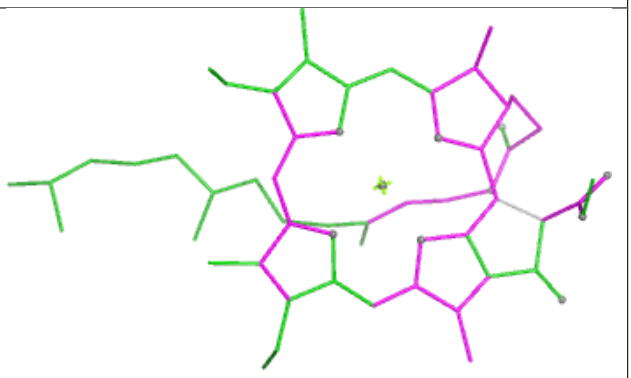

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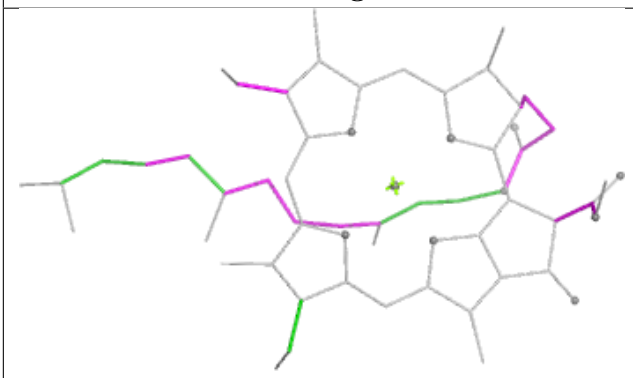
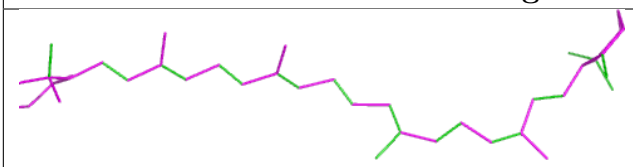


Torsions

Rings

Ligand BCR A 844



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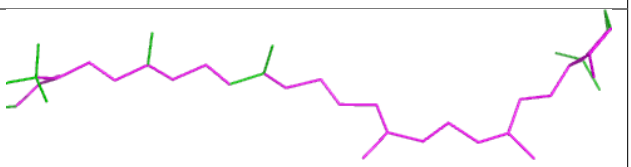
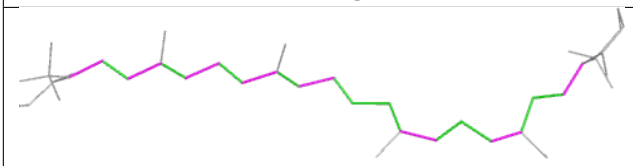


Bond angles



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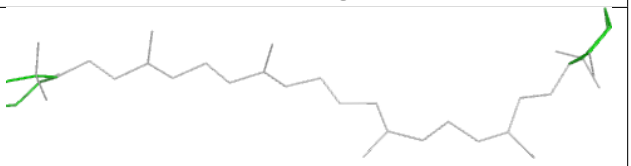
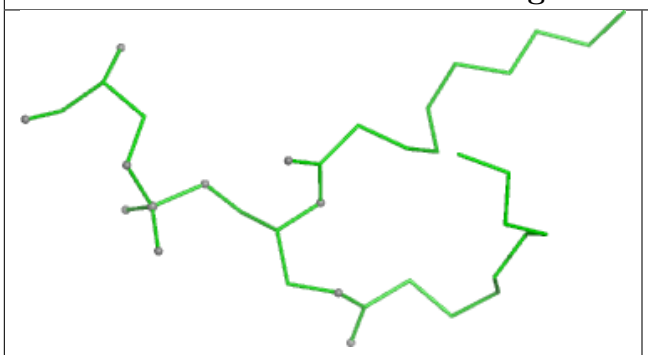


Rings

Ligand LHG 5 324



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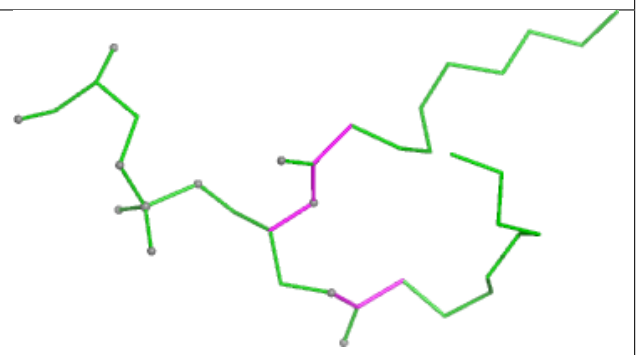

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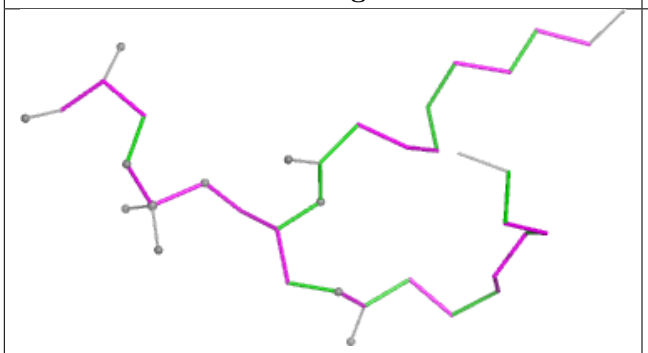

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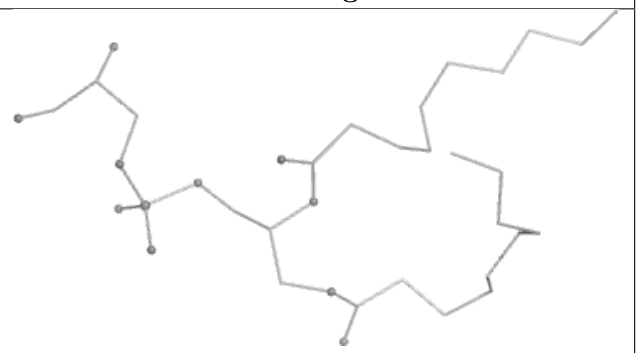
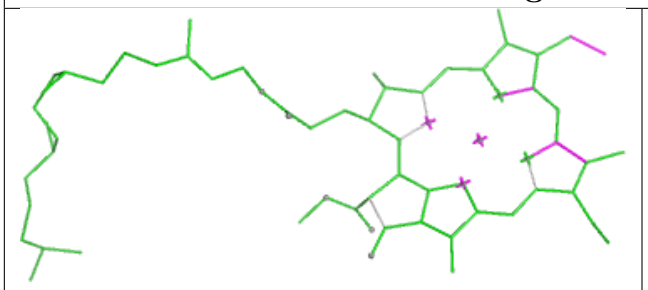


Rings

Ligand CLA B 828



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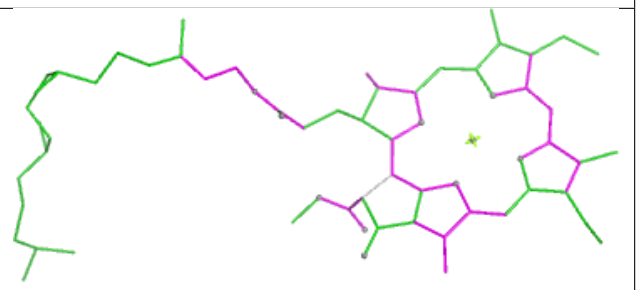

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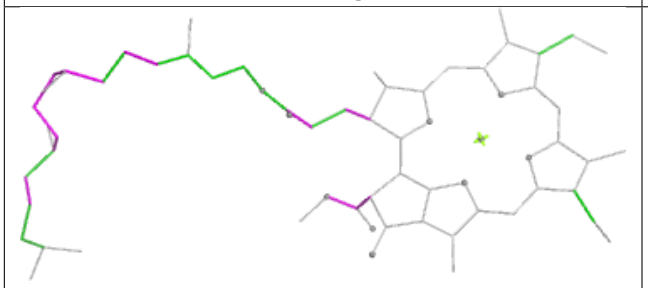

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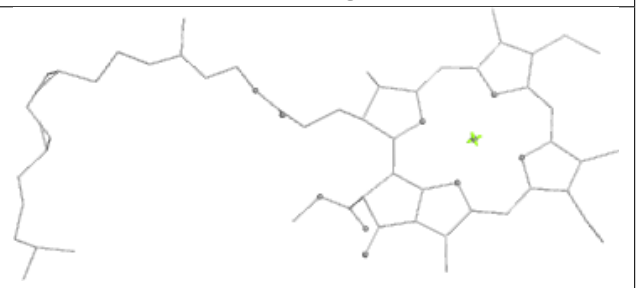
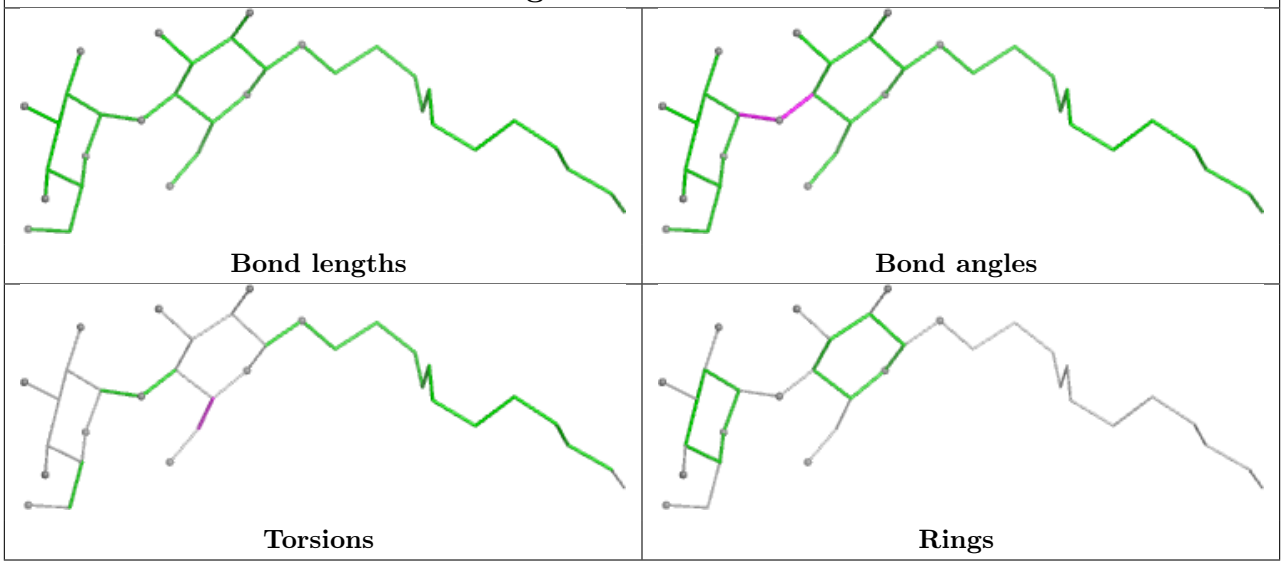
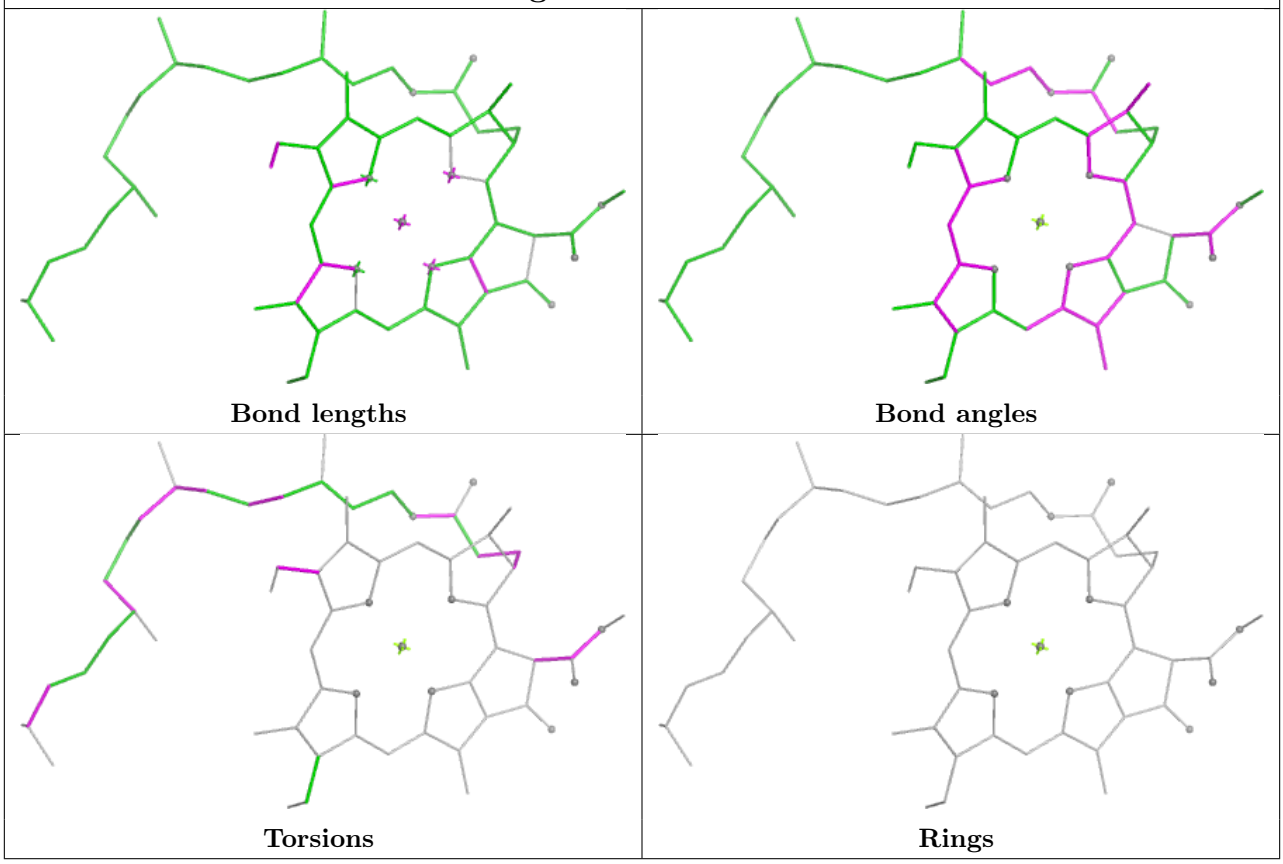


Rings

Ligand LMT 4 801



Ligand CLA 6 310



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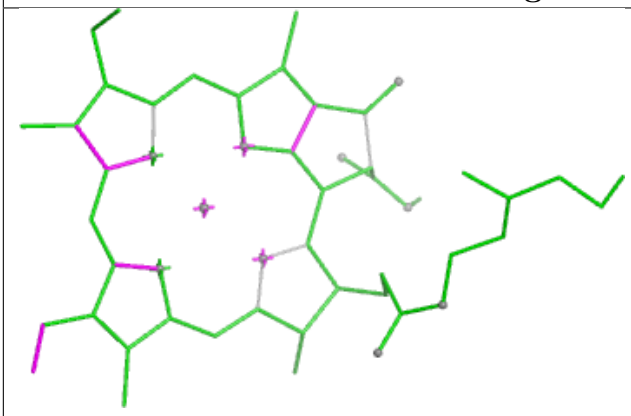
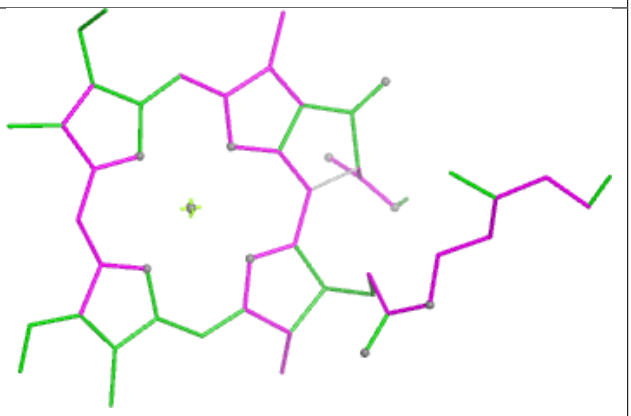
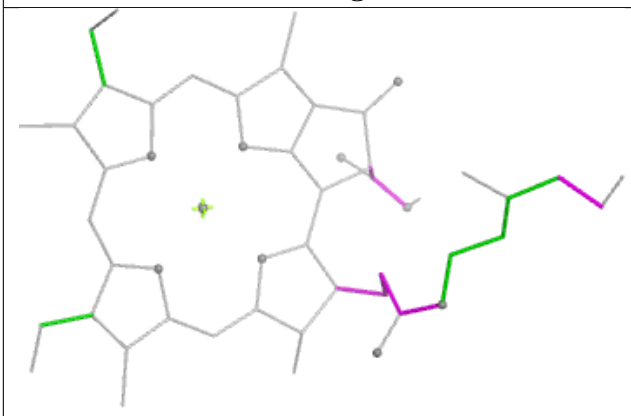
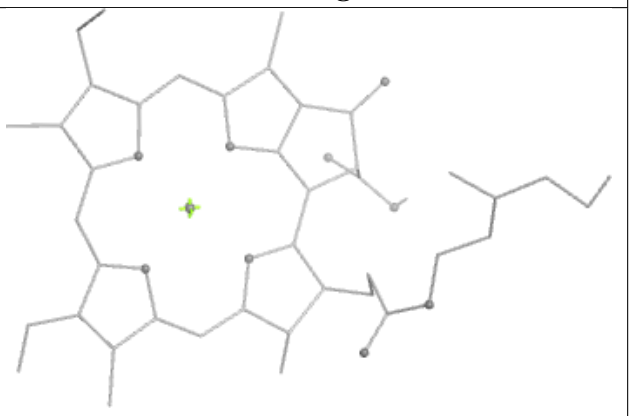
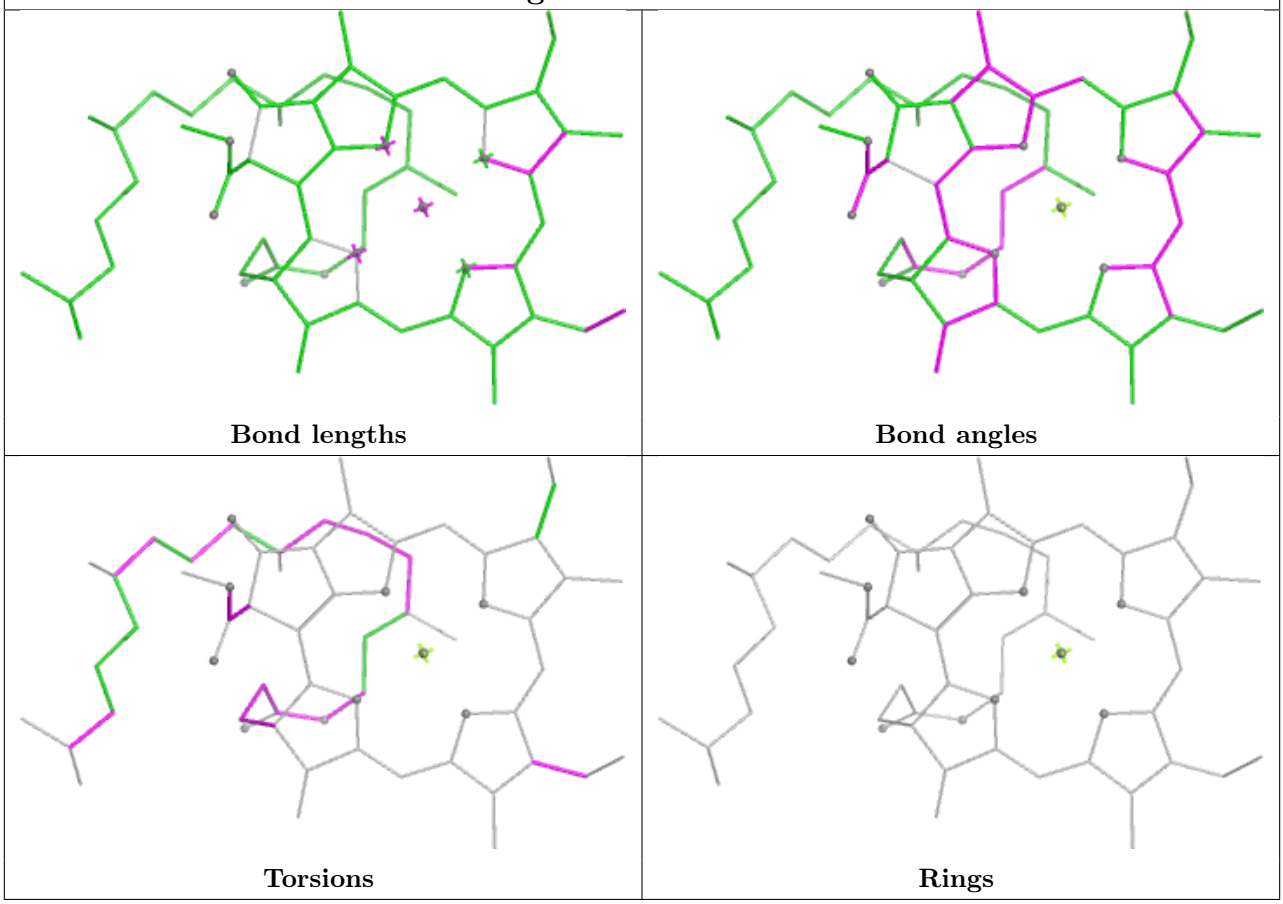
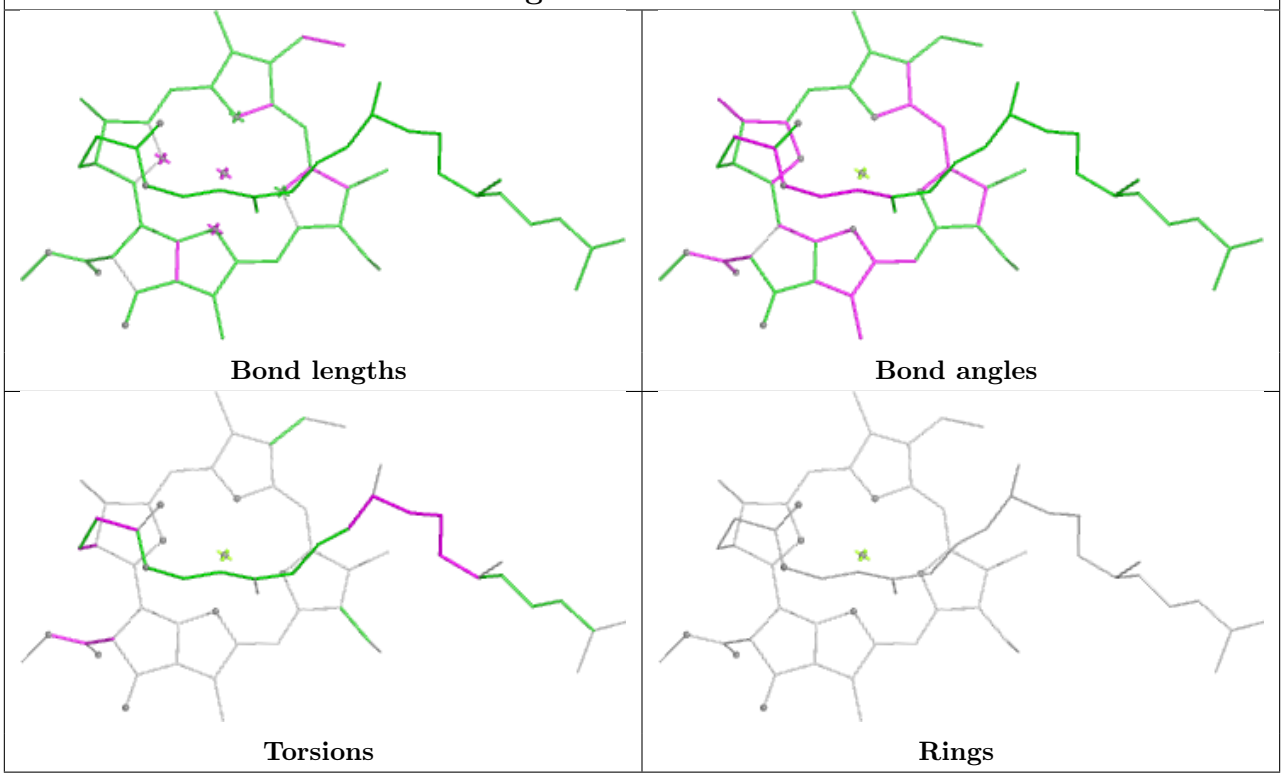
 Bond lengths	 Bond angles
 Torsions	 Rings

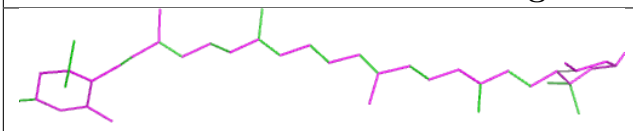
Ligand CLA F 304



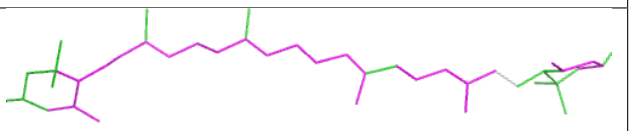
Ligand CLA B 818



Ligand LUT 6 303



Bond lengths



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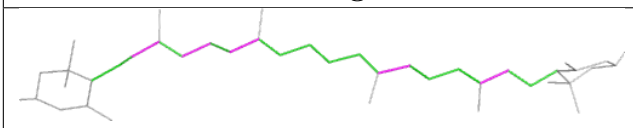
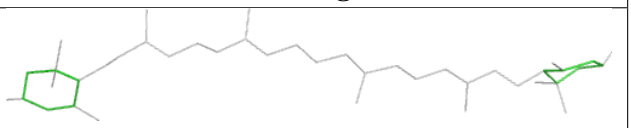
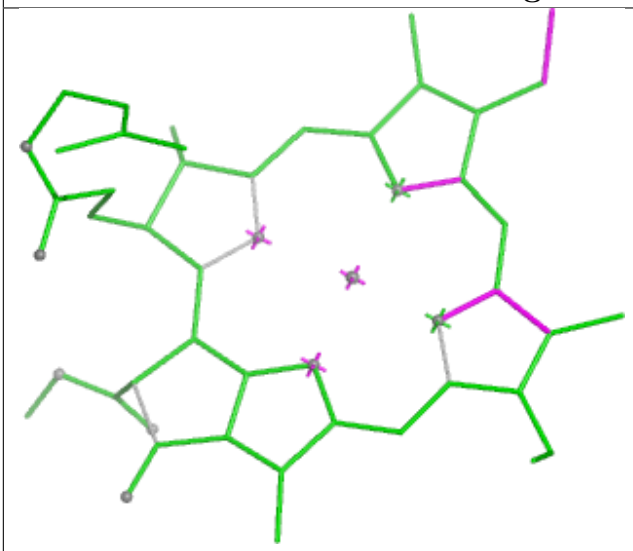


Torsions



Rings

Ligand CLA A 831



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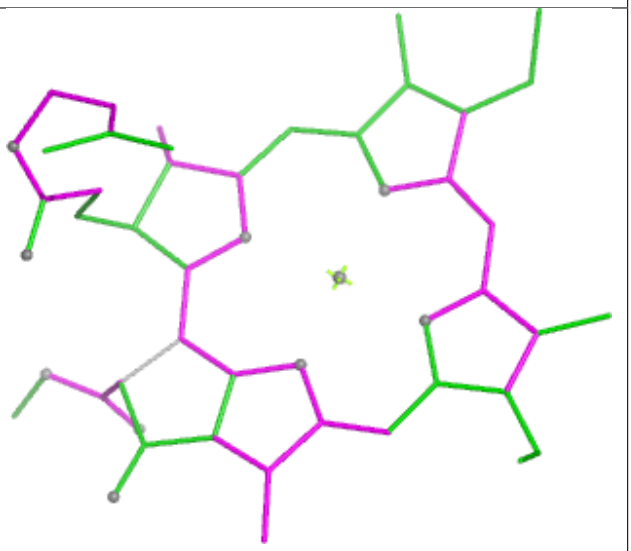
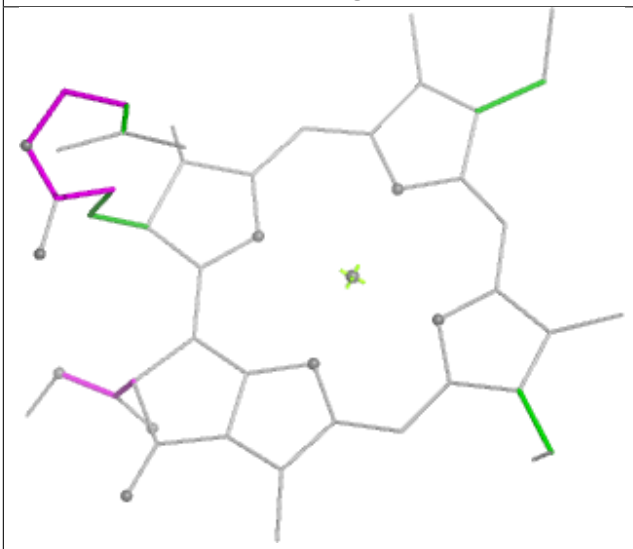


Bond angles



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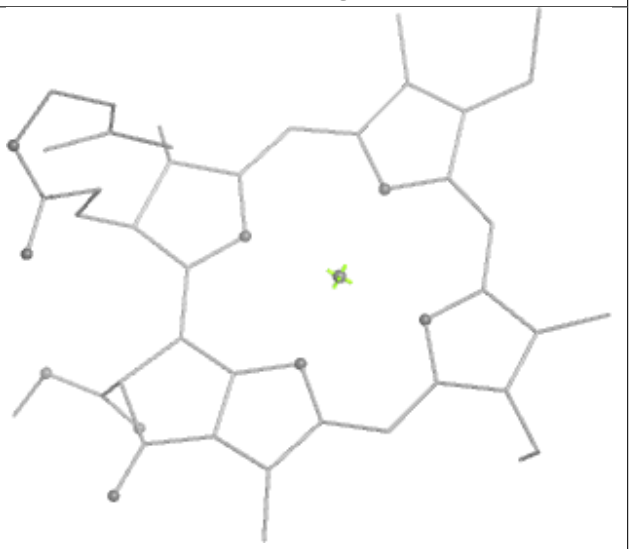
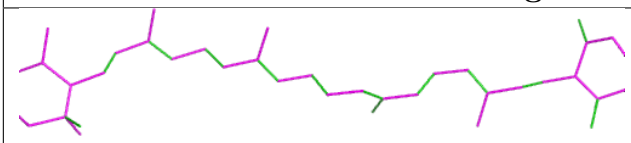


Rings

Ligand BCR L 204



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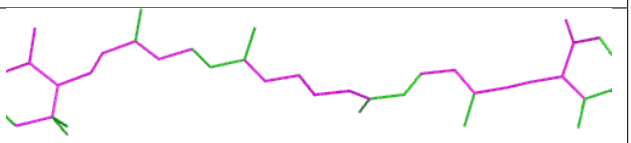
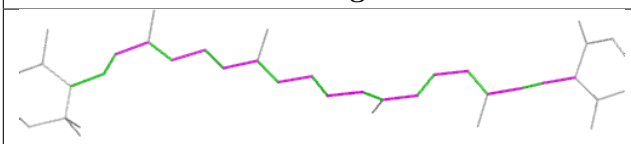


Bond angles



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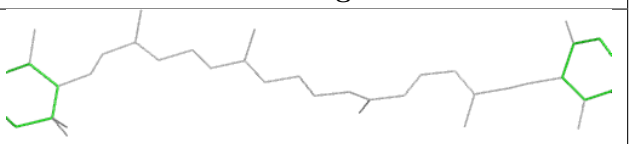
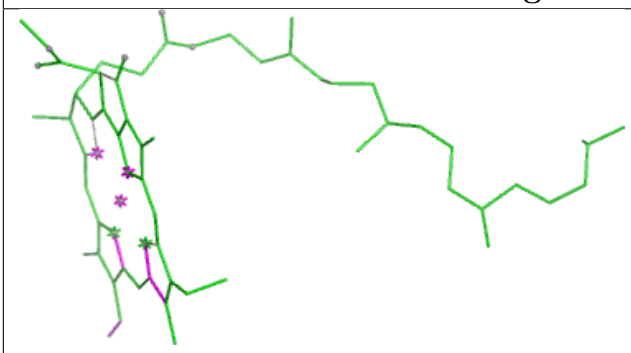


Rings

Ligand CLA A 830



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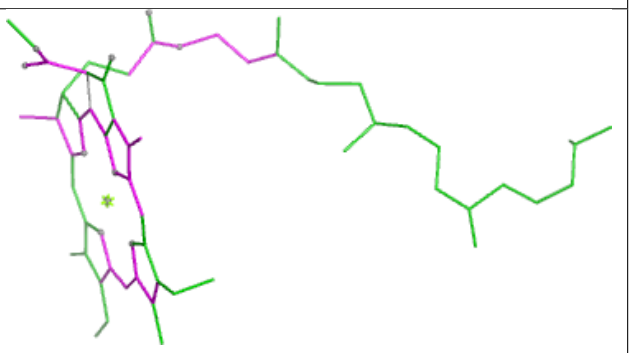
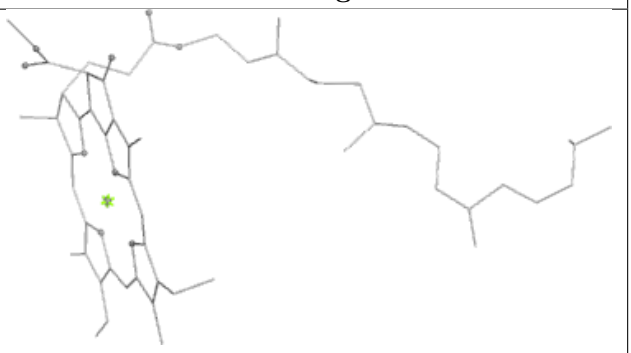


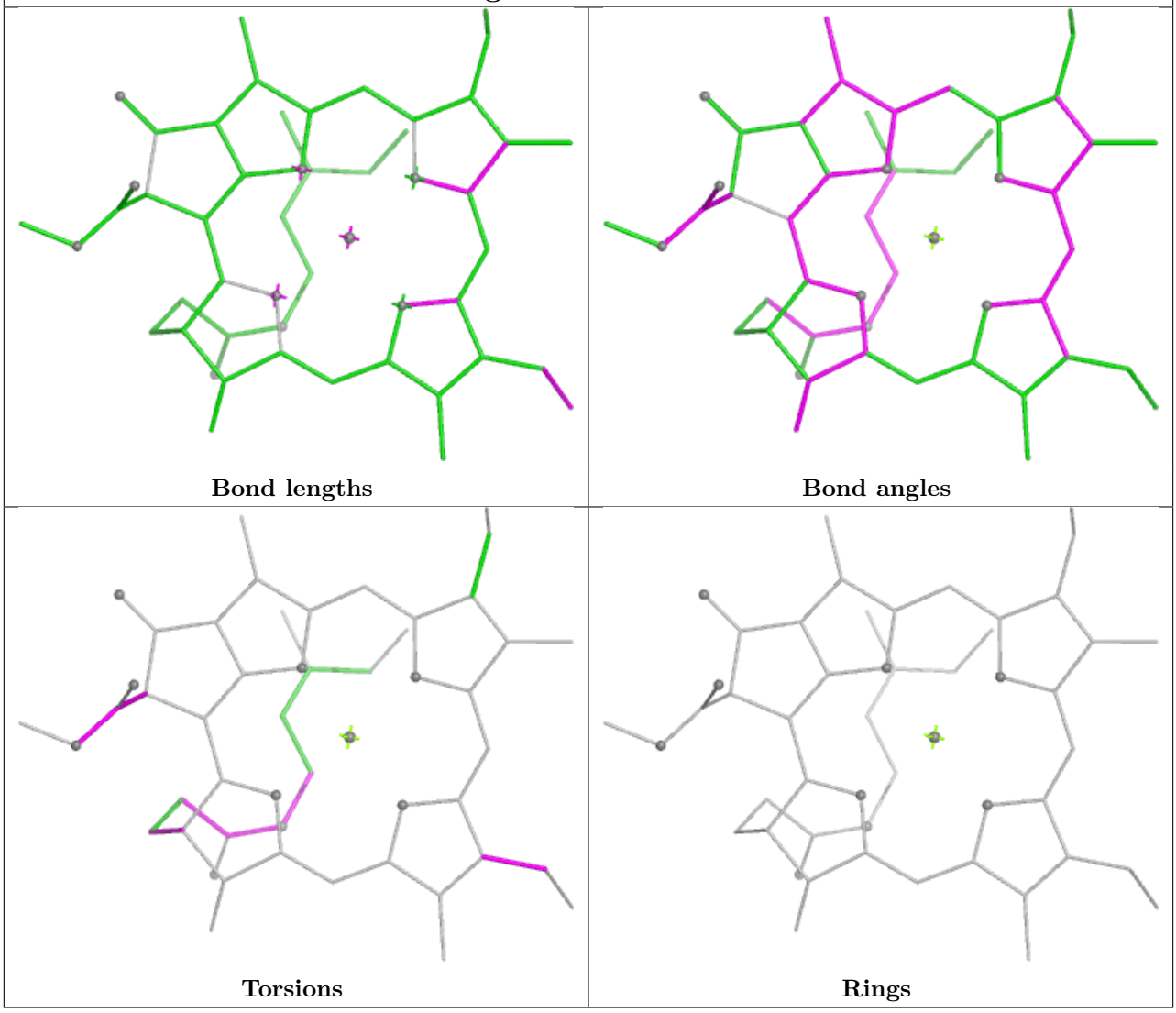
Bond angles

Torsions

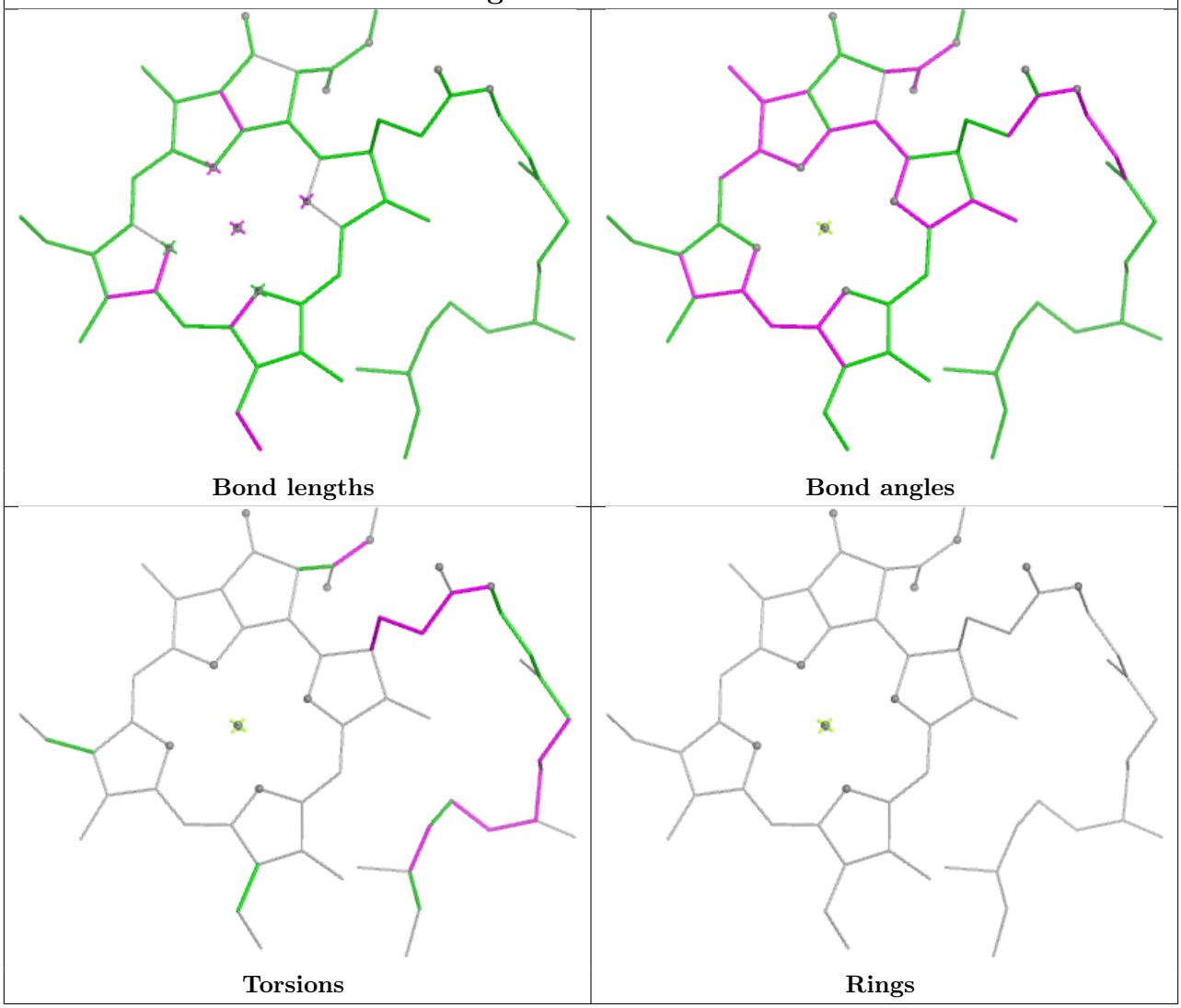


Rings

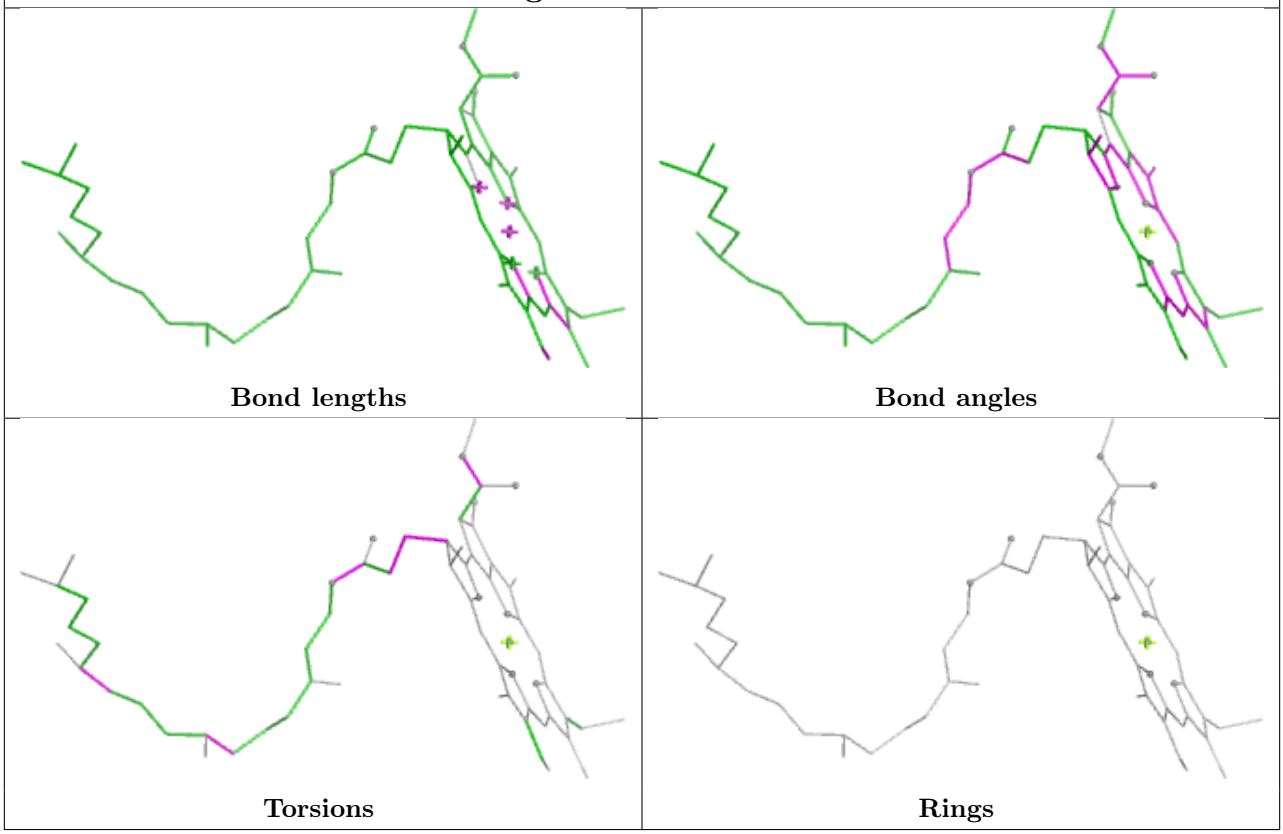
Ligand CLA 4 818



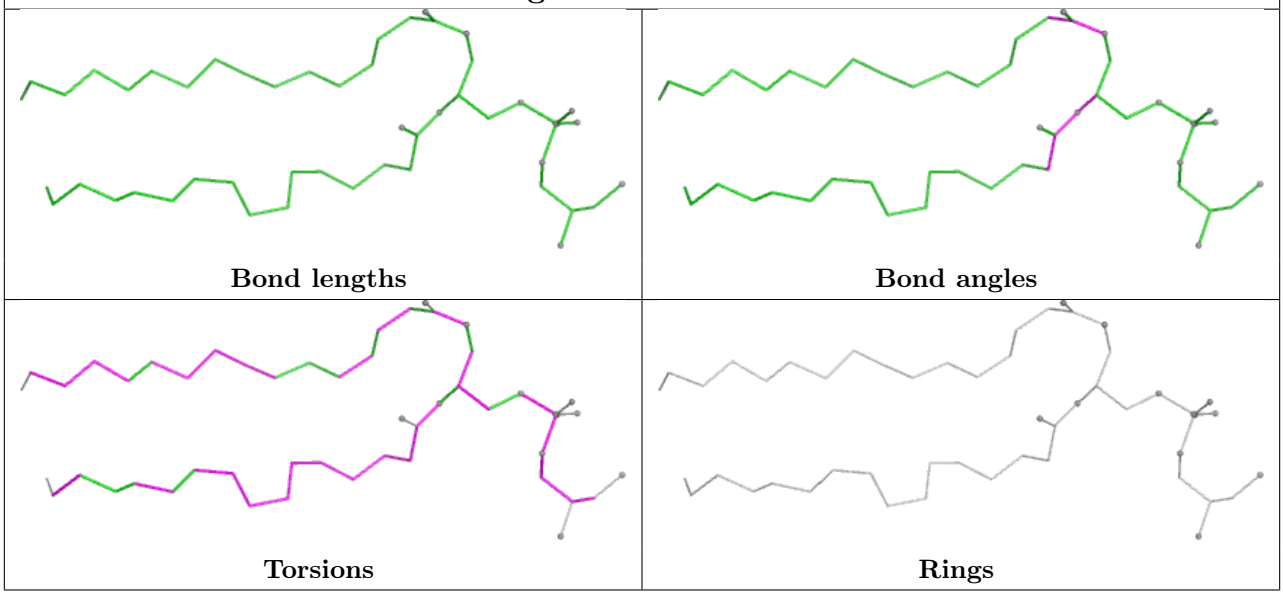
Ligand CLA 5 308



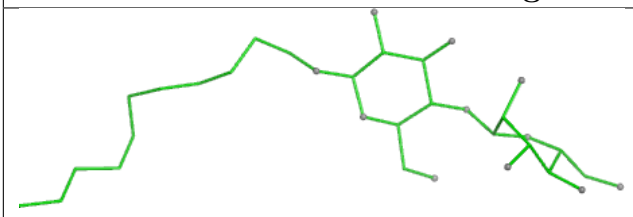
Ligand CLA B 840



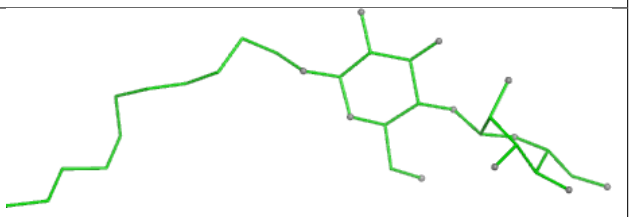
Ligand LHG 6 323



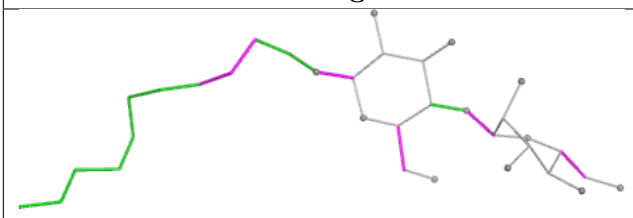
Ligand LMT F 307



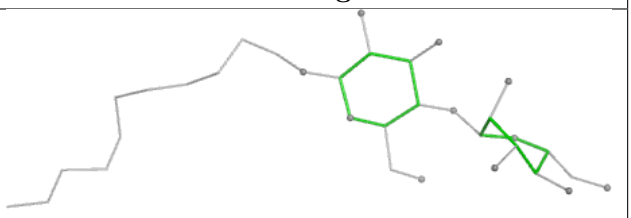
Bond lengths



Bond angles

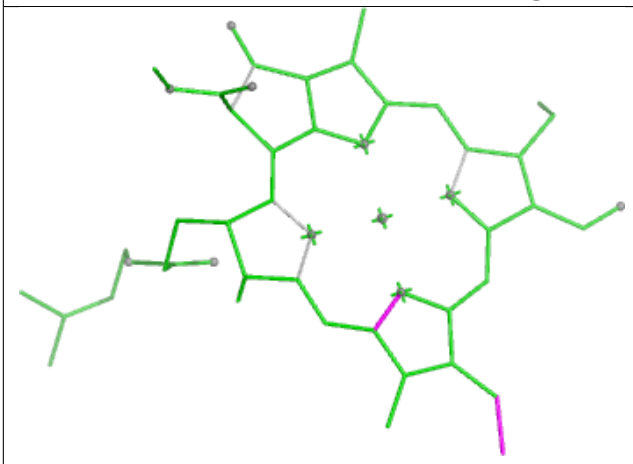


Torsions

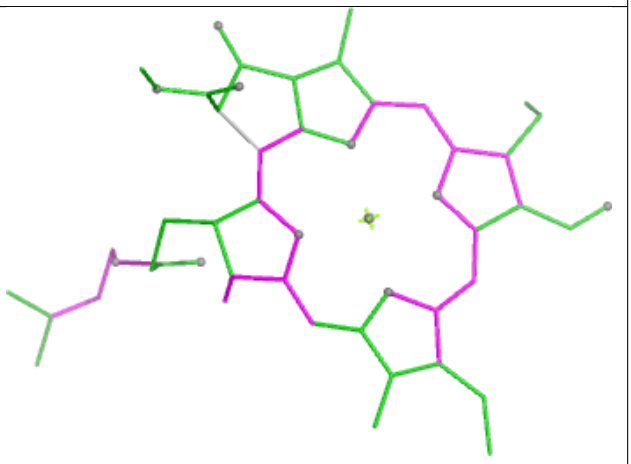


Rings

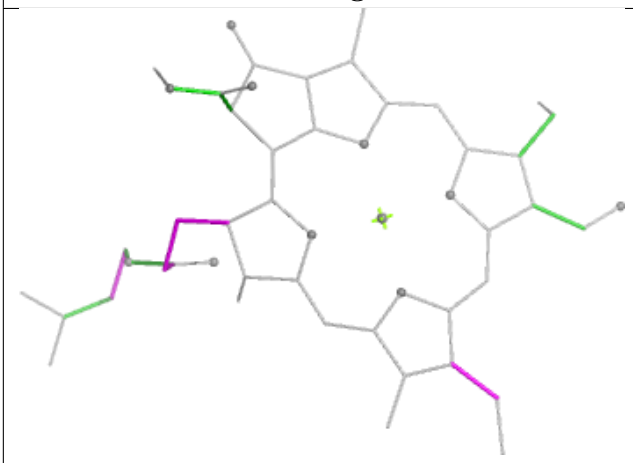
Ligand CHL 5 317



Bond lengths



Bond angles



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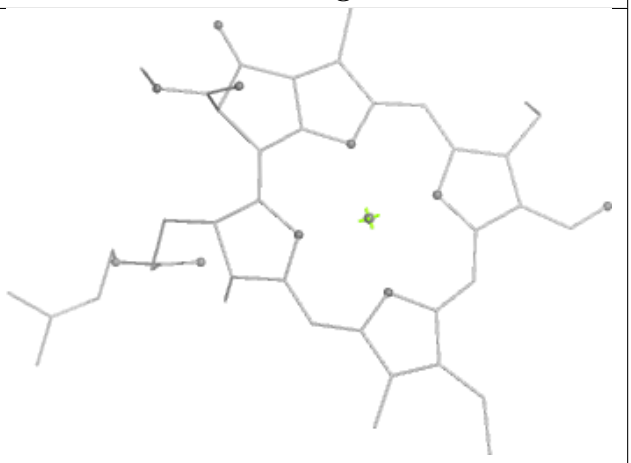
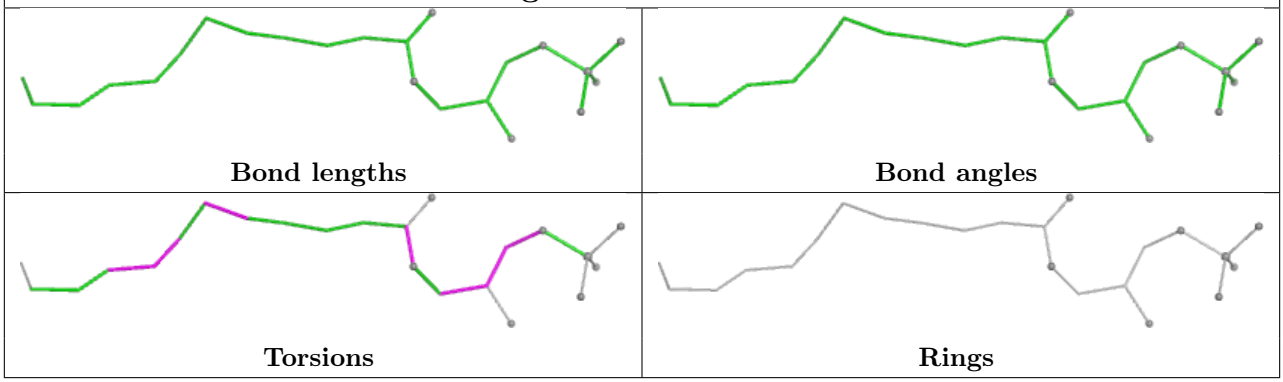
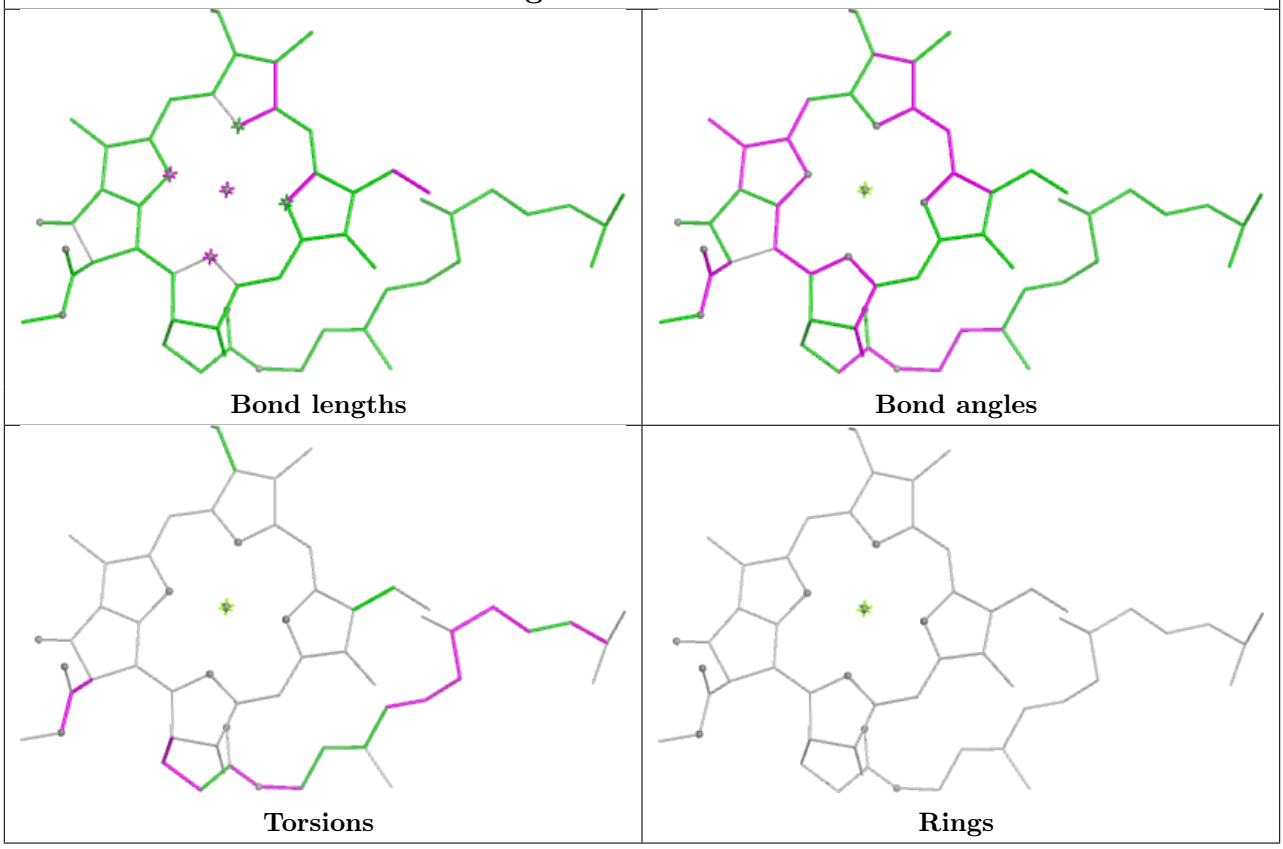


Rings

Ligand NKP A 851



Ligand CLA B 820



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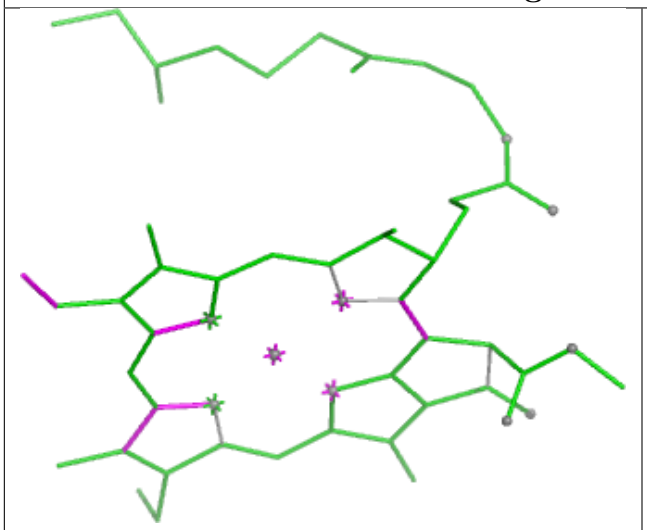

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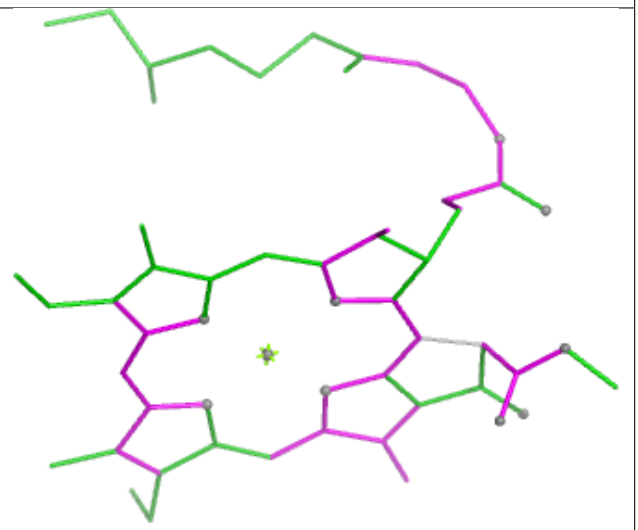
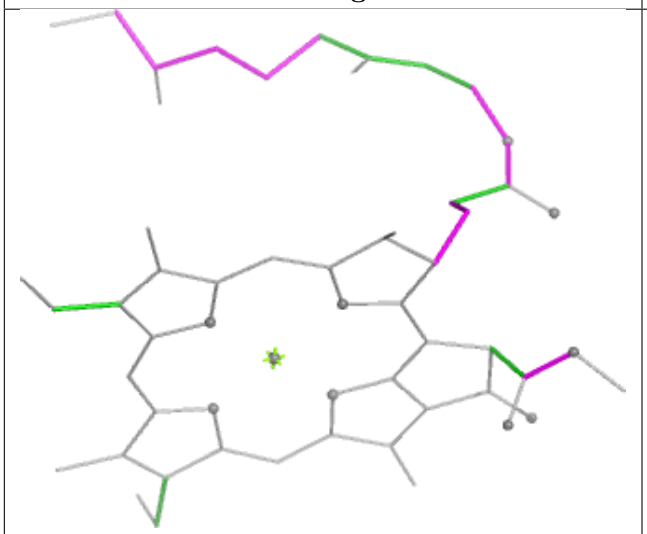
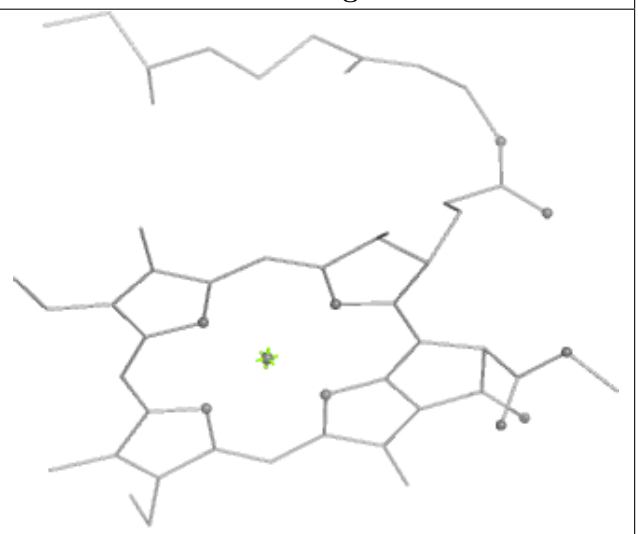


Bond angles

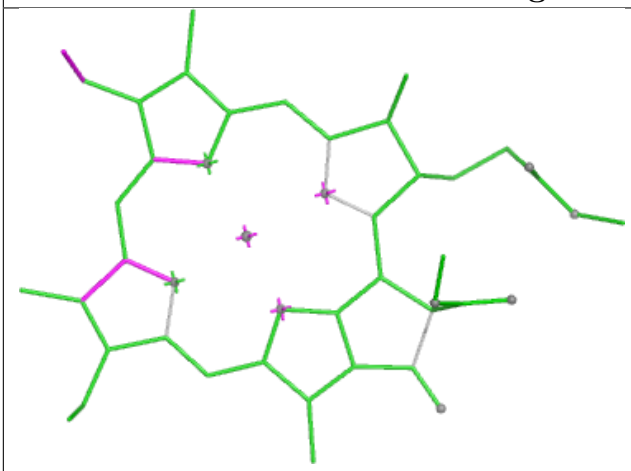


Torsions

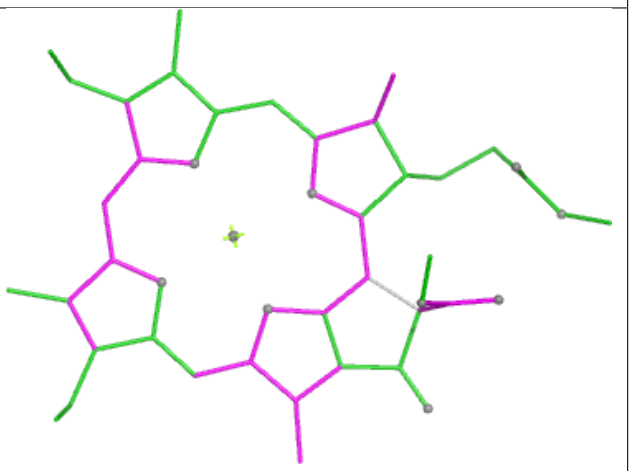


Rings

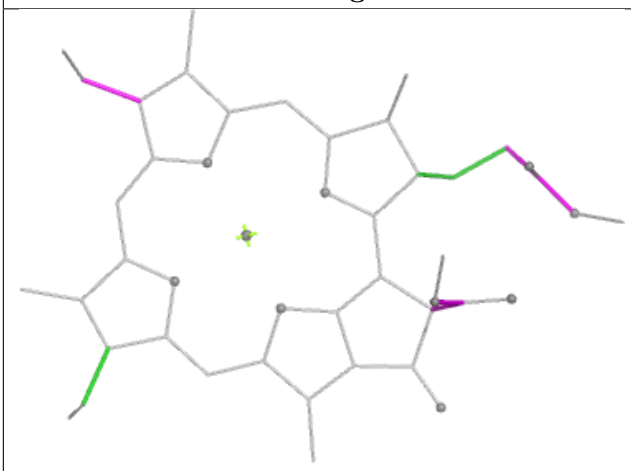
Ligand CLA 5 323



Bond lengths



Bond angles



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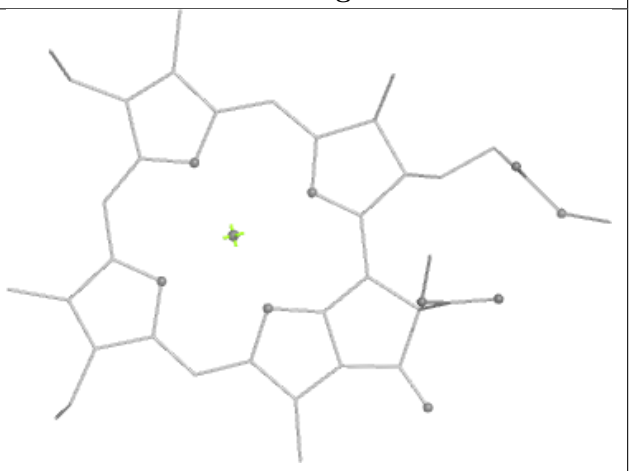
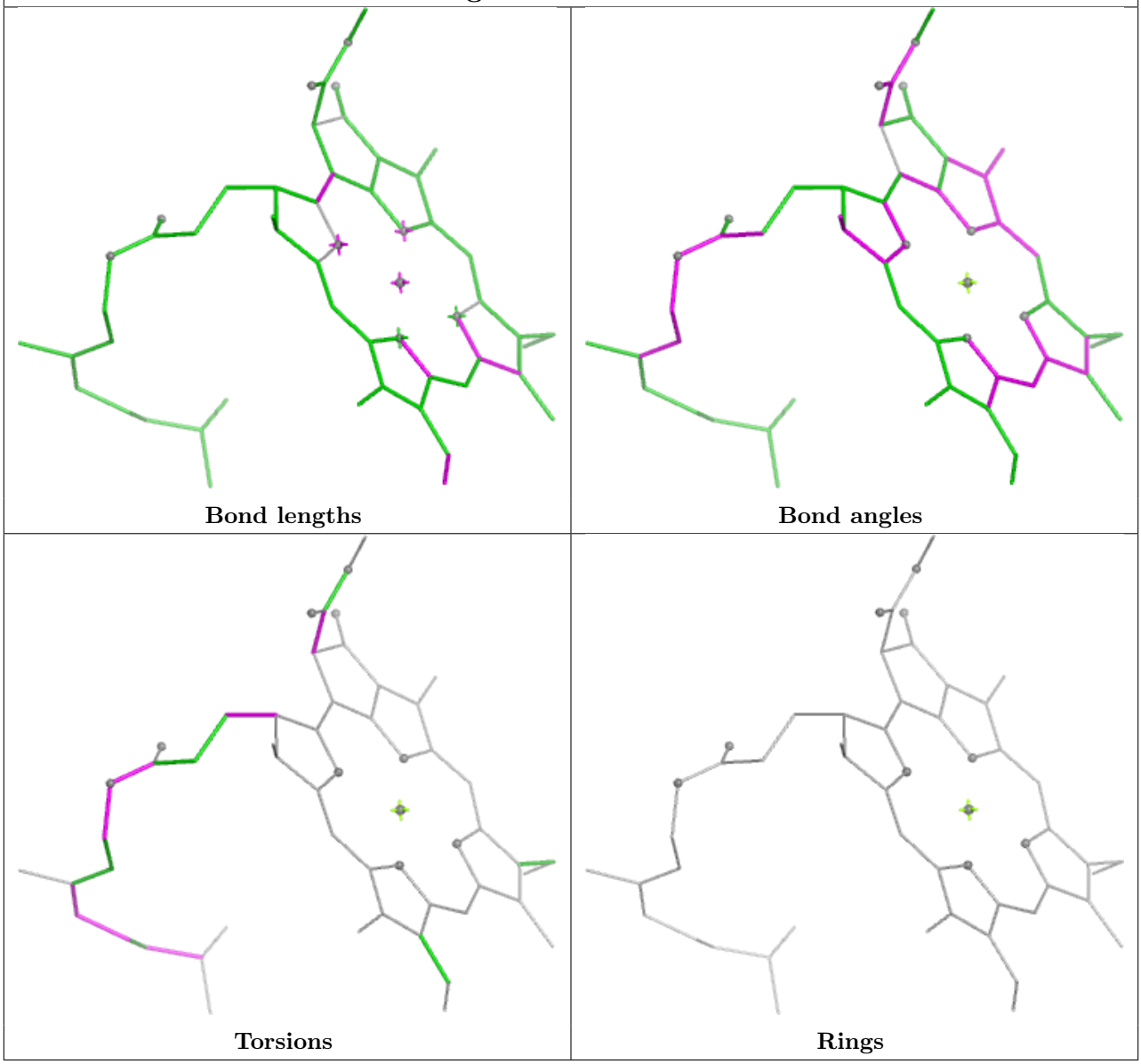
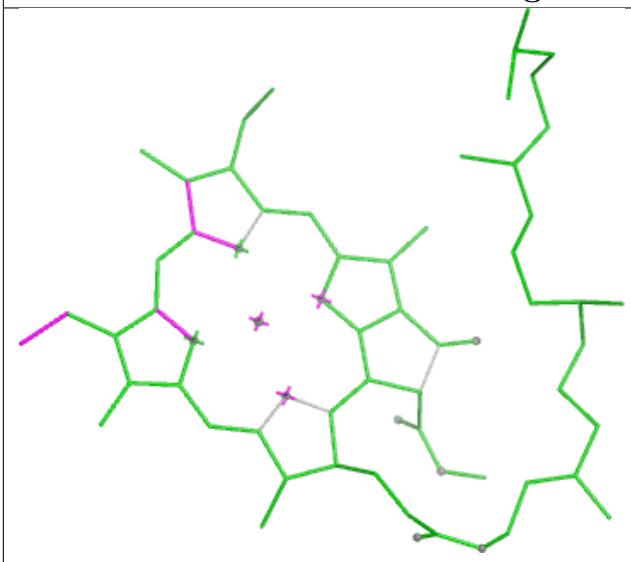


Rings

Ligand CLA A 822



Ligand CLA A 825



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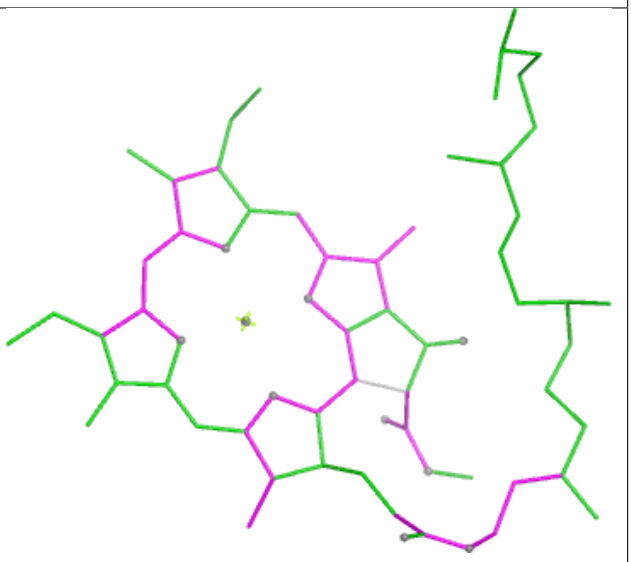
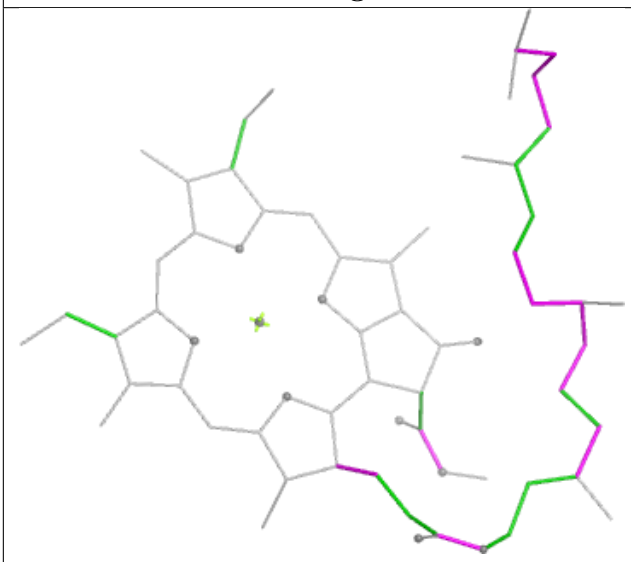


Bond angles



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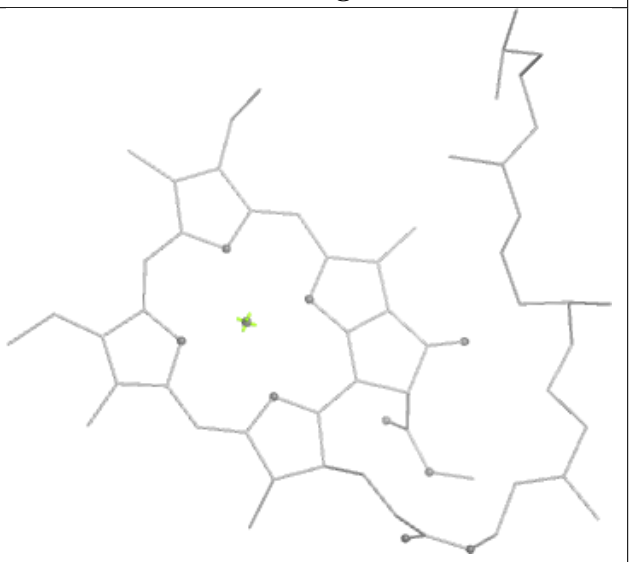
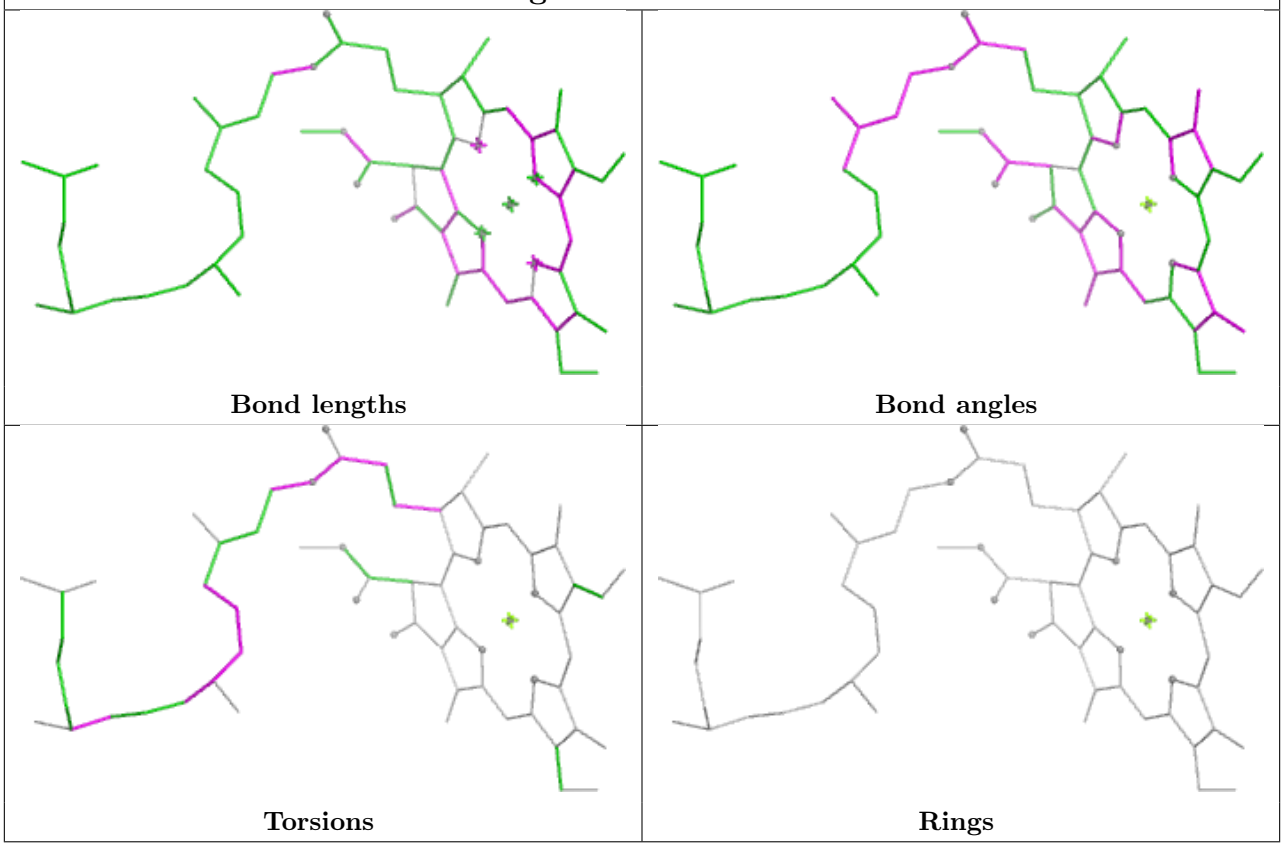
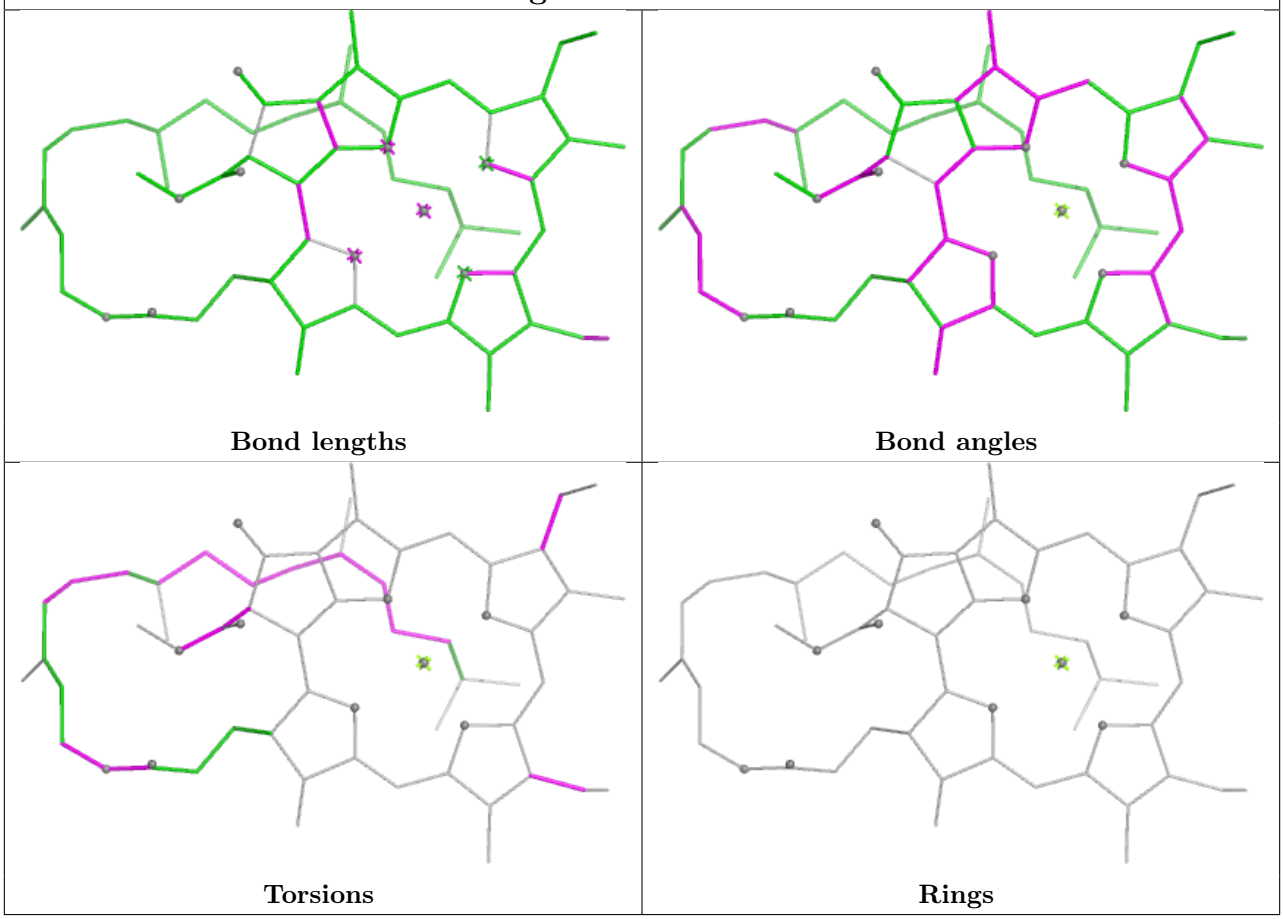


Rings

Ligand CL0 A 801



Ligand CLA 1 316



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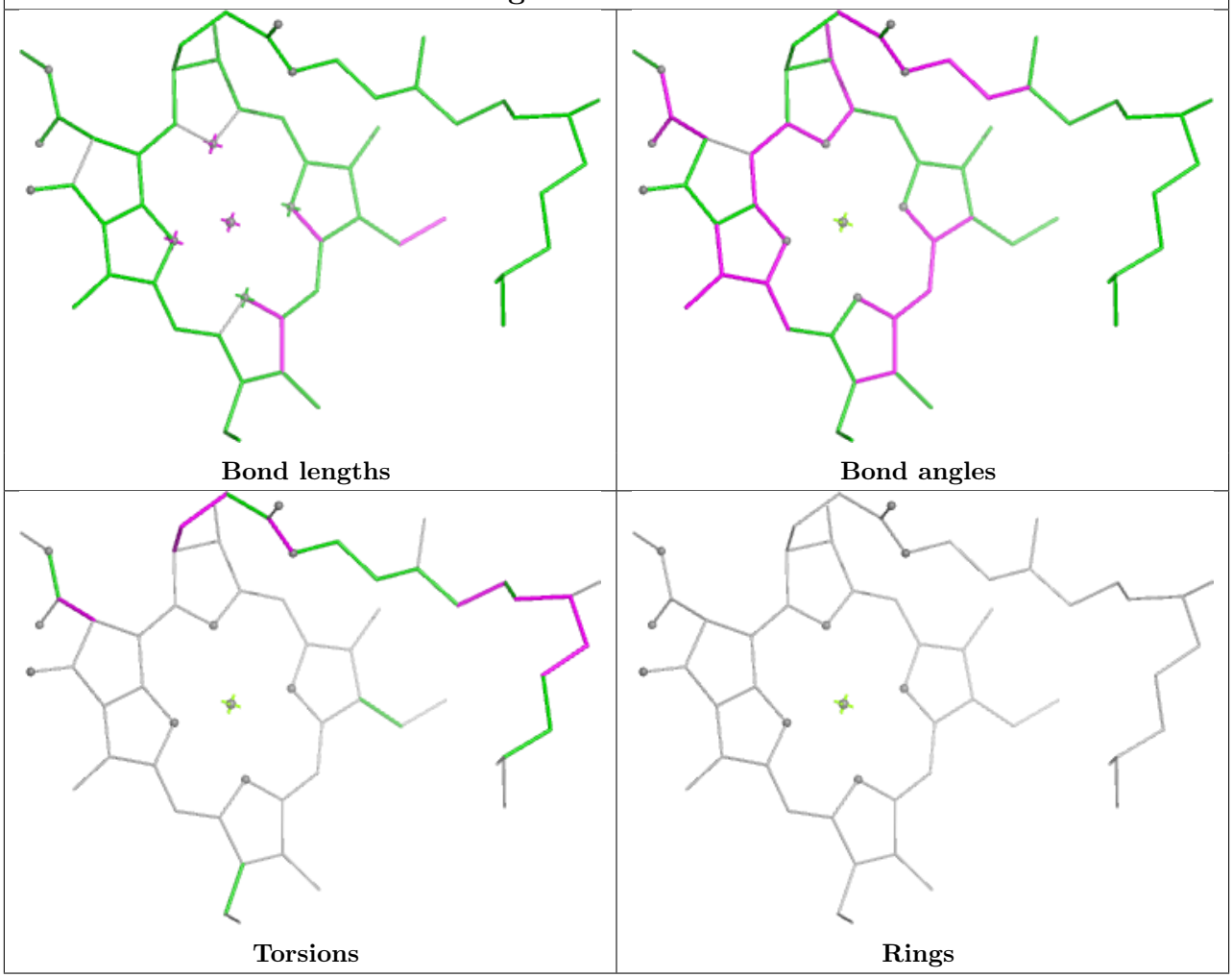
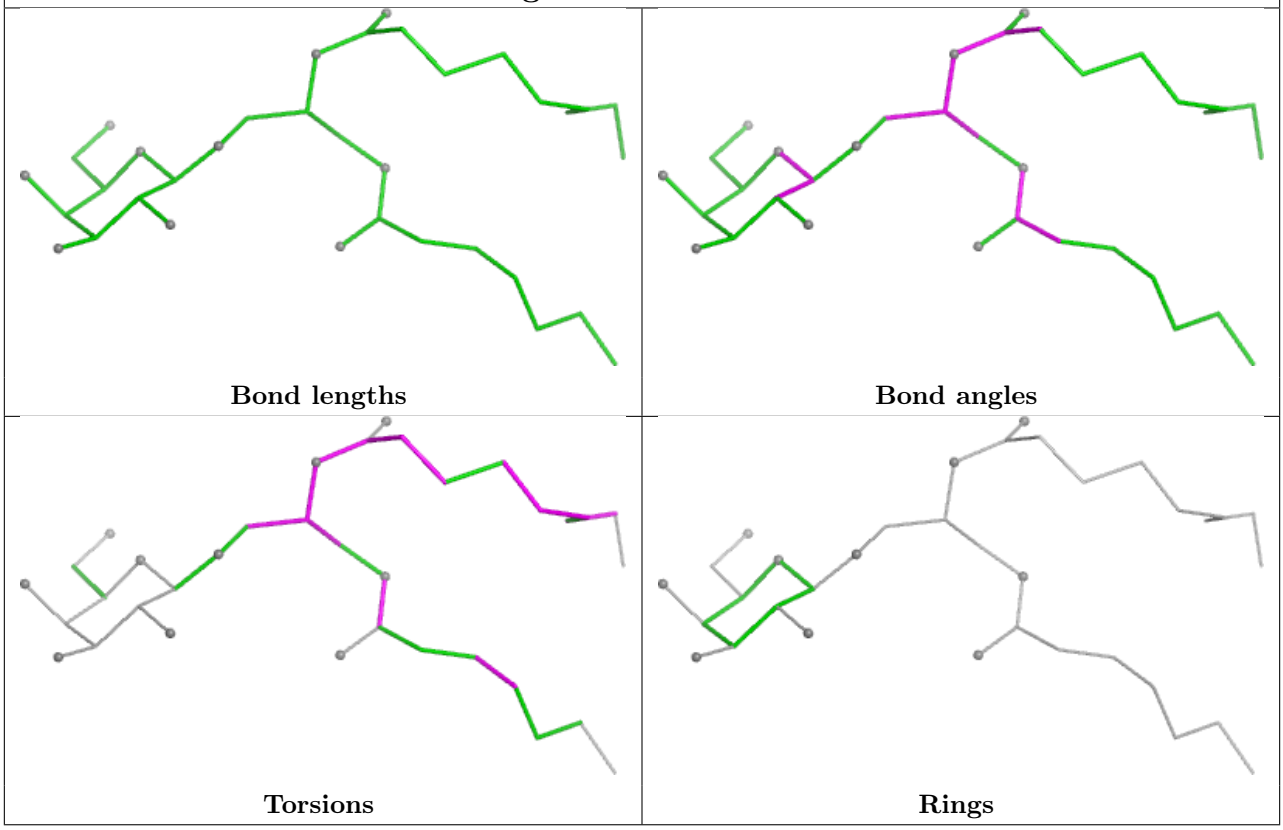


Ligand LMG F 308



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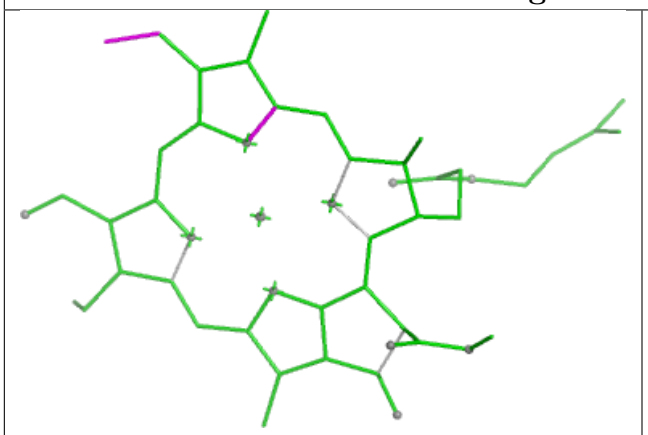

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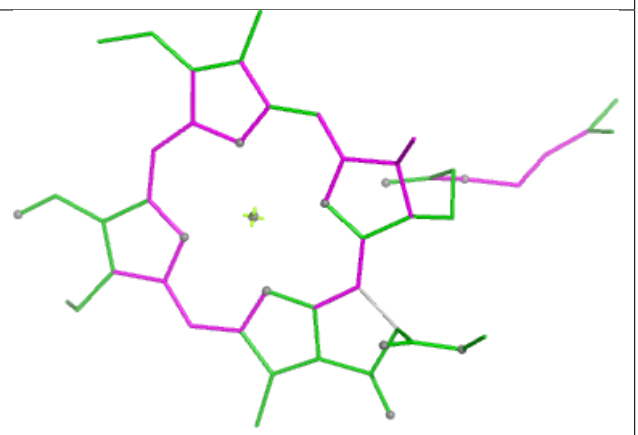
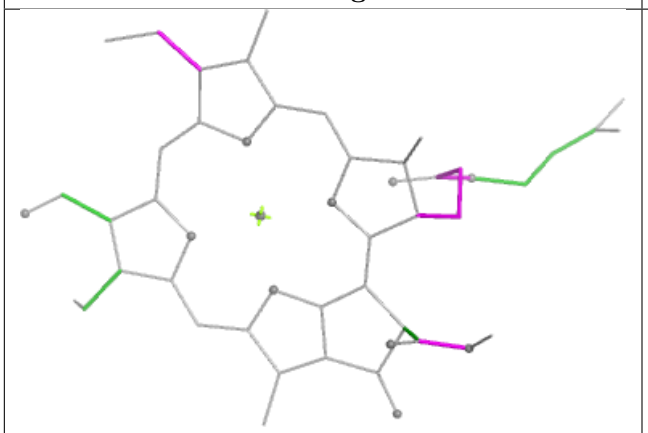
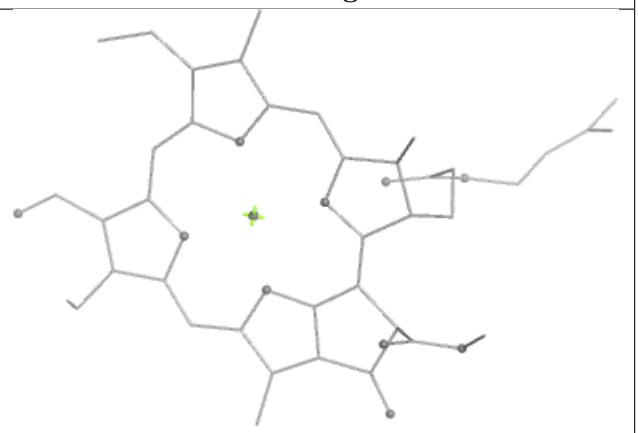


Bond angles

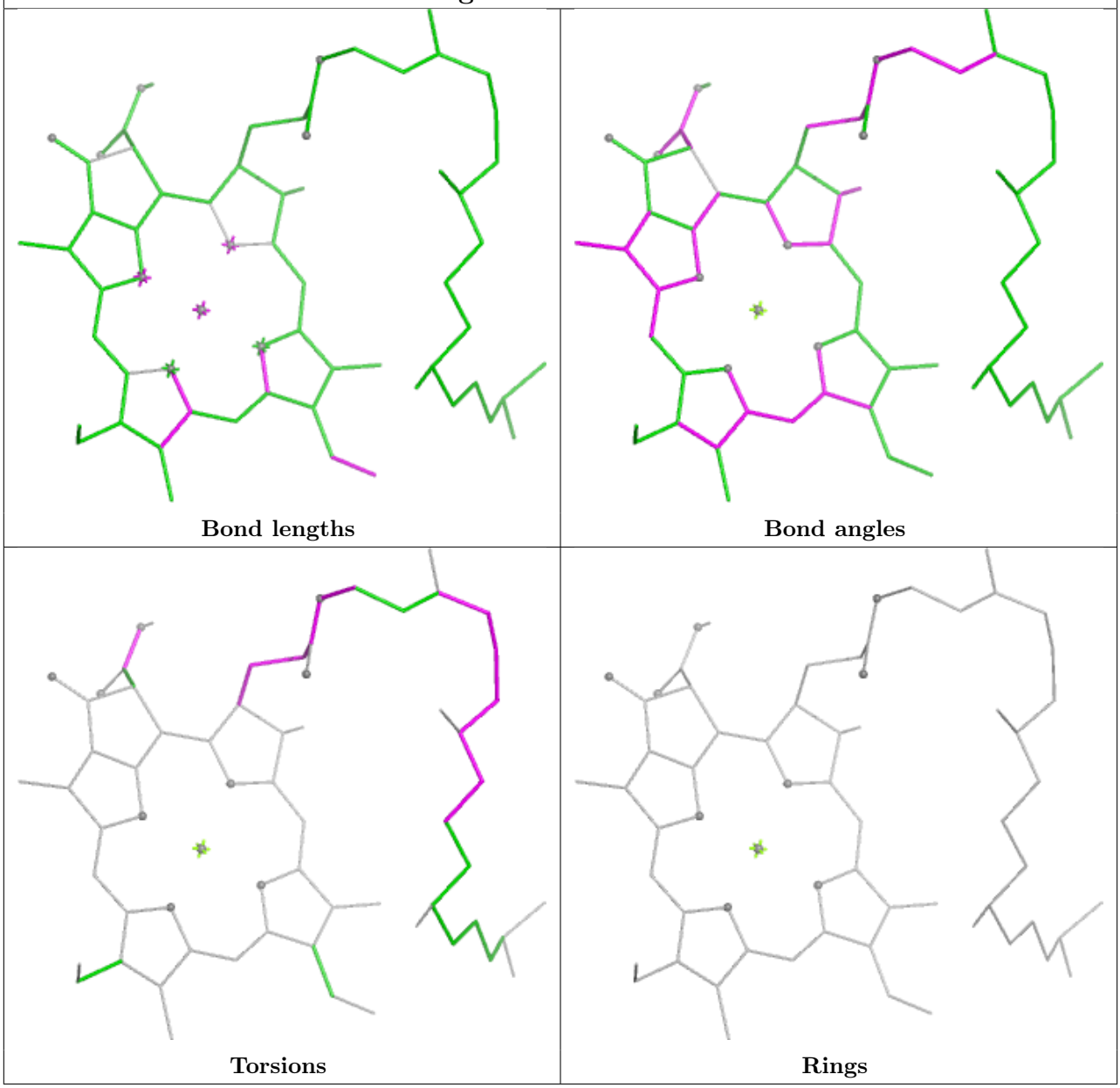


Torsions



Rings

Ligand CLA B 825



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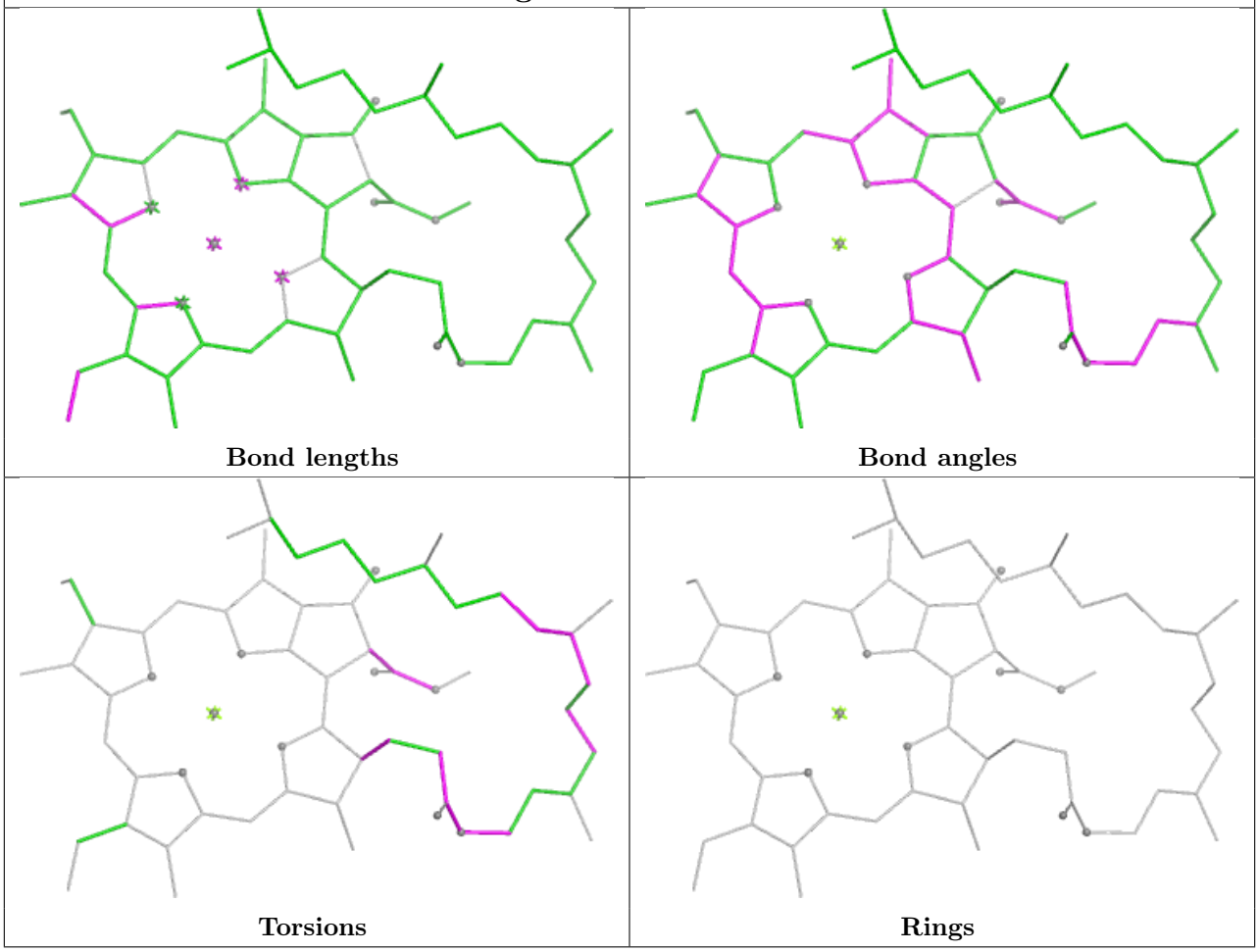

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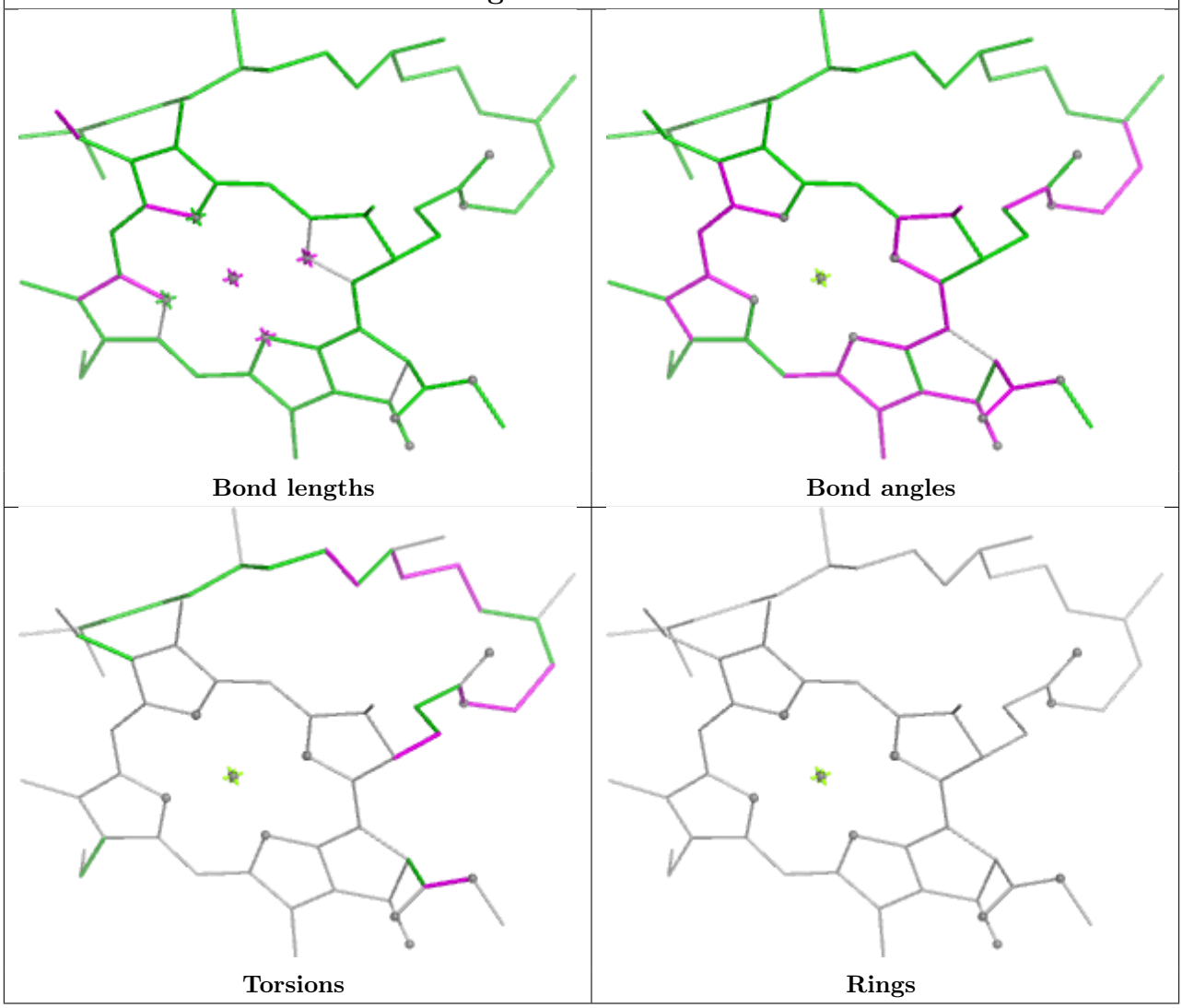

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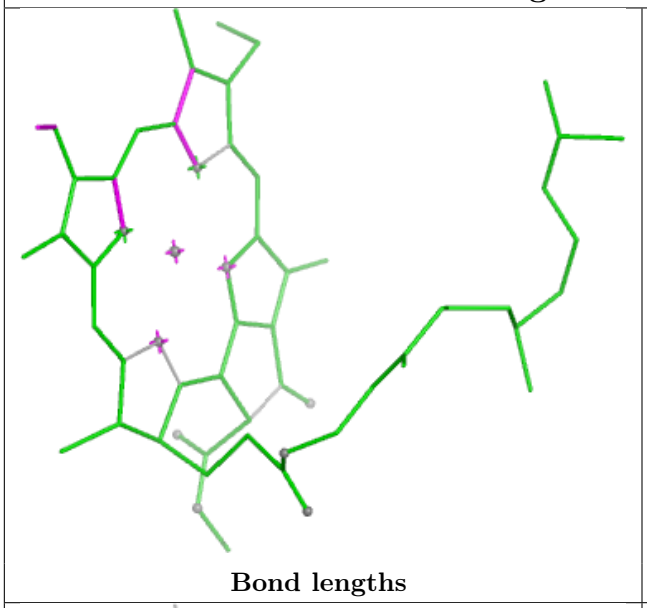
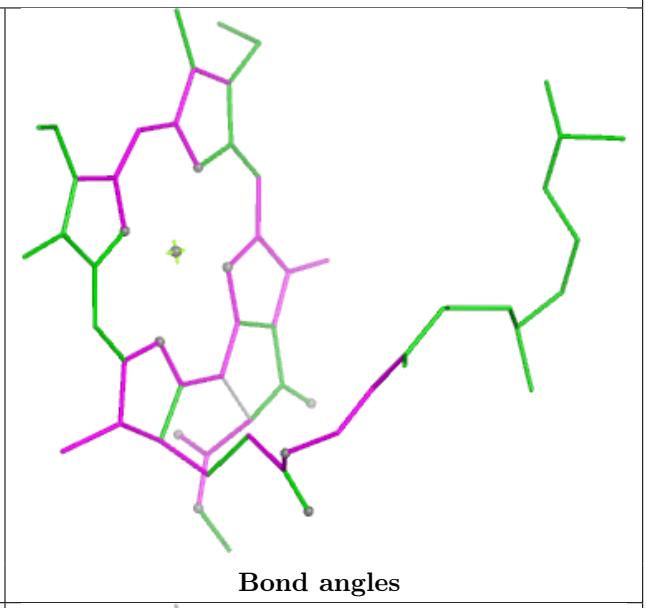
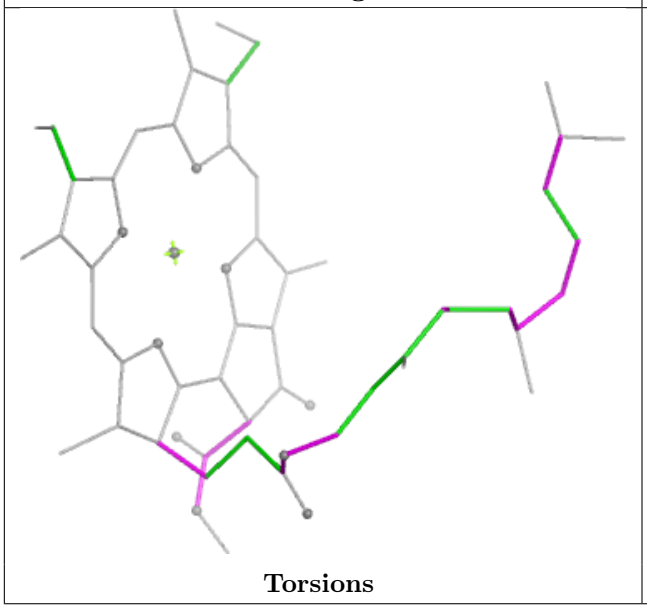


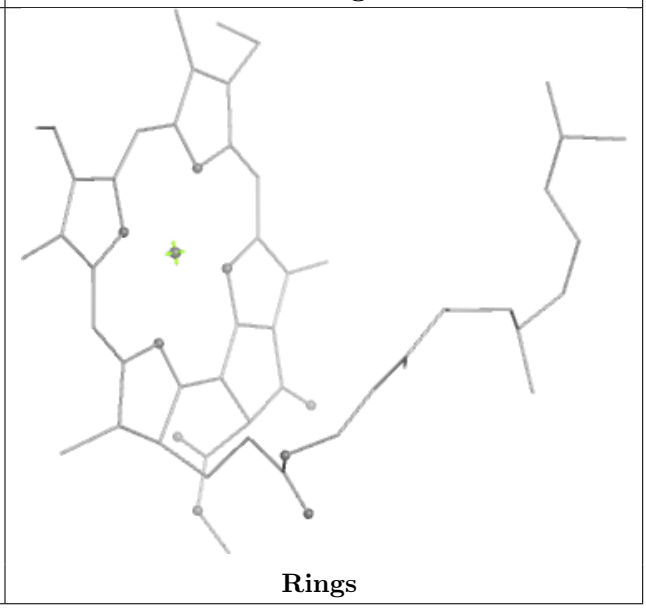
Bond lengths



Bond angles

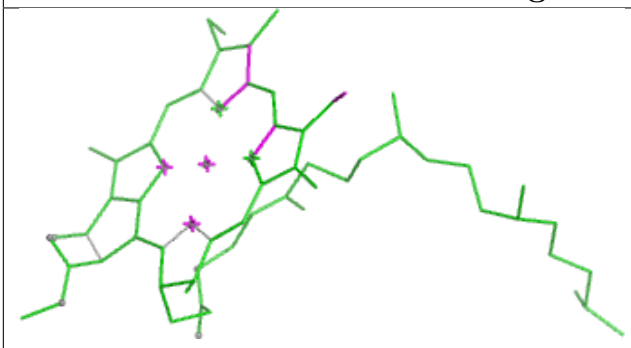


Torsions



Rings

Ligand CLA 1 306



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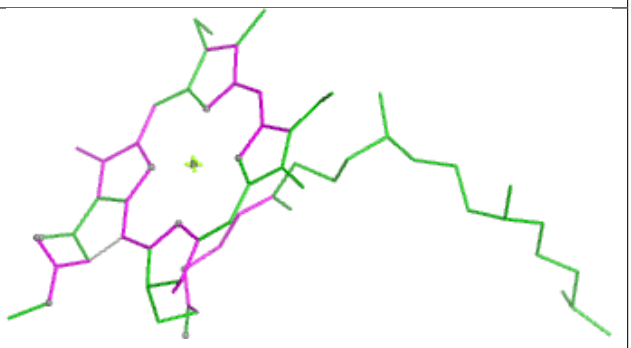
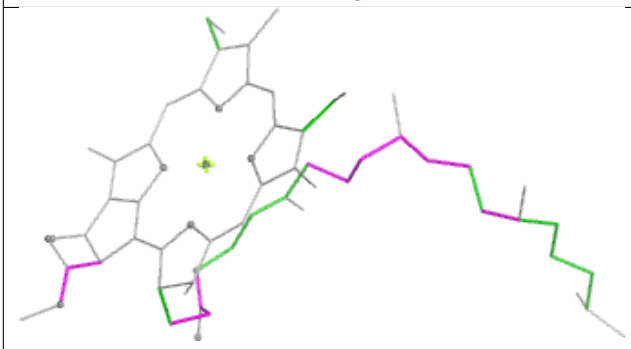


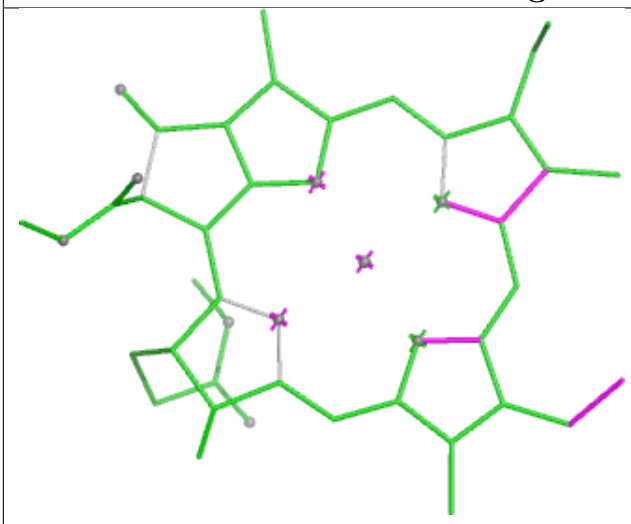
Bond angles



Torsions

Rings

Ligand CLA 2 304



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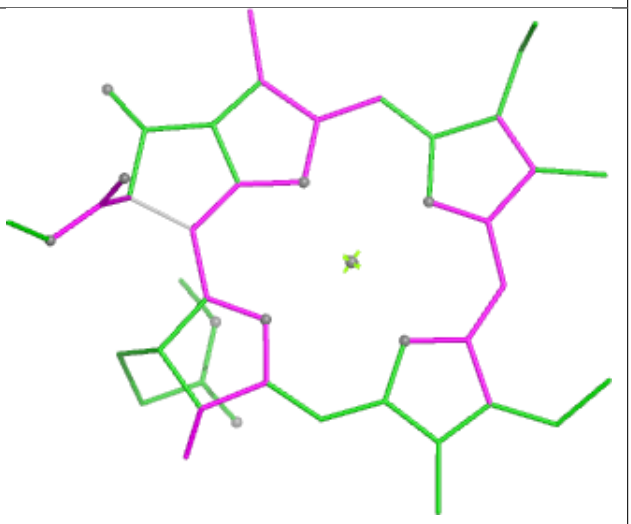
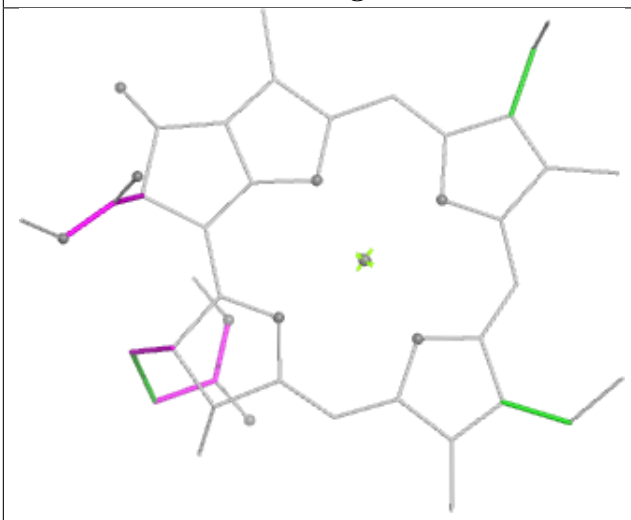
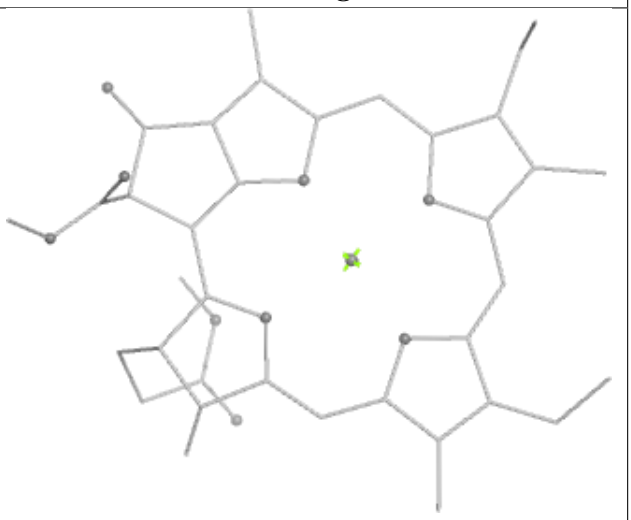


Bond angles

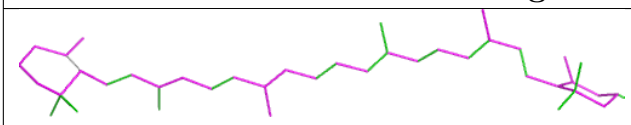


Torsions

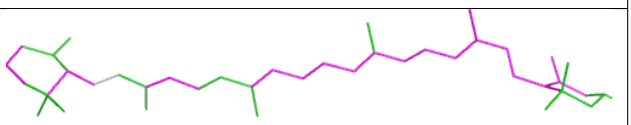


Rings

Ligand LUT 5 303

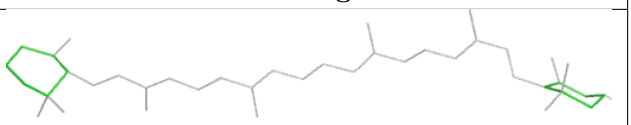


Bond lengths



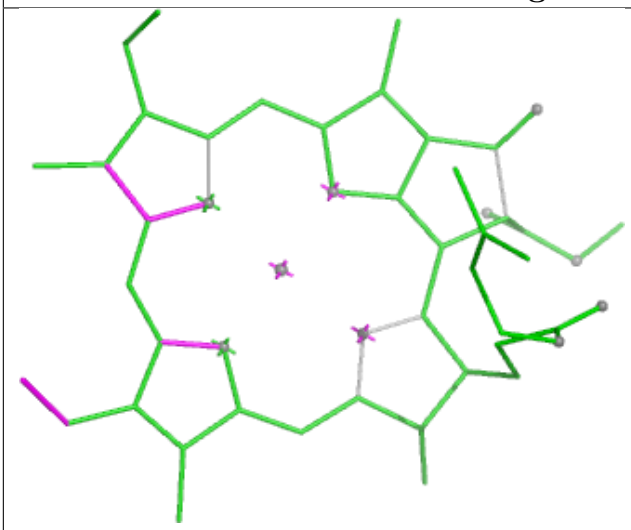
Bond angles

Torsions



Rings

Ligand CLA 9 313



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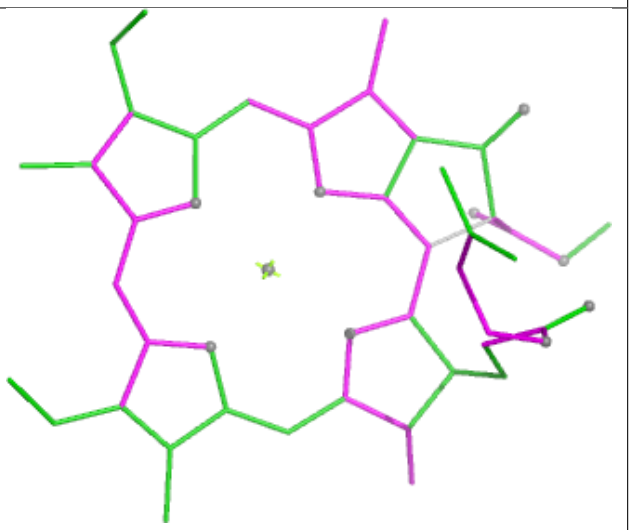

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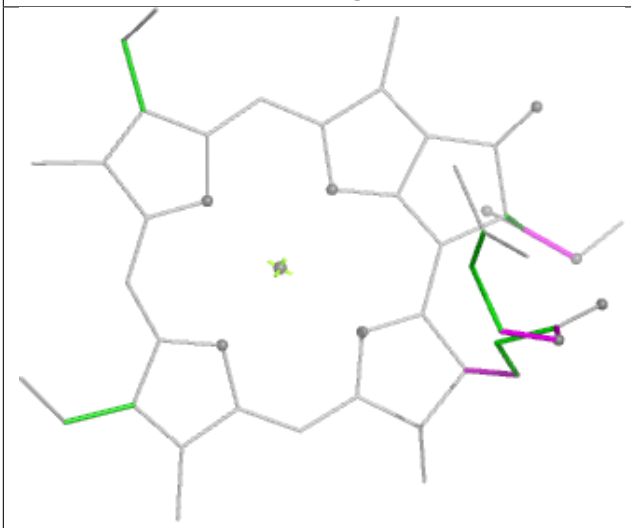

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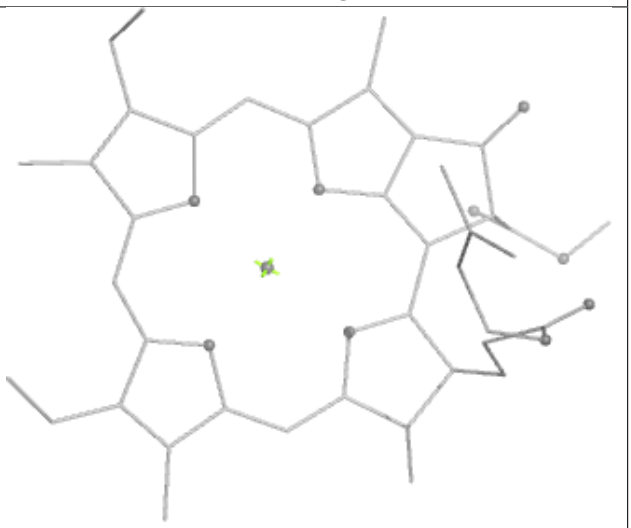
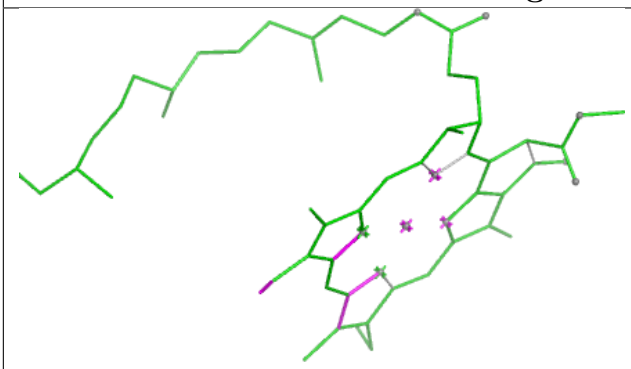


Rings

Ligand CLA Z 308



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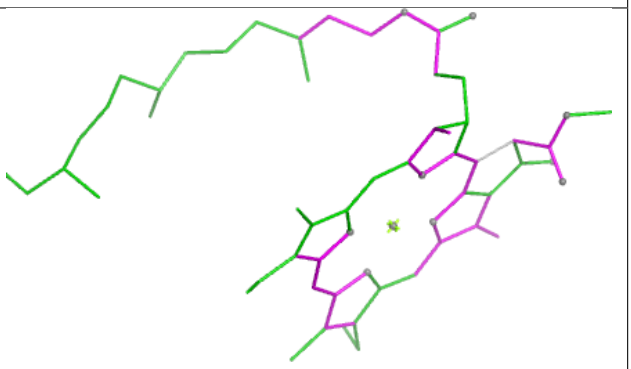
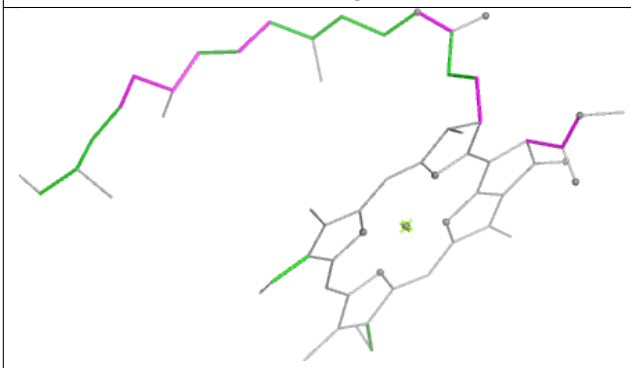


Bond angles



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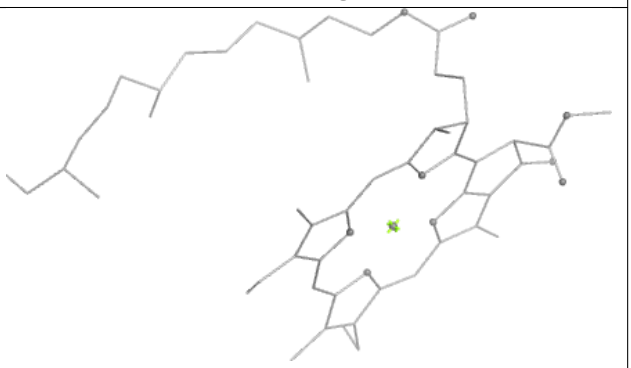
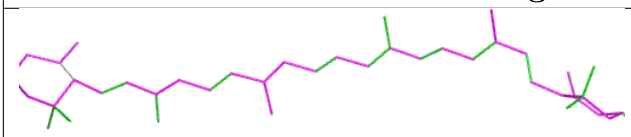


Rings

Ligand LUT 4 803



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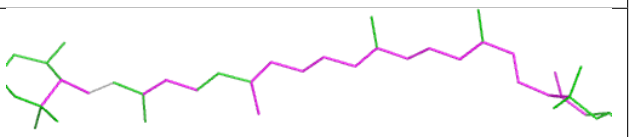
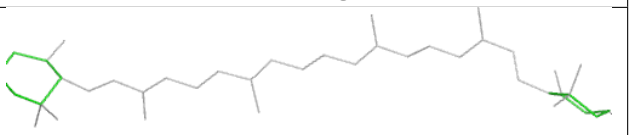


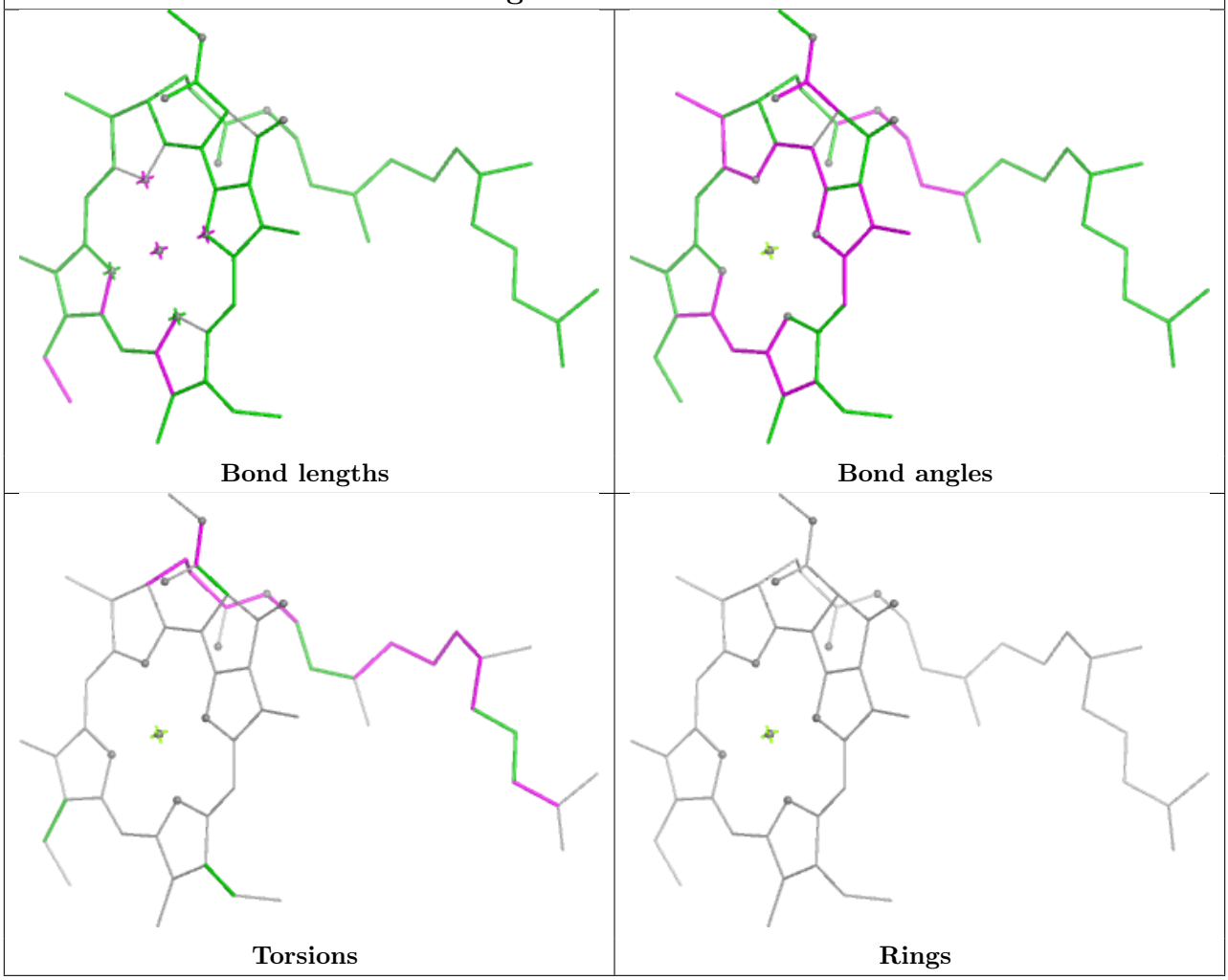
Bond angles

Torsions



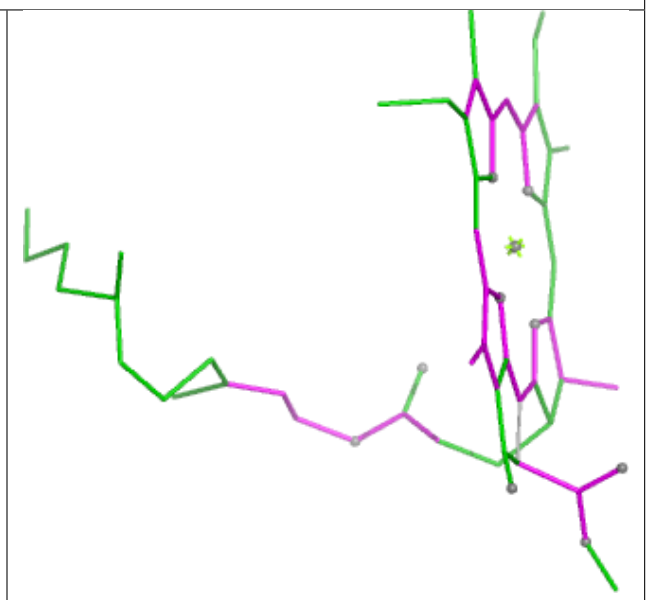
Rings

Ligand CLA 3 314

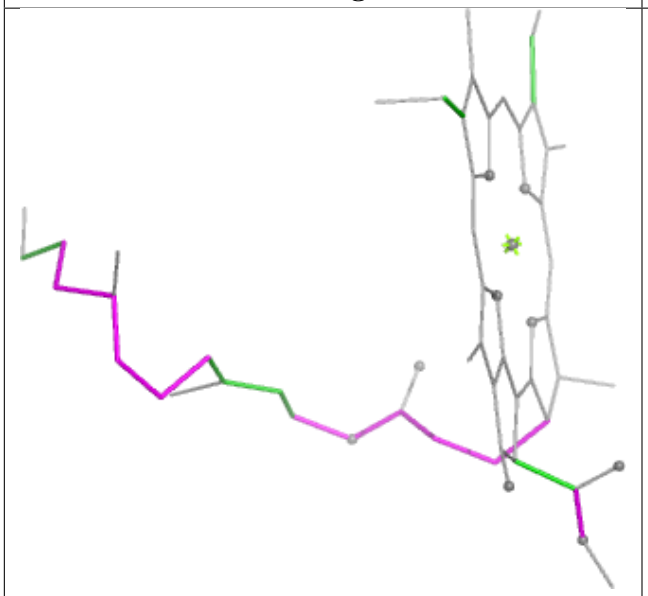


Ligand CLA B 831

Bond lengths



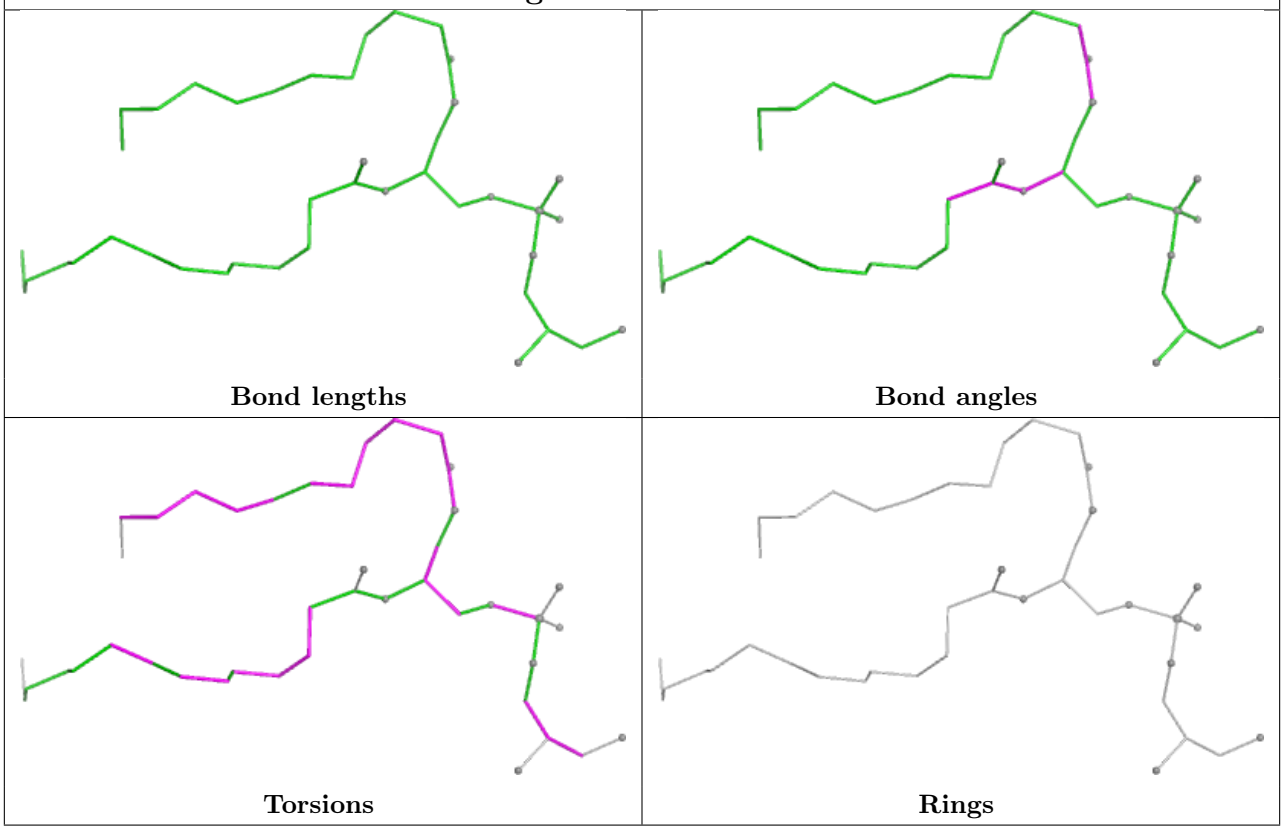
Bond angles



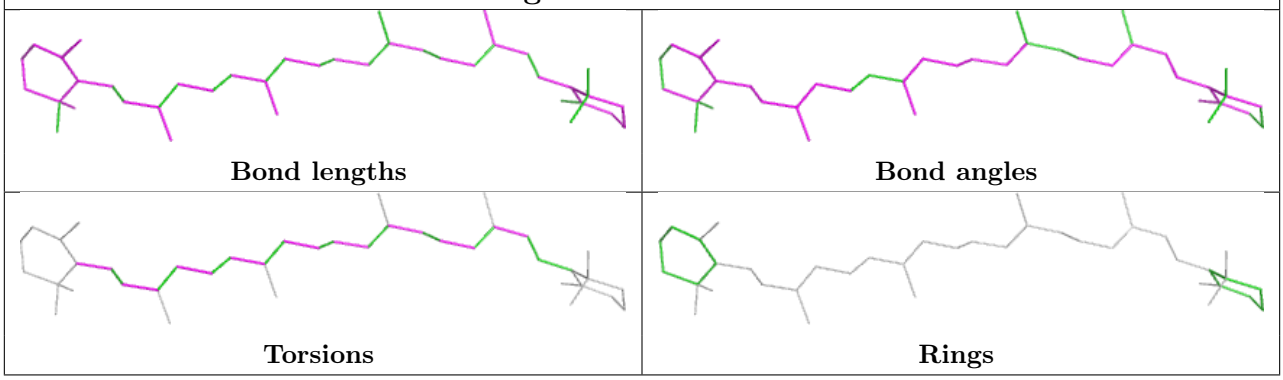
Torsions

Rings

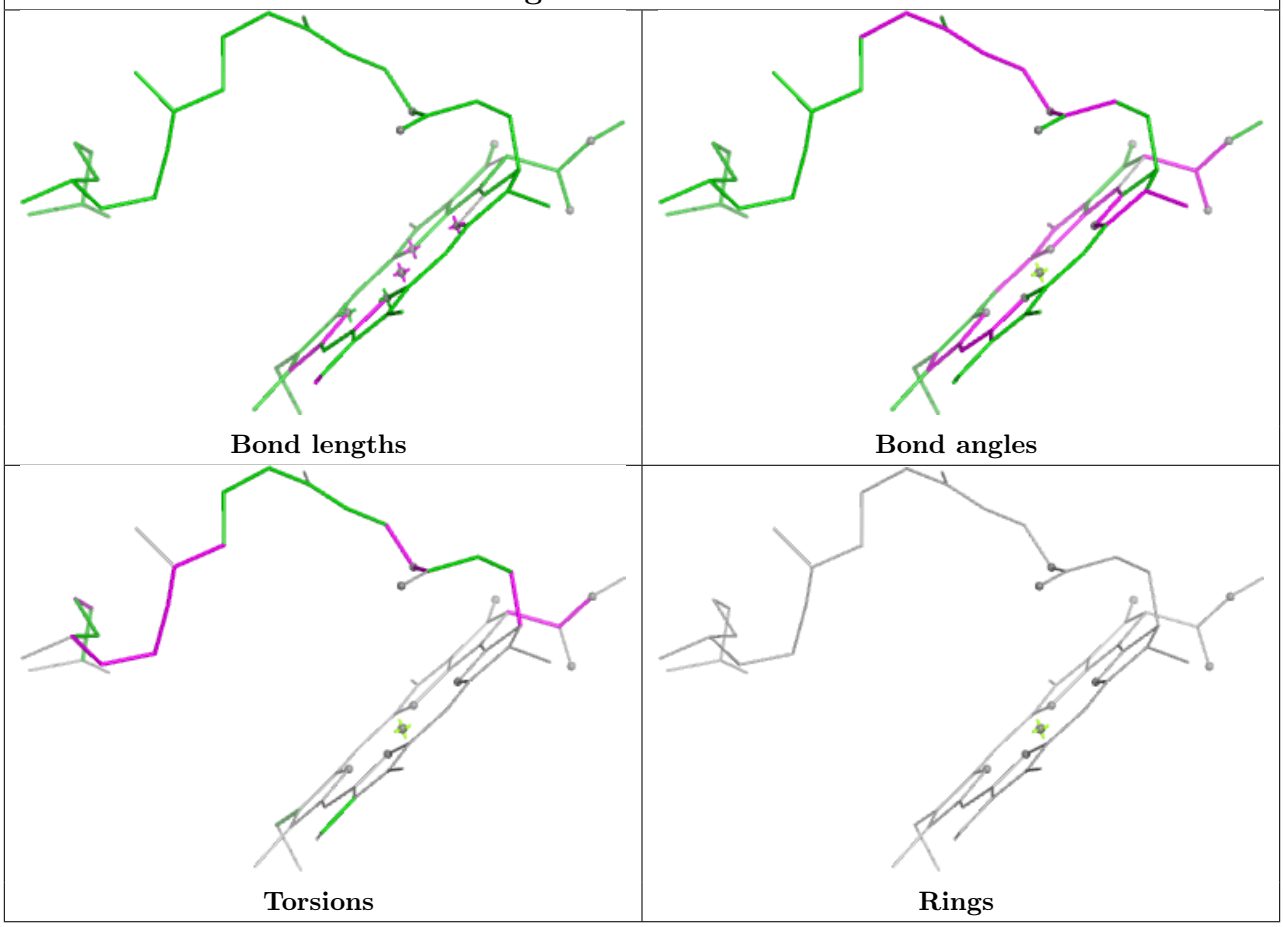
Ligand LHG Z 317



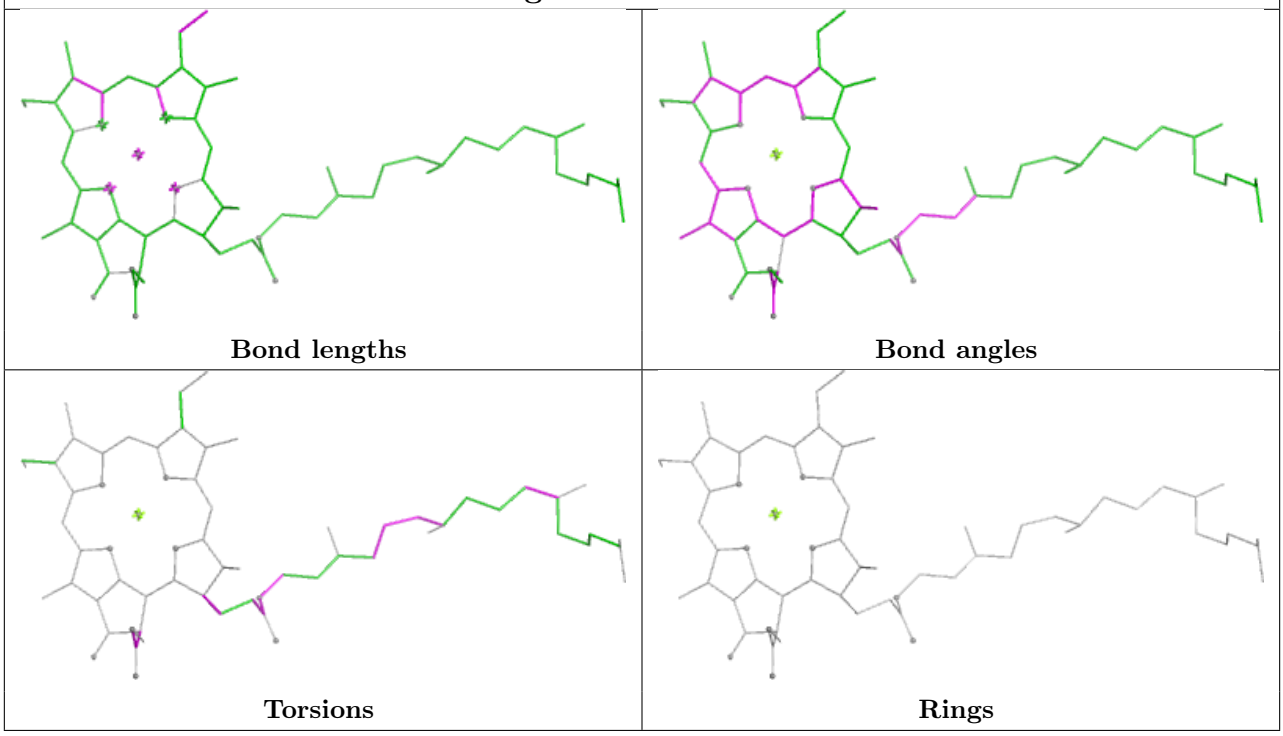
Ligand BCR B 849



Ligand CLA A 832



Ligand CLA A 815



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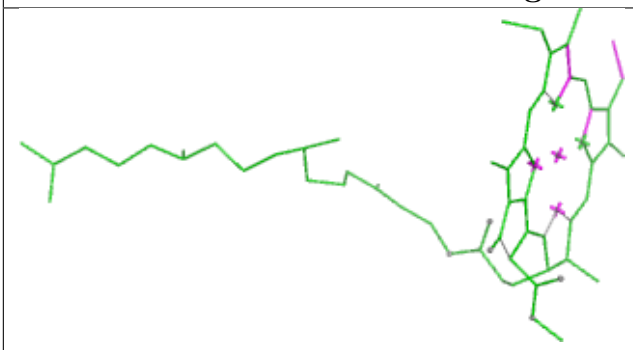
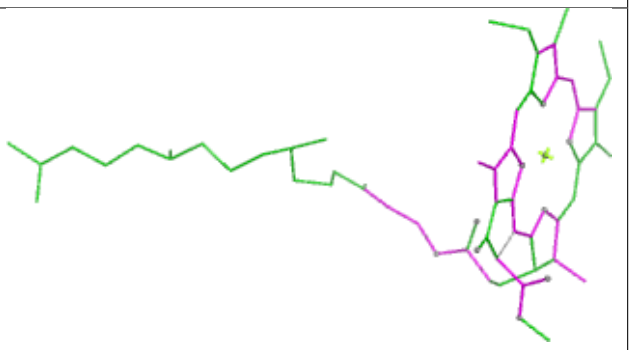
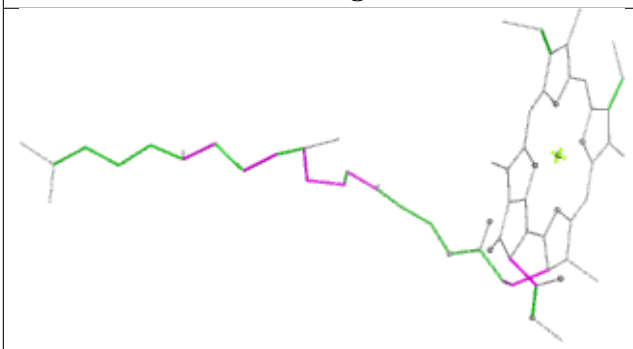


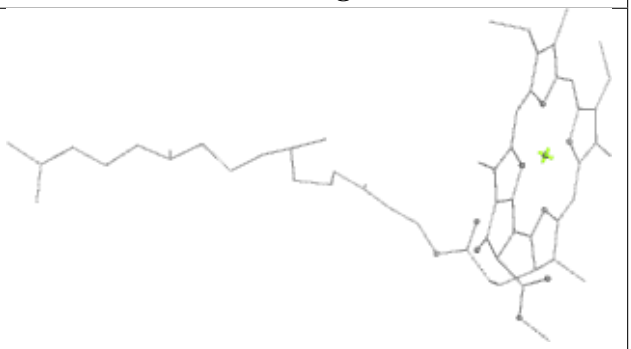
Bond lengths



Bond angles

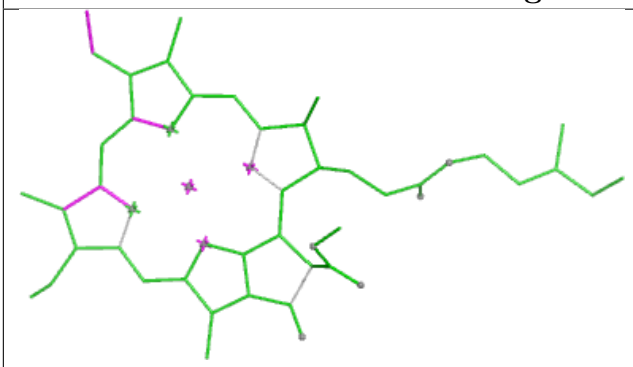


Torsions

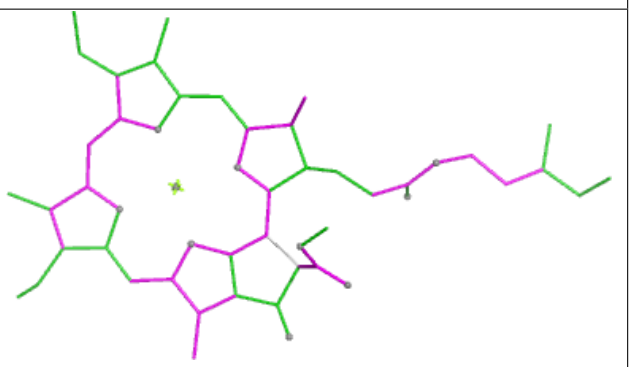


Rings

Ligand CLA B 837



Bond lengths



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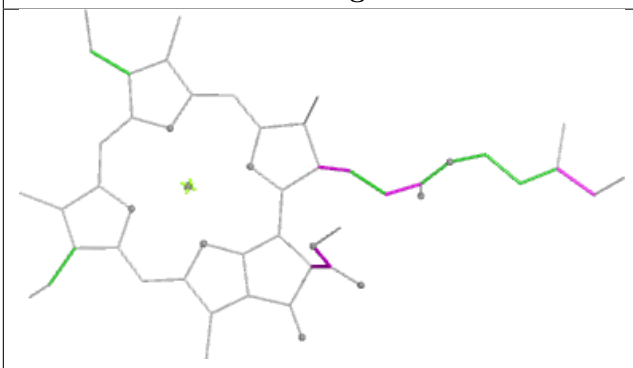

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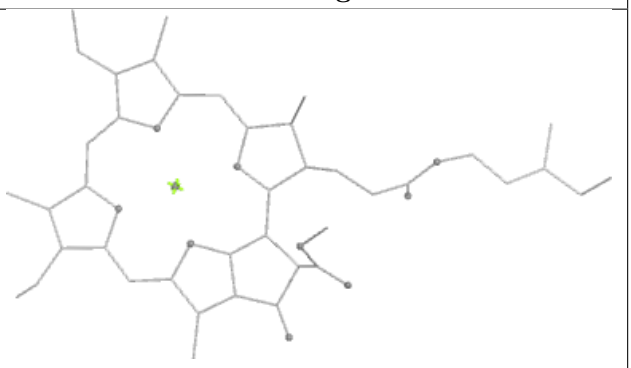
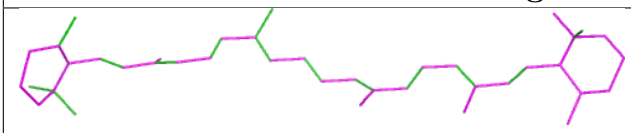


Rings

Ligand BCR 3 306



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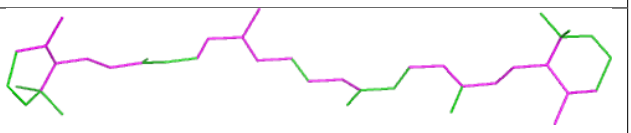

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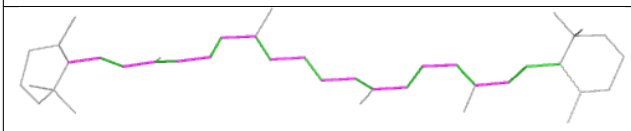

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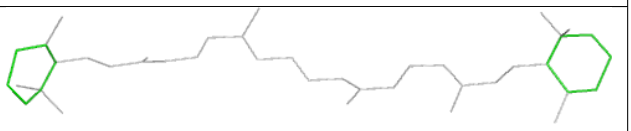
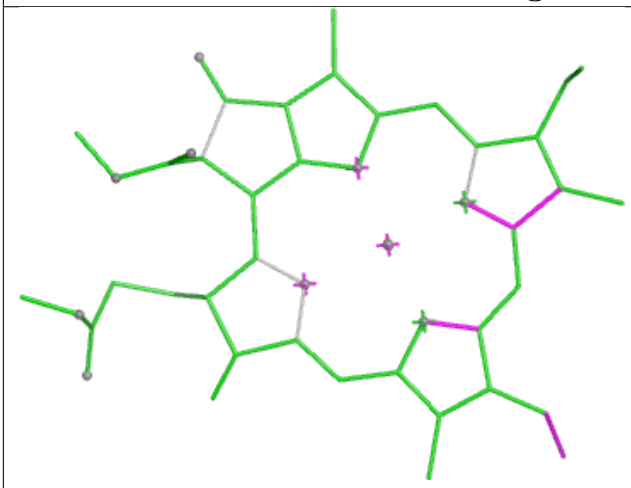


Rings

Ligand CLA Z 315



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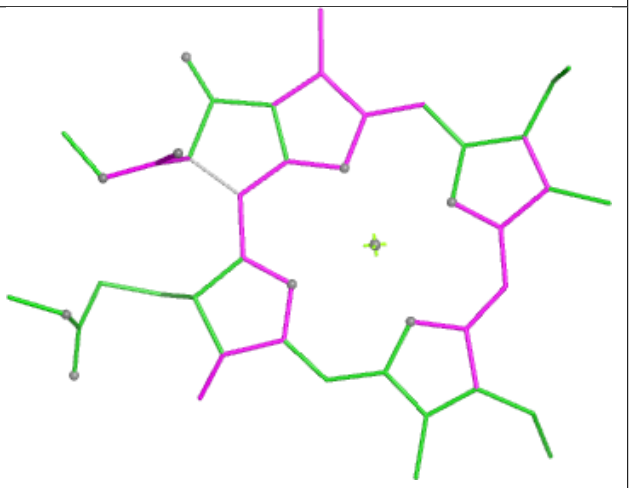

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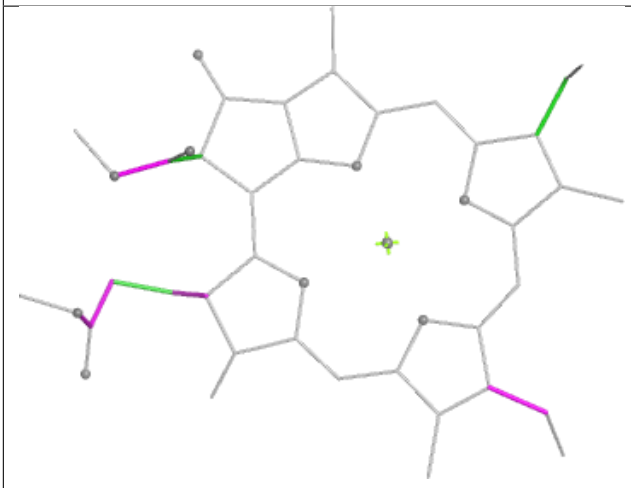

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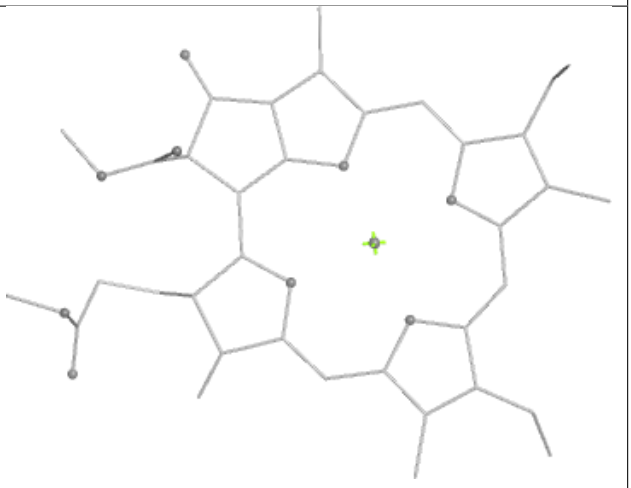

Rings

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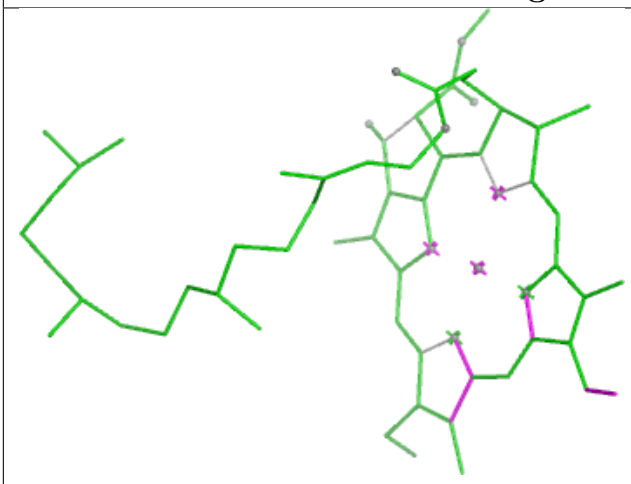
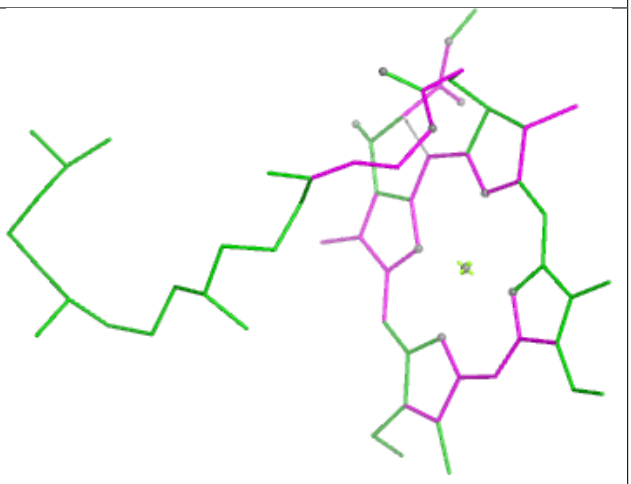
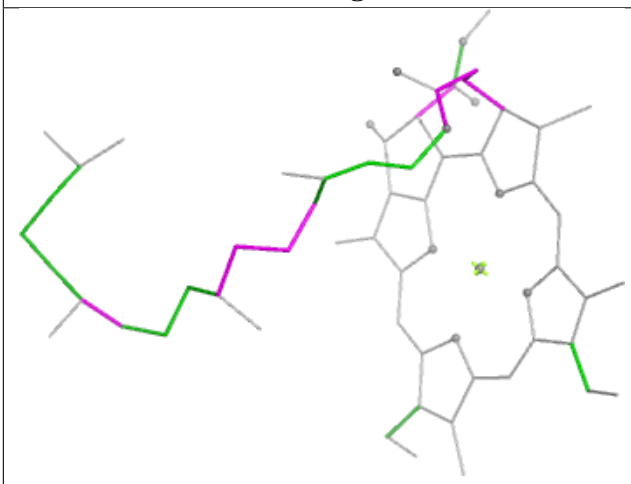
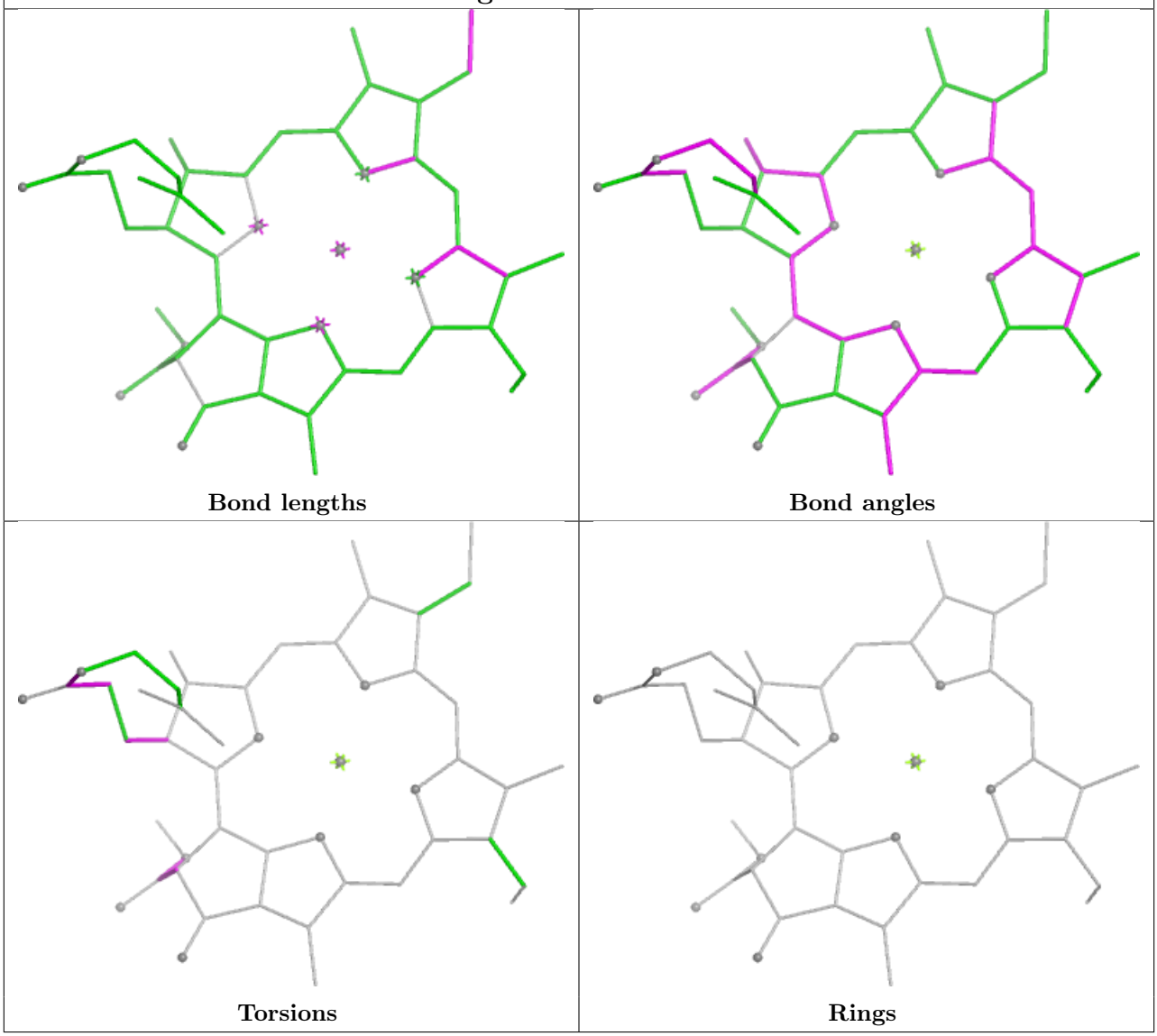
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA 6 317



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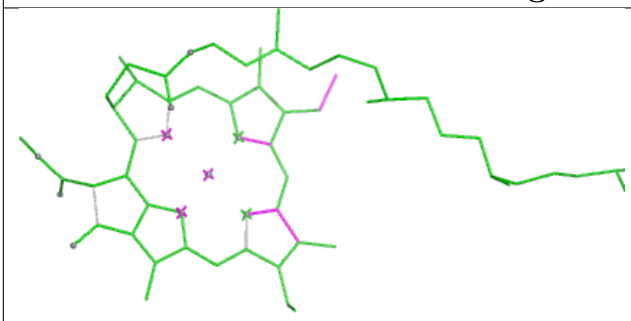
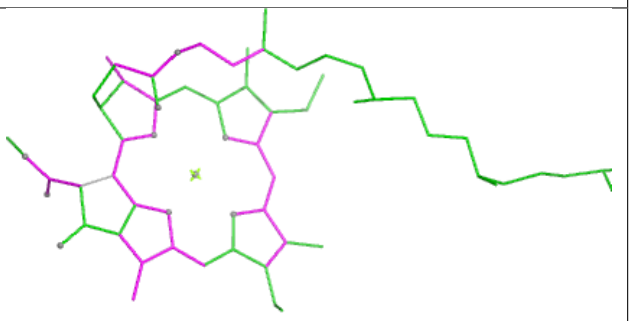
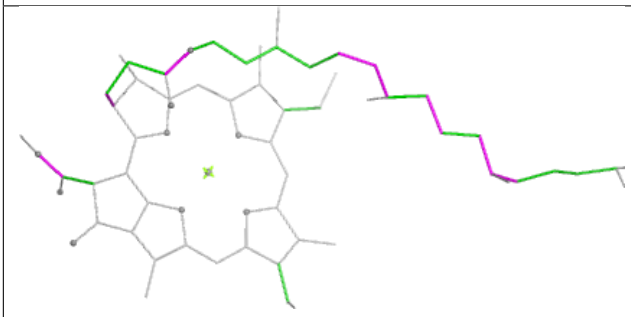
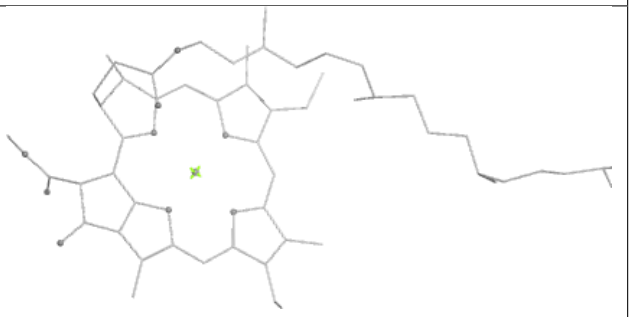
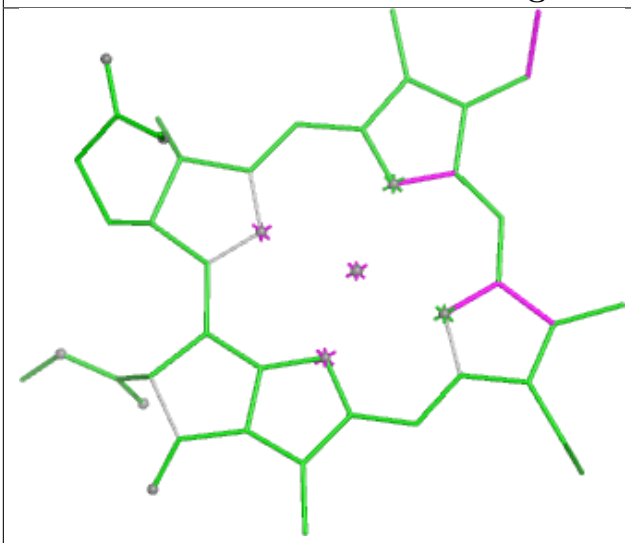
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 314



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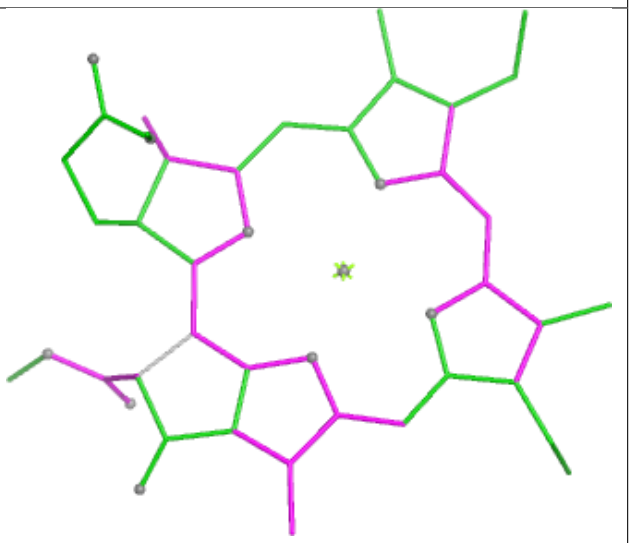

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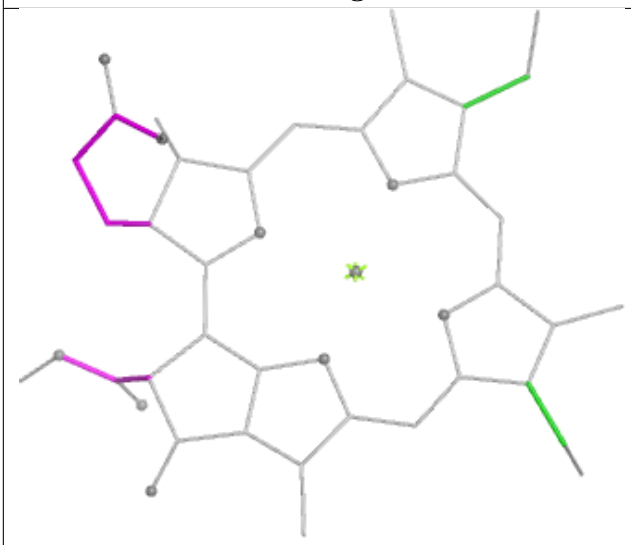

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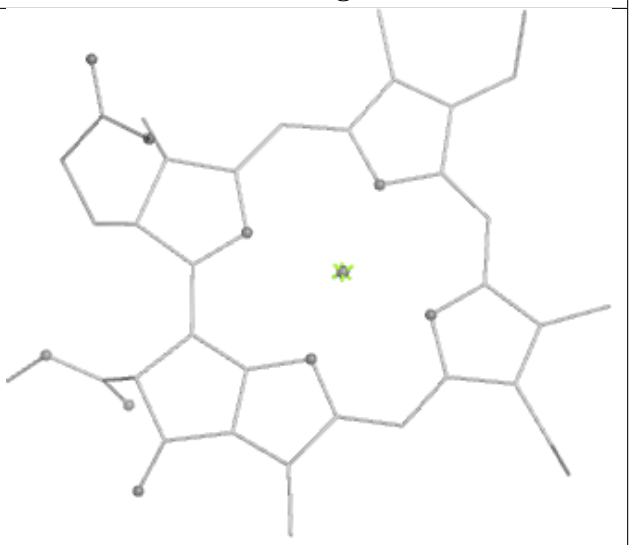

Rings

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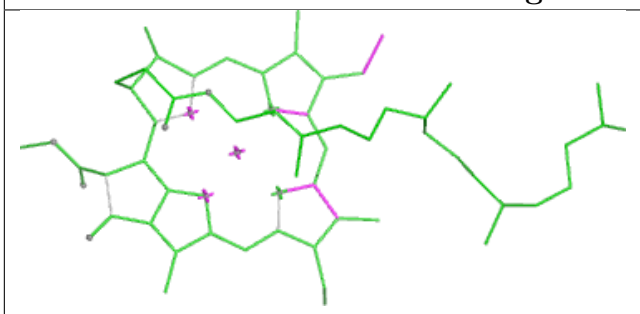
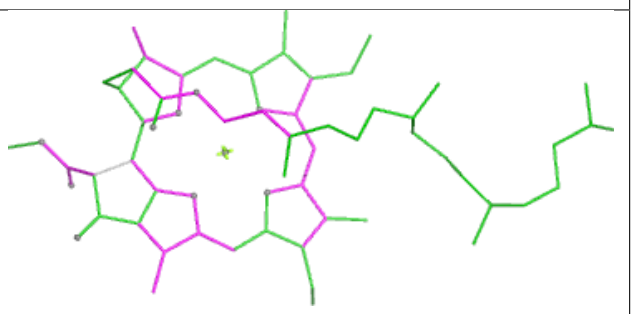
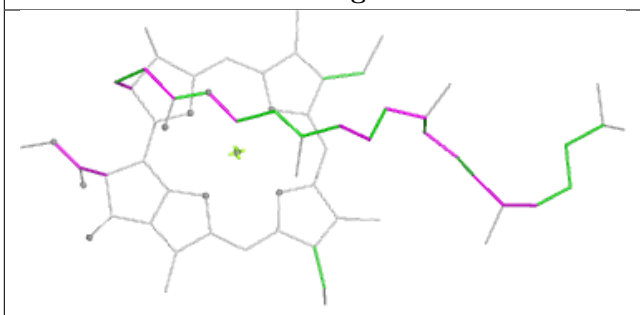
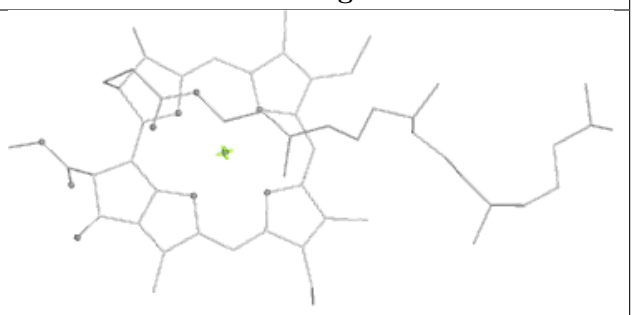
 Bond lengths	 Bond angles
 Torsions	 Rings

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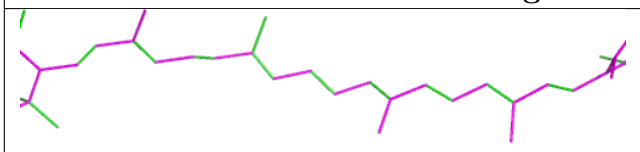
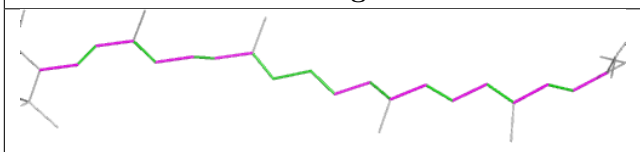
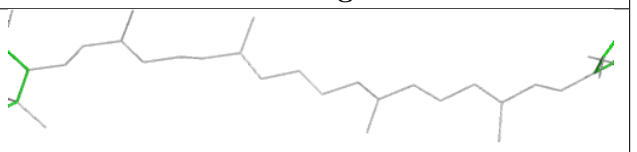
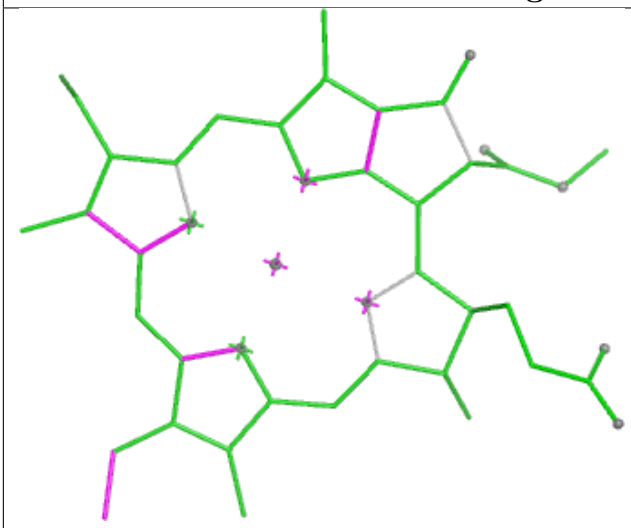
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA F 305



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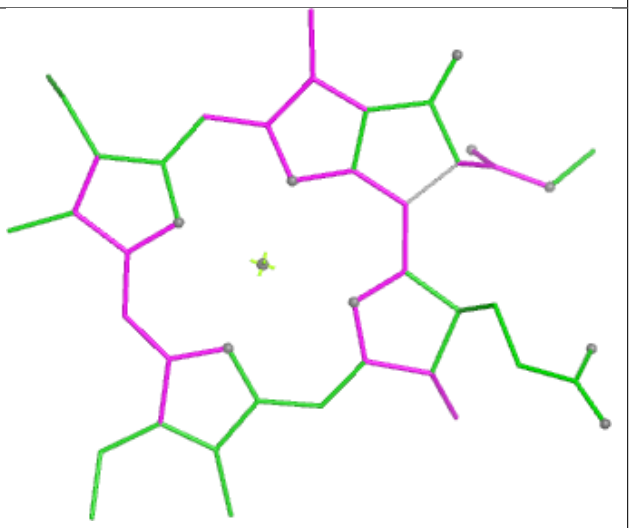

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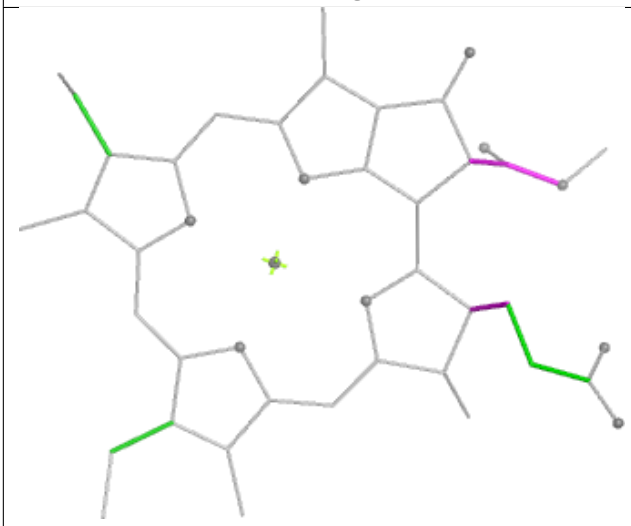

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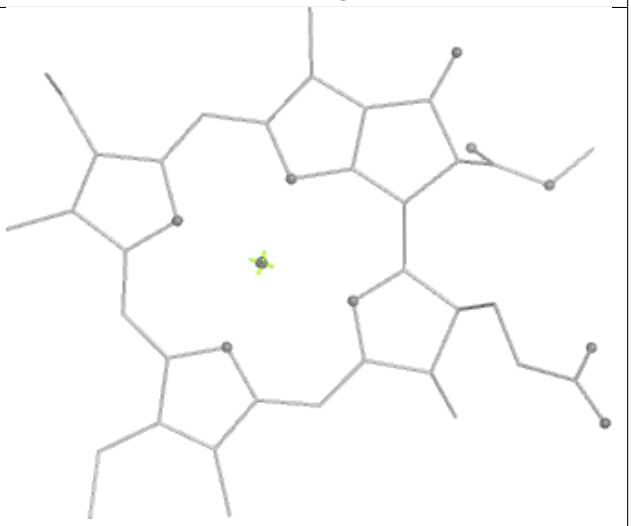
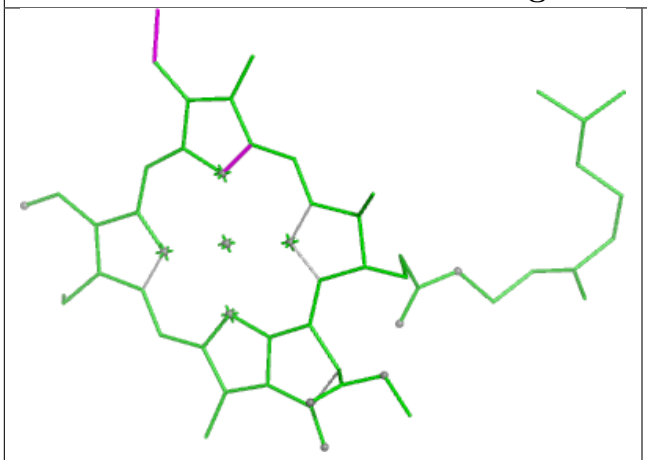


Rings

Ligand CHL 8 312



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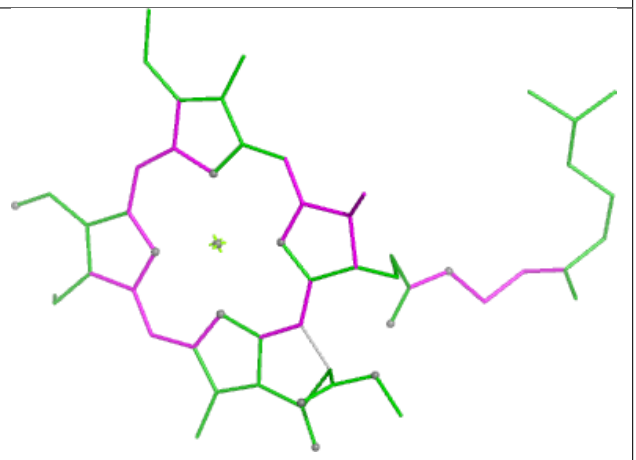

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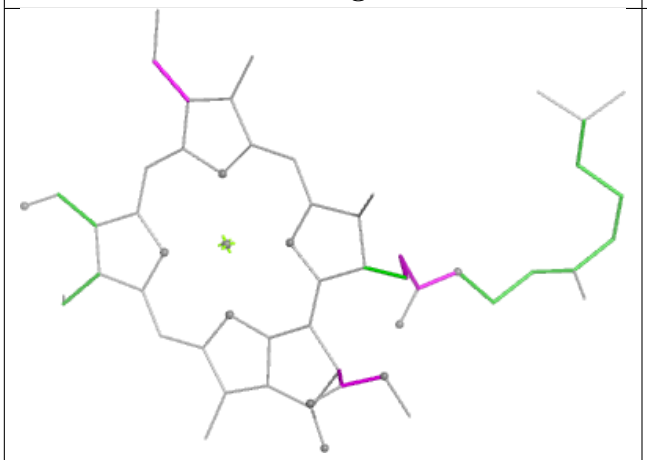

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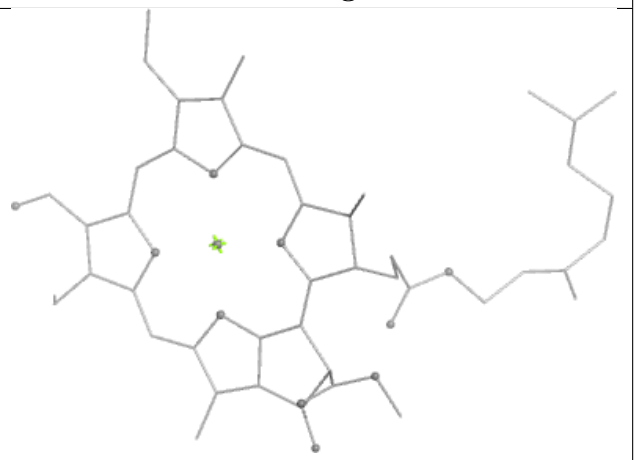
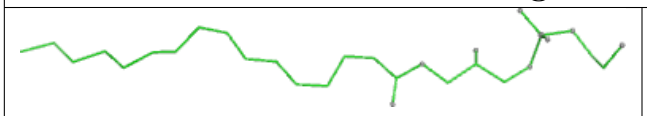


Rings

Ligand LPX 8 319



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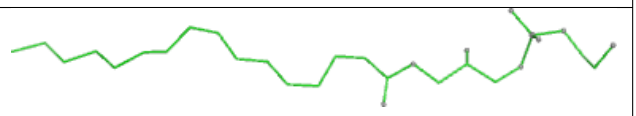

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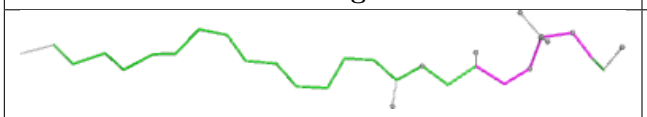

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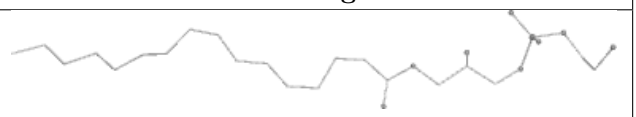
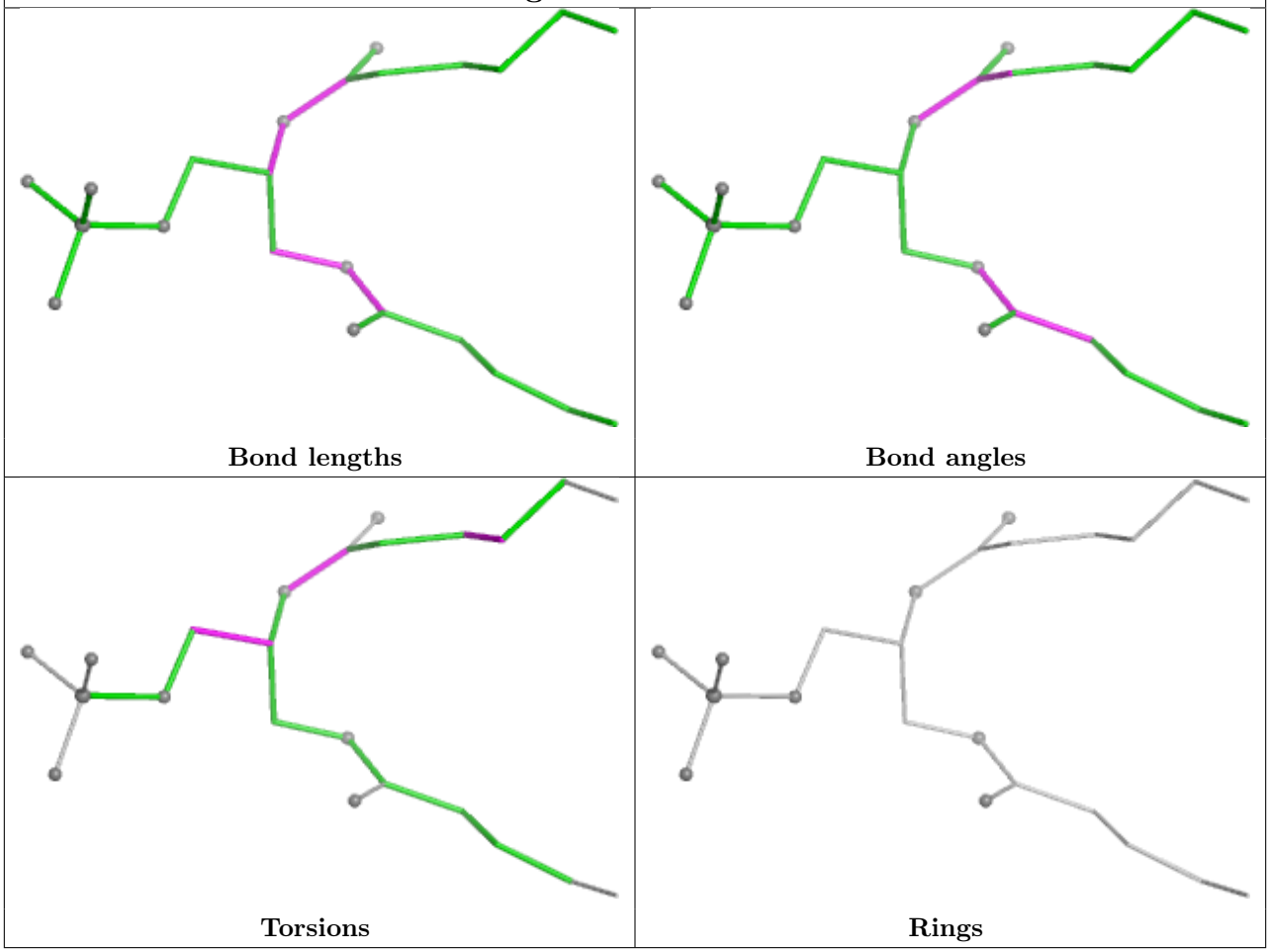
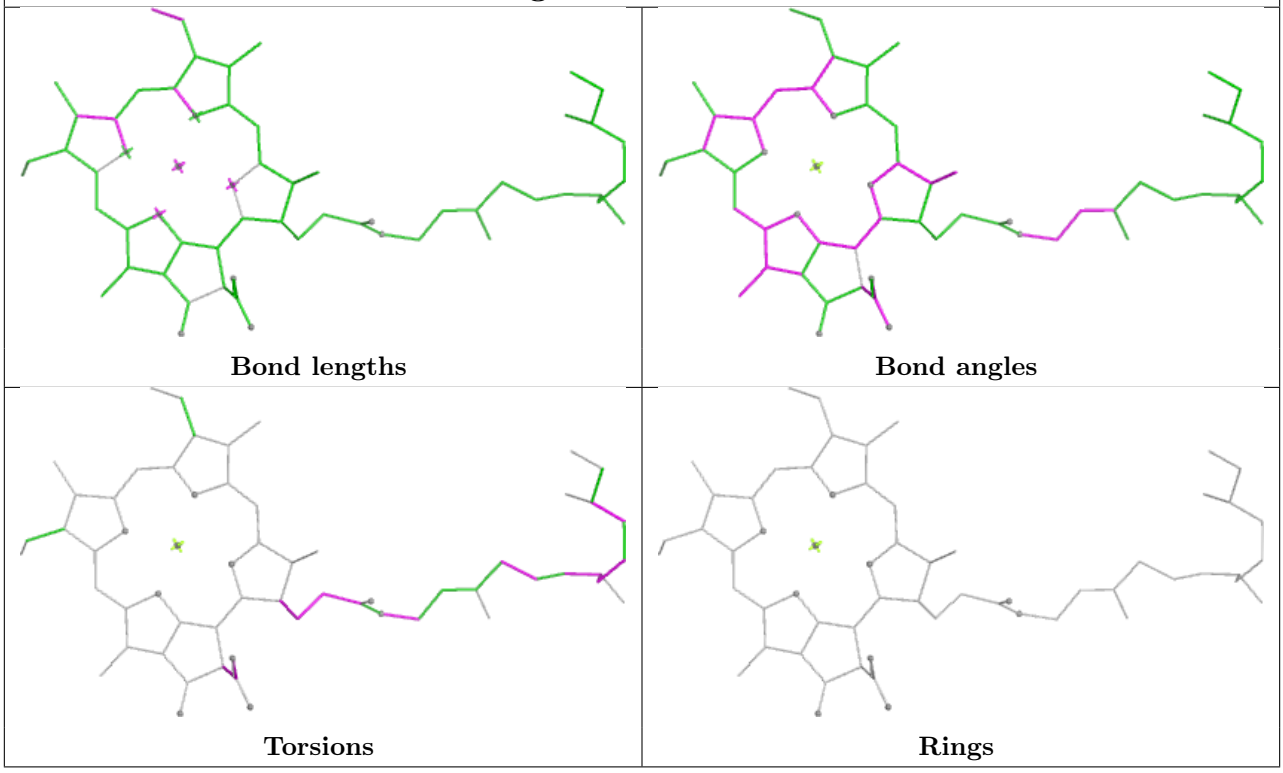


Rings

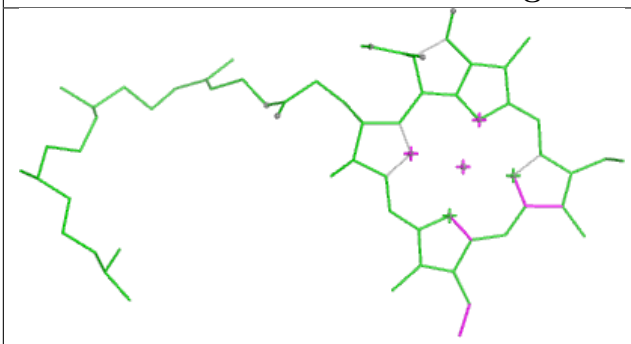
Ligand 3PH 5 325



Ligand CLA 6 319



Ligand CLA A 827



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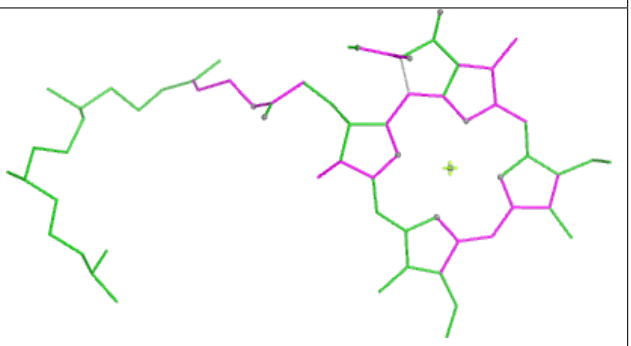
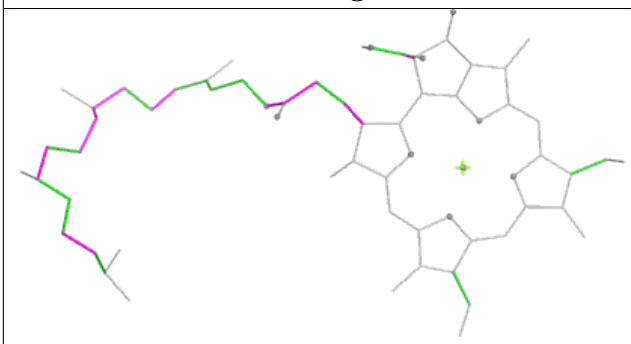


Bond angles



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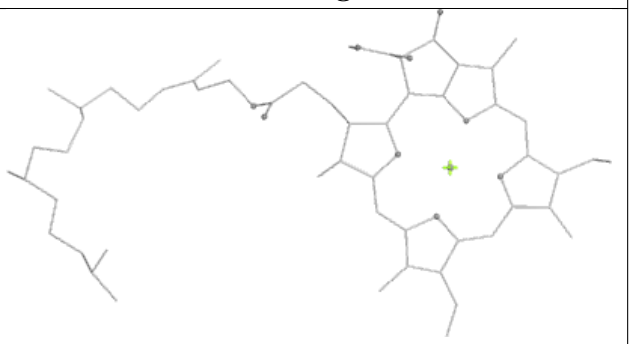
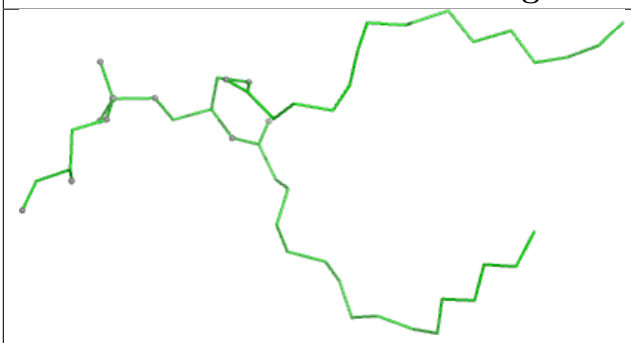


Rings

Ligand LHG A 850



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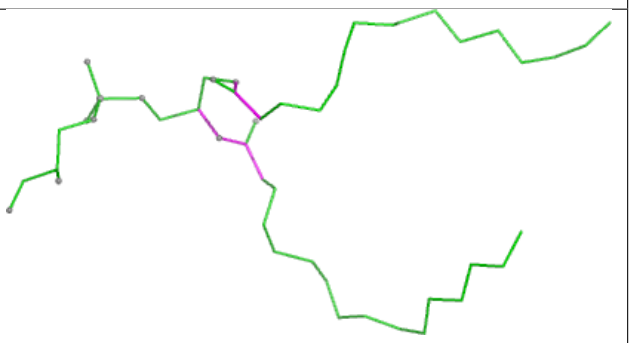
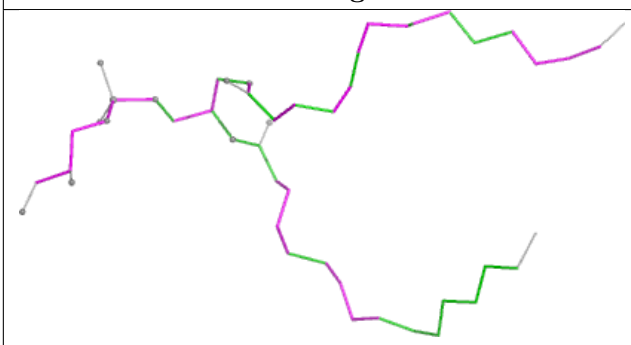


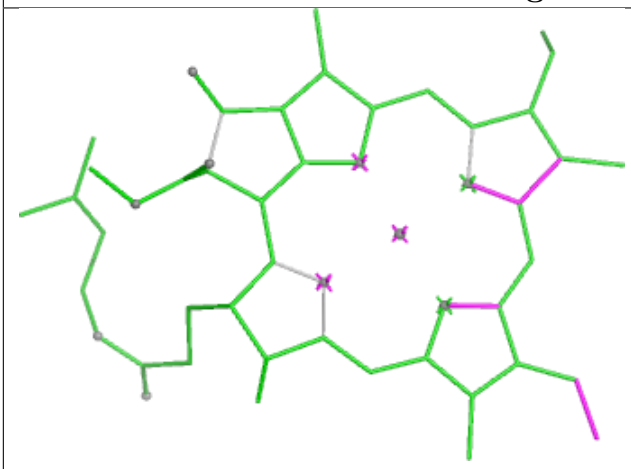
Bond angles



Torsions

Rings

Ligand CLA L 203



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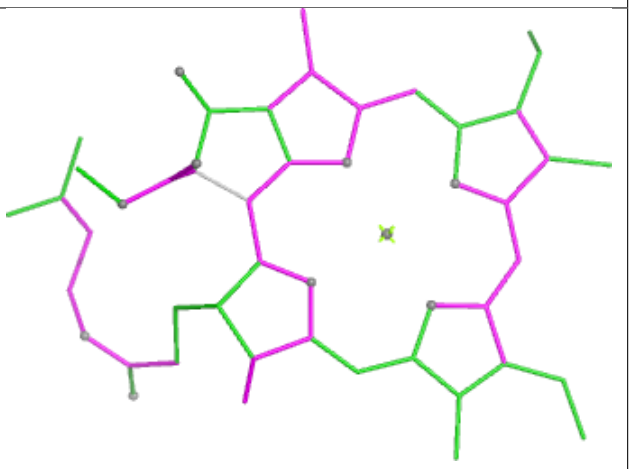
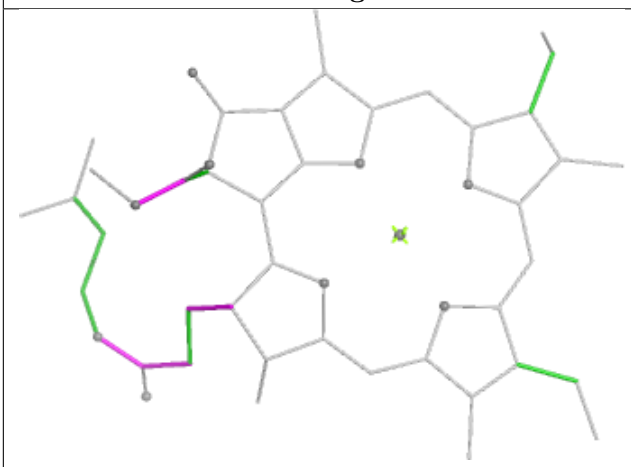


Bond angles



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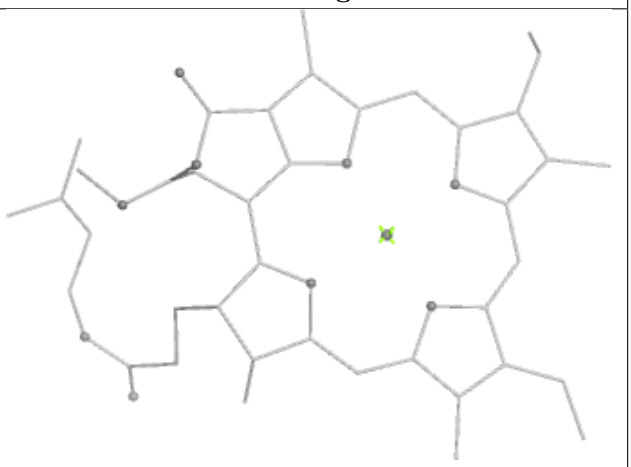
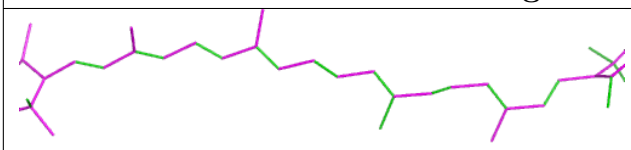
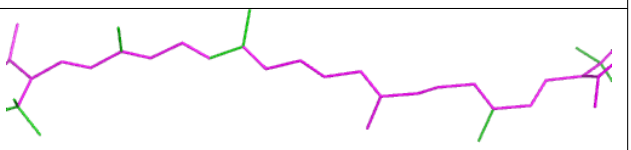


Rings

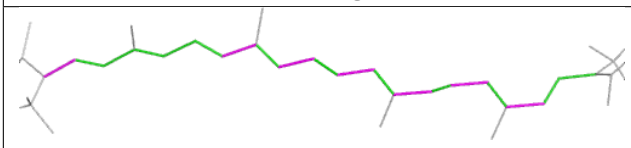
Ligand BCR B 847



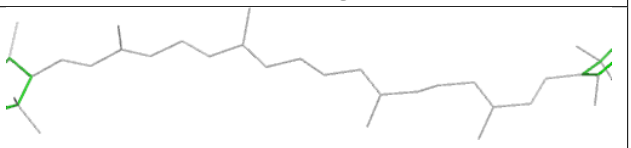
Bond lengths



Bond angles

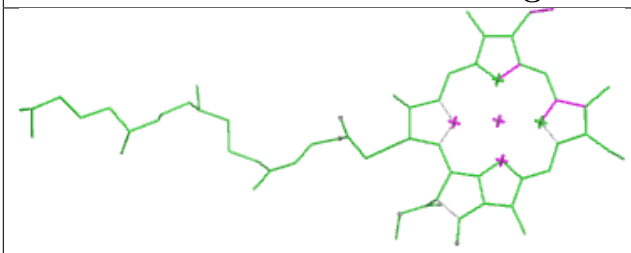


Torsions



Rings

Ligand CLA A 833



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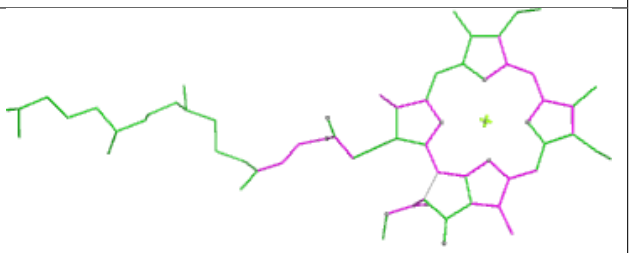

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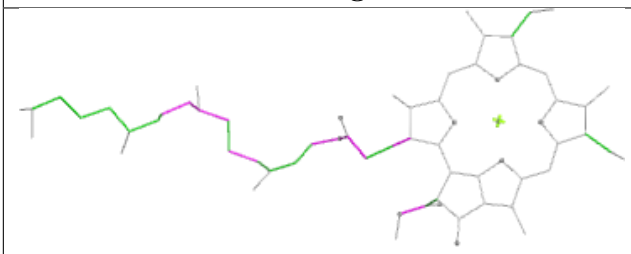

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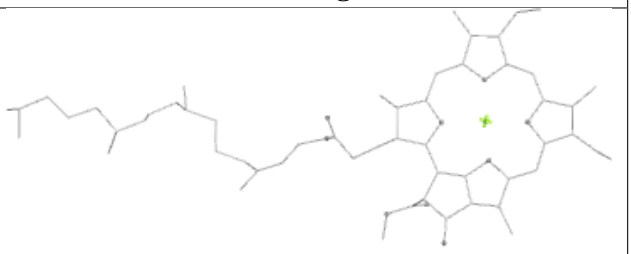
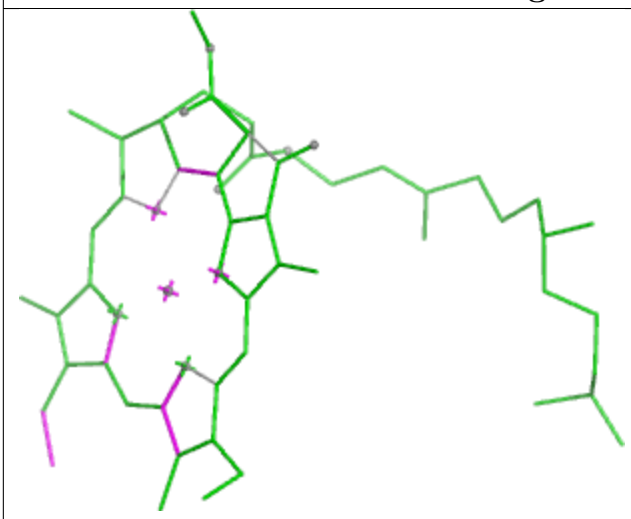


Rings

Ligand CLA 1 310



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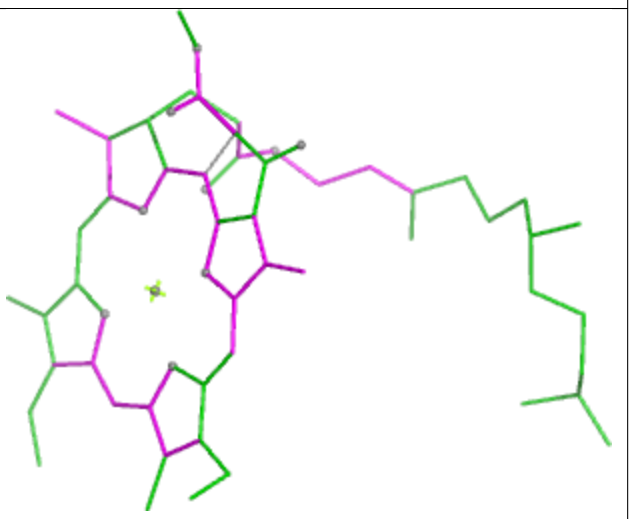

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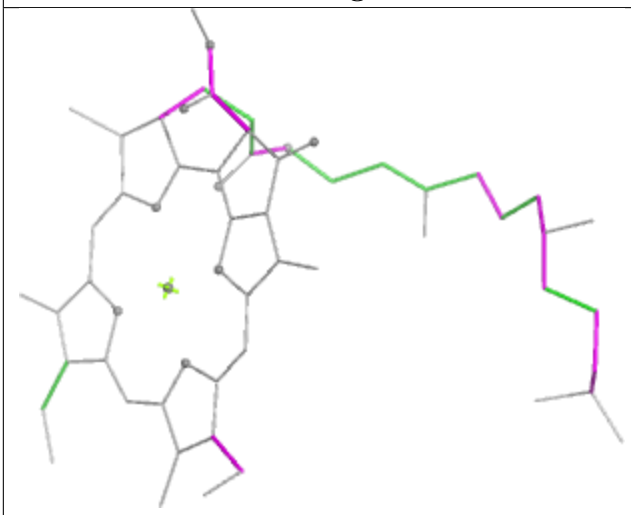

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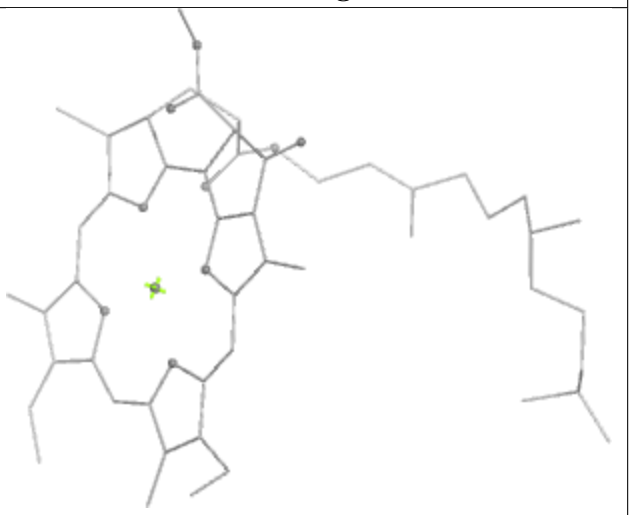

Rings

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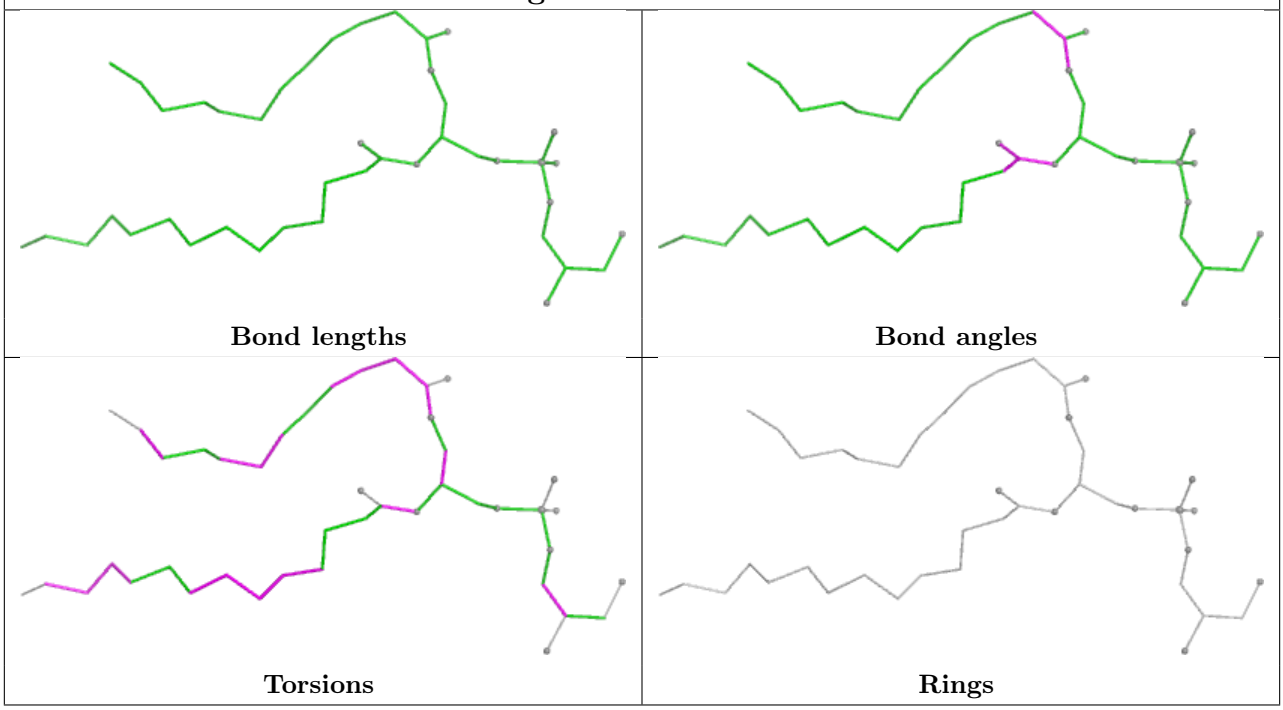

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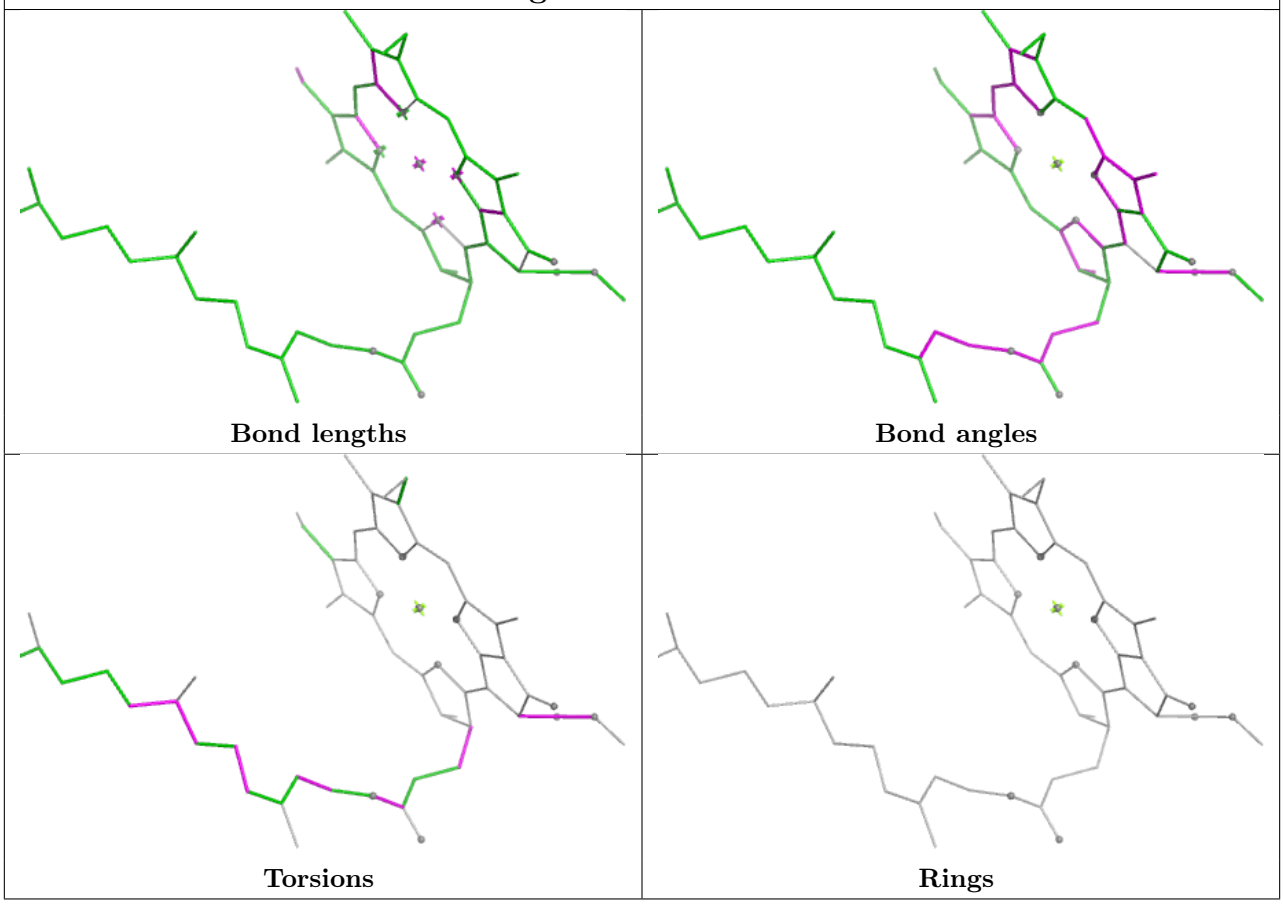
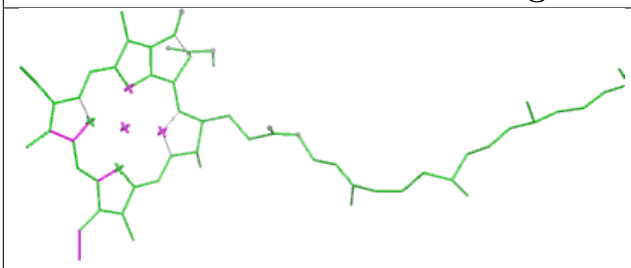


Ligand CLA 5 322



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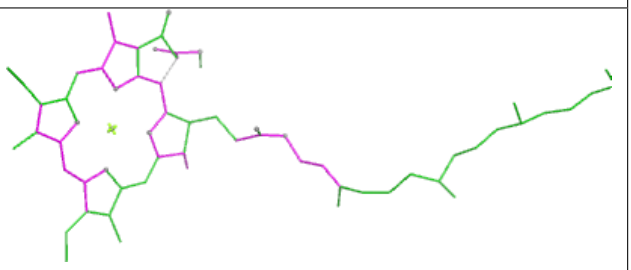
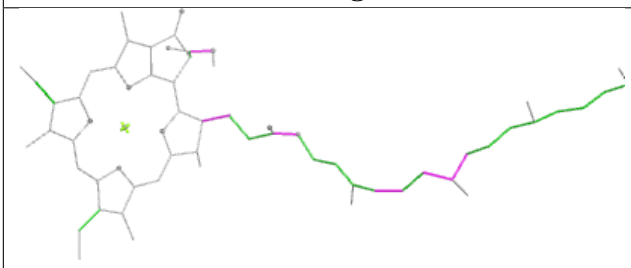


Bond angles



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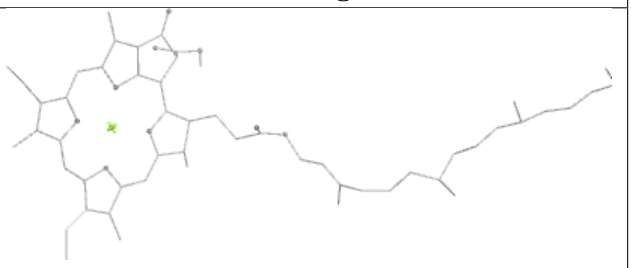

Rings

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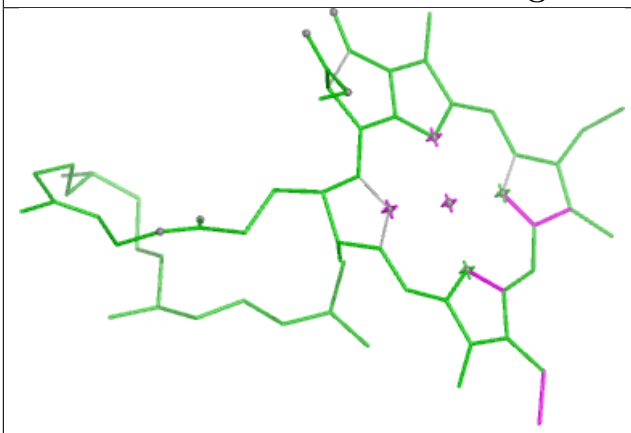

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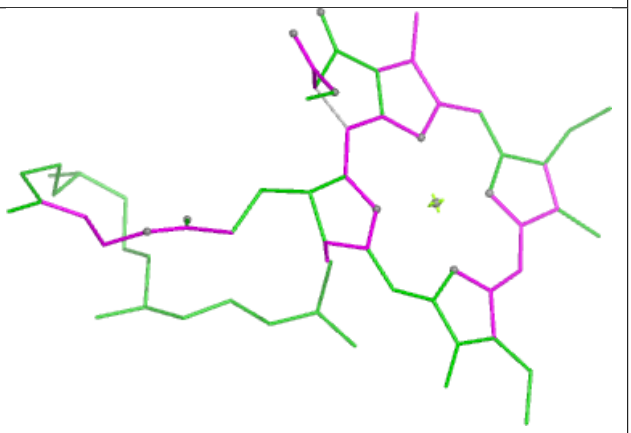

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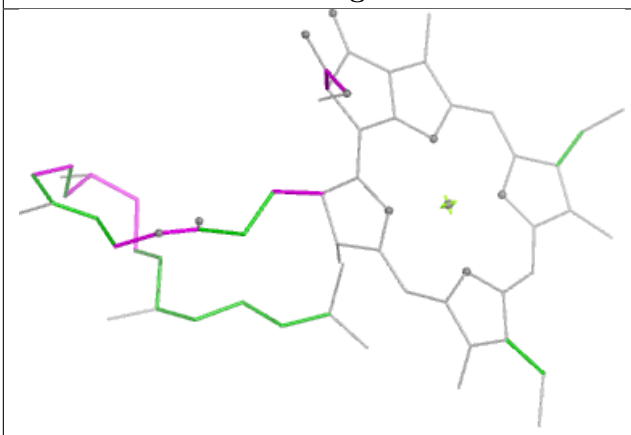

Torsions

Rings

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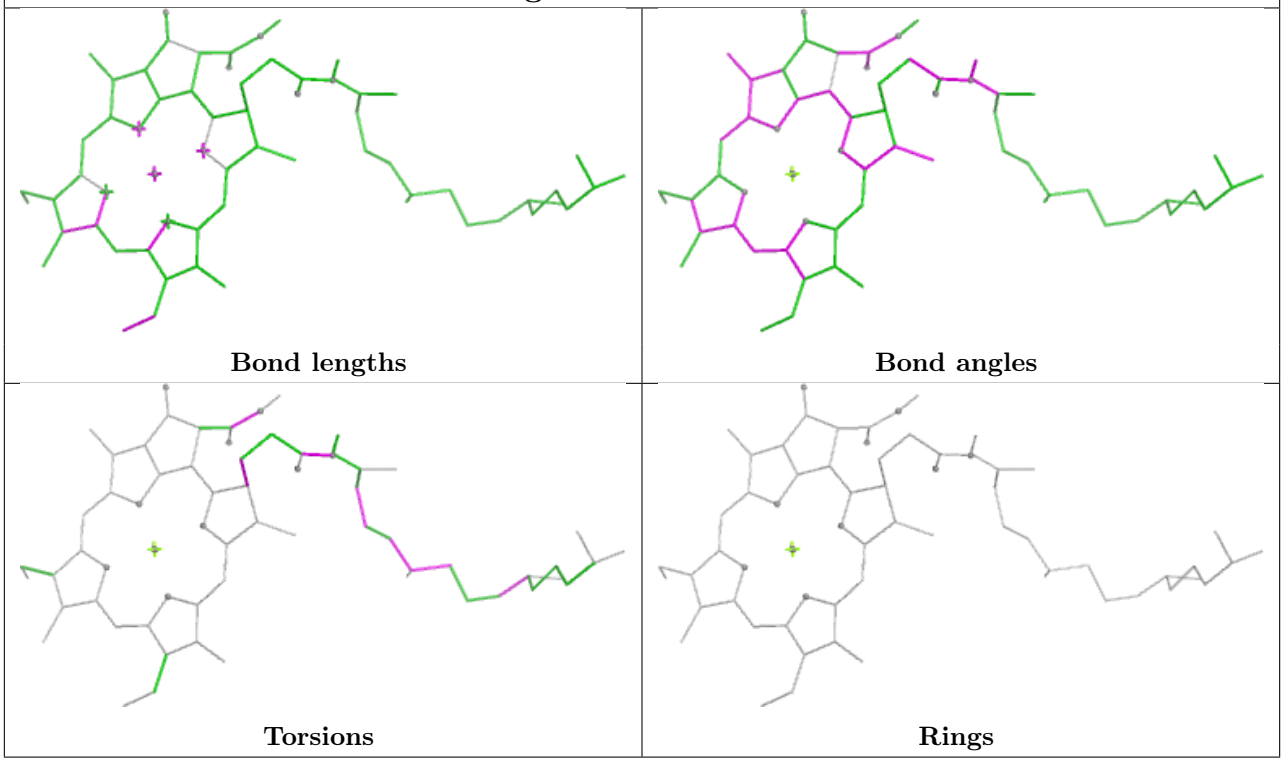
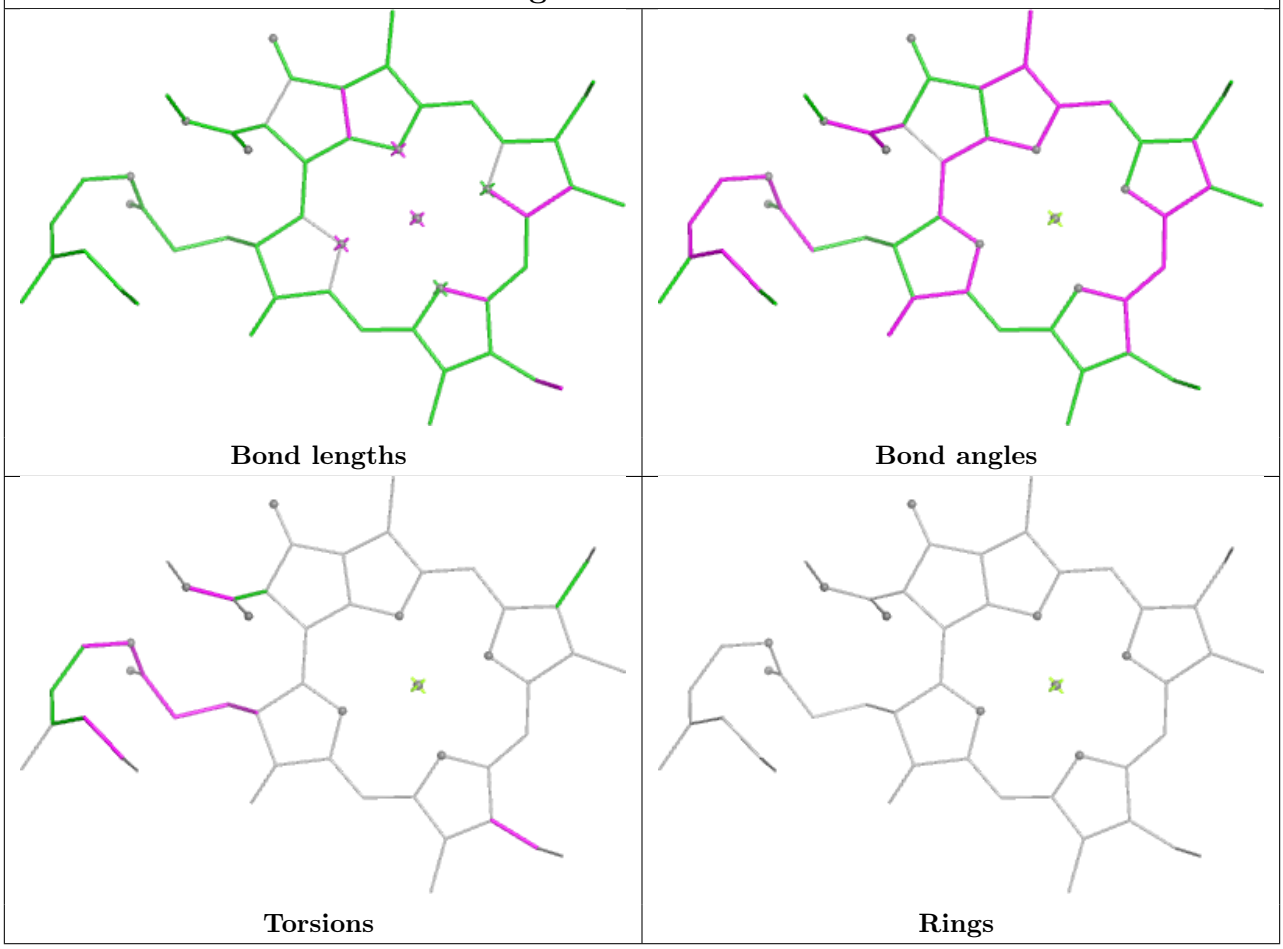


Ligand CLA 4 806



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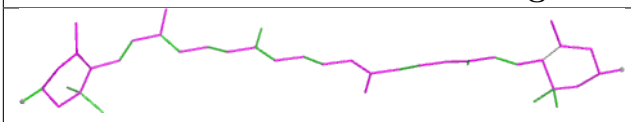
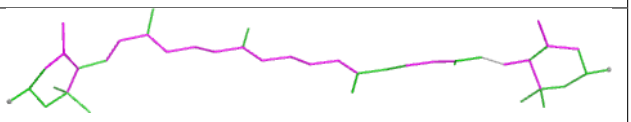
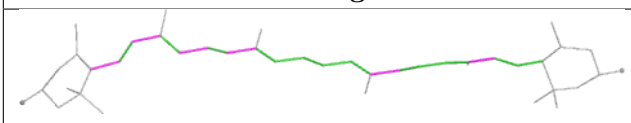
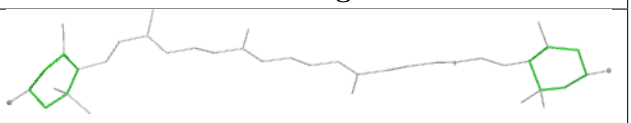
 Bond lengths	 Bond angles
 Torsions	 Rings

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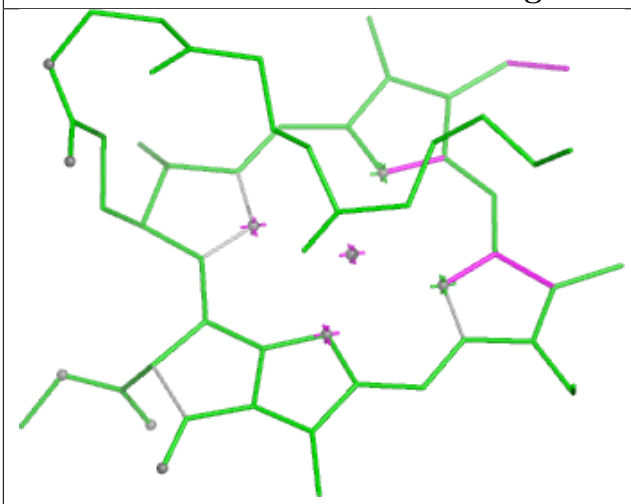
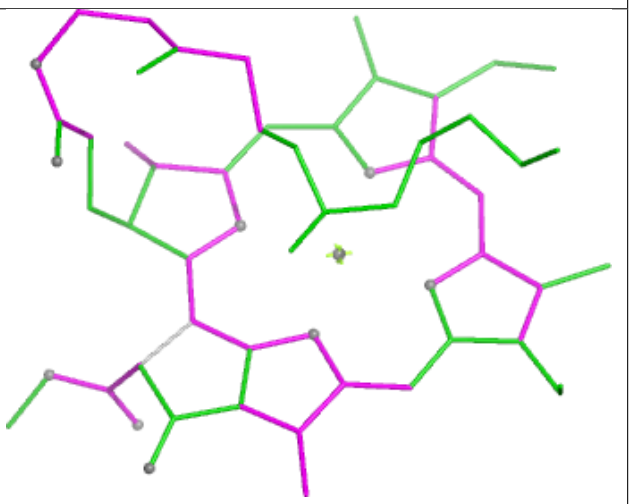
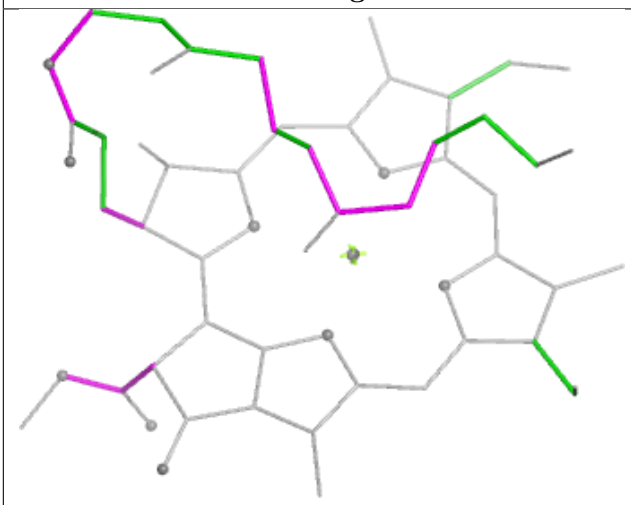
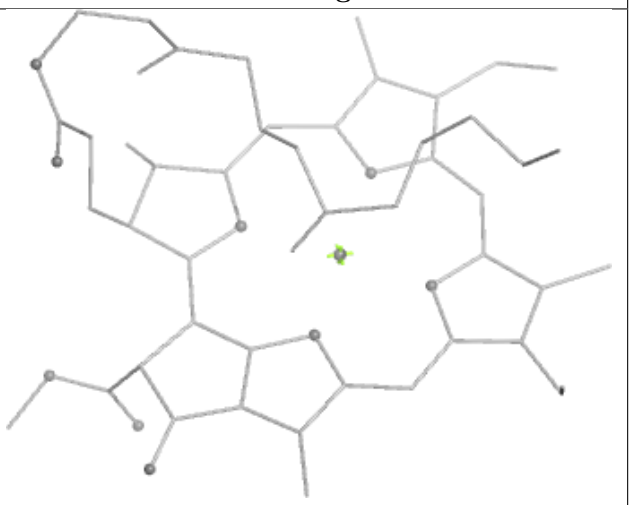
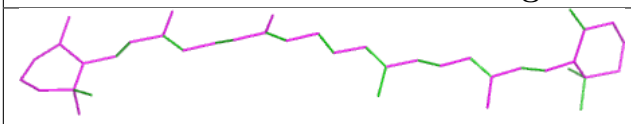
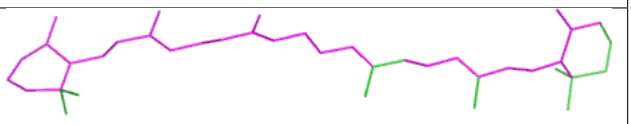
 Bond lengths	 Bond angles
 Torsions	 Rings

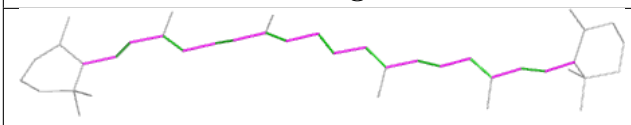
Ligand BCR A 856



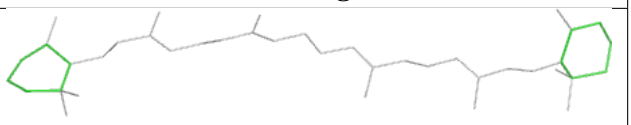
Bond lengths



Bond angles

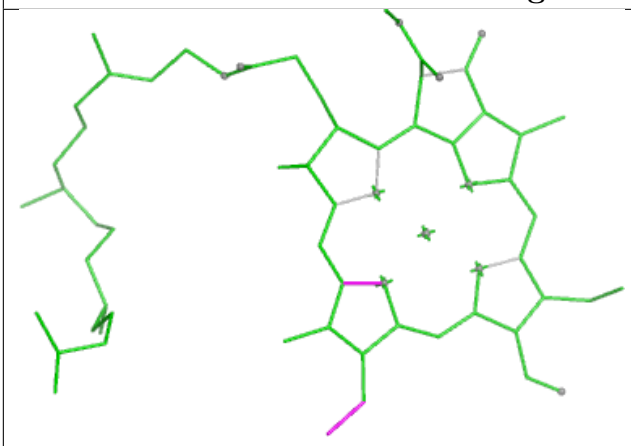


Torsions



Rings

Ligand CHL 8 315



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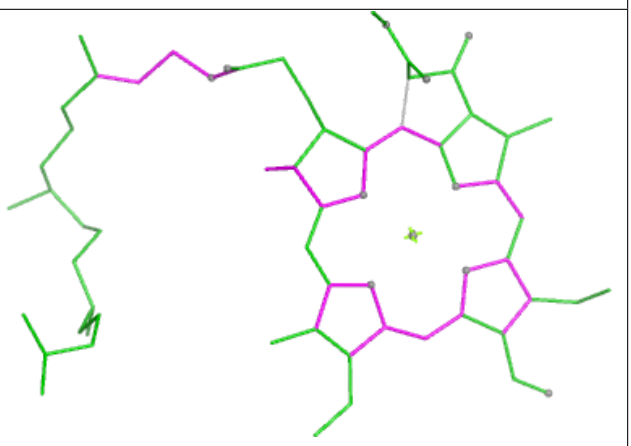

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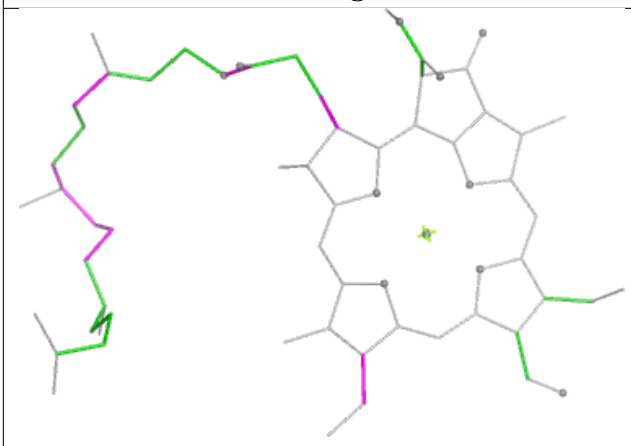

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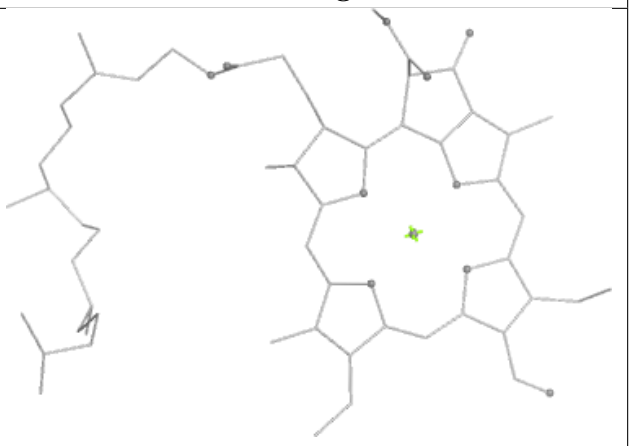
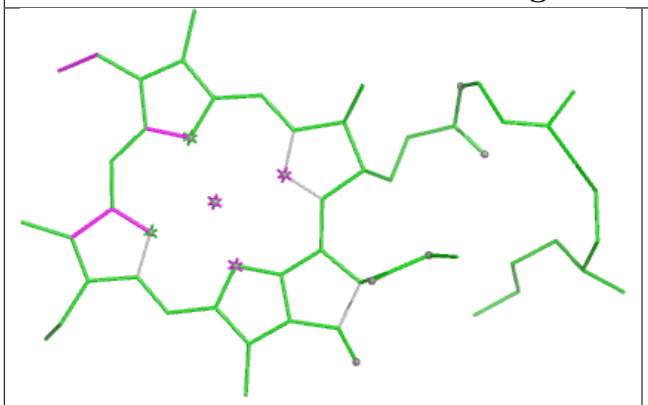


Rings

Ligand CLA 7 317



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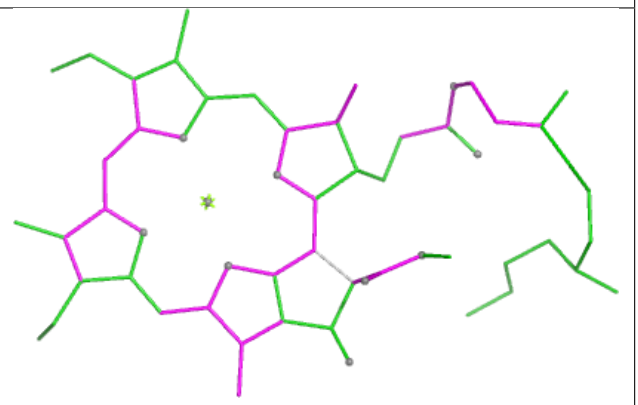

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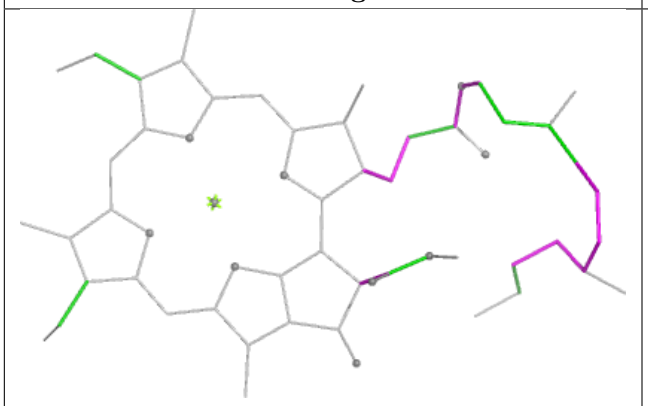

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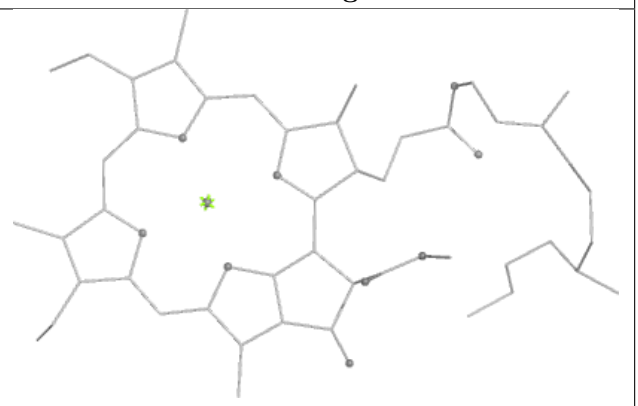
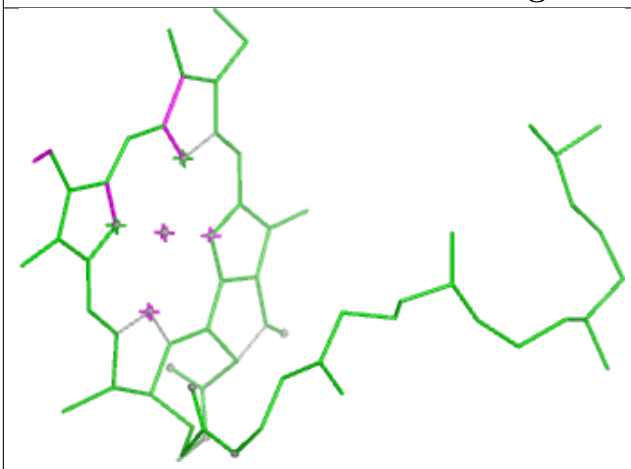


Rings

Ligand CLA 1 314



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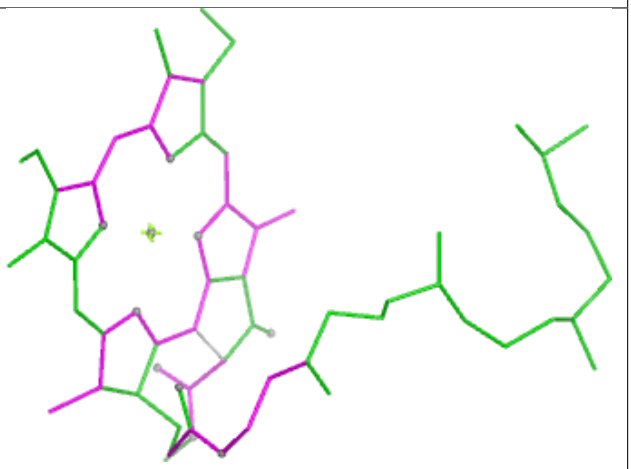

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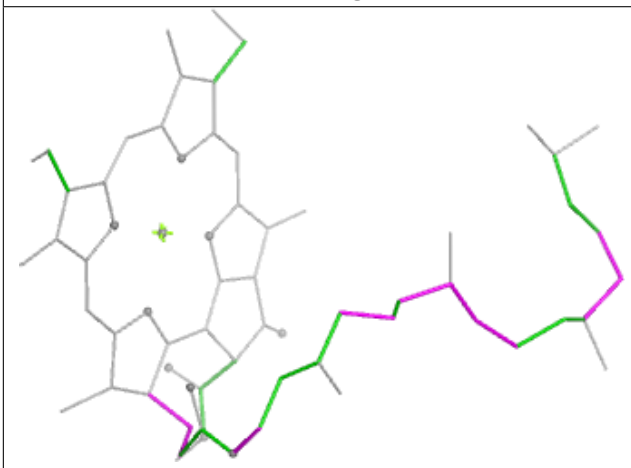
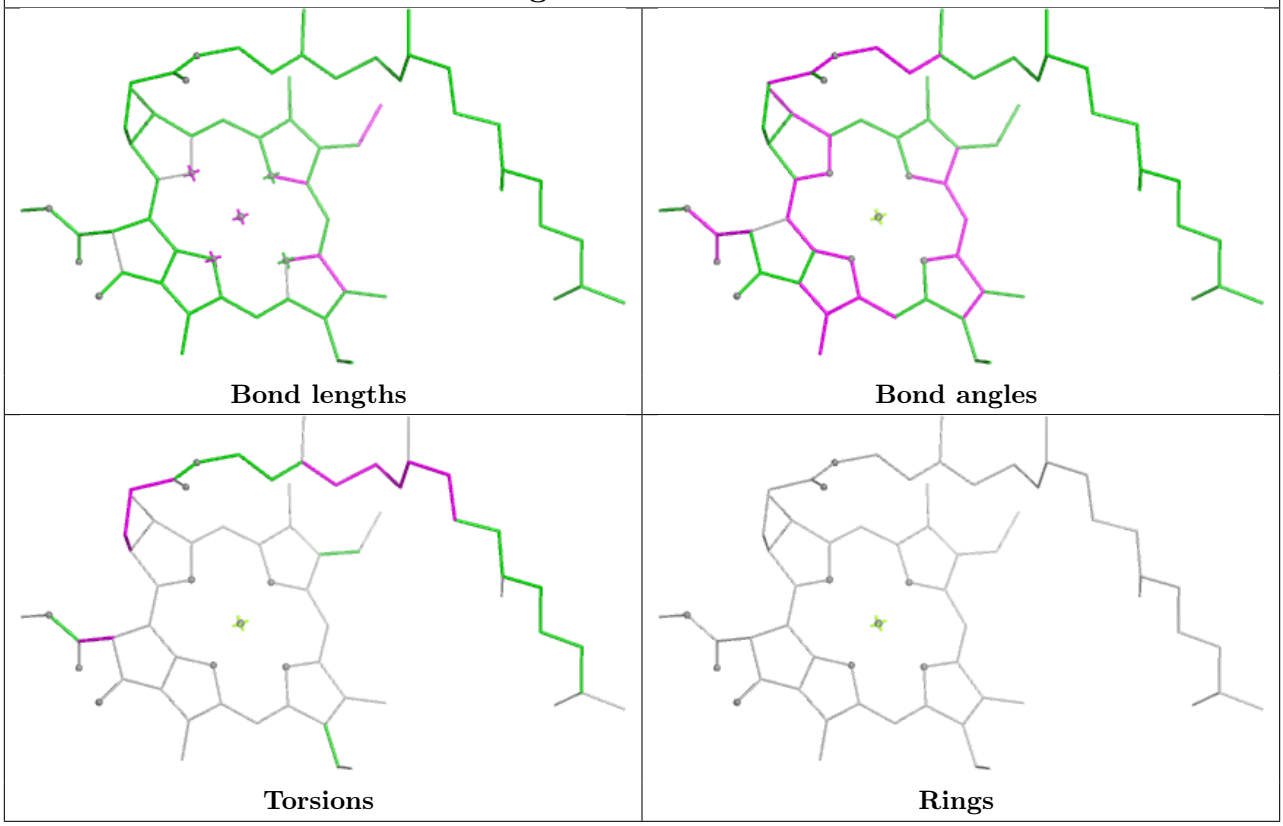


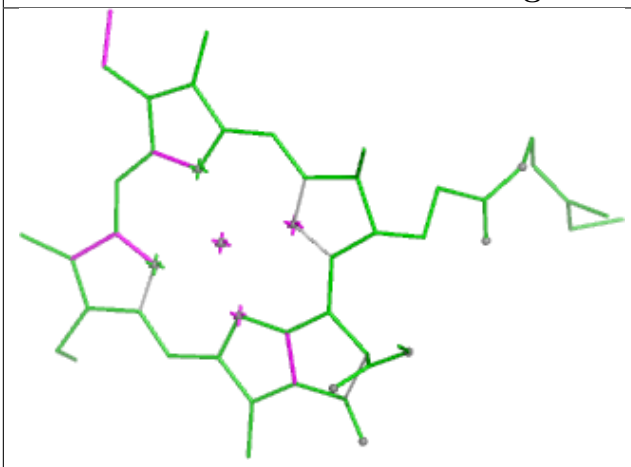
Torsions

Rings

Ligand CLA 5 310



Ligand CLA A 839



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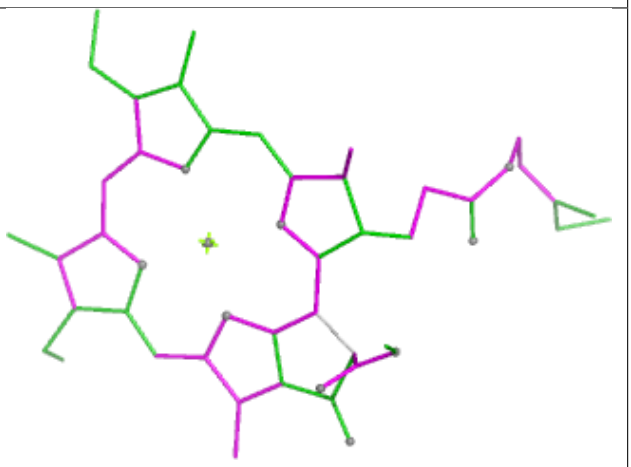

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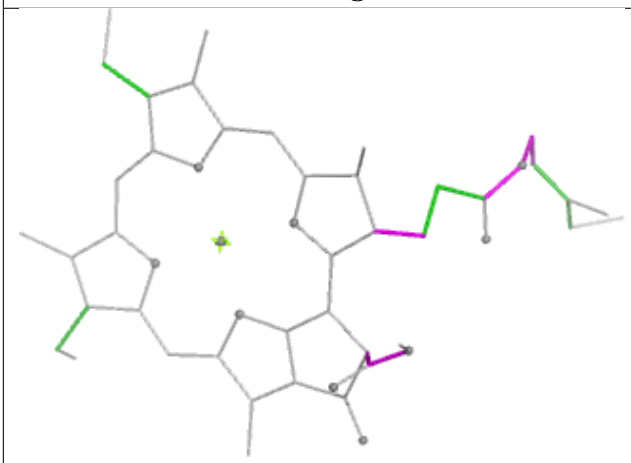
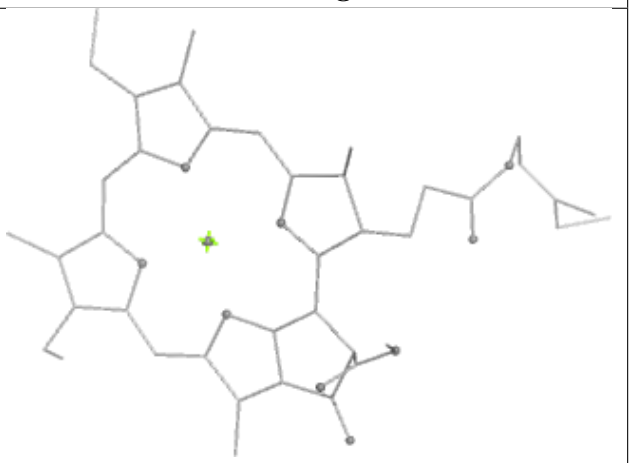
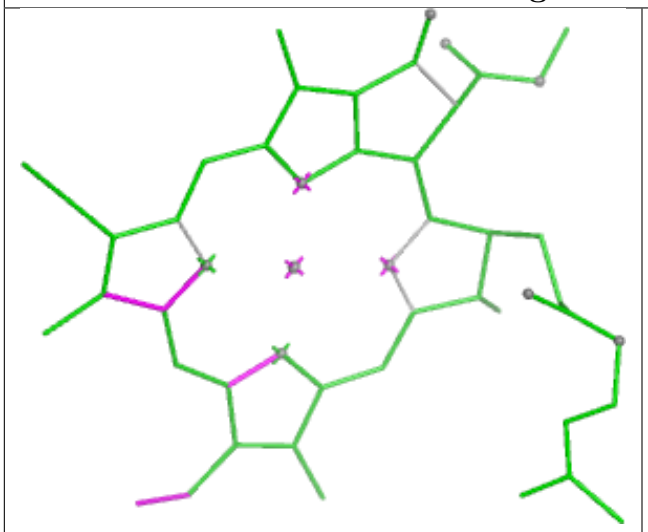


Torsions



Rings

Ligand CLA 8 311



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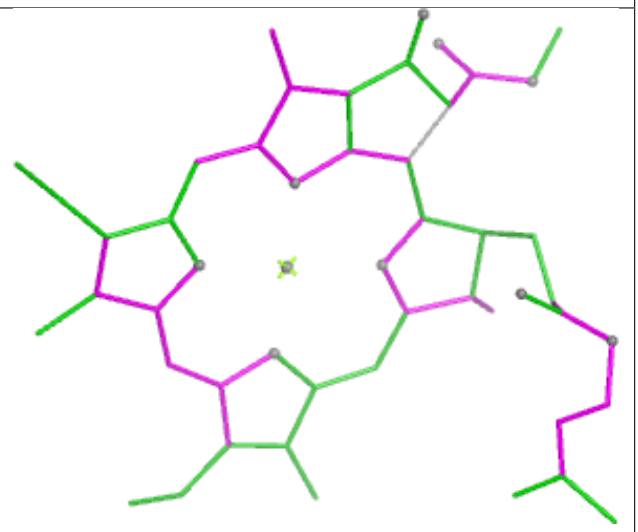
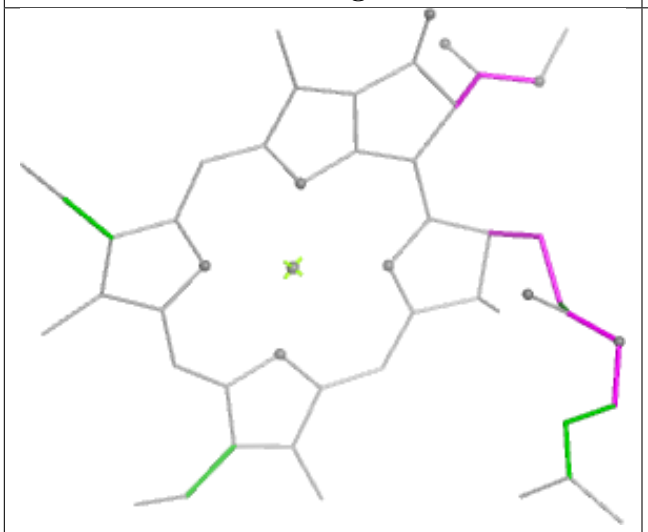


Bond angles



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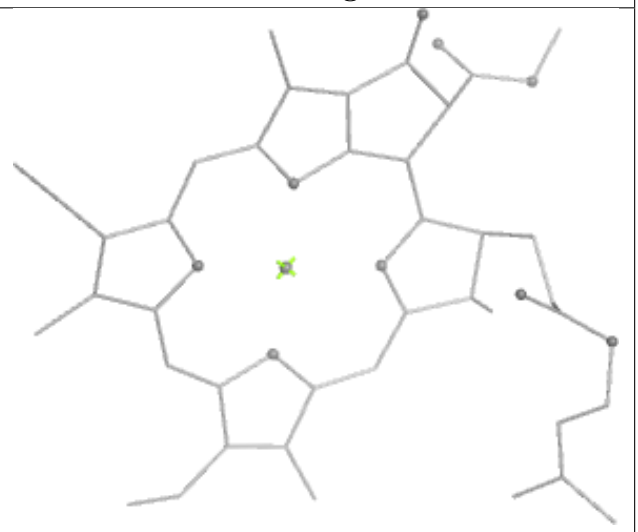
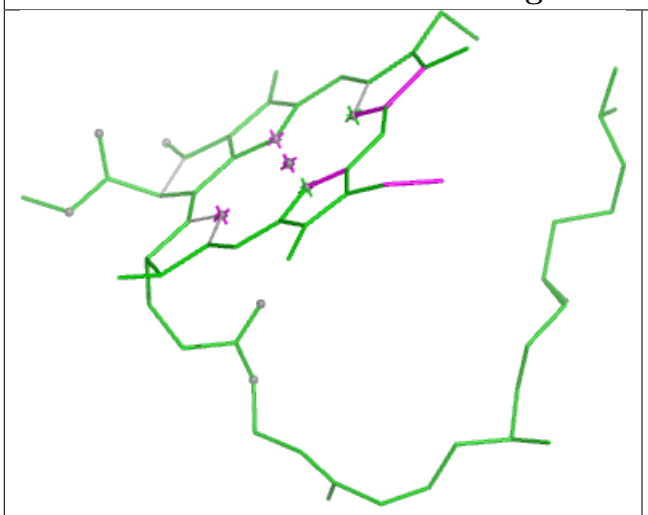
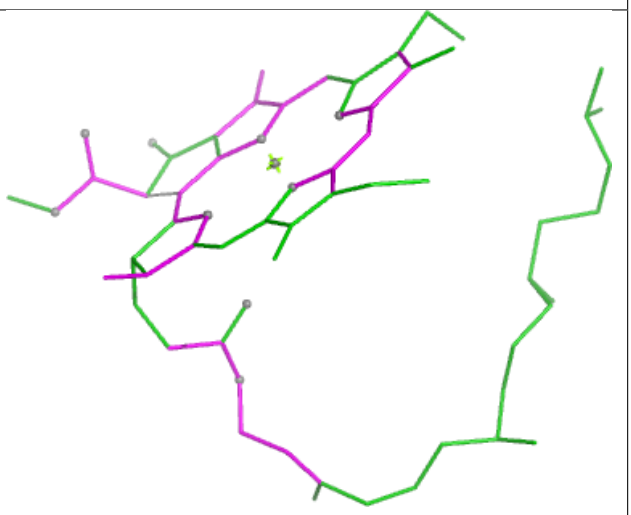


Rings

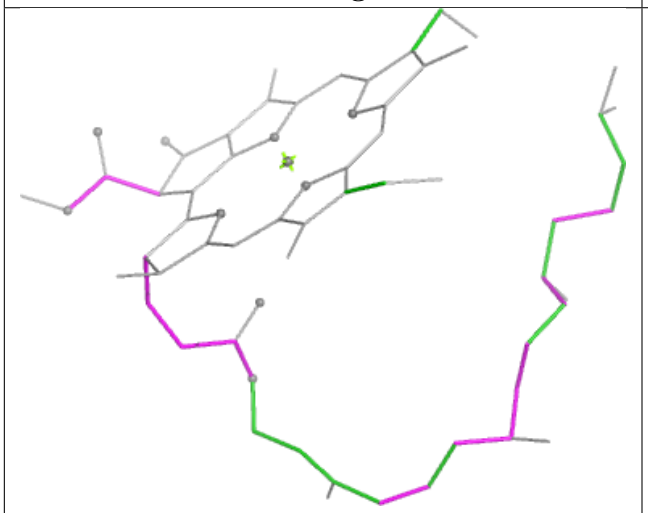
Ligand CLA B 821



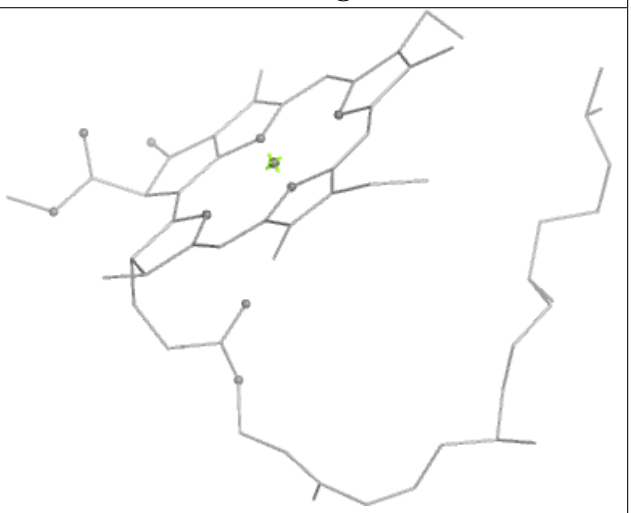
Bond lengths



Bond angles

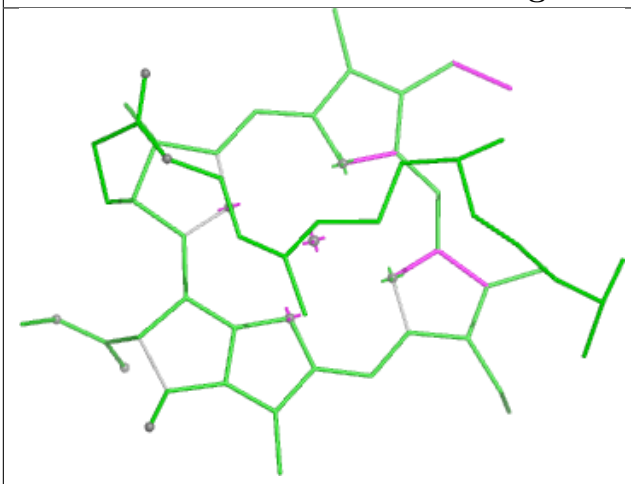


Torsions



Rings

Ligand CLA 7 312



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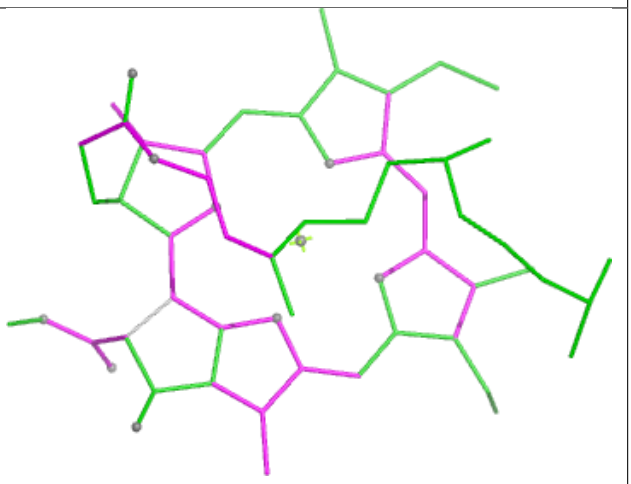

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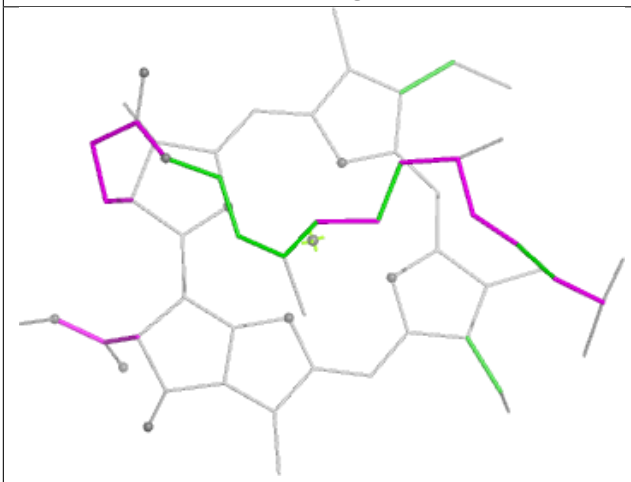

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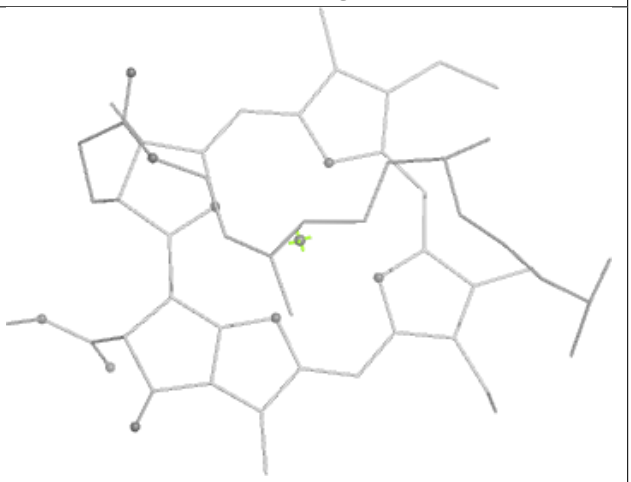
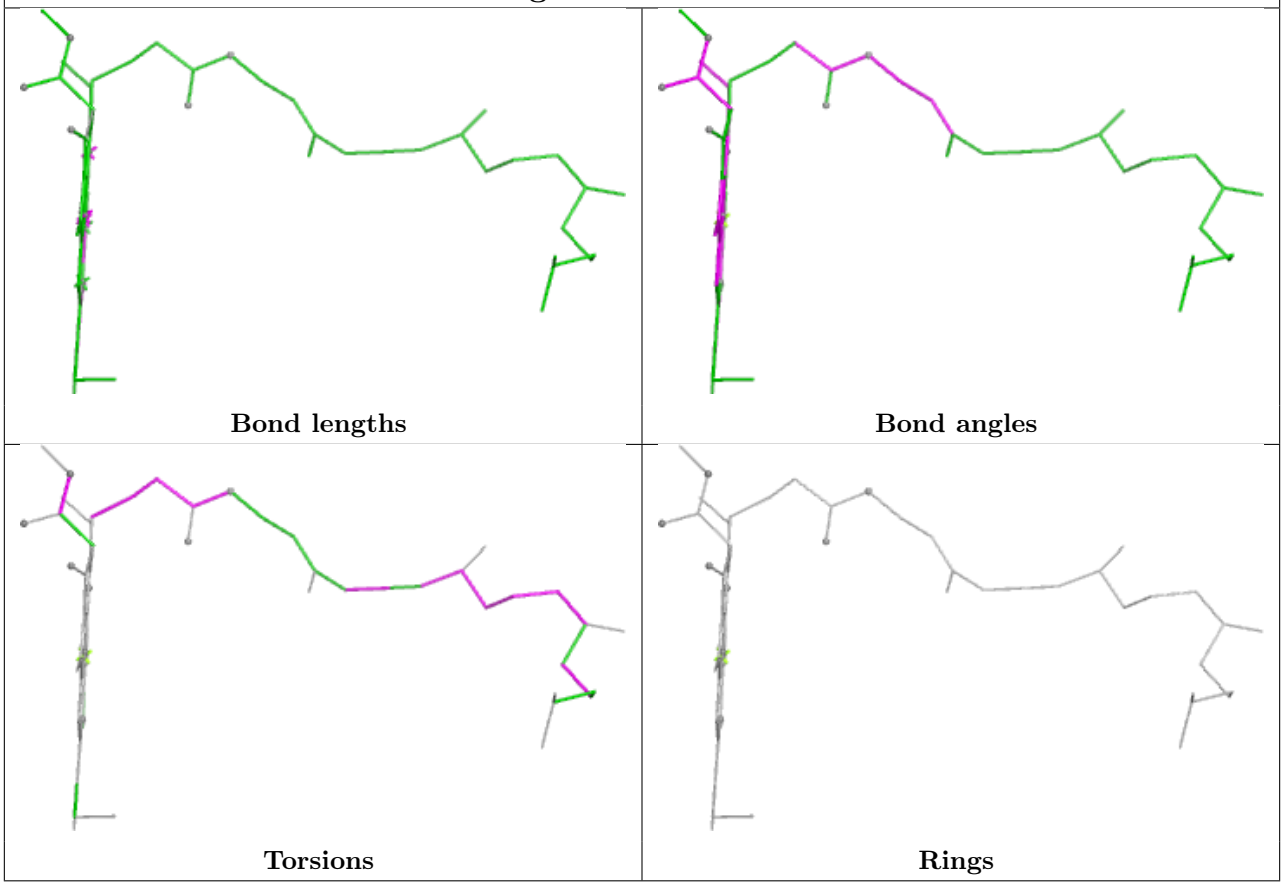
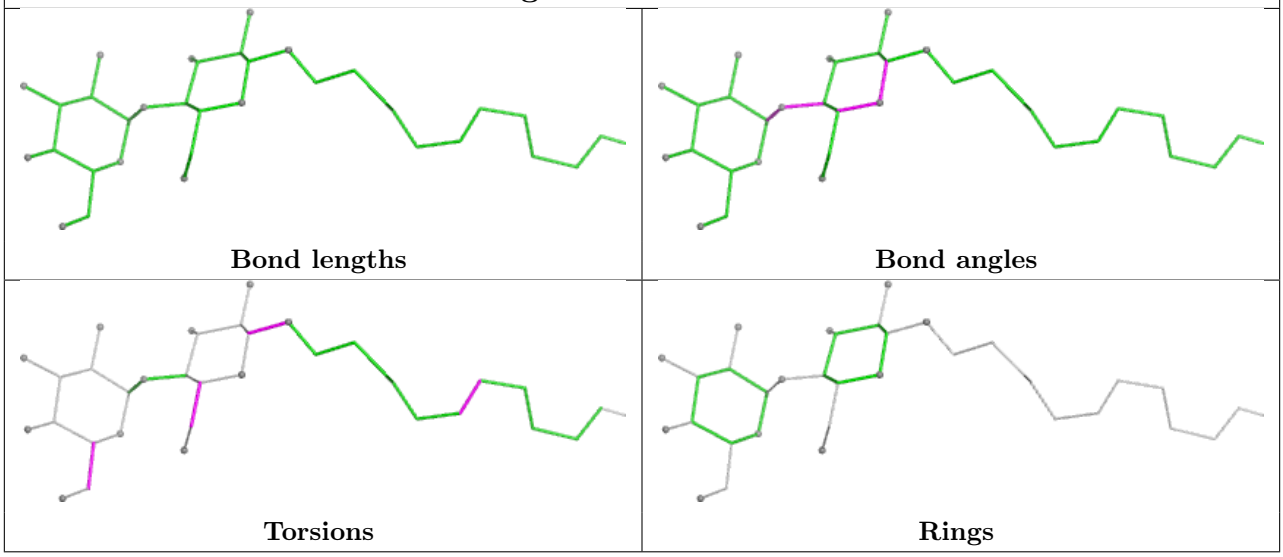


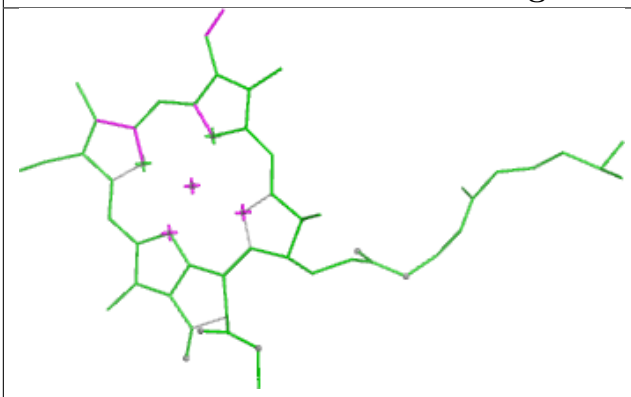
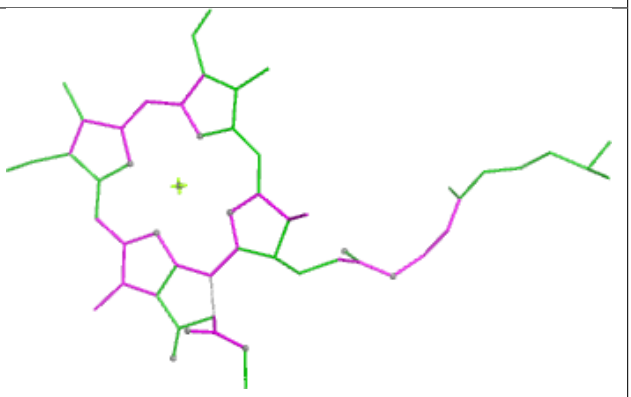
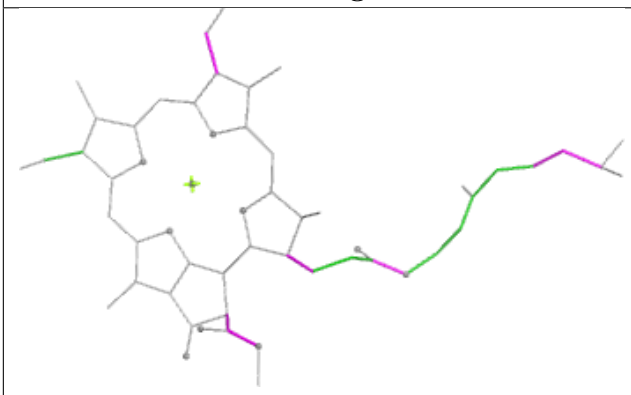
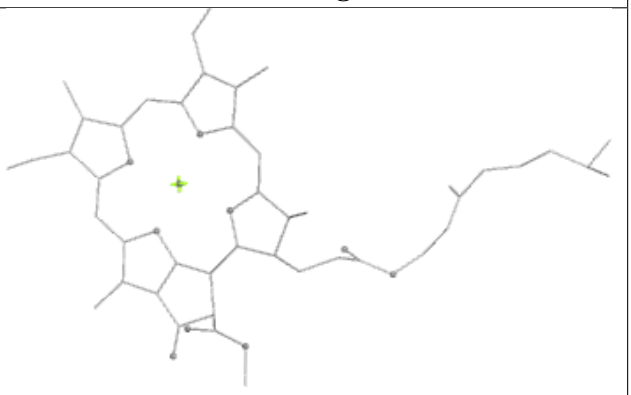
Rings

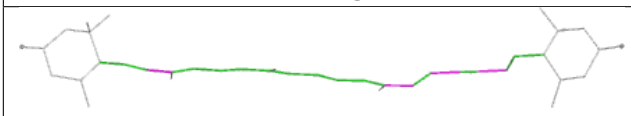
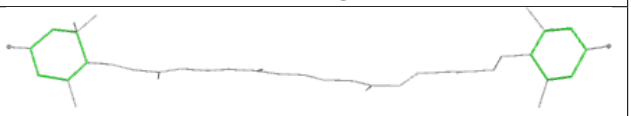
Ligand CLA 3 313



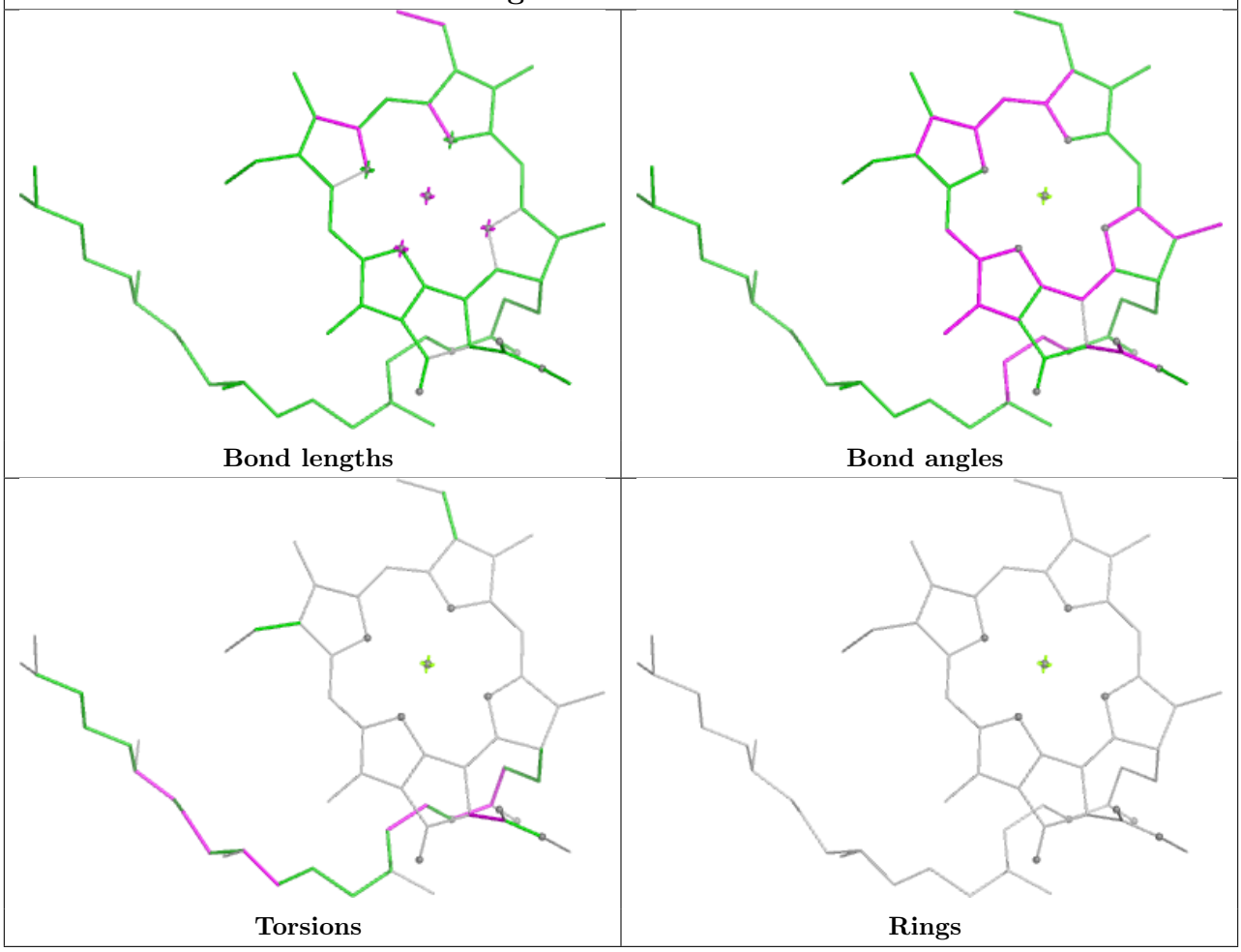
Ligand LMT G 204

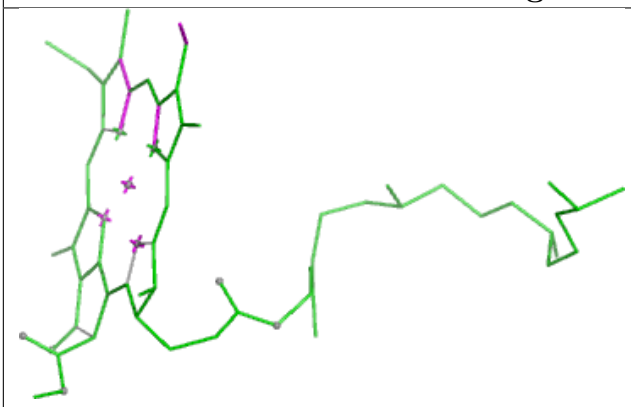
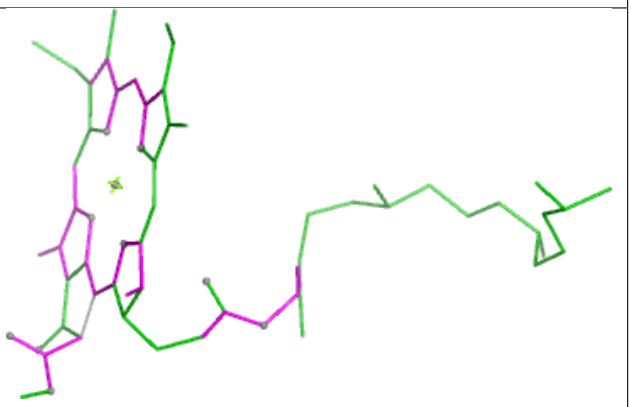
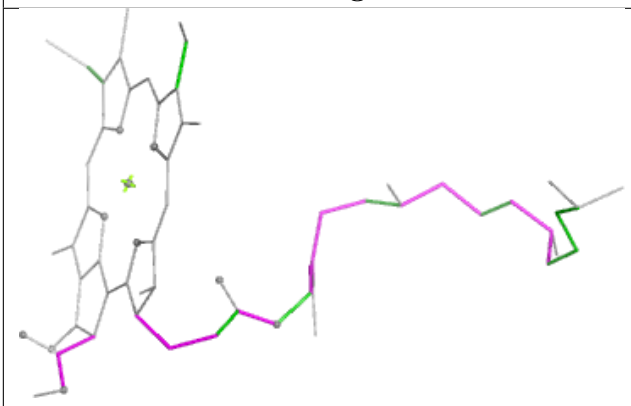


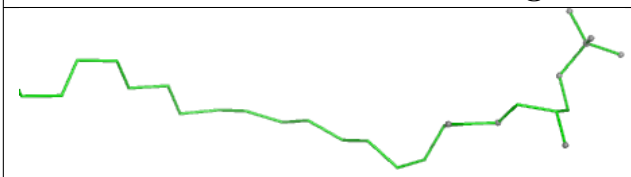
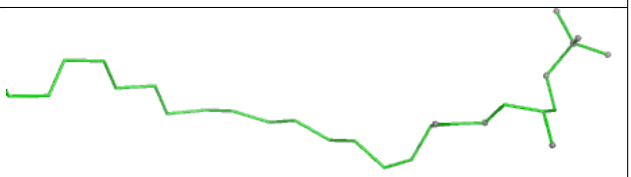
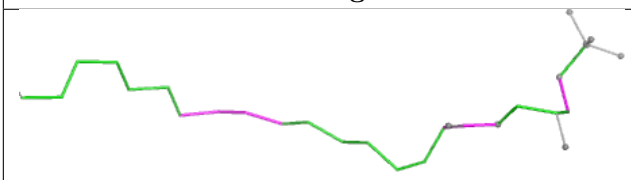
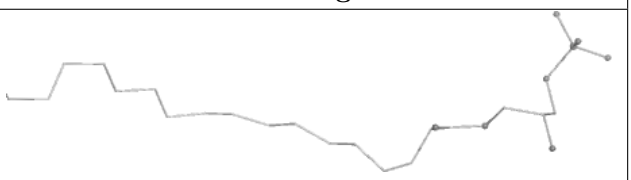
Ligand CLA 5 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT Z 301	
Bond lengths	Bond angles
 Torsions	 Rings

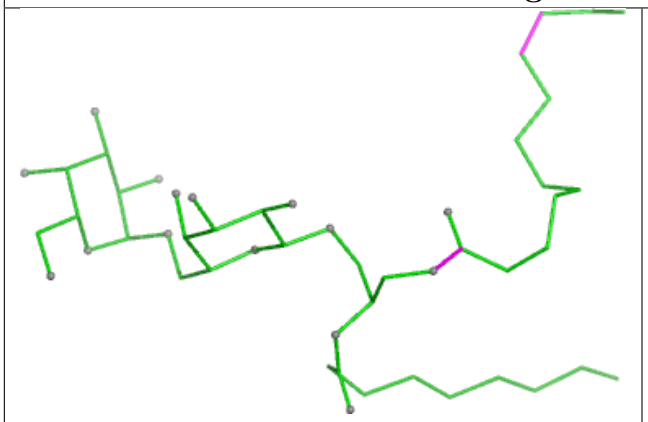
Ligand CLA A 829



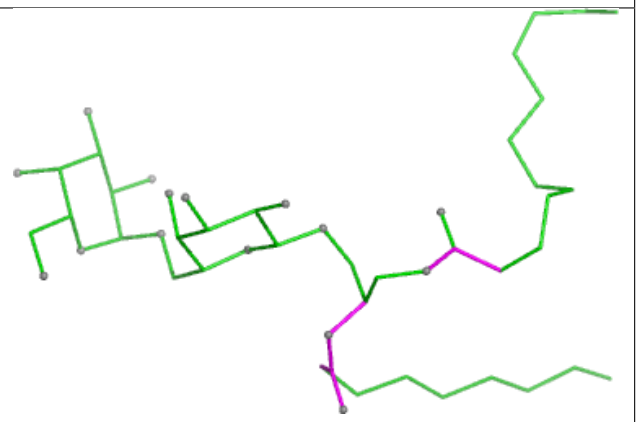
Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand NKP 8 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

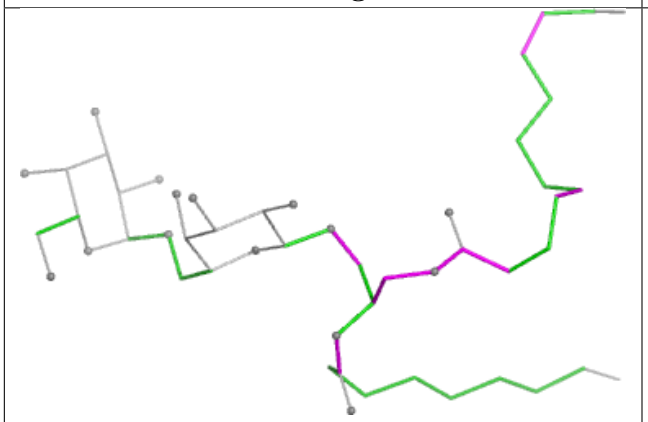
Ligand DGD 3 301



Bond lengths



Bond angles



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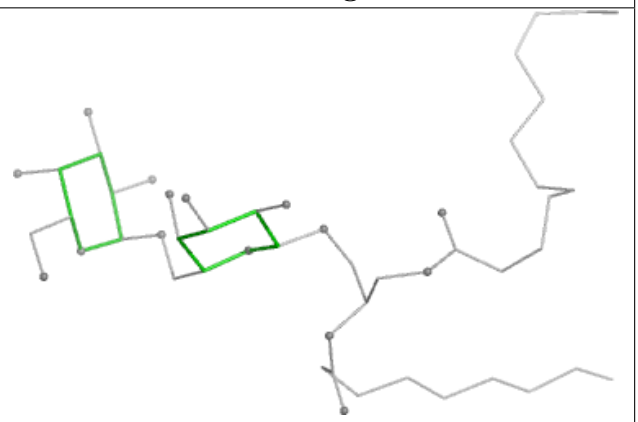
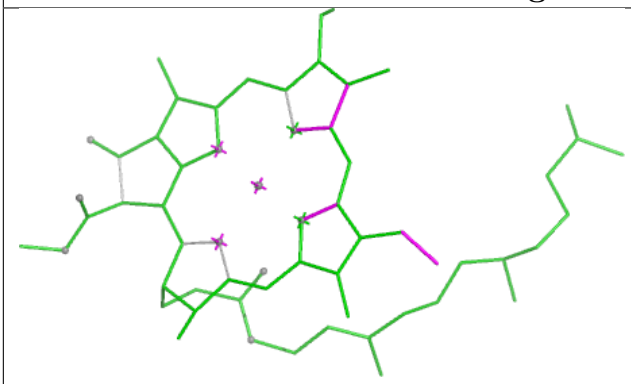
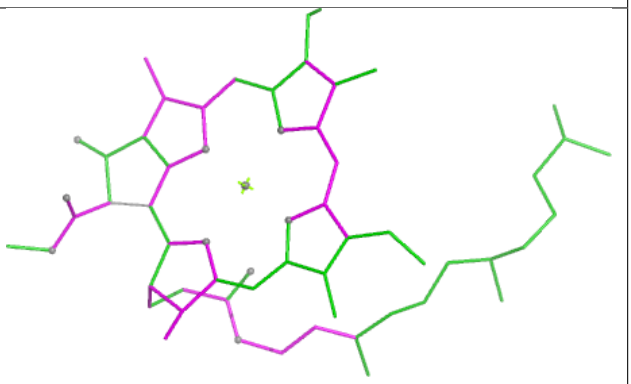
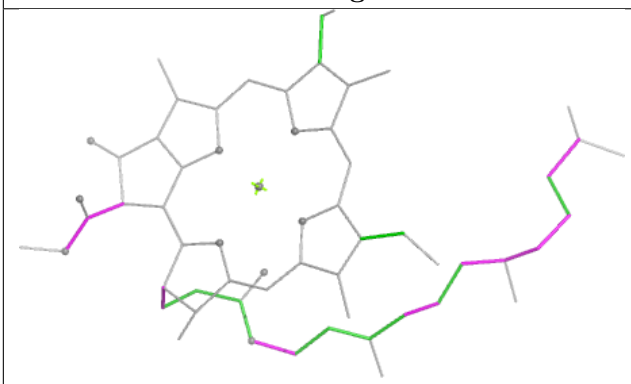
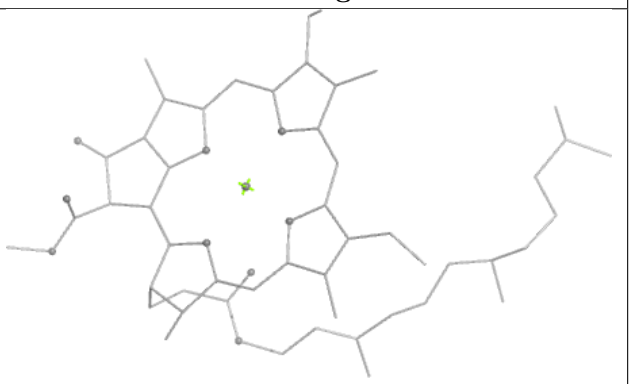
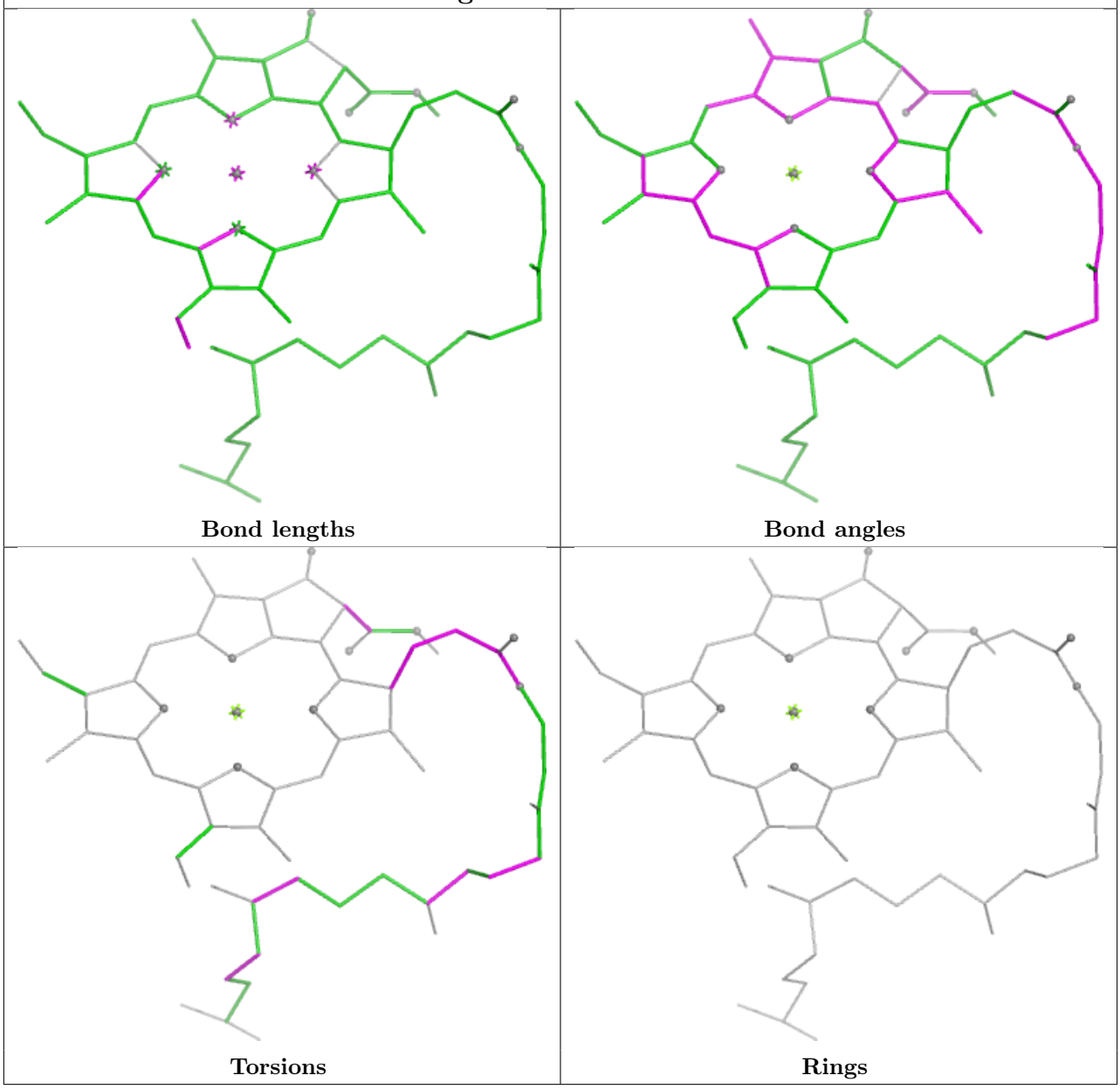


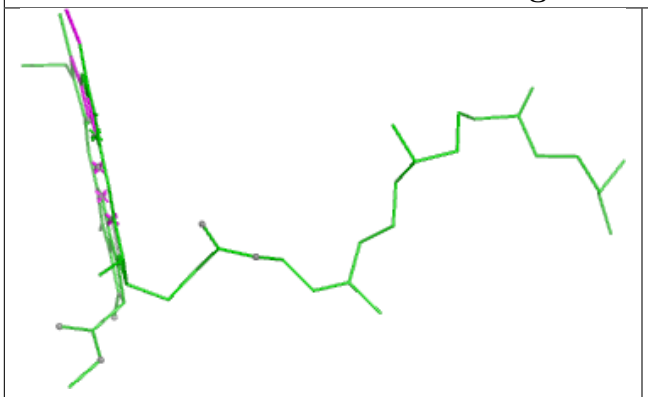
Rings

Ligand CLA 7 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

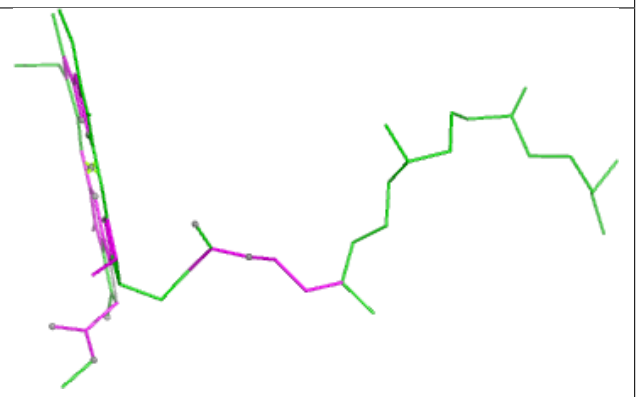
Ligand CLA A 813



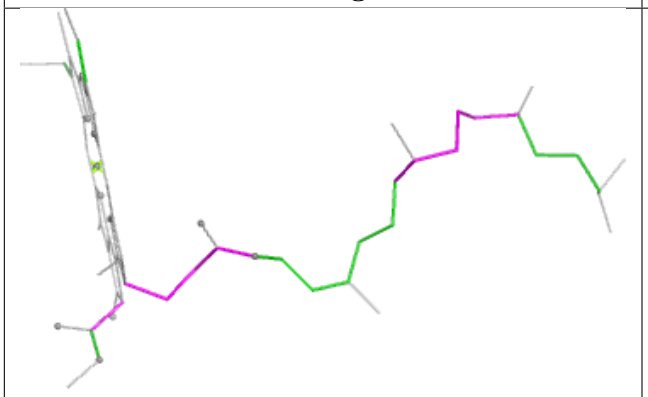
Ligand CLA 6 314



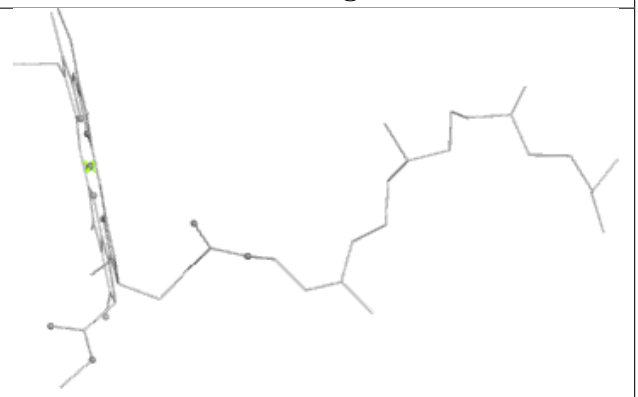
Bond lengths



Bond angles

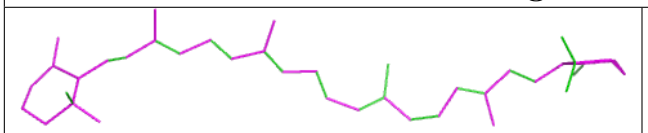


Torsions

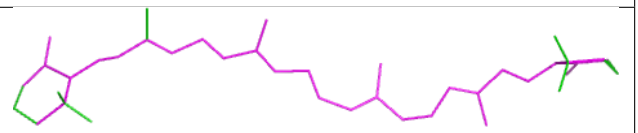


Rings

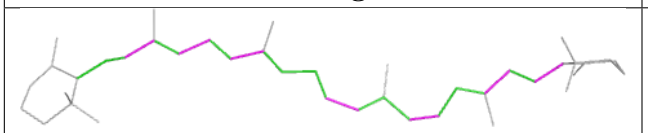
Ligand BCR 3 304



Bond lengths



Bond angles



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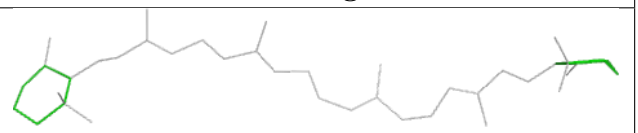
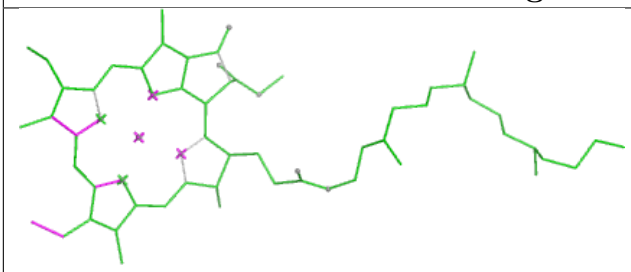
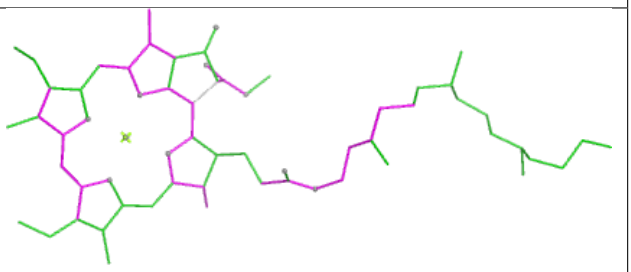
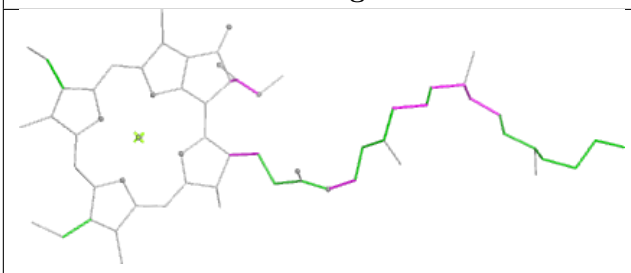
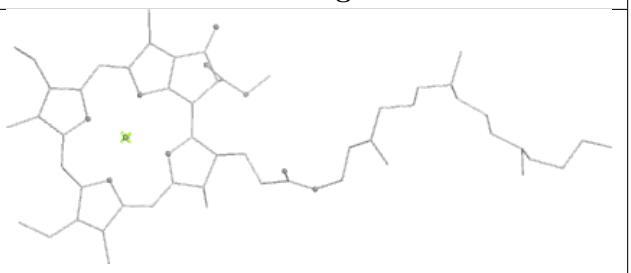


Rings

Ligand CLA F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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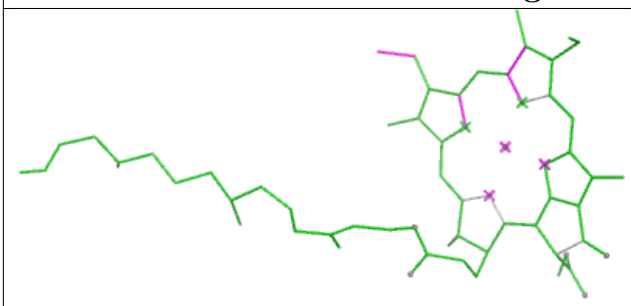
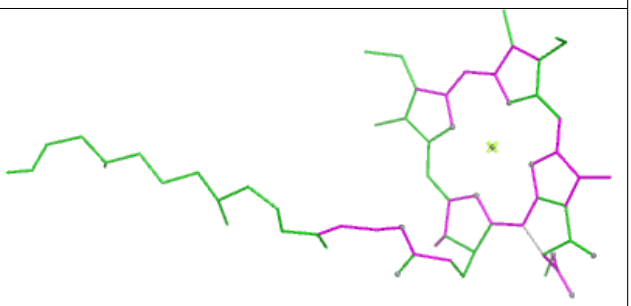
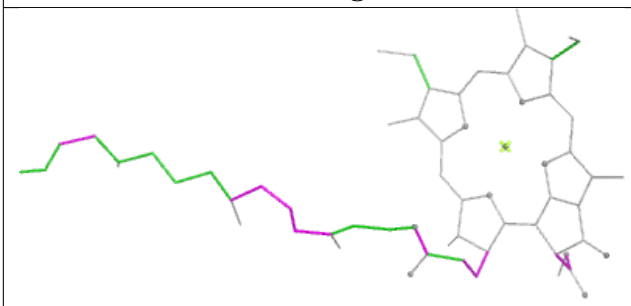
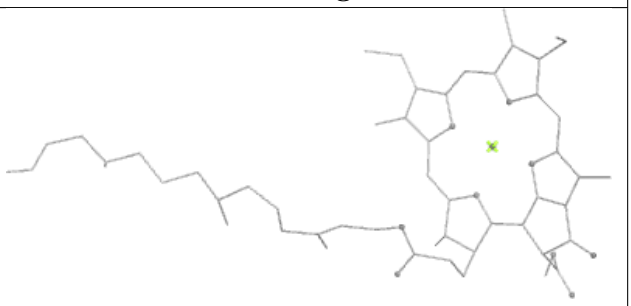
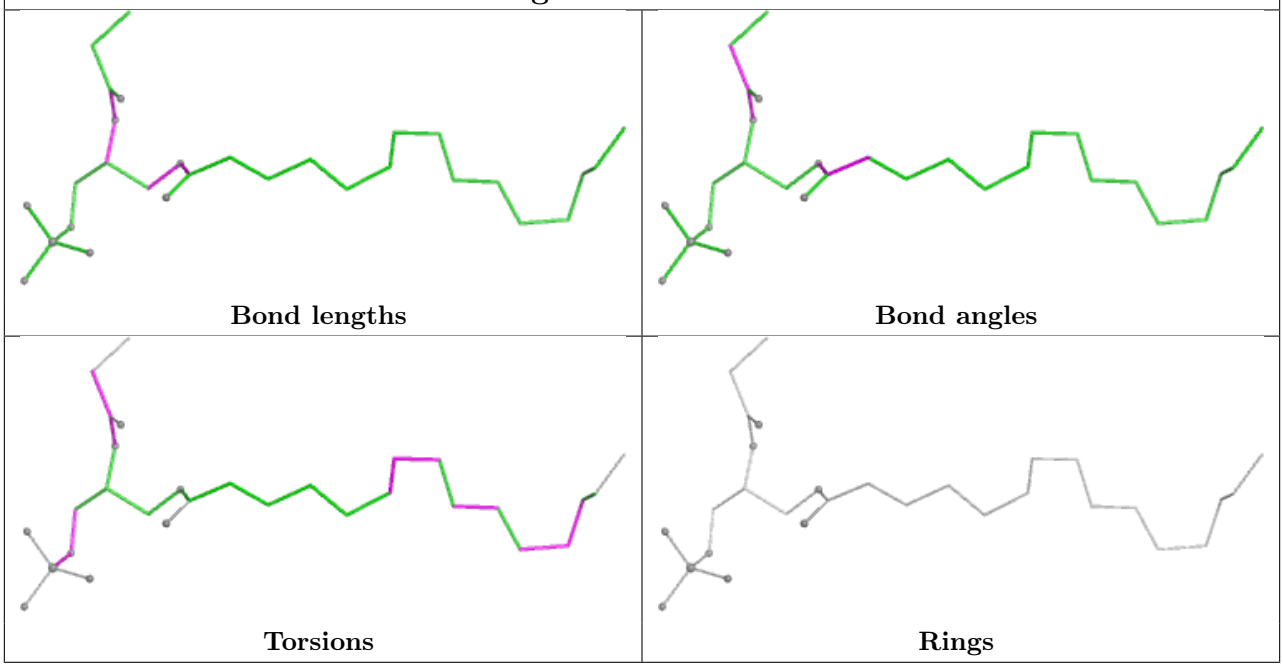
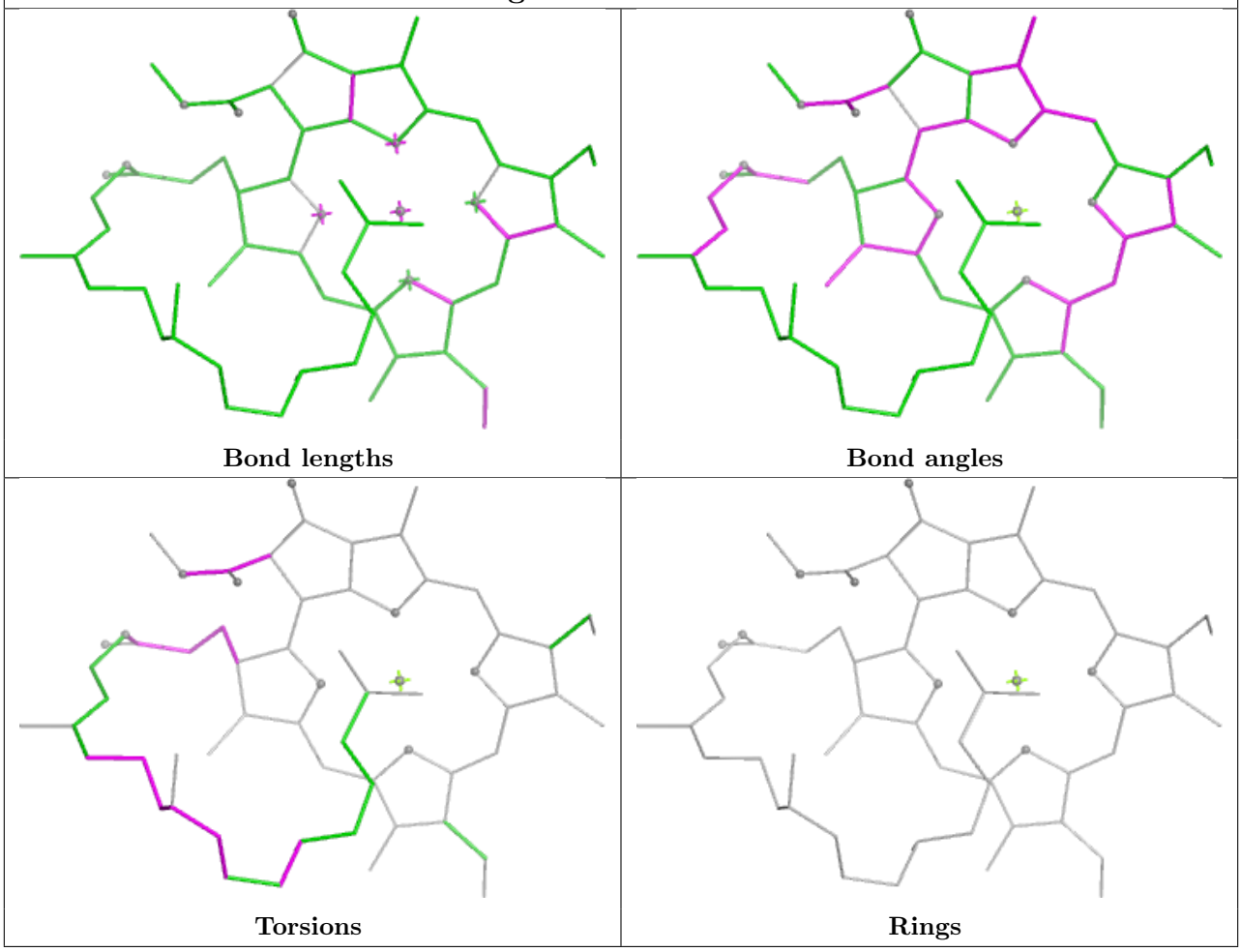
 Bond lengths	 Bond angles
 Torsions	 Rings

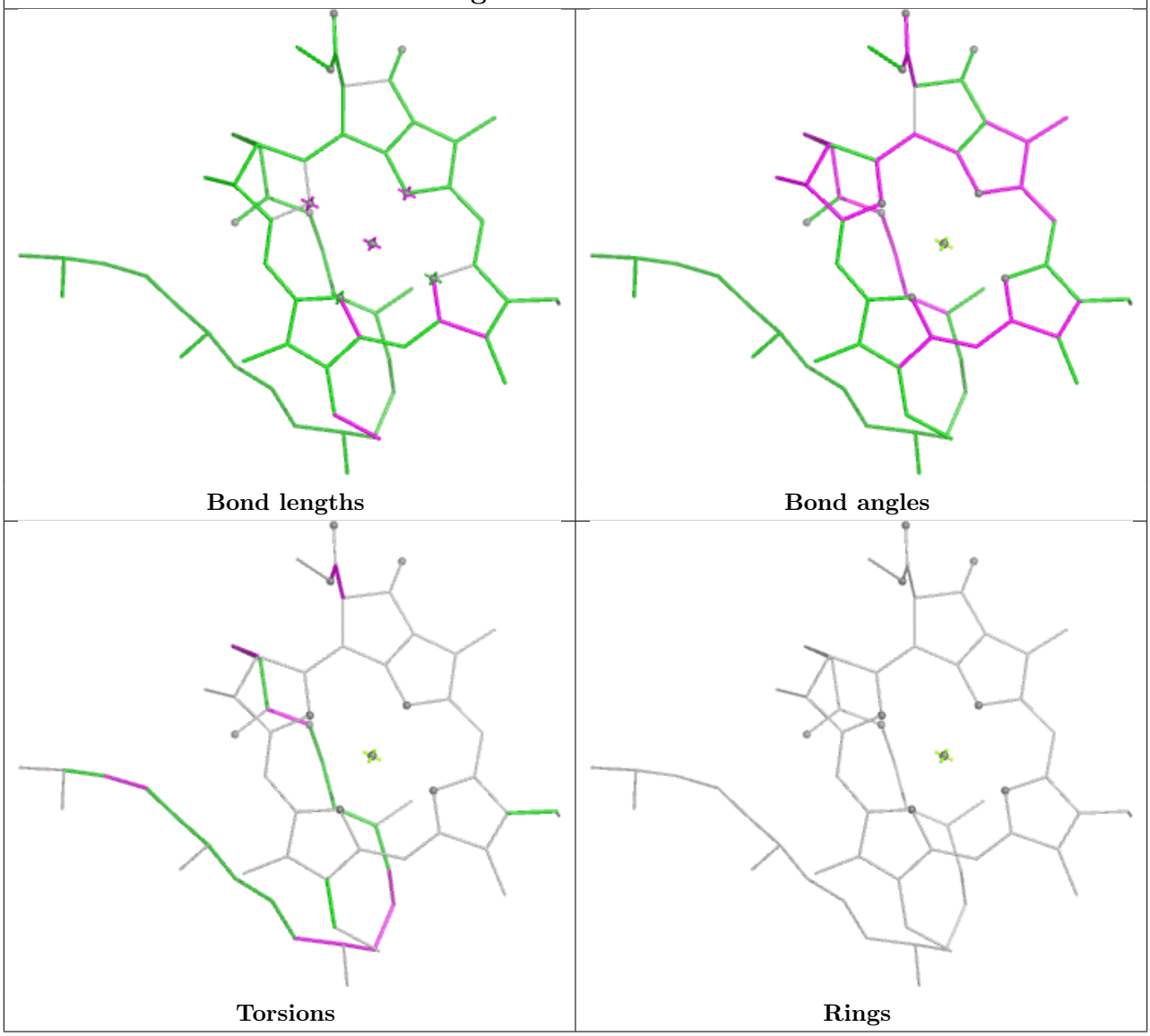
Ligand 3PH 8 320

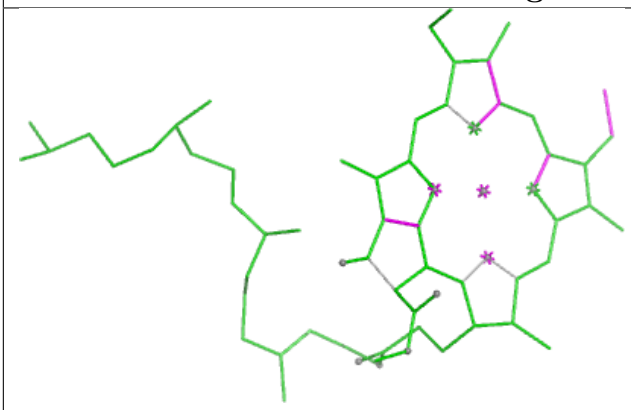
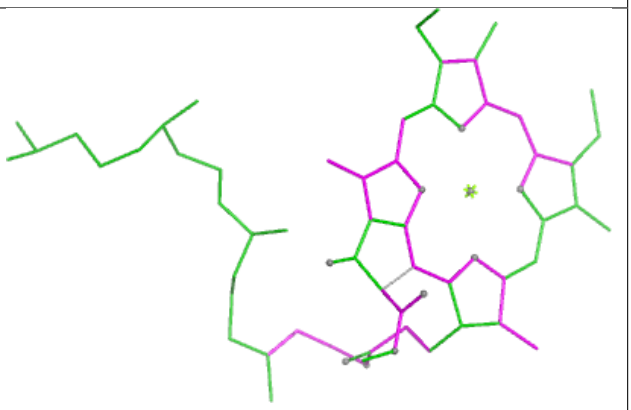
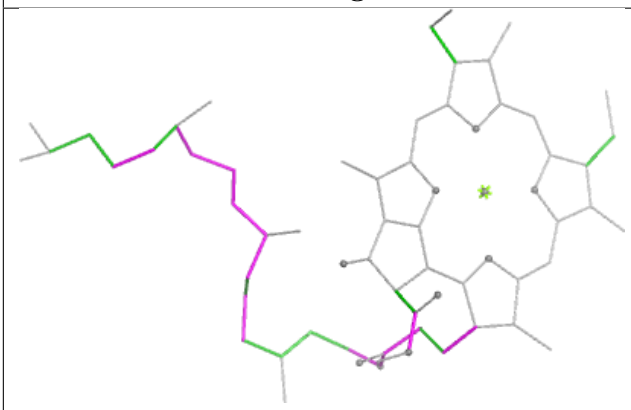
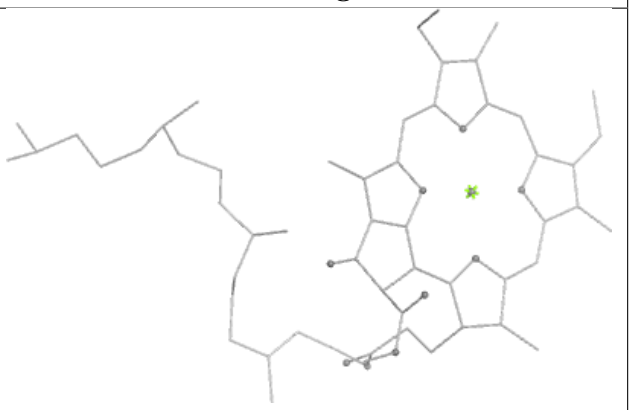


Ligand CLA B 809

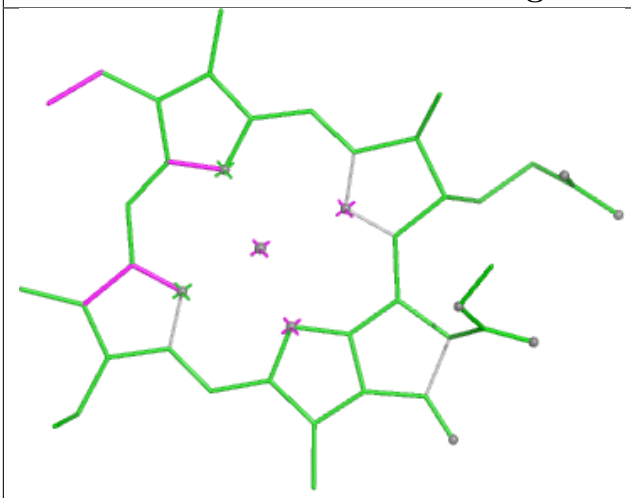


Ligand CLA B 811

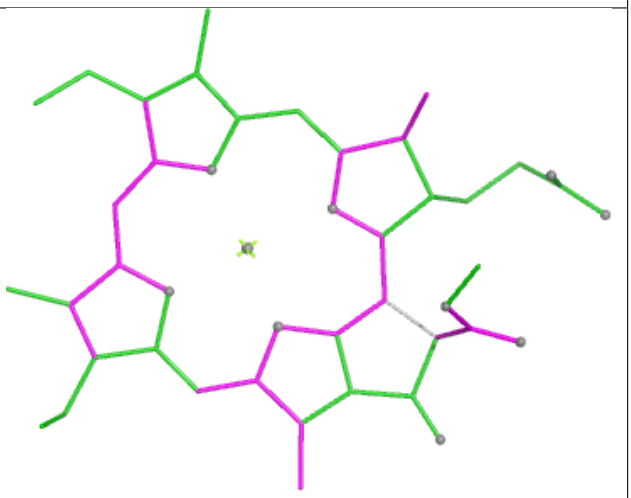


Ligand CLA F 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

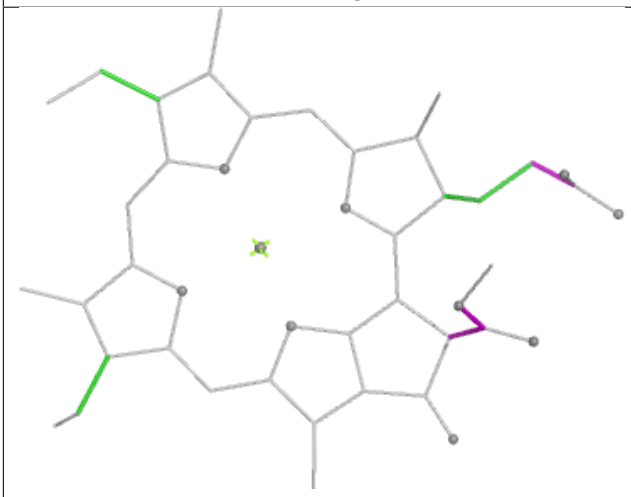
Ligand CLA Z 304



Bond lengths



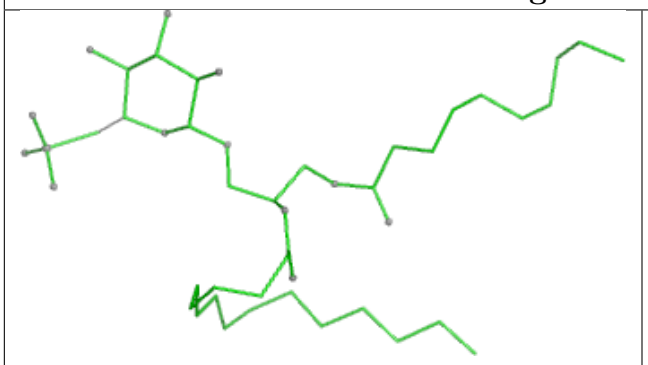
Bond angles



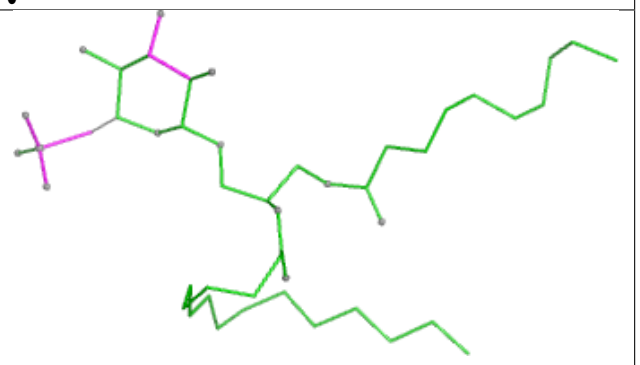
Torsions

Rings

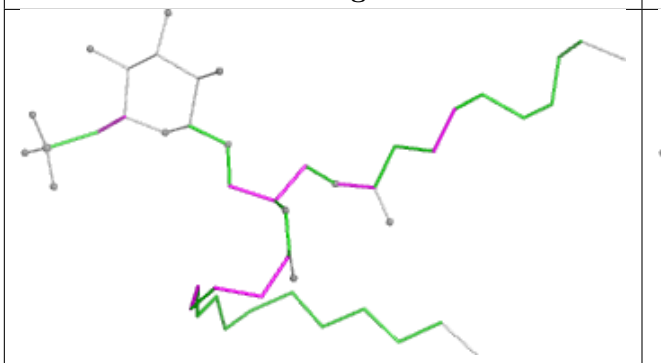
Ligand SQD 1 318



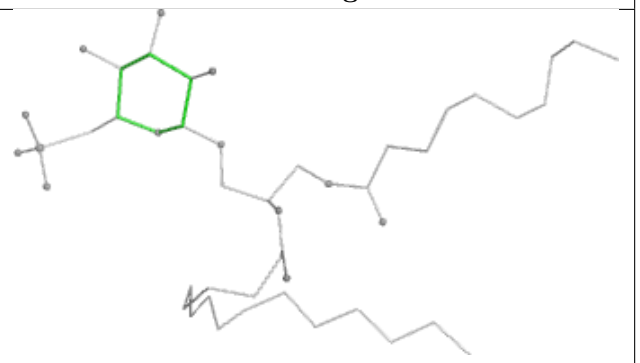
Bond lengths



Bond angles

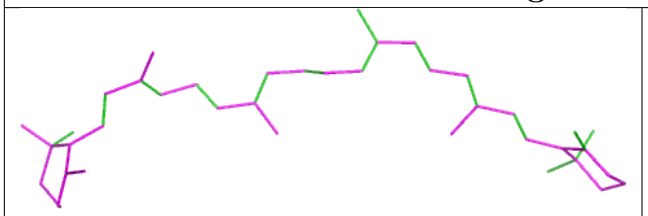


Torsions



Rings

Ligand BCR 6 306



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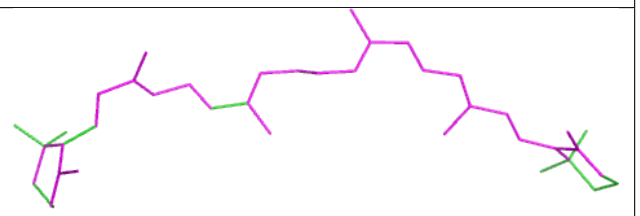

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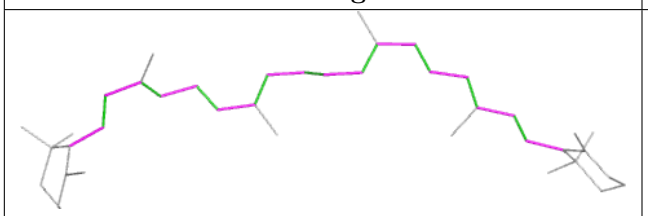

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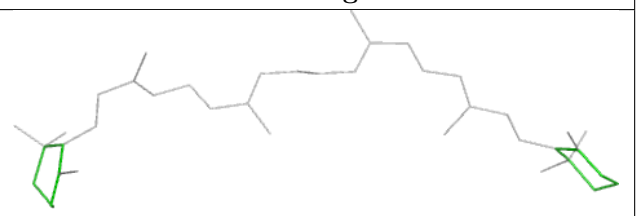
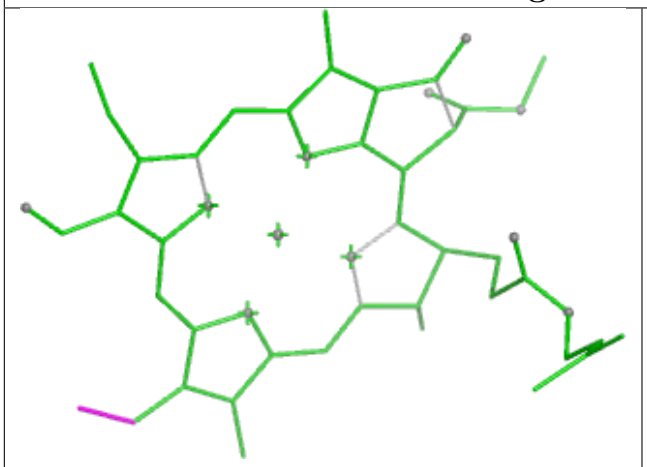


Rings

Ligand CHL 2 303



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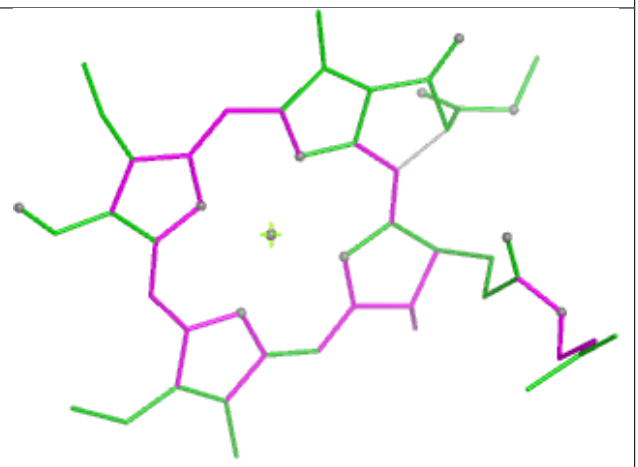

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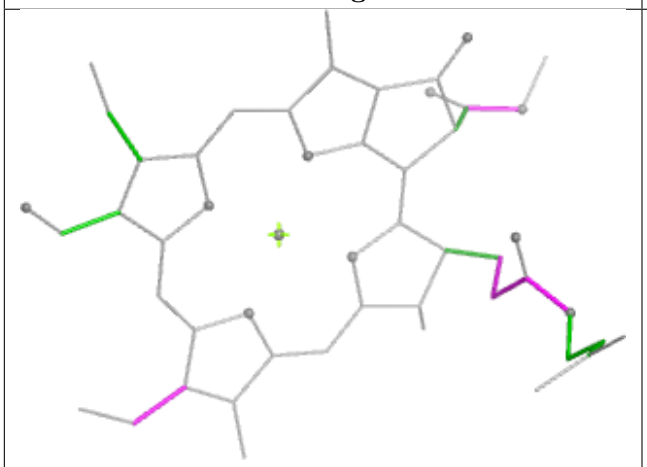

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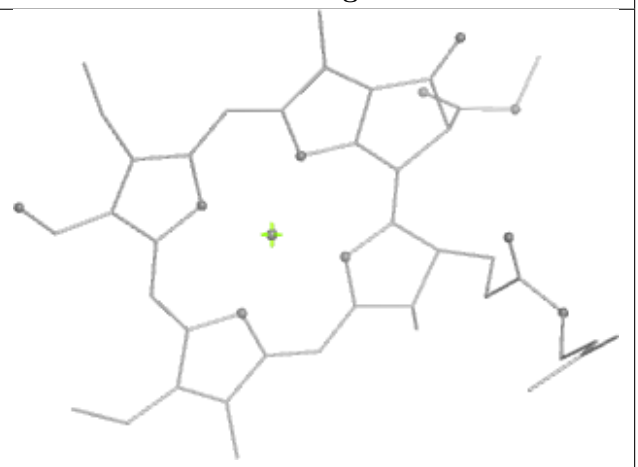
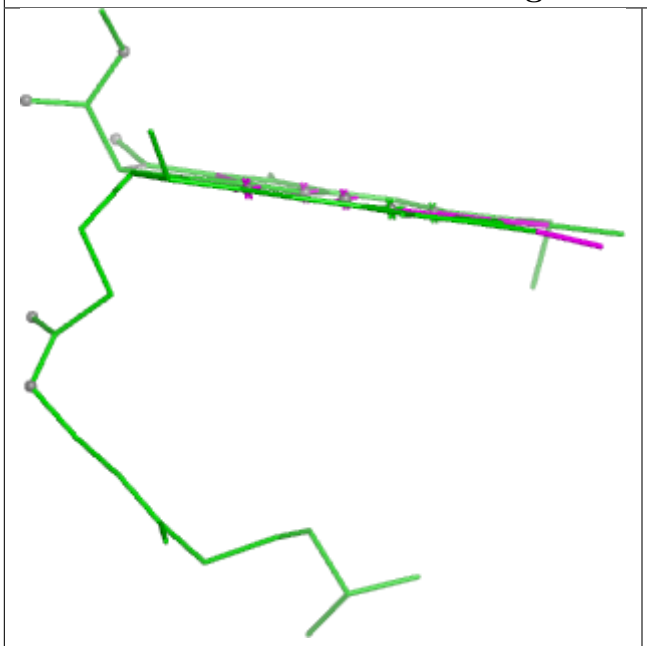


Rings

Ligand CLA B 823



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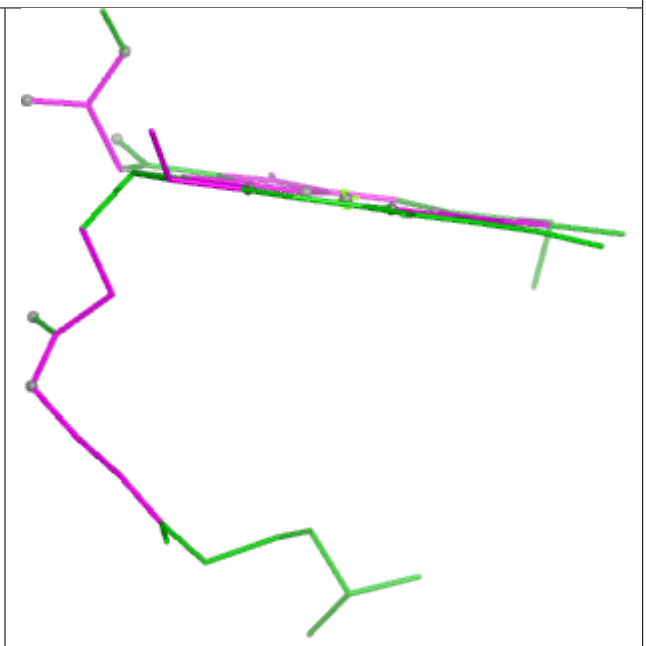
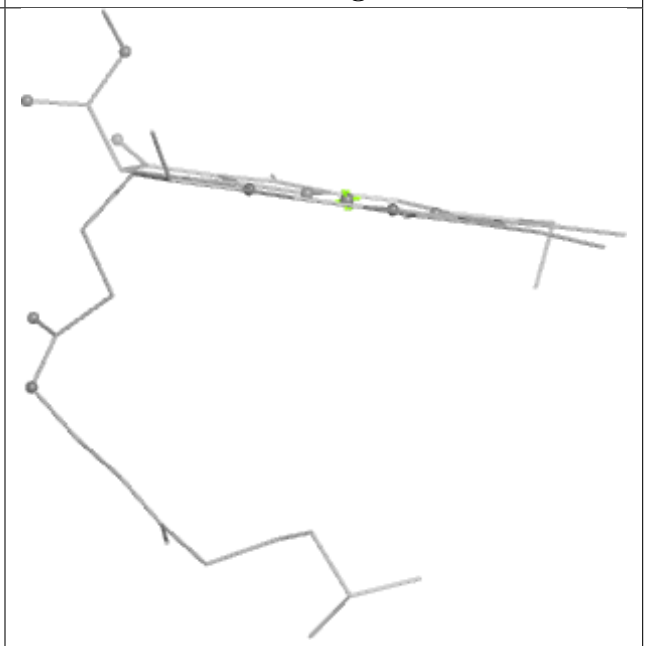


Bond angles

Torsions

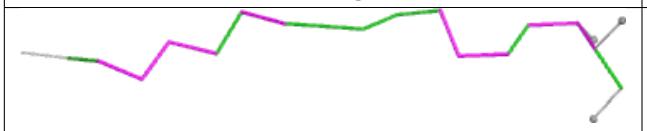


Rings

Ligand SPH 7 321

Bond lengths

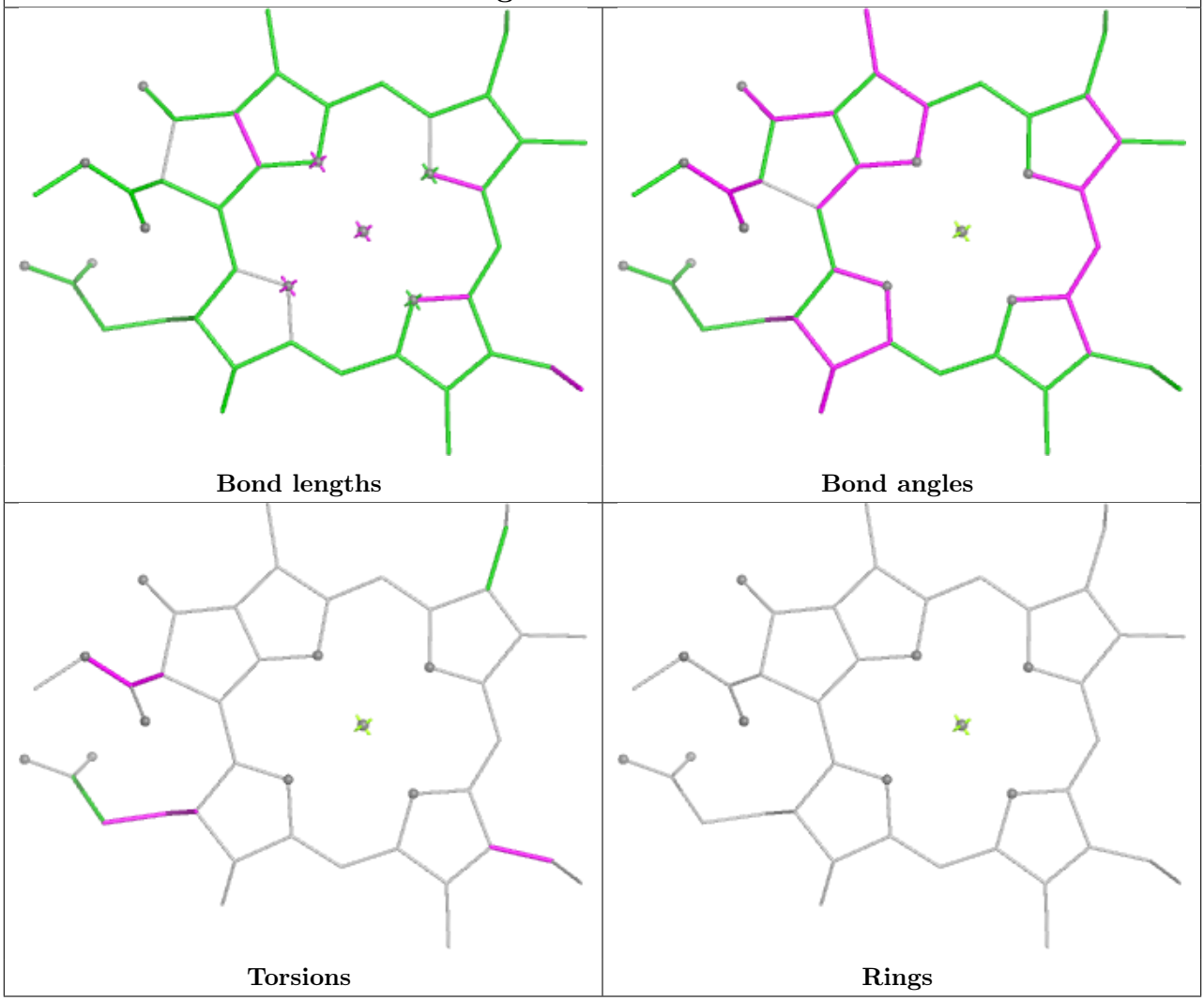
Bond angles



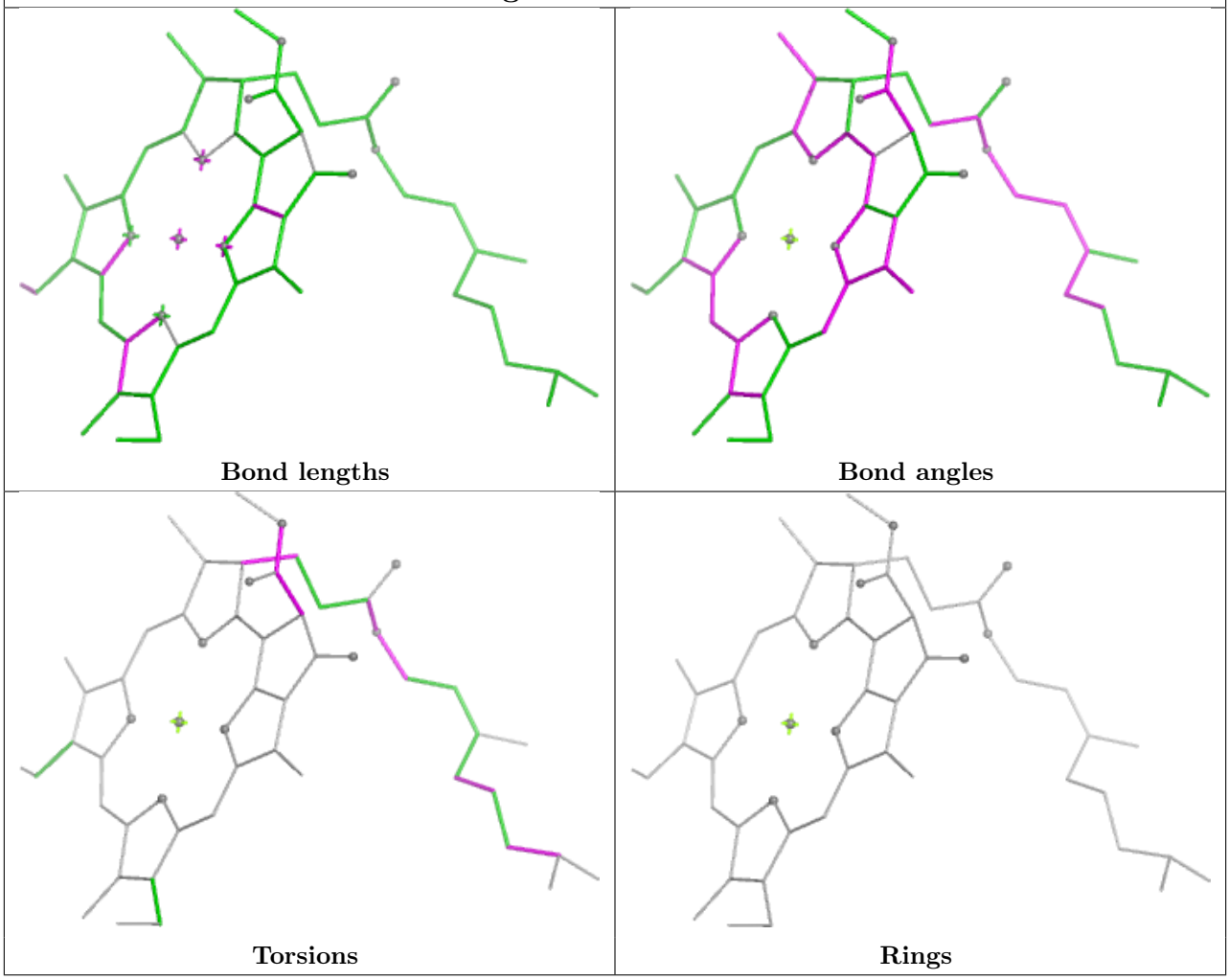
Torsions

Rings

Ligand CLA 3 315



Ligand CLA A 836



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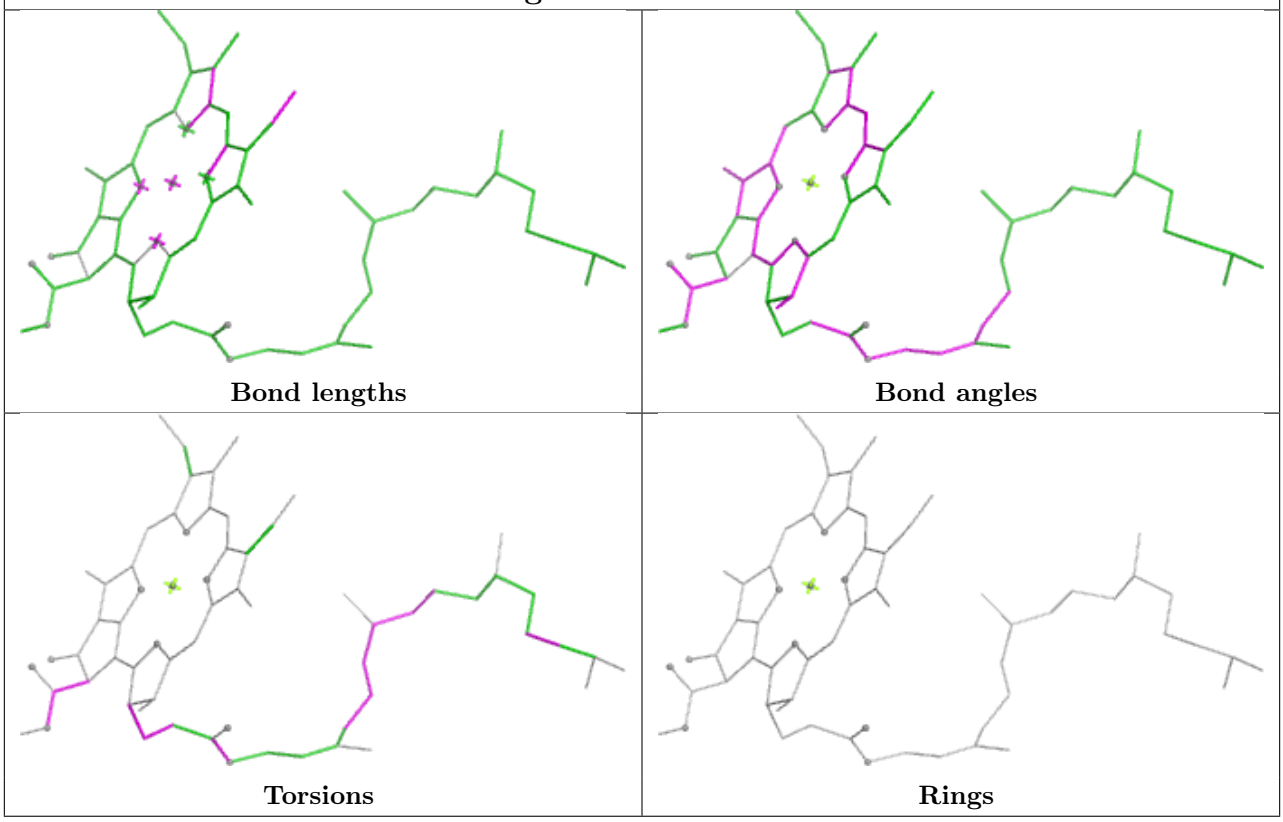

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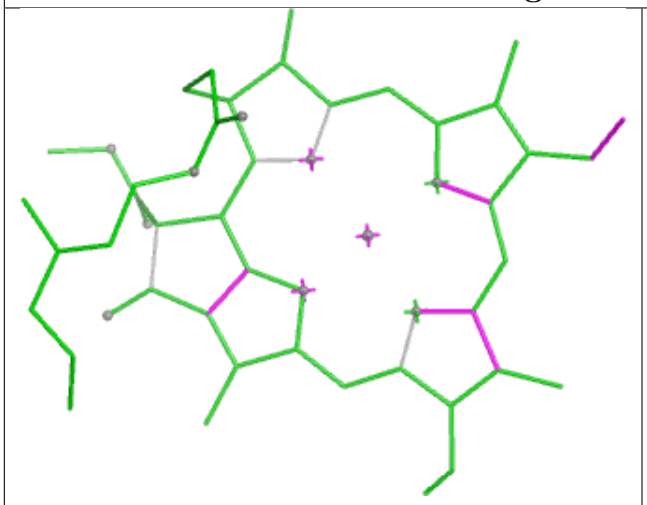

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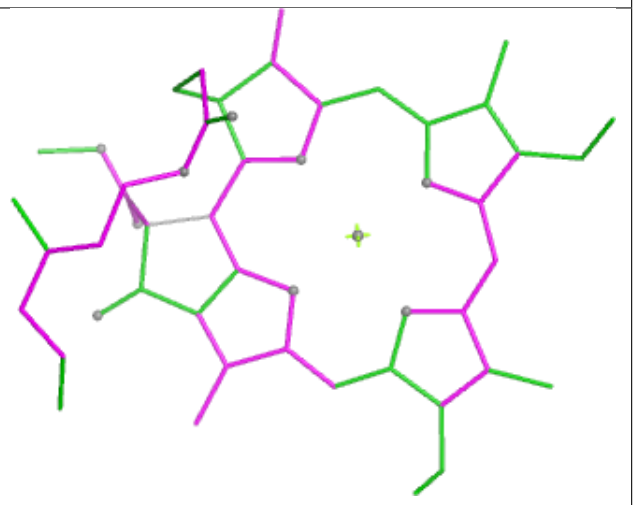
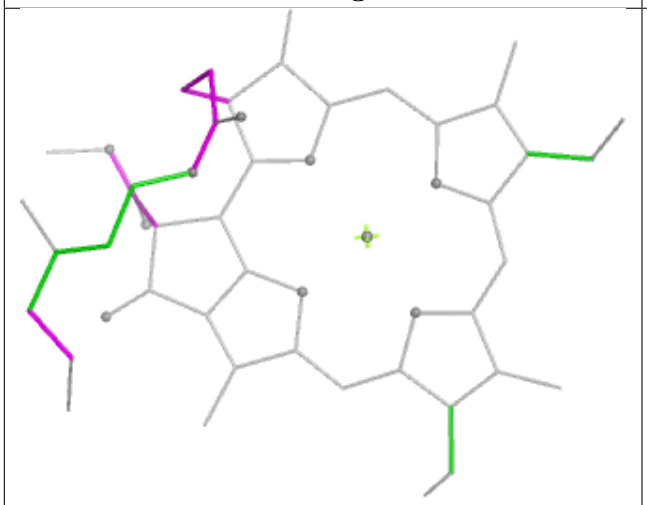


Bond angles



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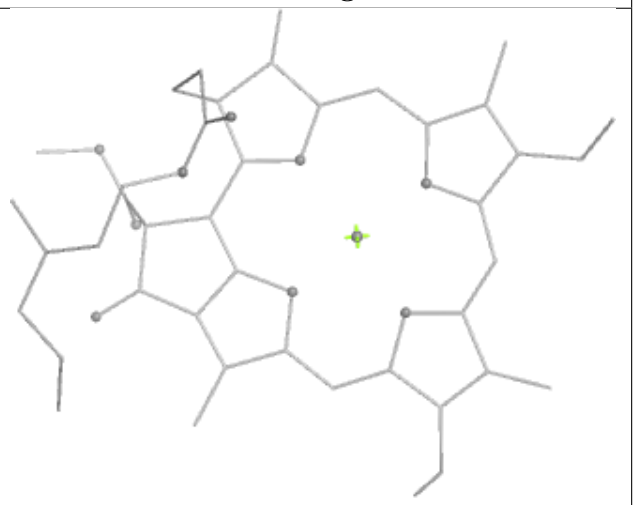
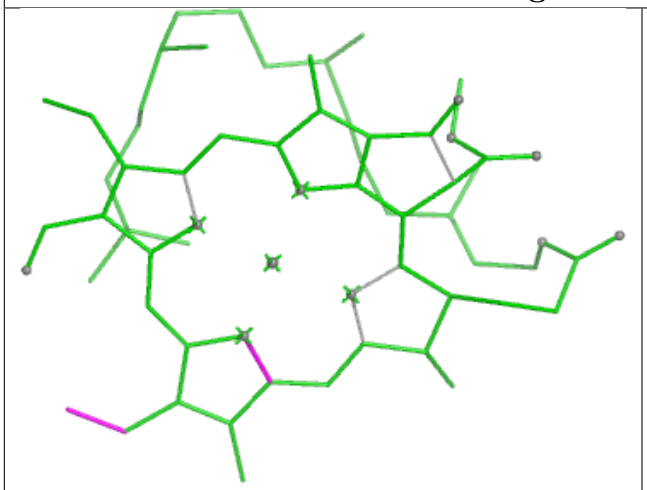


Rings

Ligand CHL 9 312



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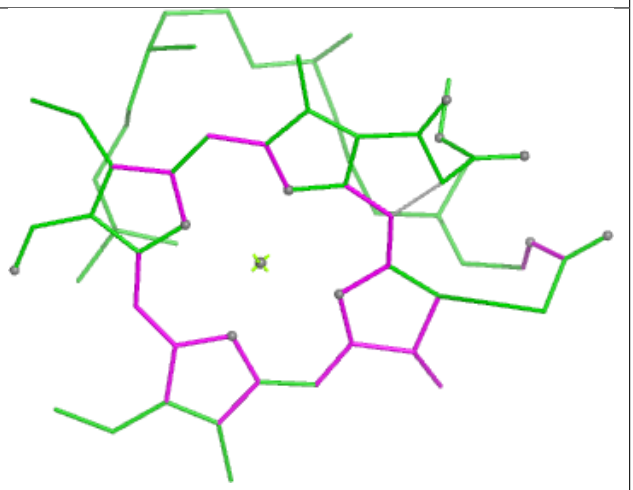
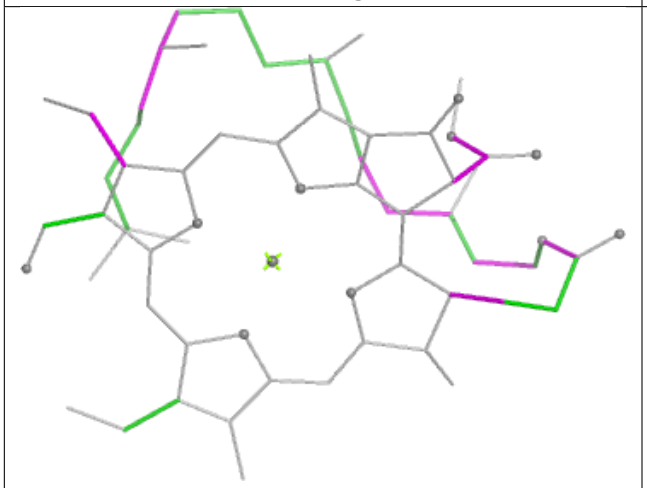


Bond angles



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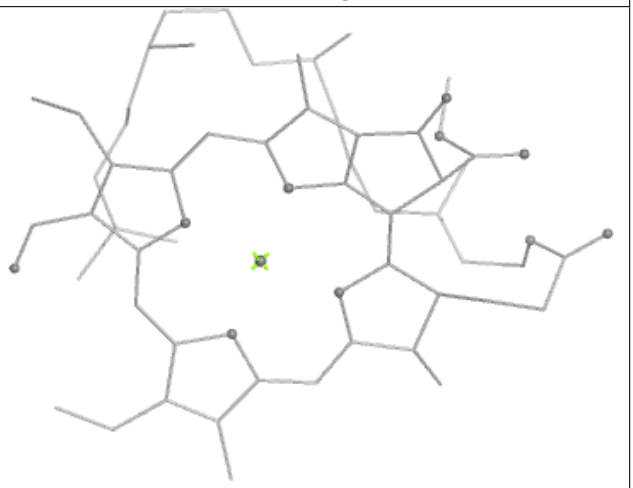
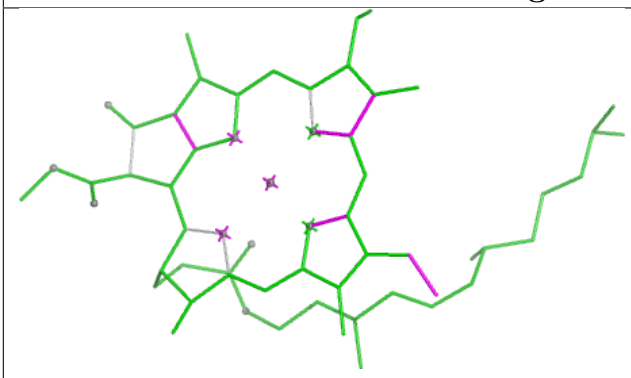
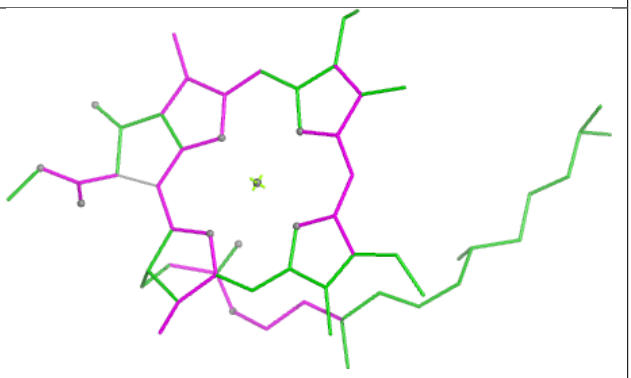
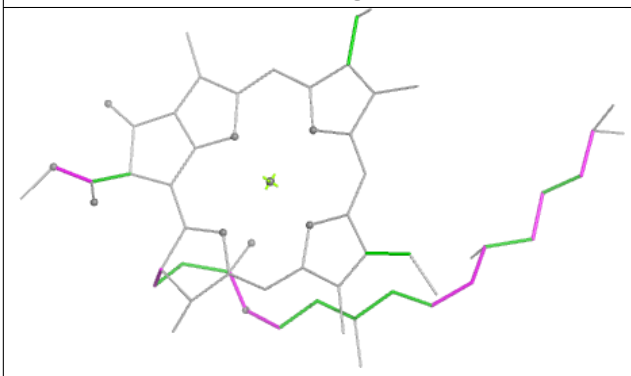
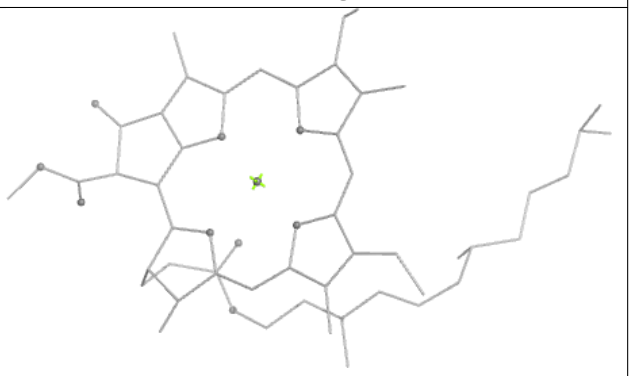


Rings

Ligand CLA 6 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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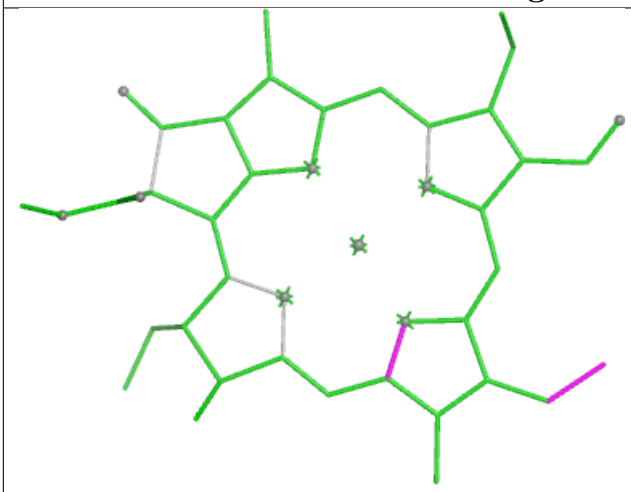
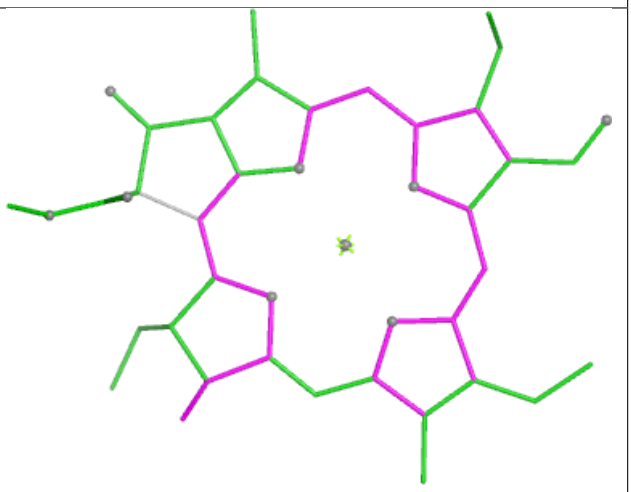
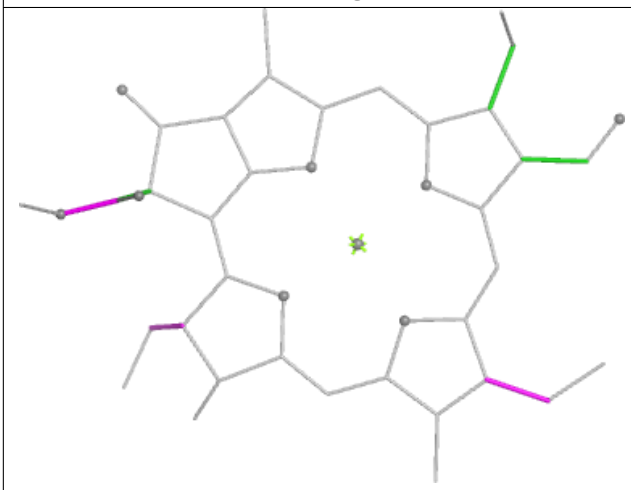
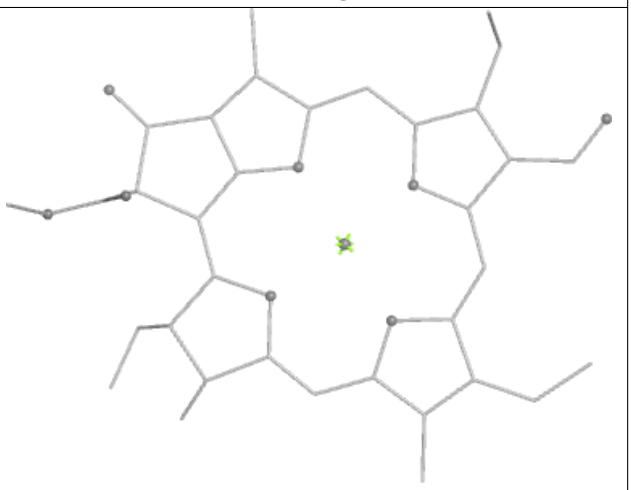
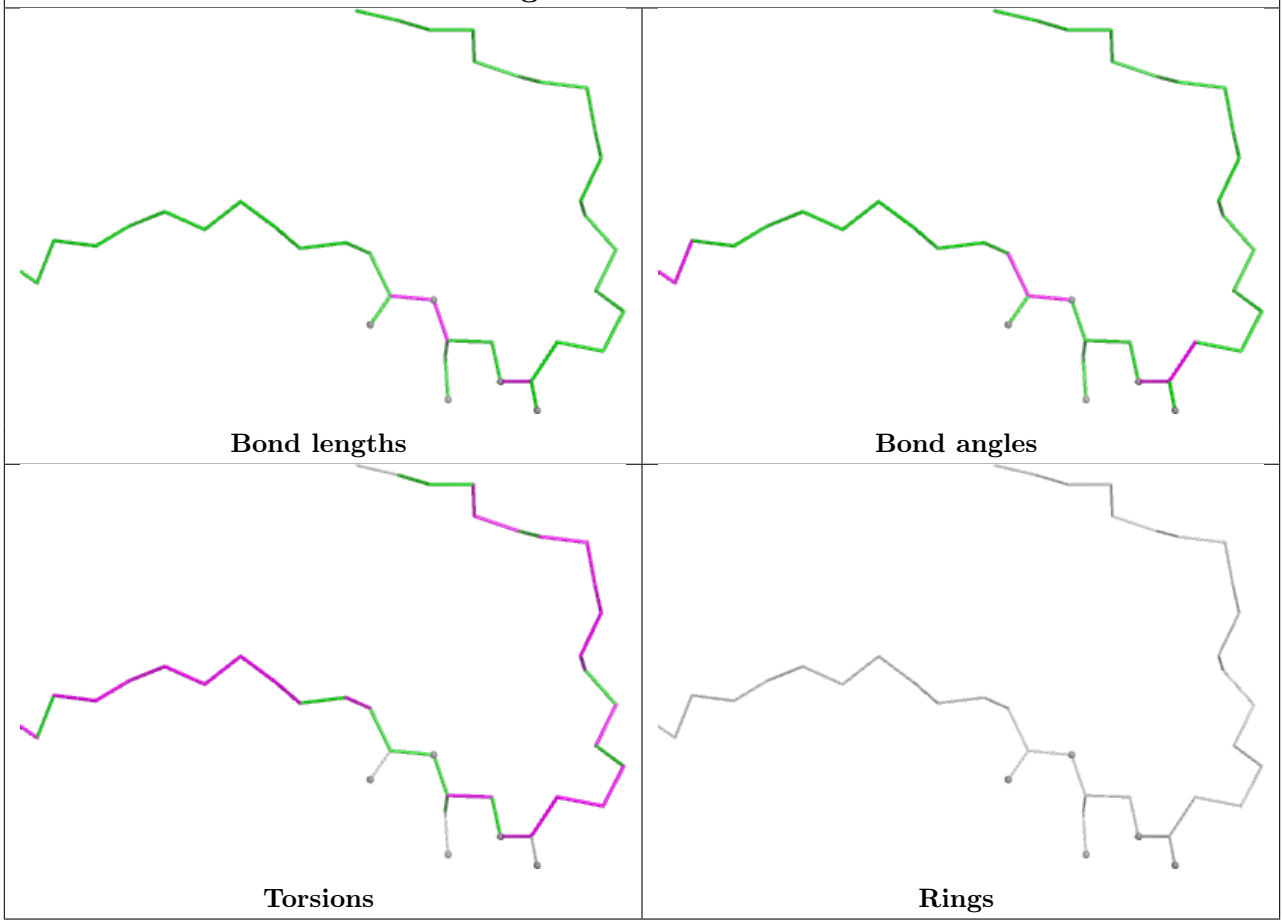
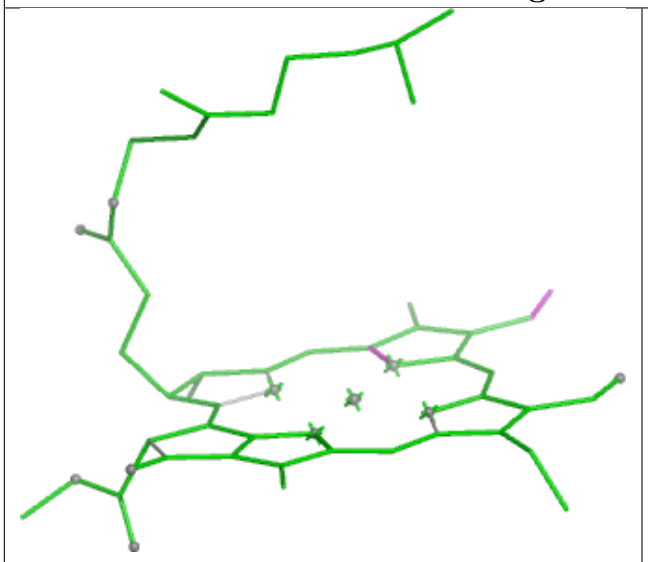
 Bond lengths	 Bond angles
 Torsions	 Rings

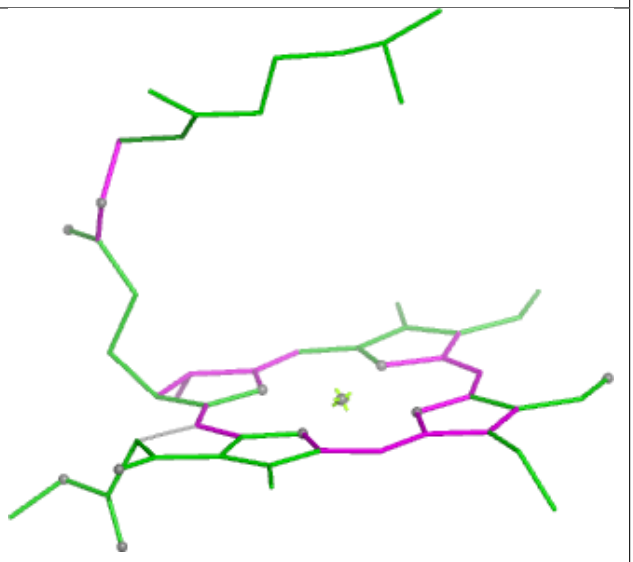
Ligand DGA A 852



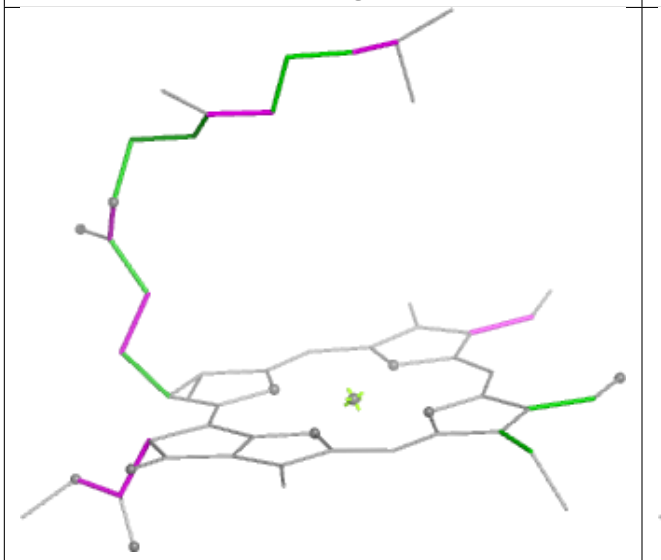
Ligand CHL 6 315



Bond lengths



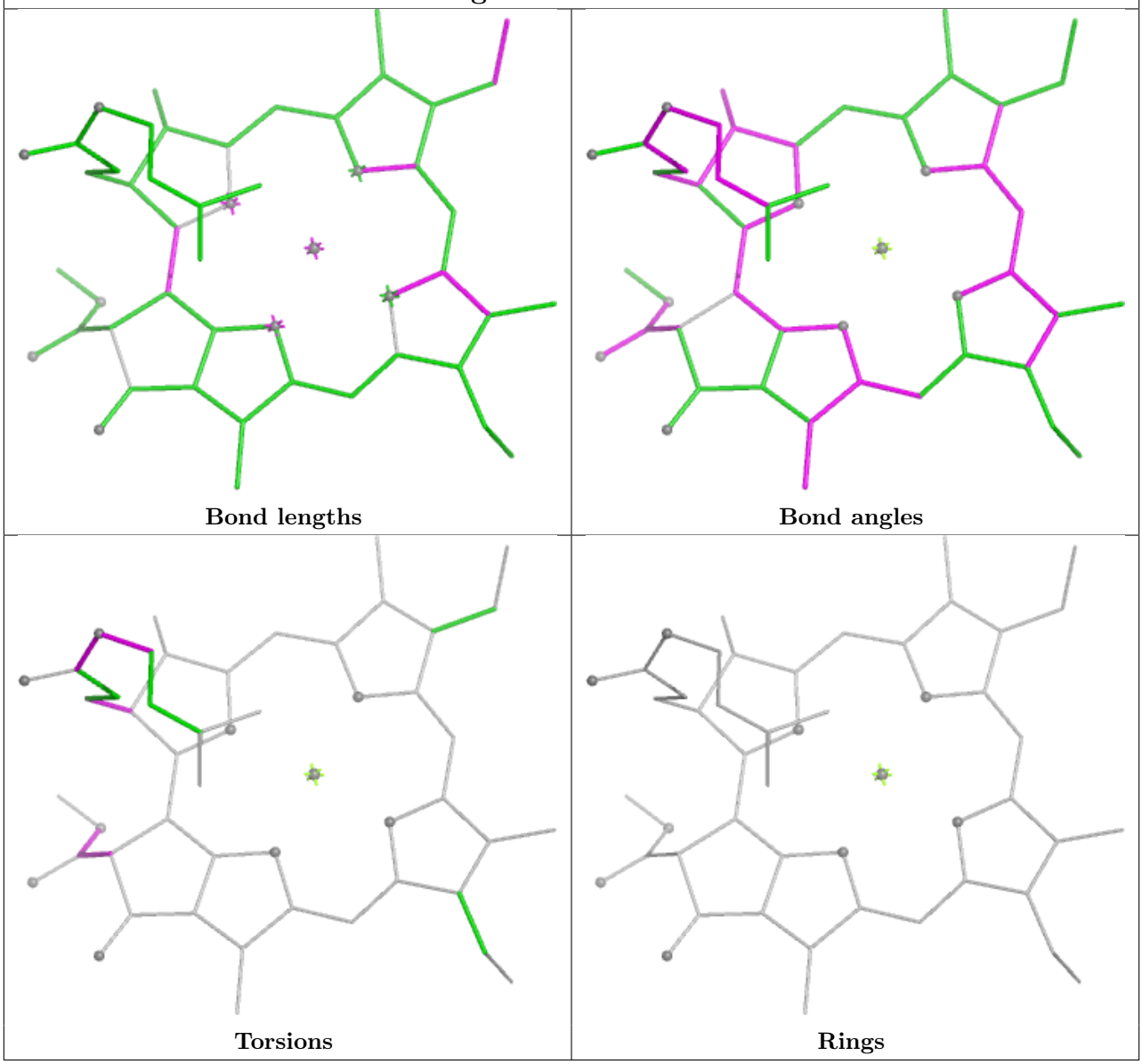
Bond angles



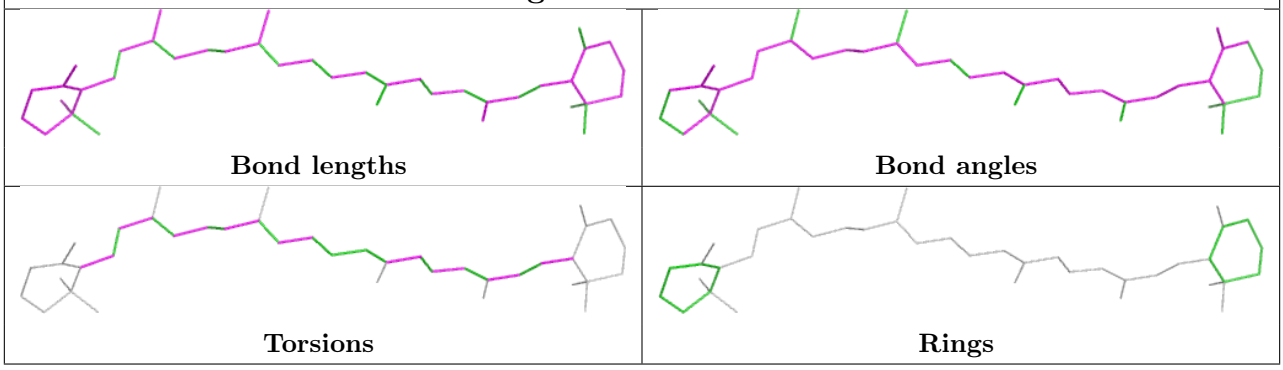
Torsions

Rings

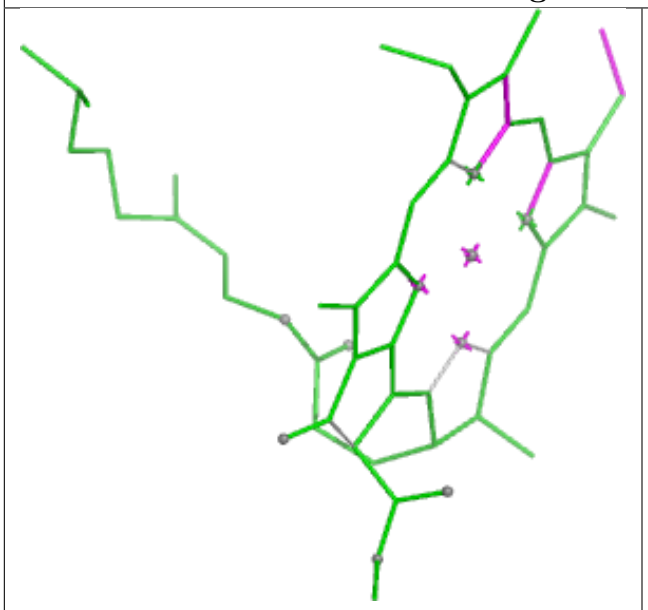
Ligand CLA 7 315



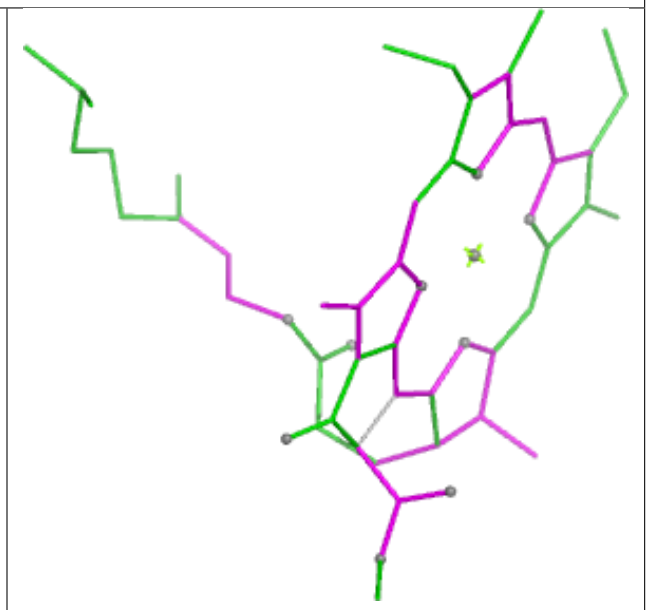
Ligand BCR 3 305



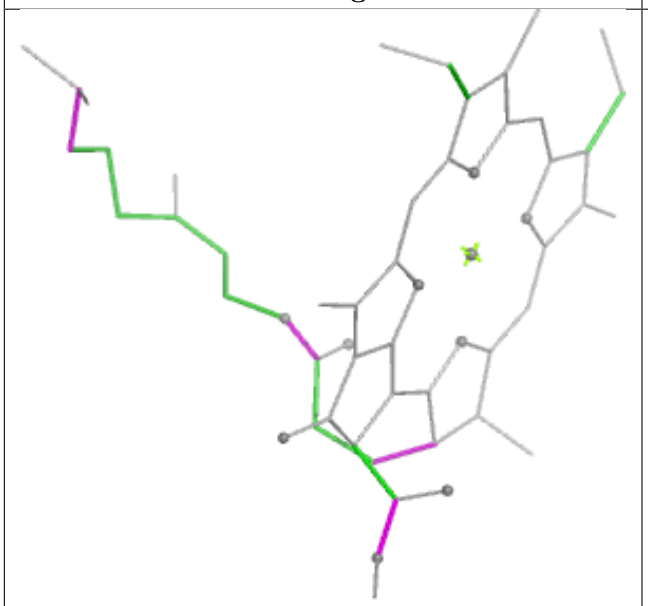
Ligand CLA 5 326



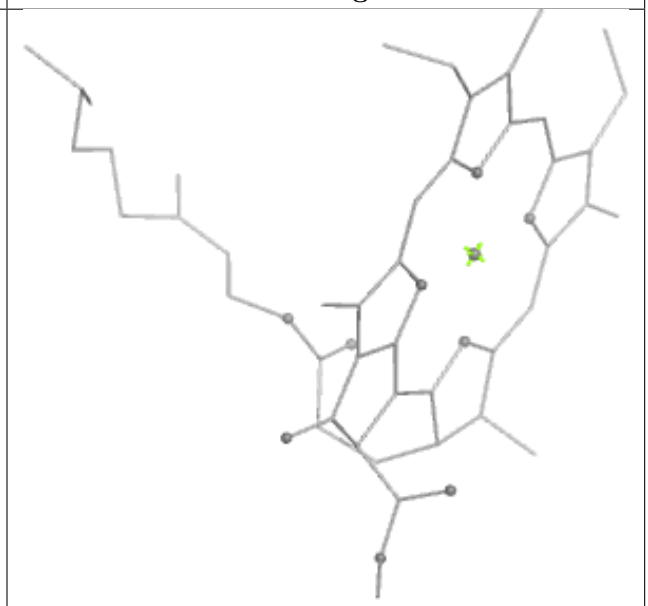
Bond lengths



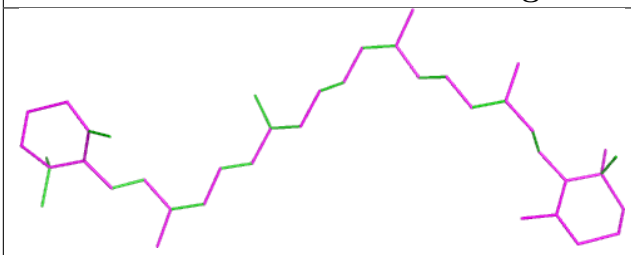
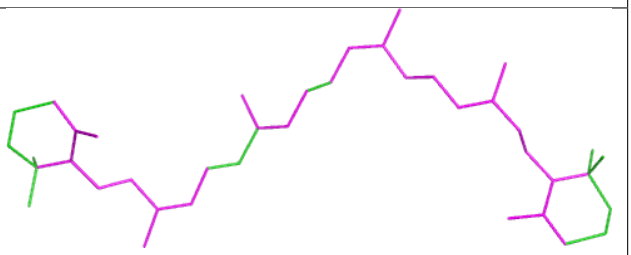
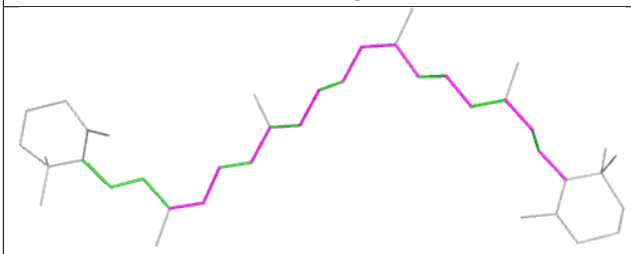
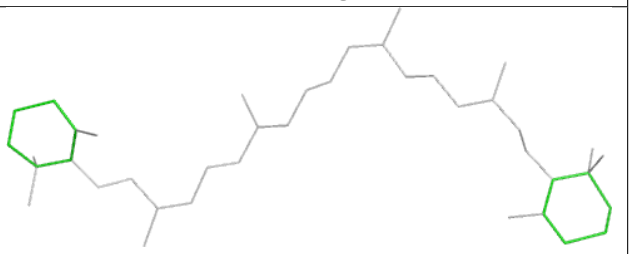
Bond angles



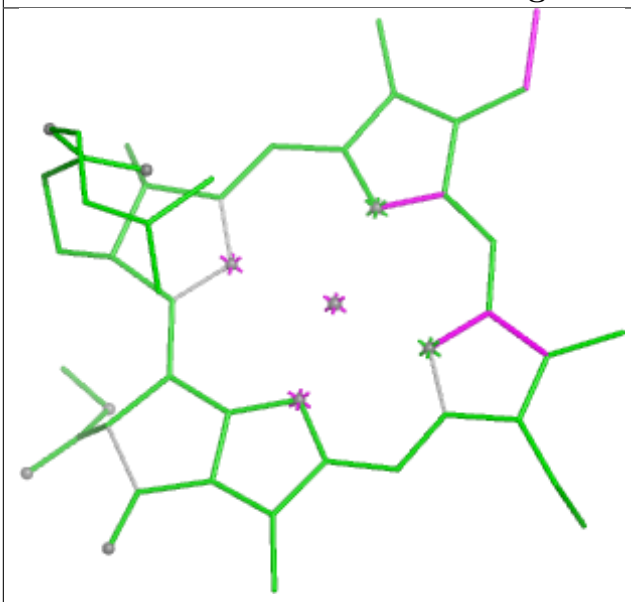
Torsions



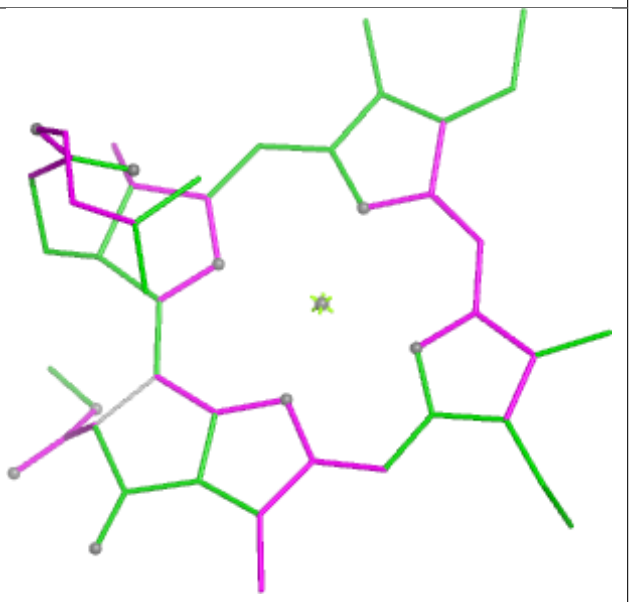
Rings

Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

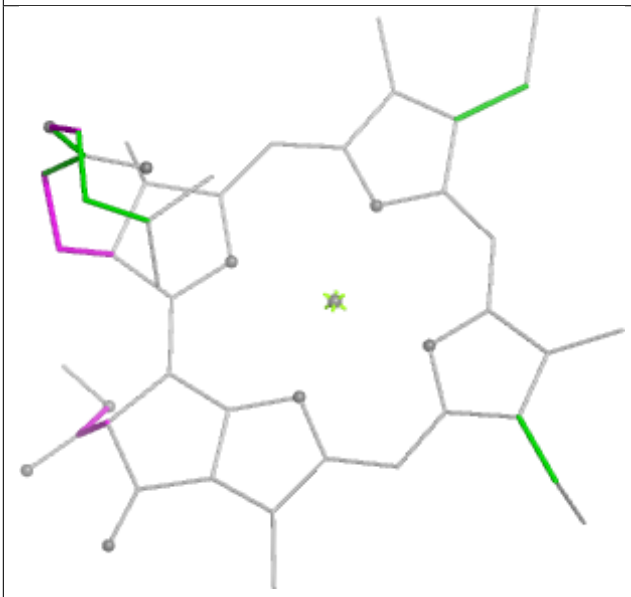
Ligand CLA 4 815



Bond lengths



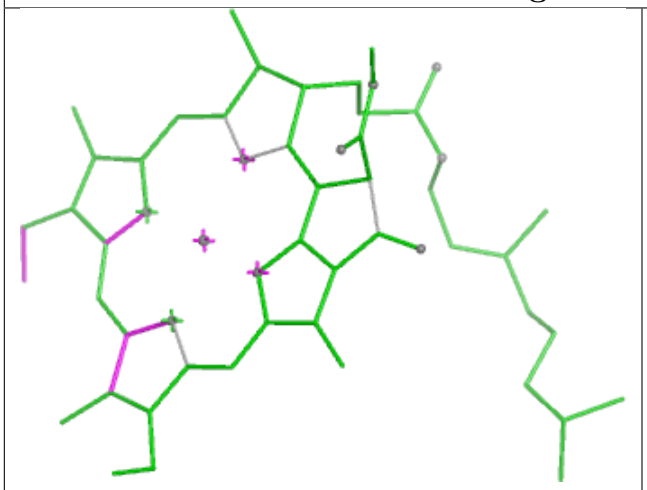
Bond angles



Torsions

Rings

Ligand CLA 6 313



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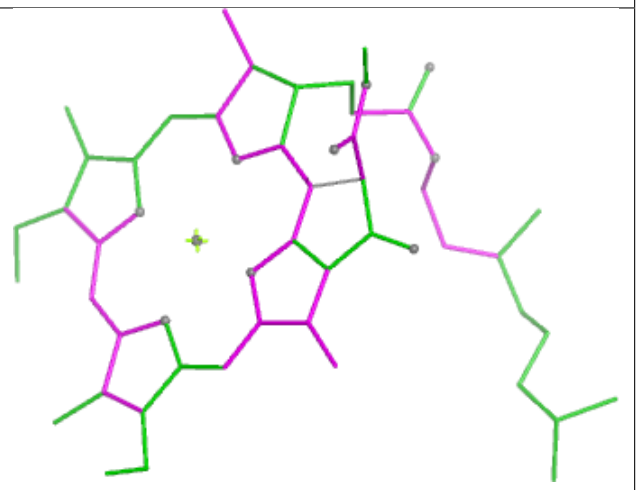
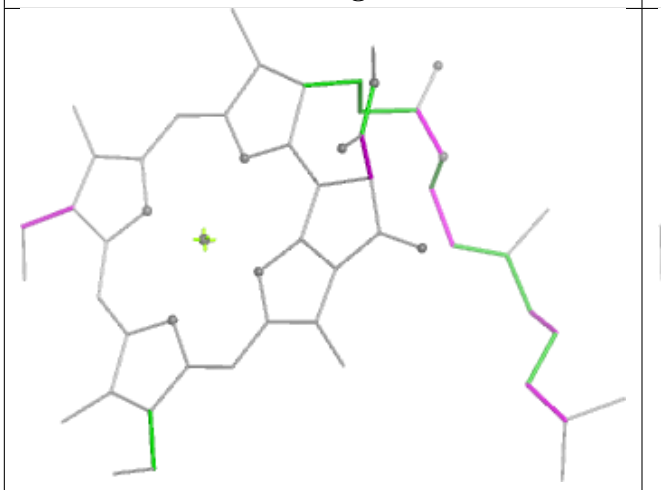


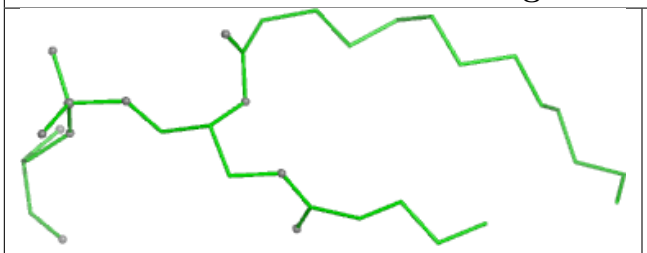
Bond angles



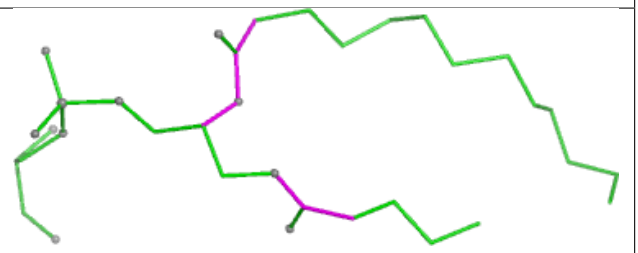
Torsions

Rings

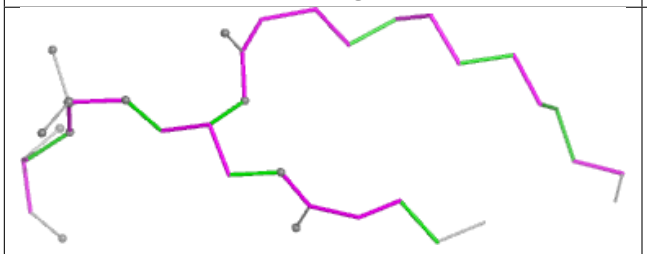
Ligand LHG A 849



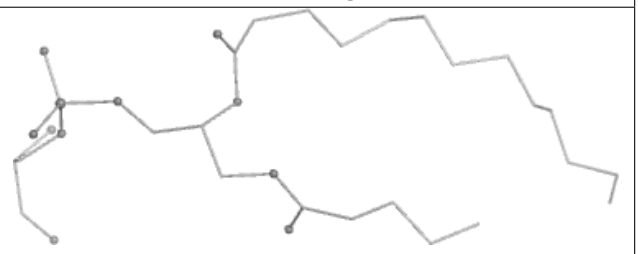
Bond lengths



Bond angles

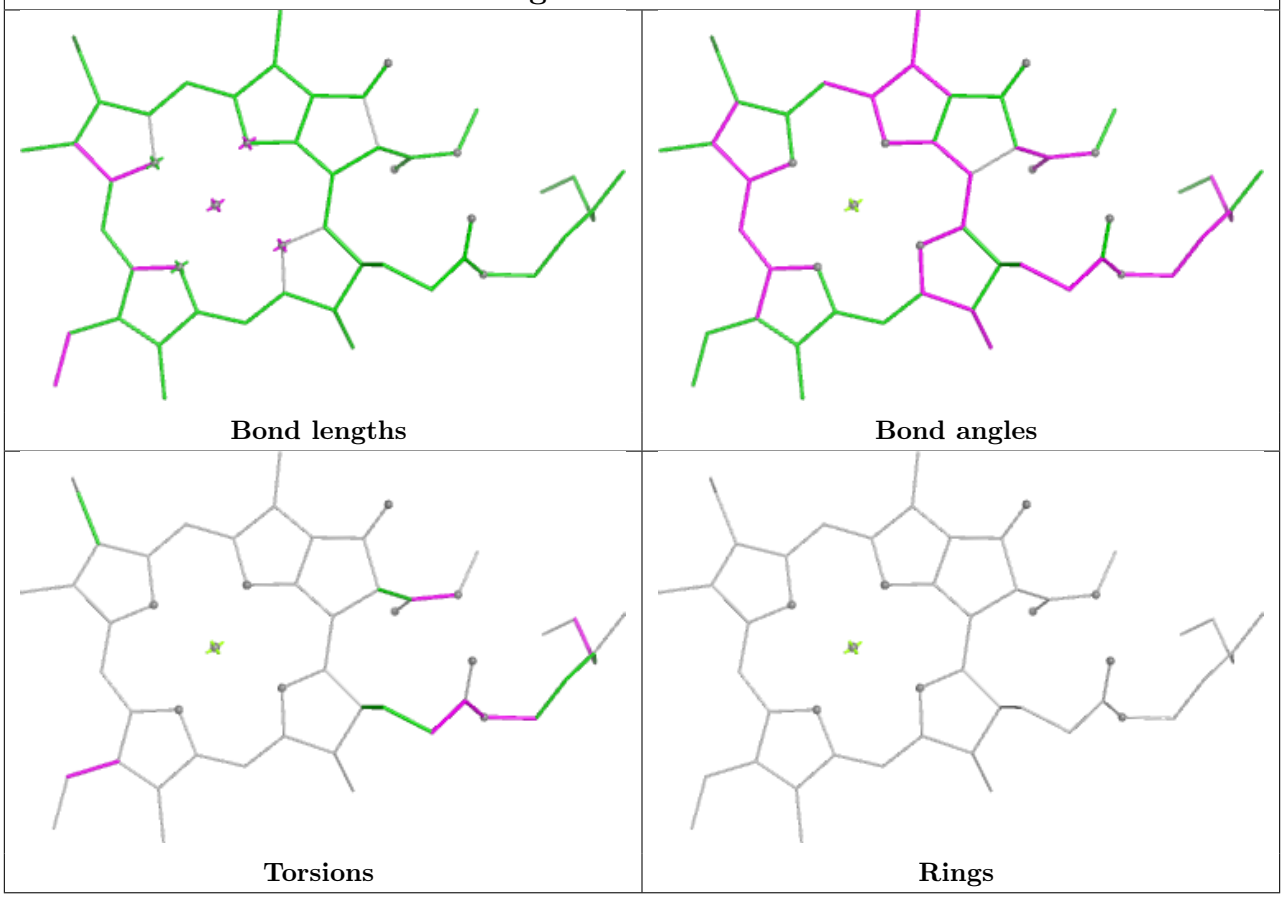


Torsions

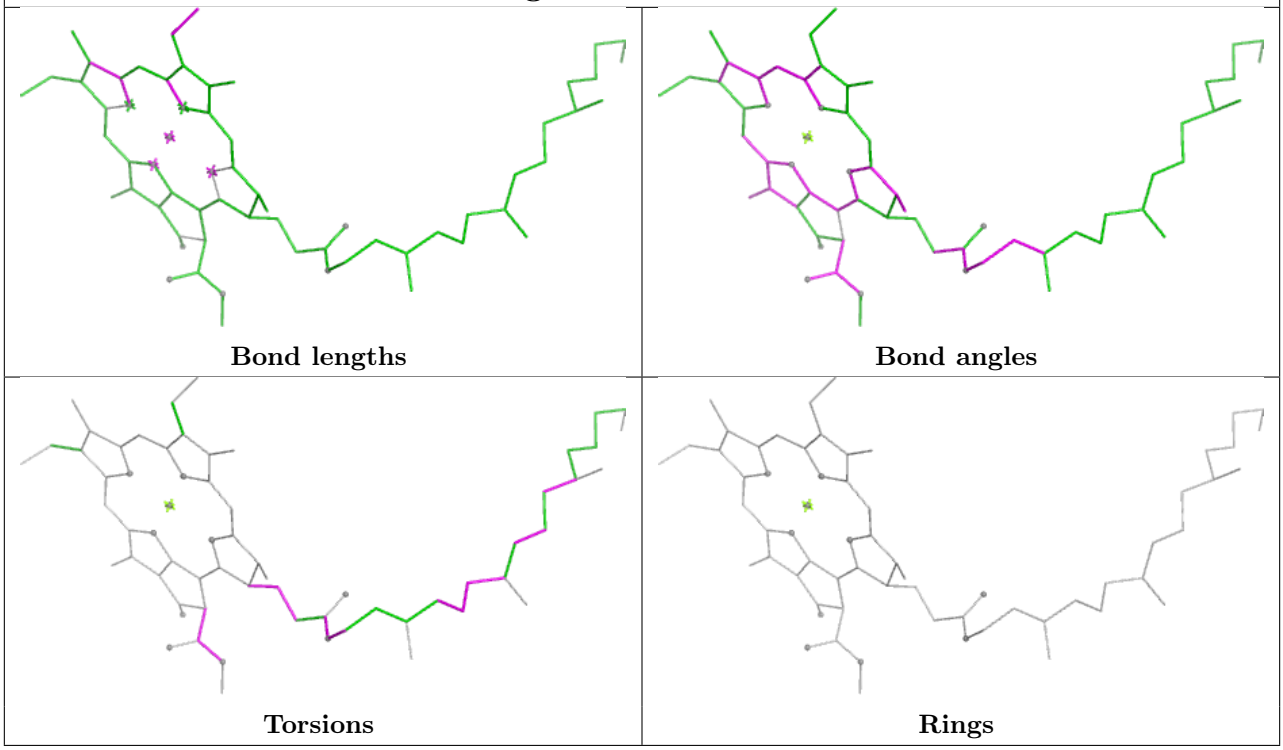


Rings

Ligand CLA 6 308



Ligand CLA A 802



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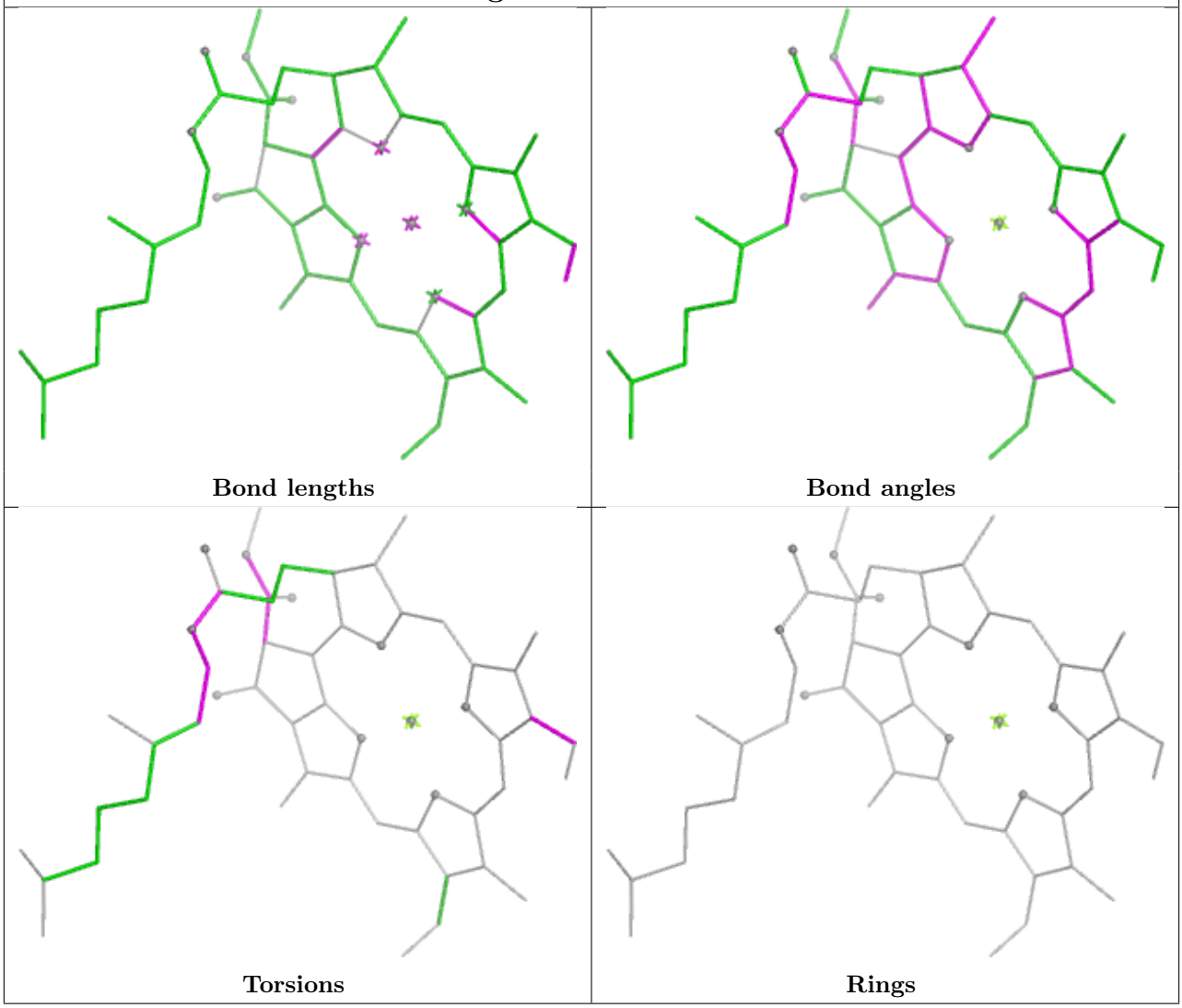

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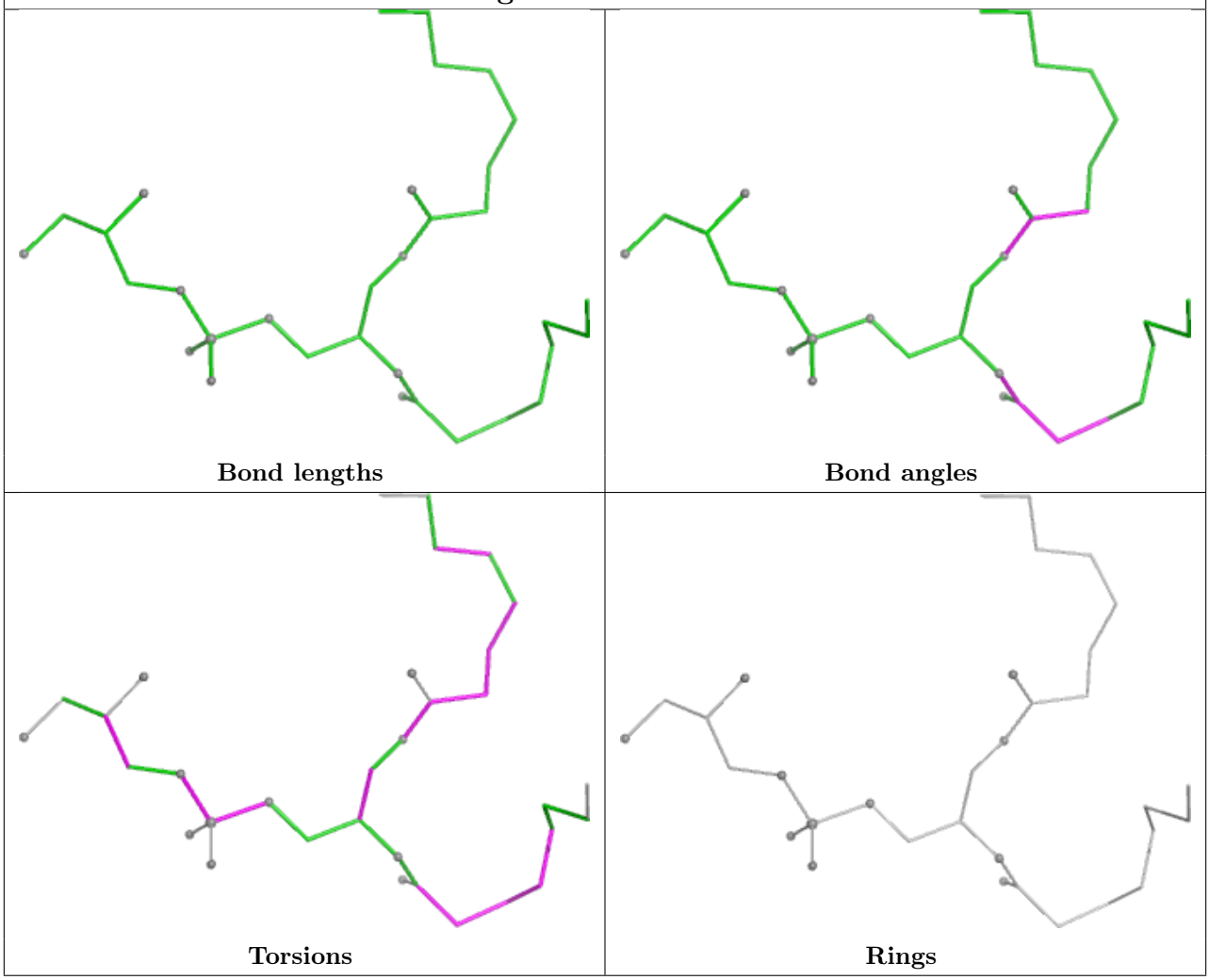

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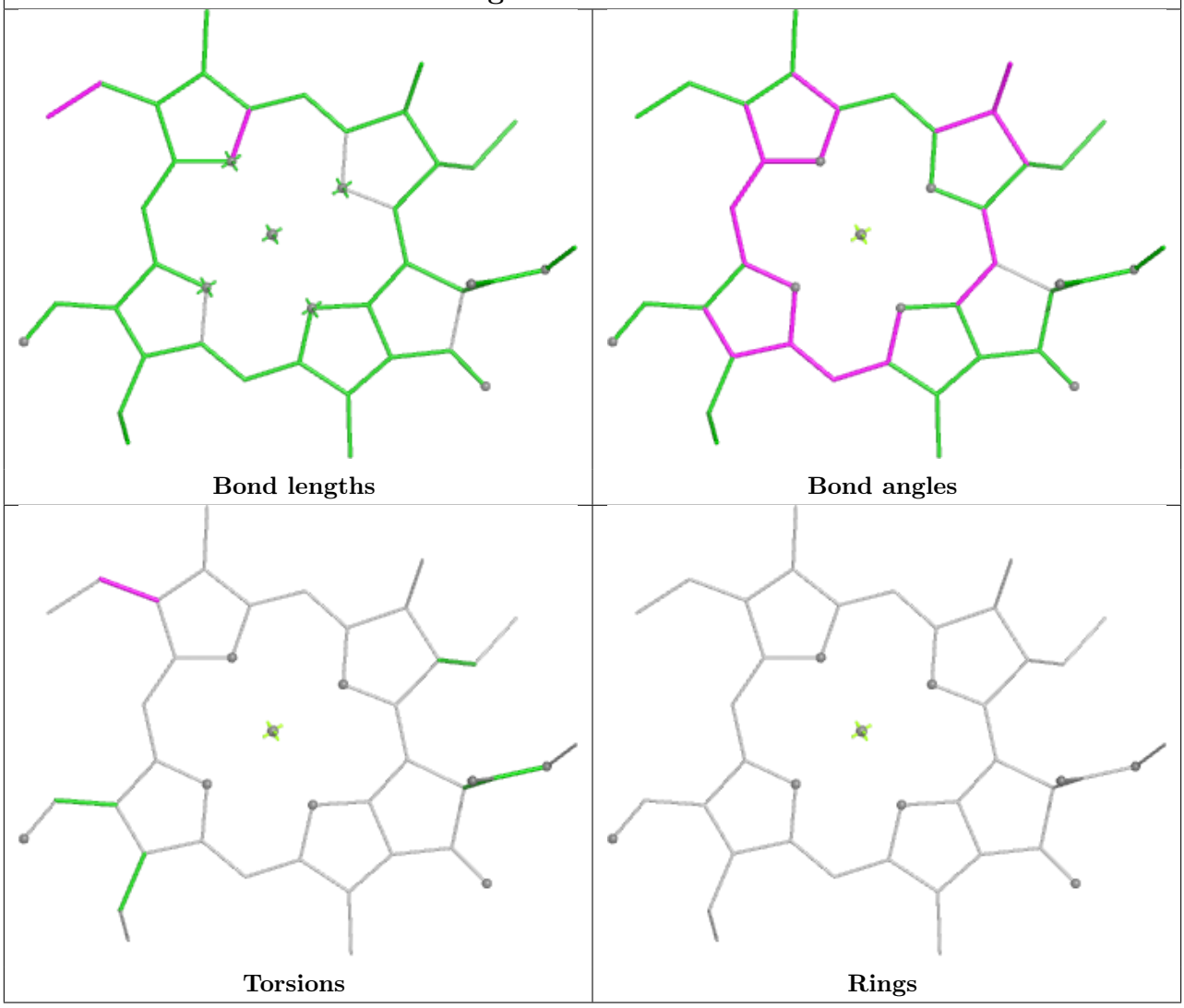

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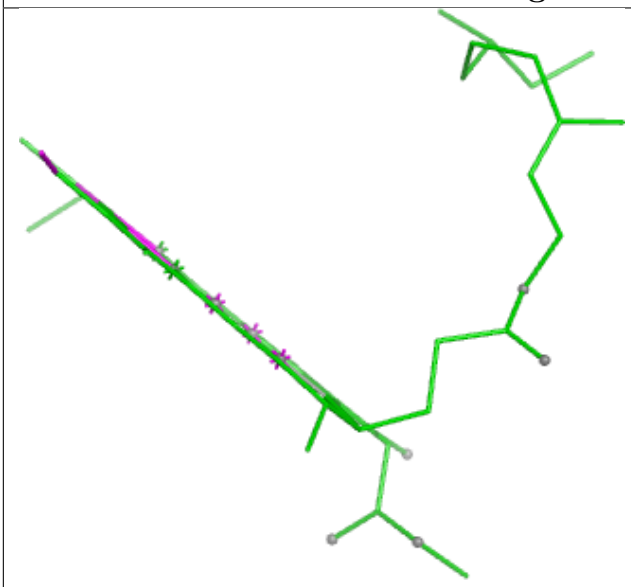
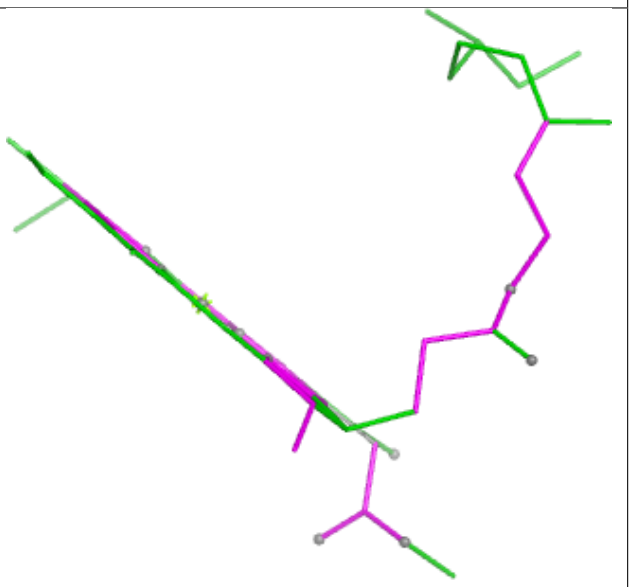
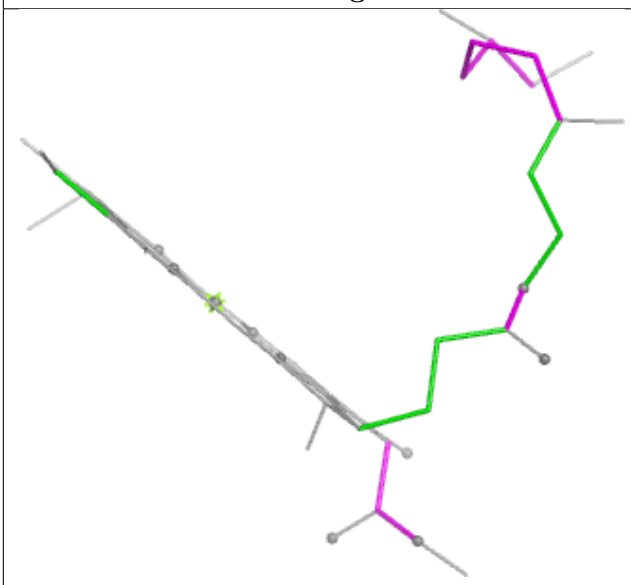
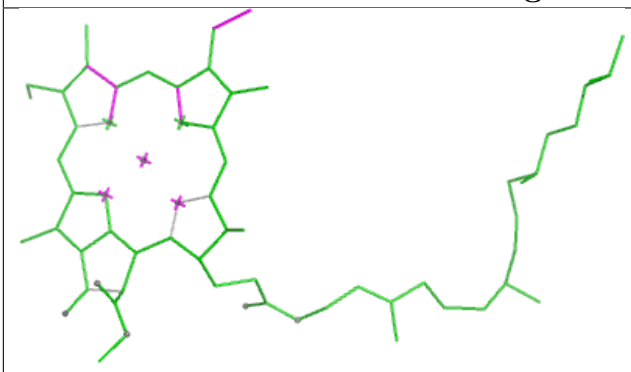
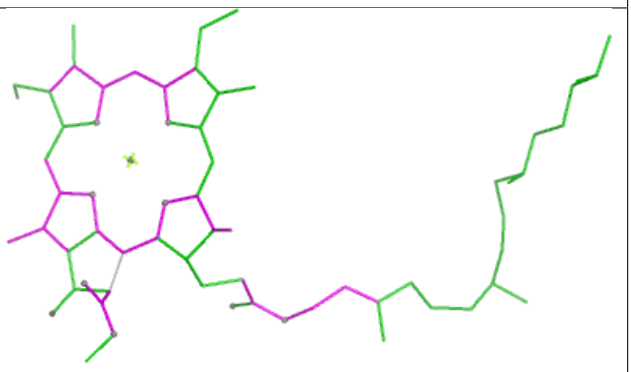
 Bond lengths	 Bond angles
 Torsions	Rings

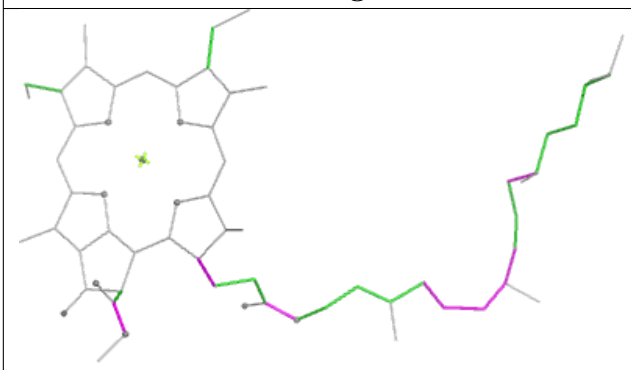
Ligand CLA B 827



Bond lengths



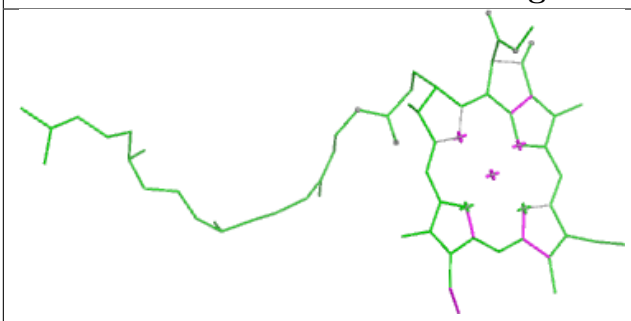
Bond angles



Torsions

Rings

Ligand CLA 3 322



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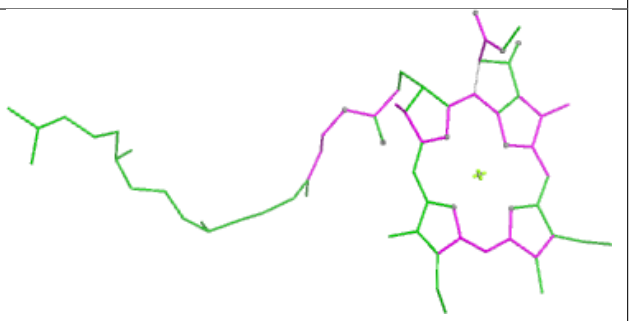
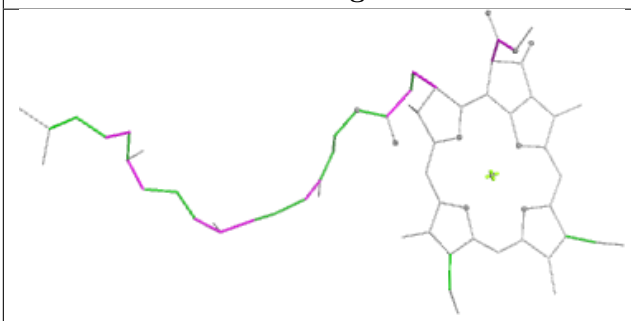


Bond angles



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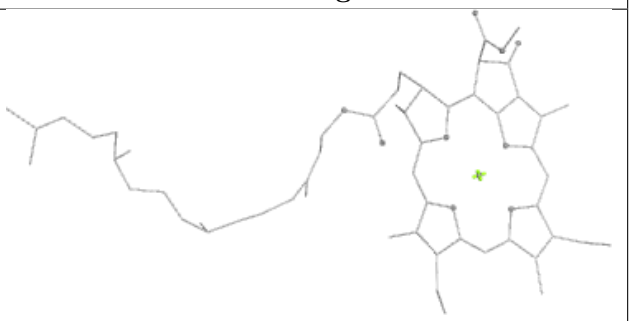
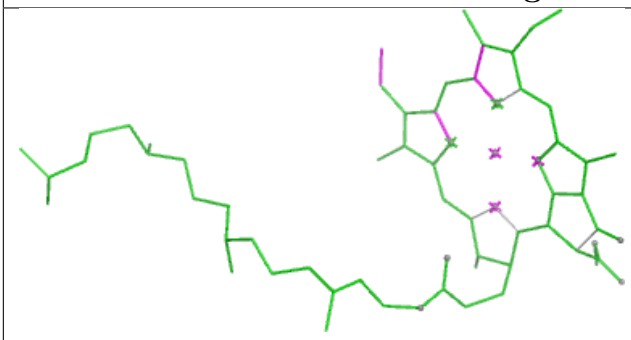
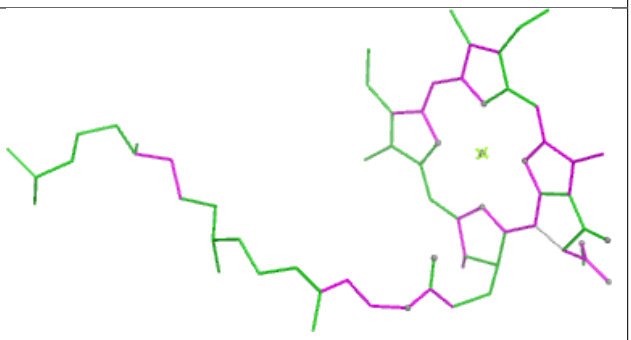
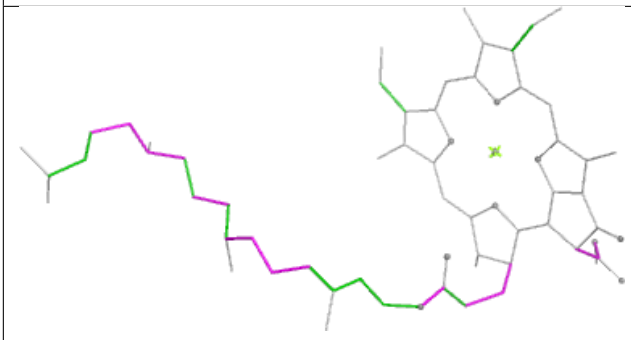
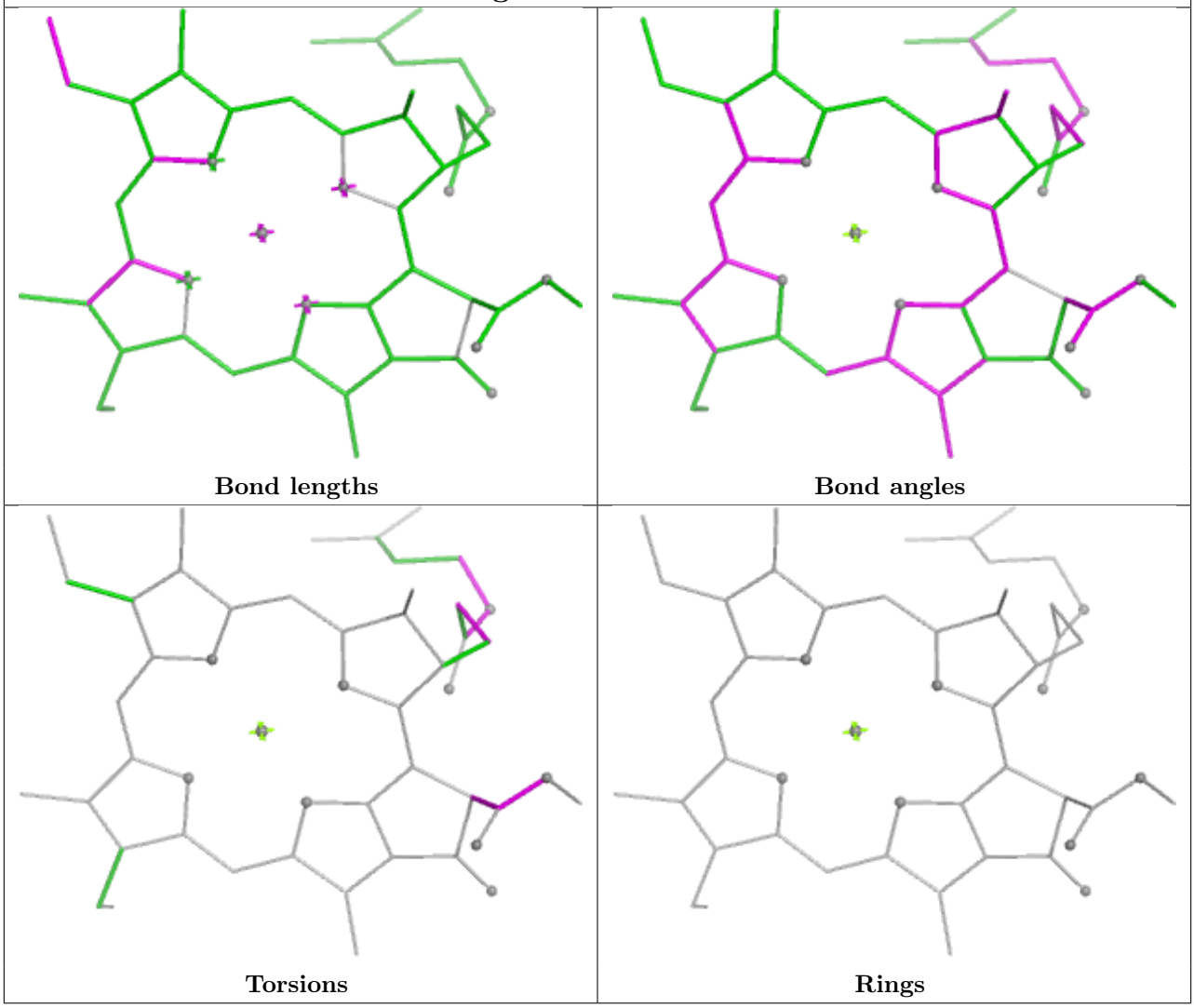


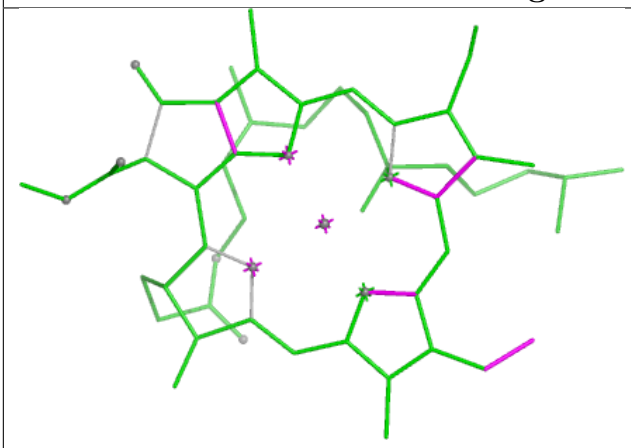
Rings

Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	Rings

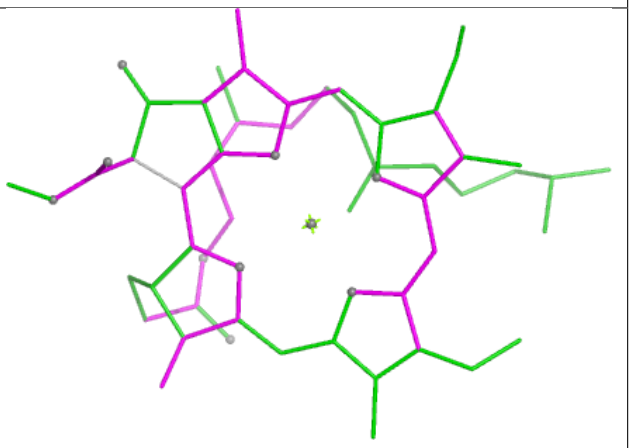
Ligand CLA 4 810



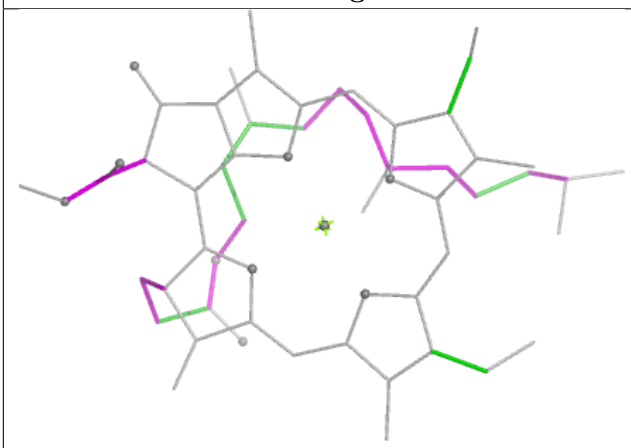
Ligand CLA 6 301



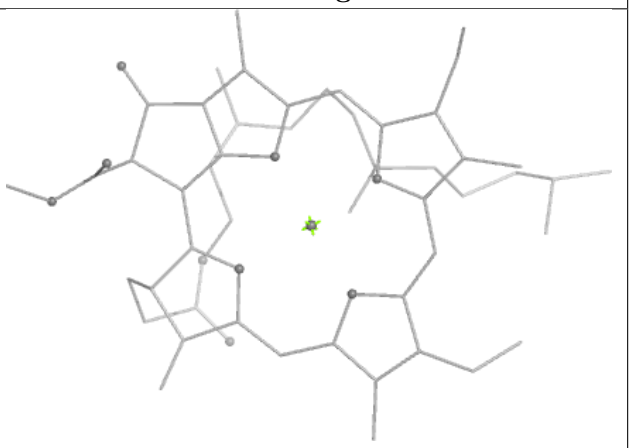
Bond lengths



Bond angles

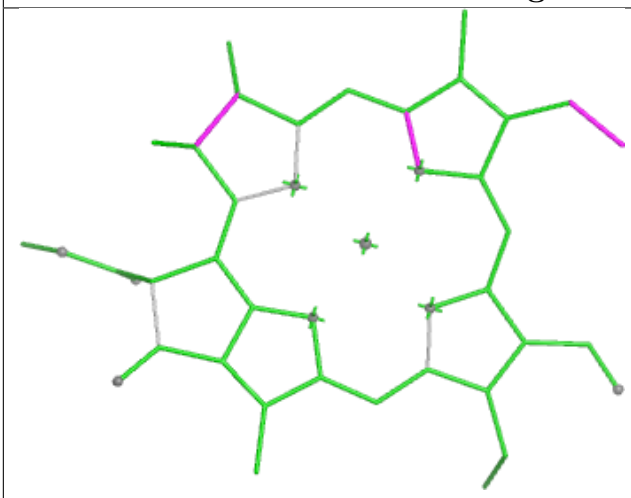


Torsions



Rings

Ligand CHL 9 314



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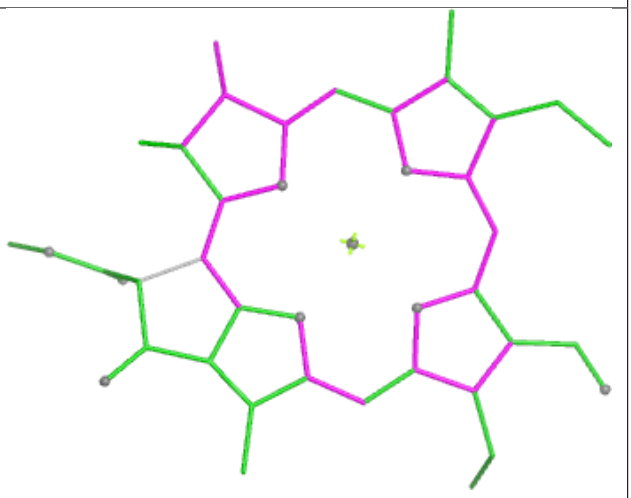

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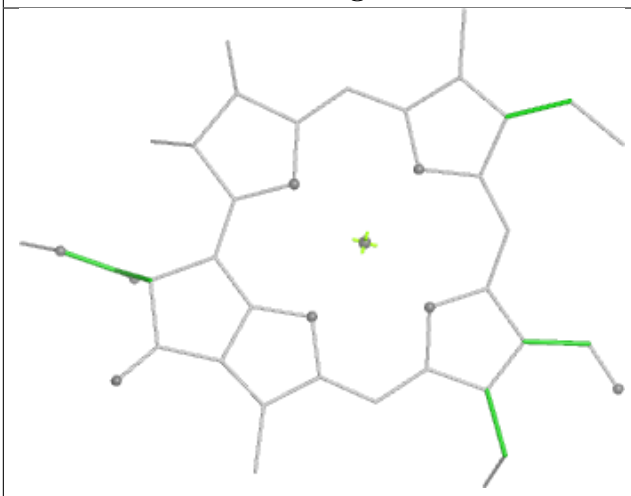

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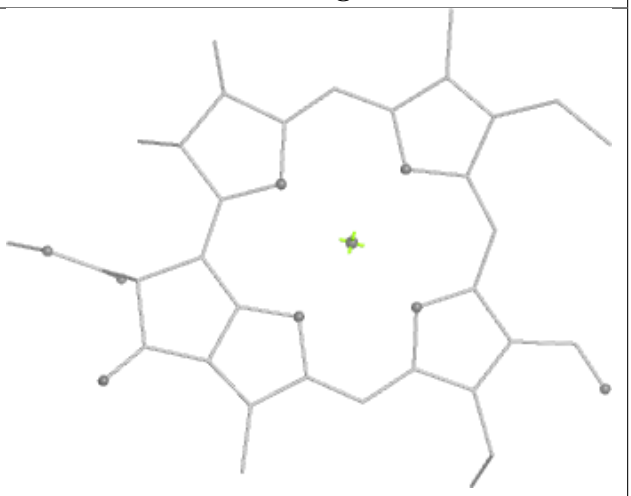
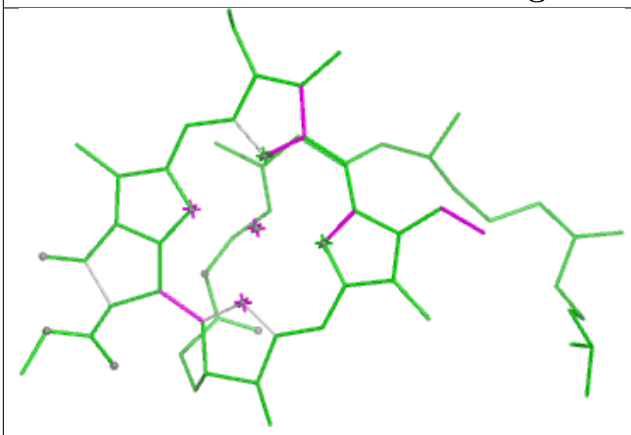


Rings

Ligand CLA 8 307



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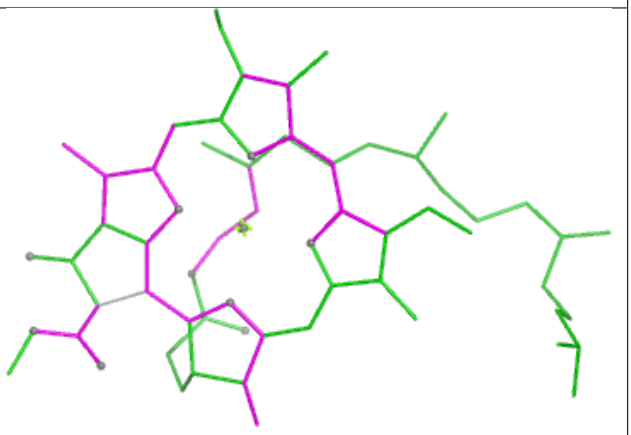
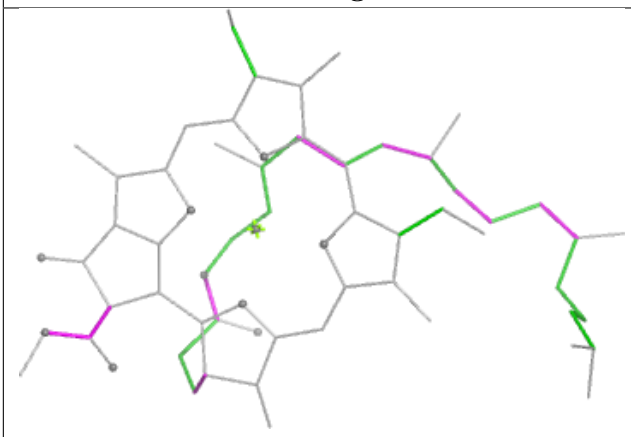


Bond angles



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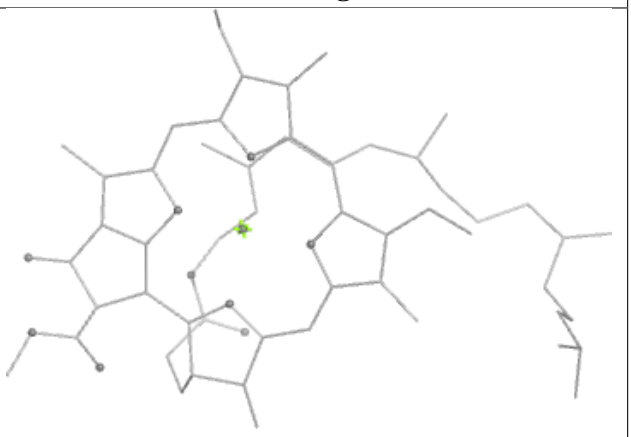
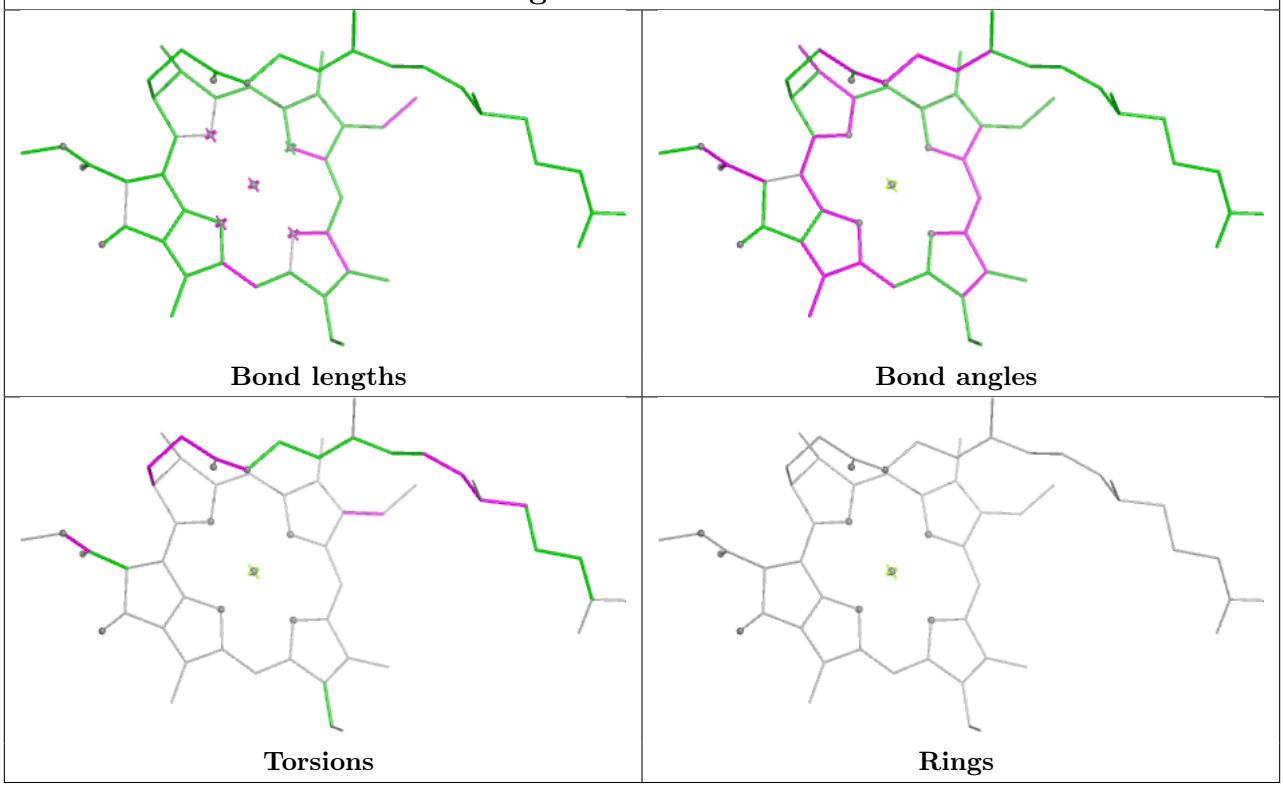
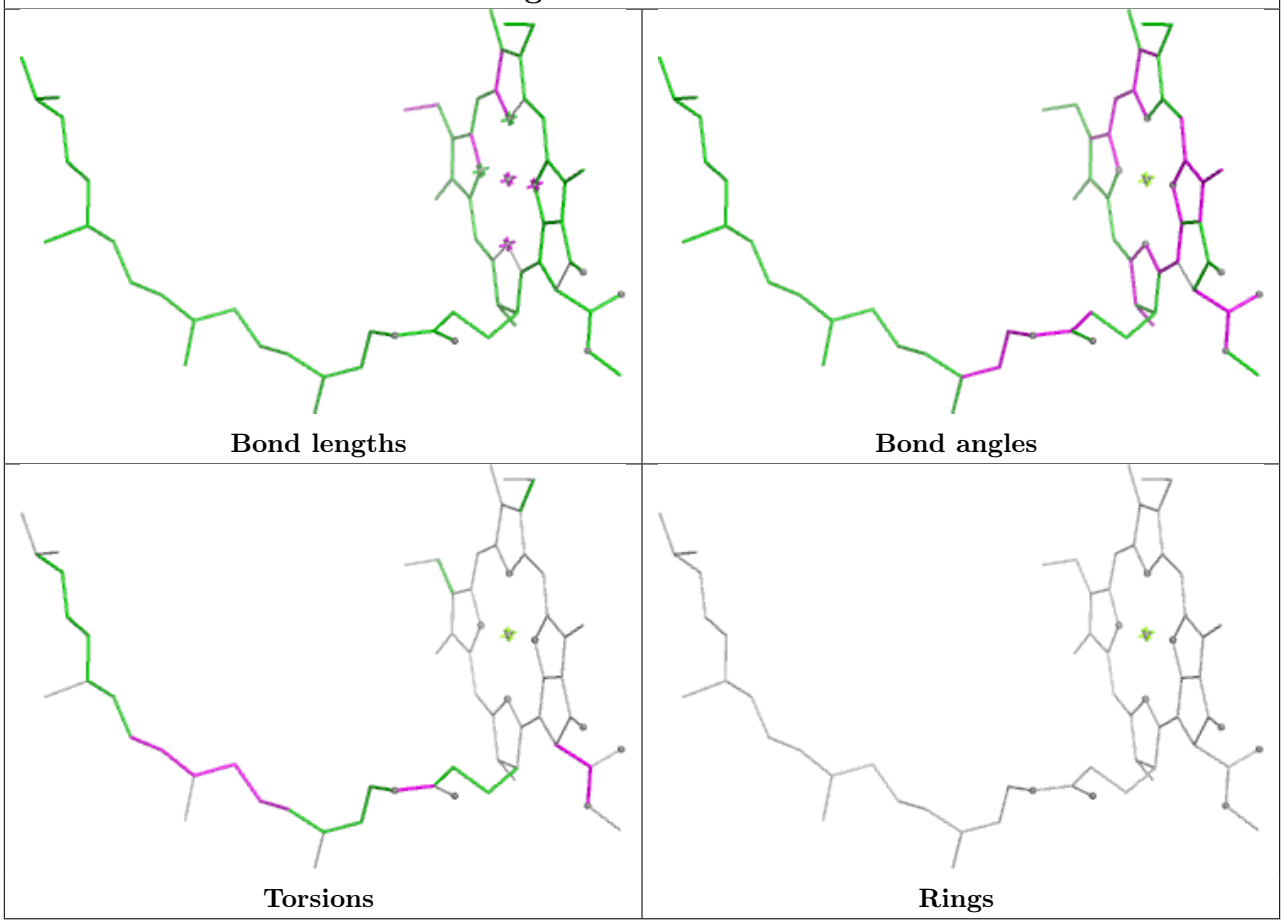


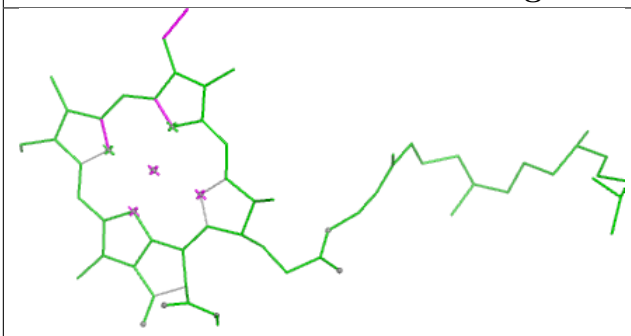
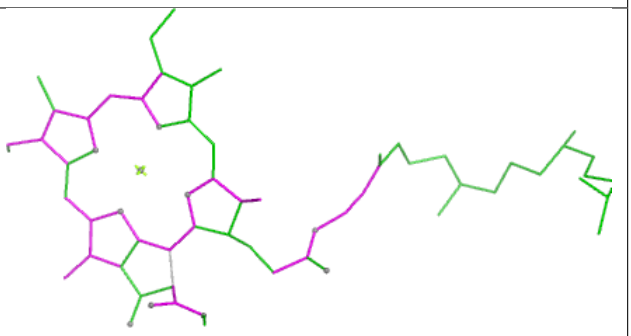
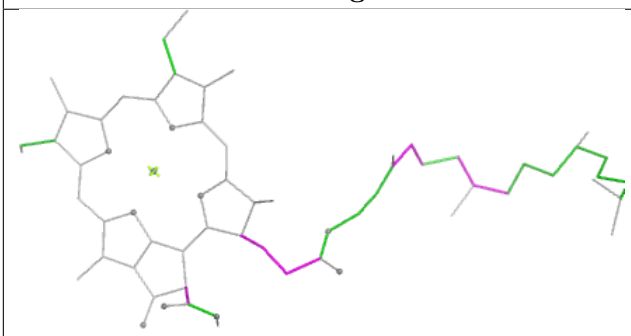
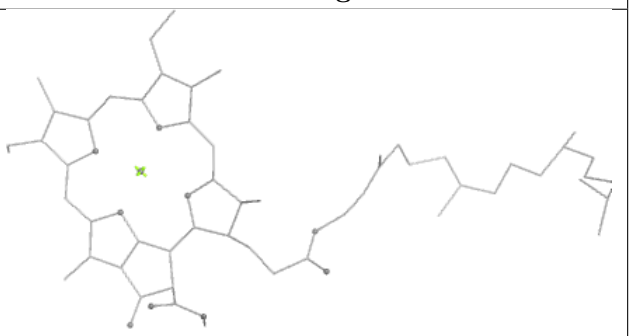
Rings

Ligand CLA 4 805

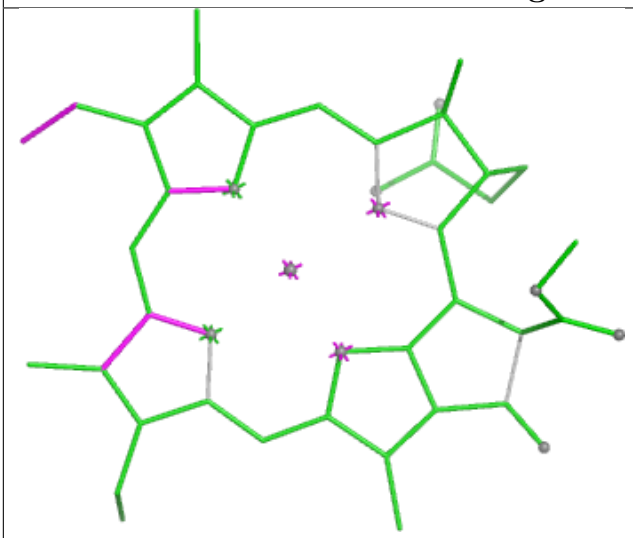


Ligand CLA A 835



Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 302



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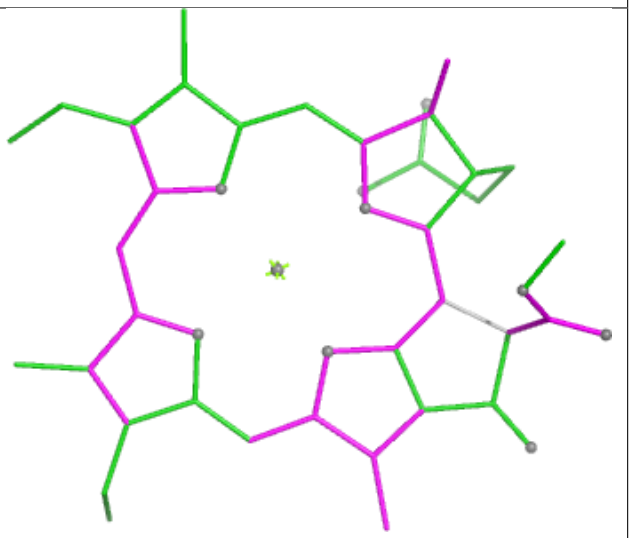
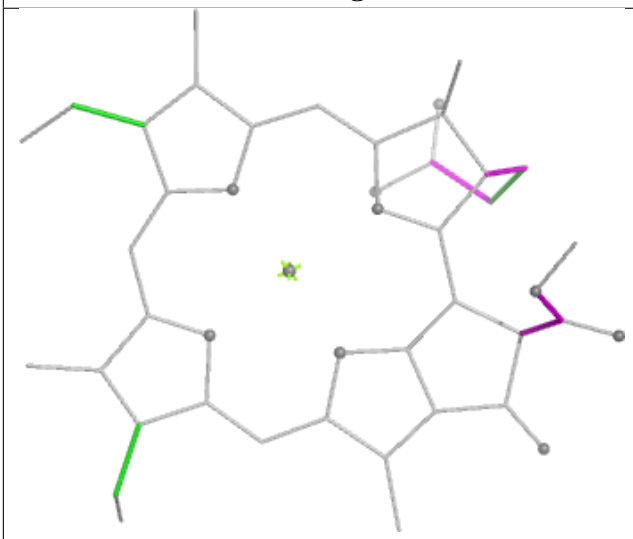


Bond angles



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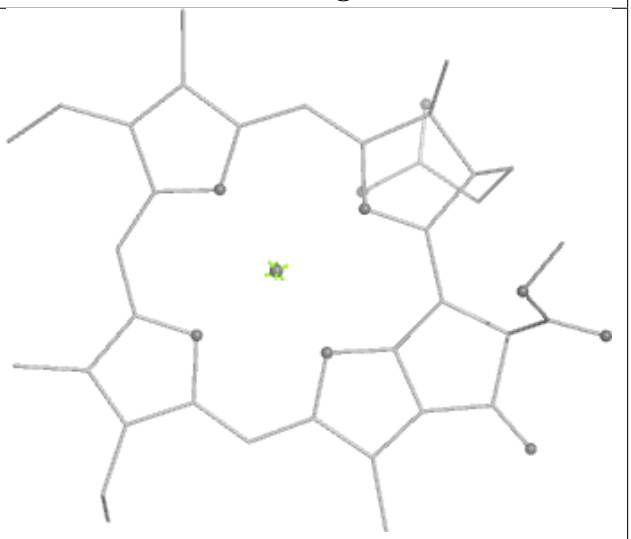
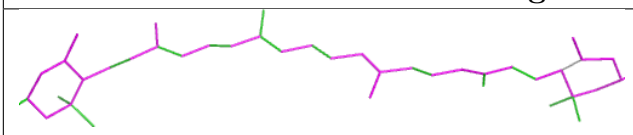


Rings

Ligand LUT 5 302



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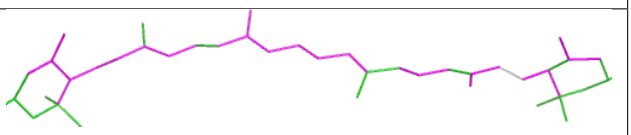
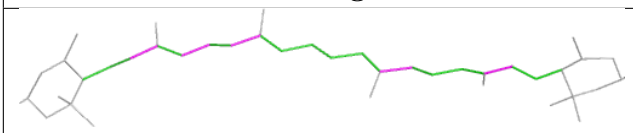


Bond angles



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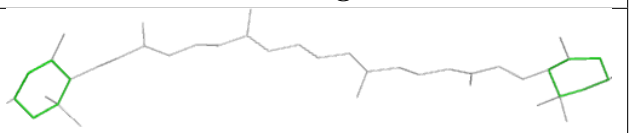
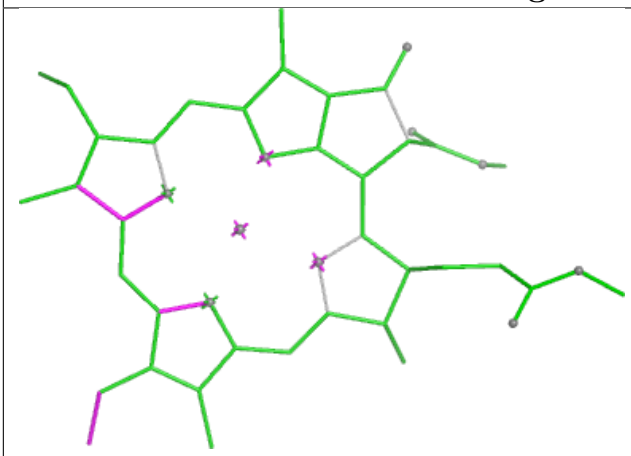
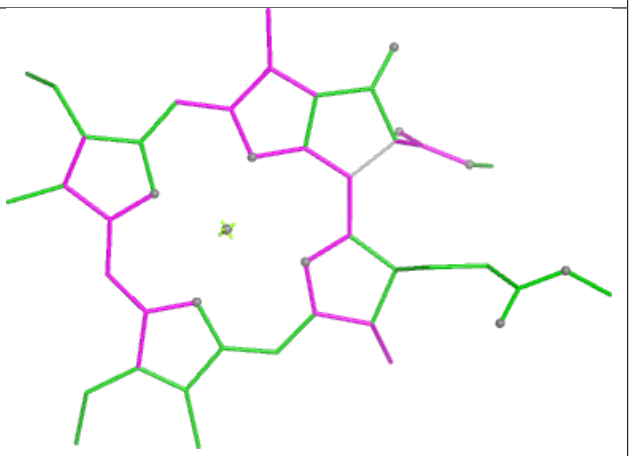


Rings

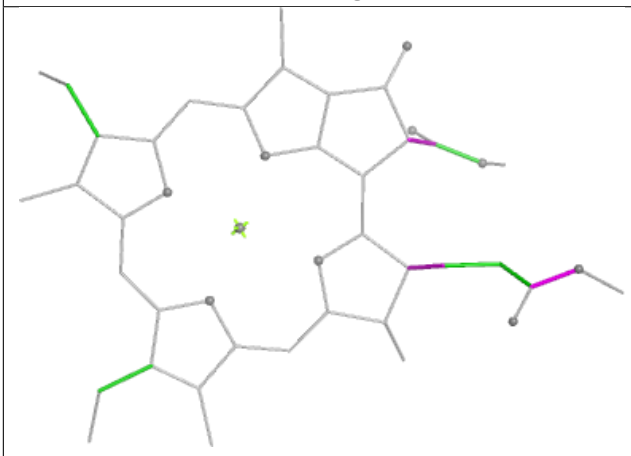
Ligand CLA 6 321



Bond lengths



Bond angles



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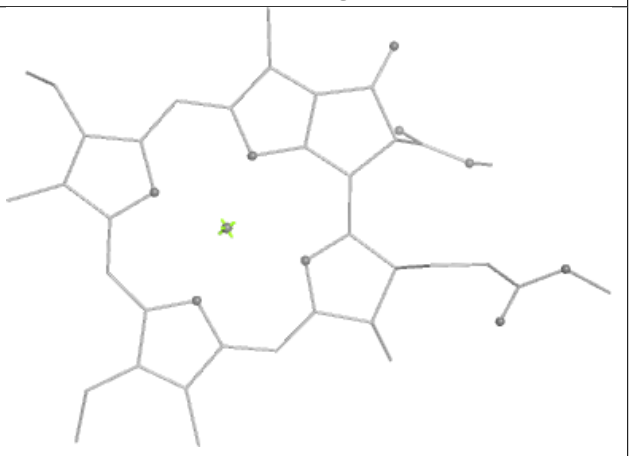
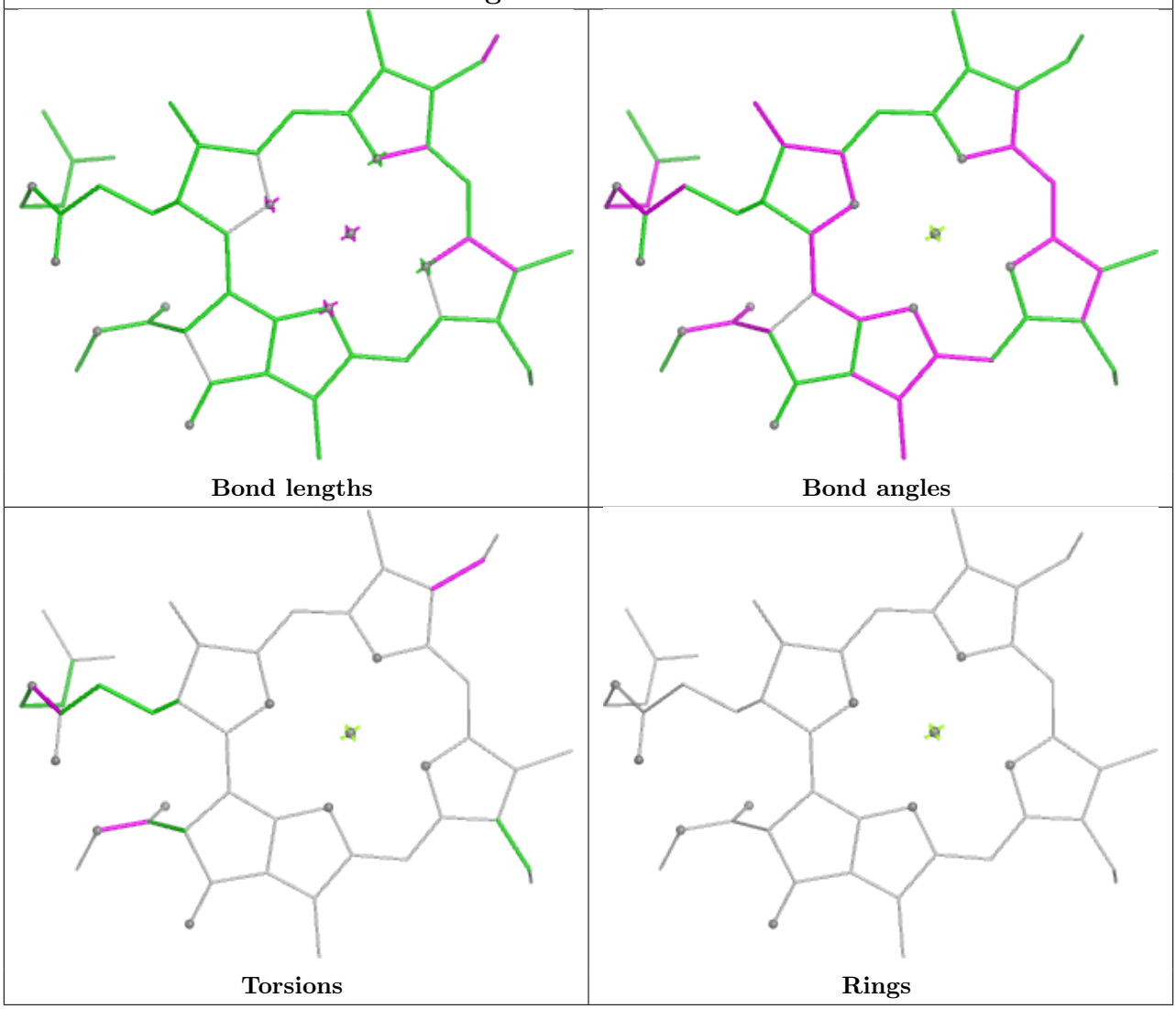
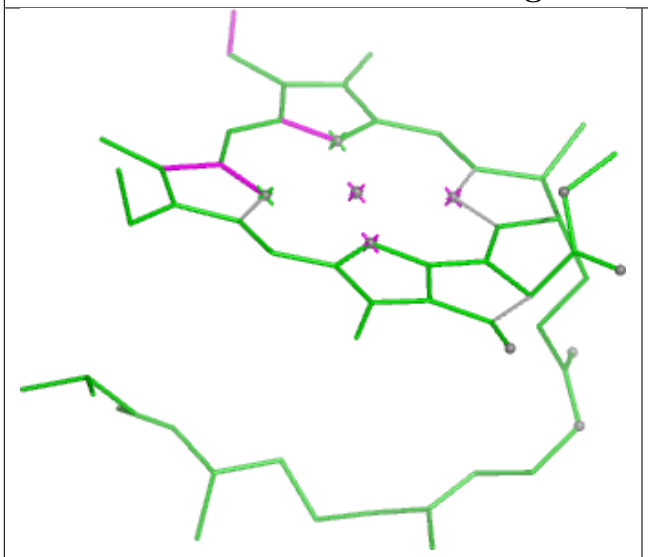


Rings

Ligand CLA 7 305



Ligand CLA A 814



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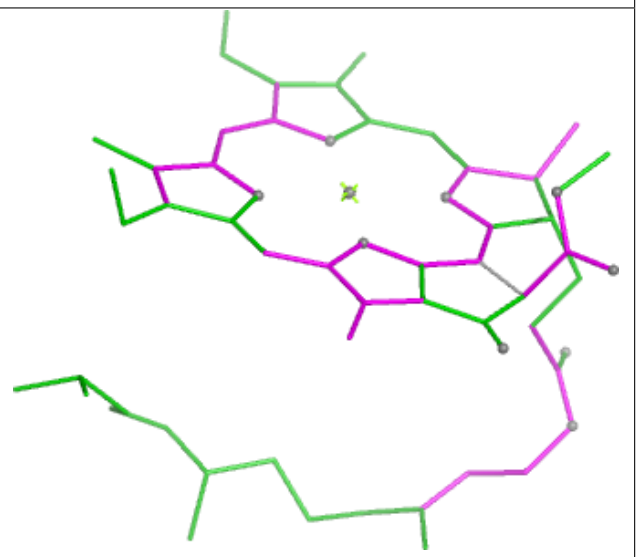
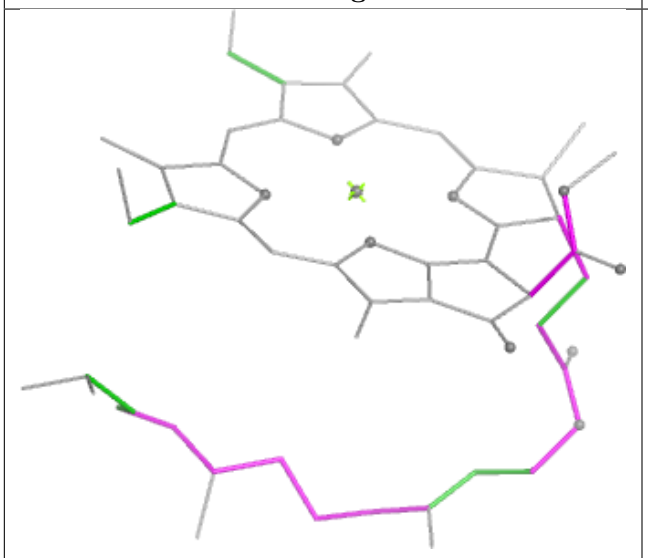


Bond angles



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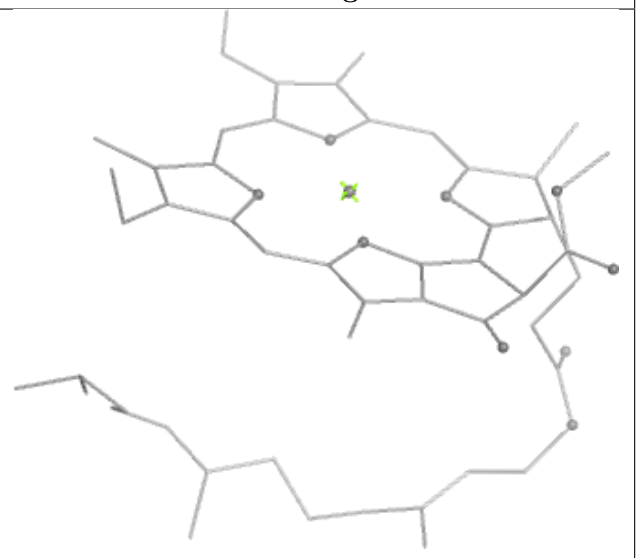
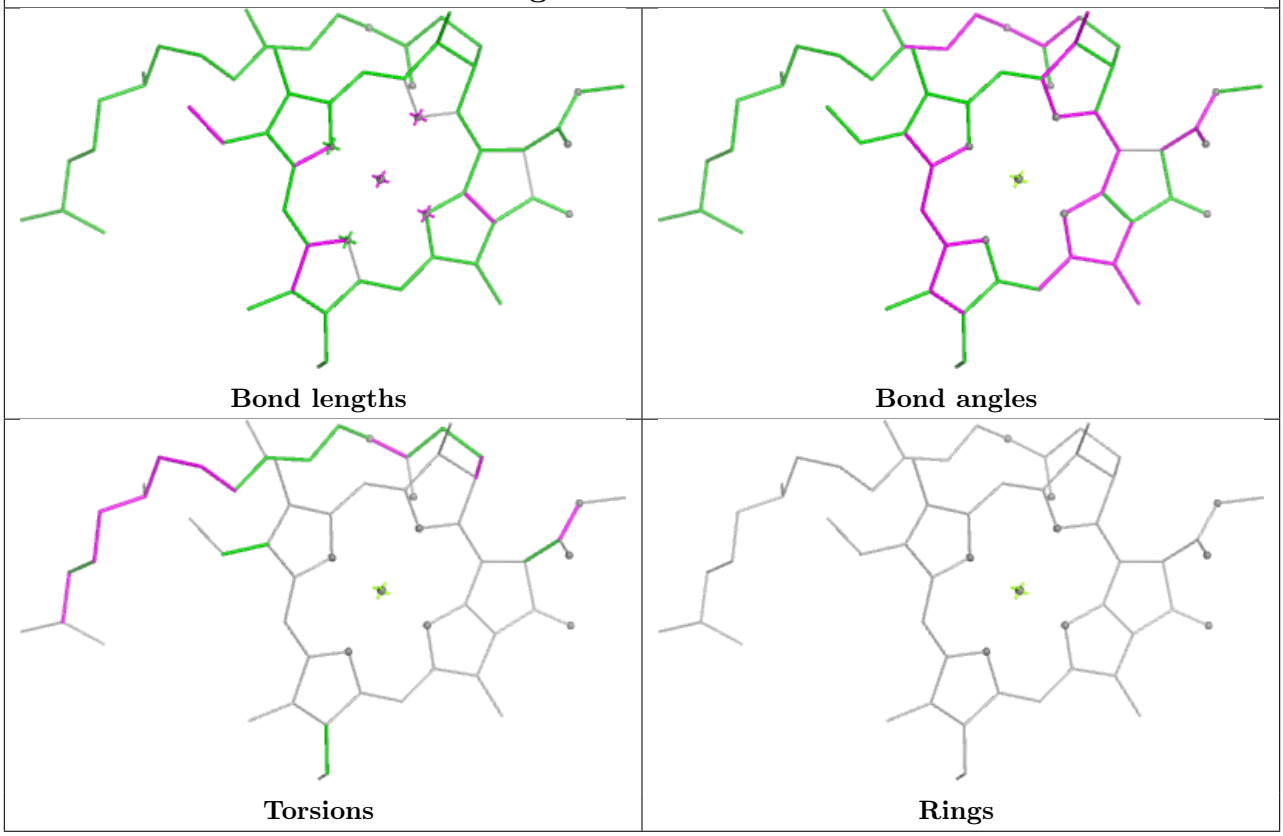
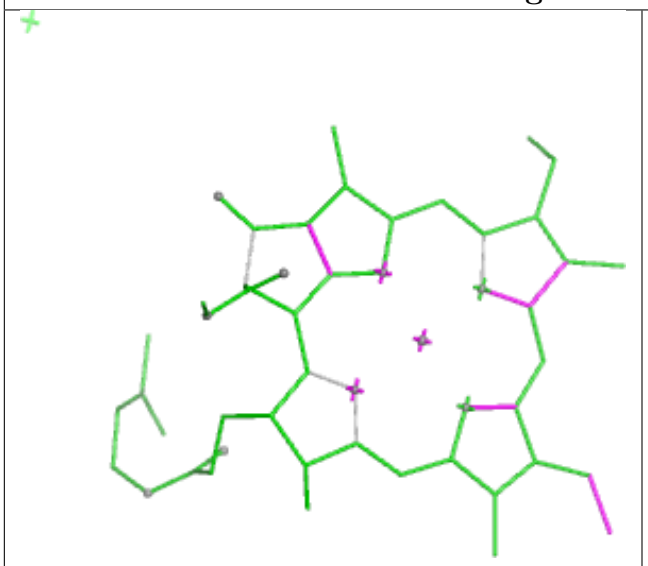


Rings

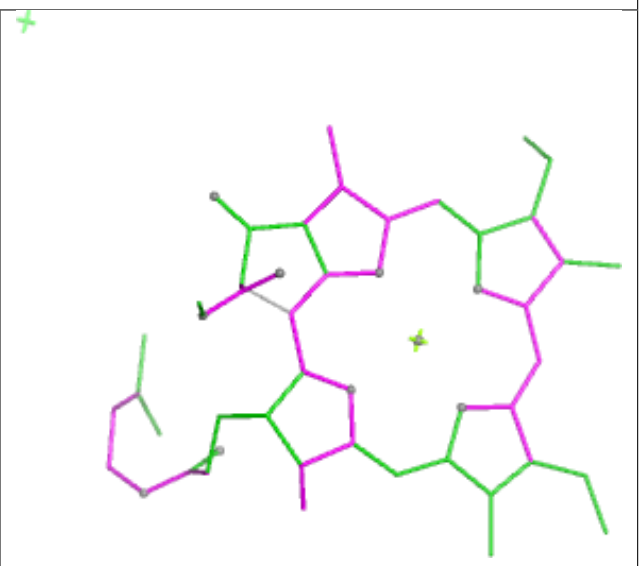
Ligand CLA 5 307



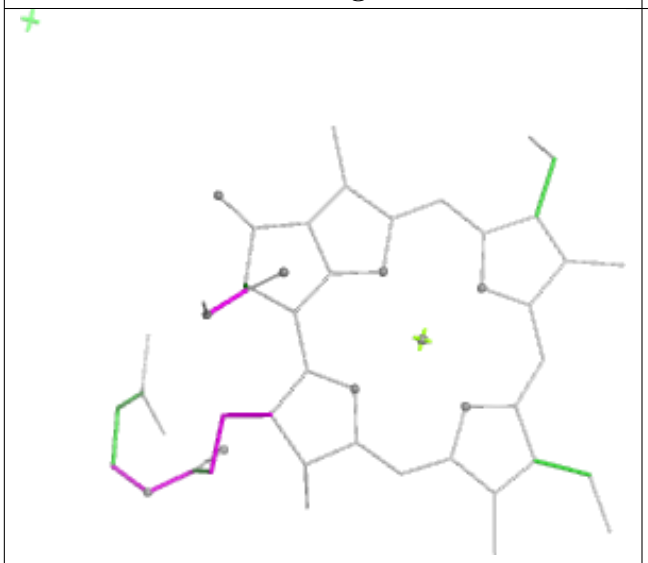
Ligand CLA B 835



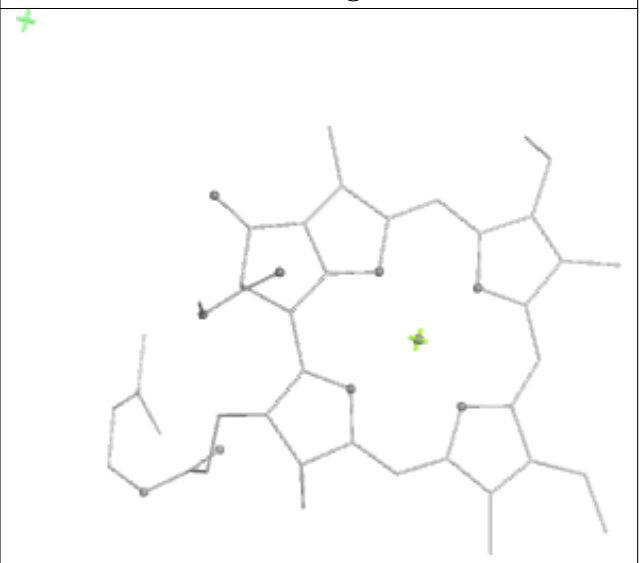
Bond lengths



Bond angles

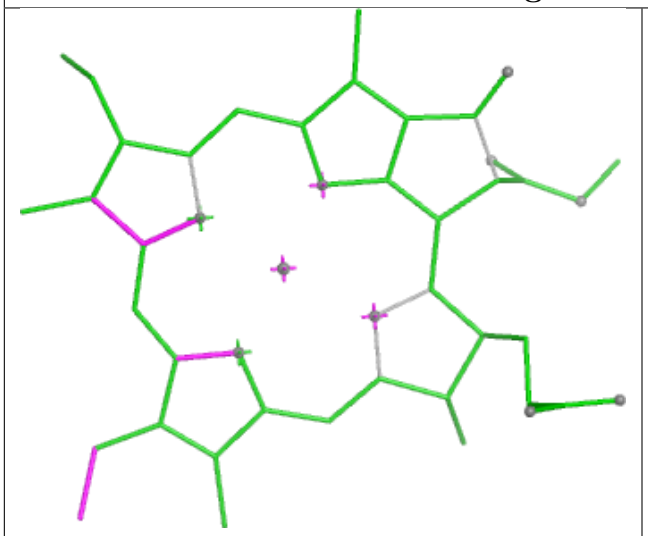


Torsions



Rings

Ligand CLA A 804



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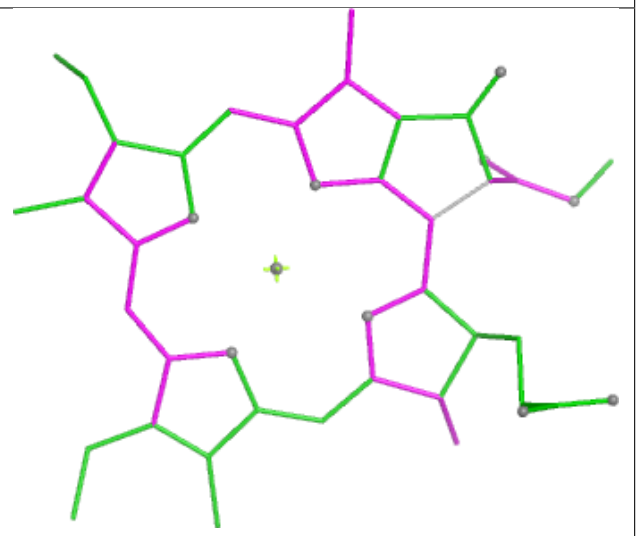

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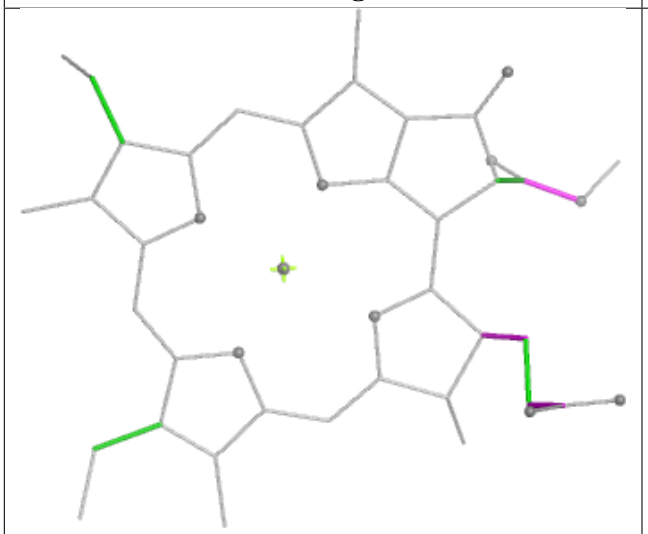

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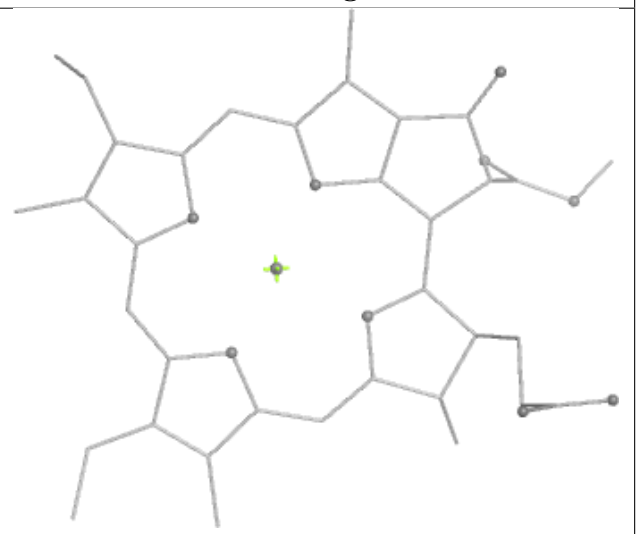
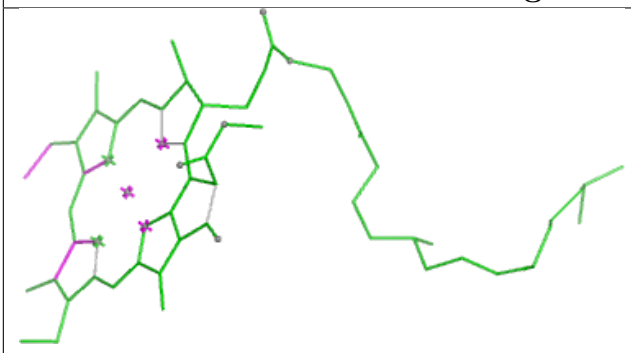


Rings

Ligand CLA B 805



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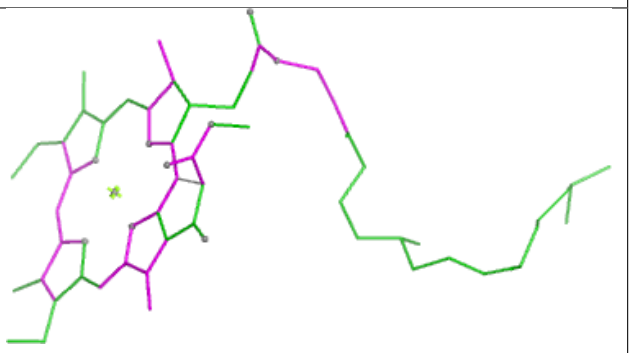
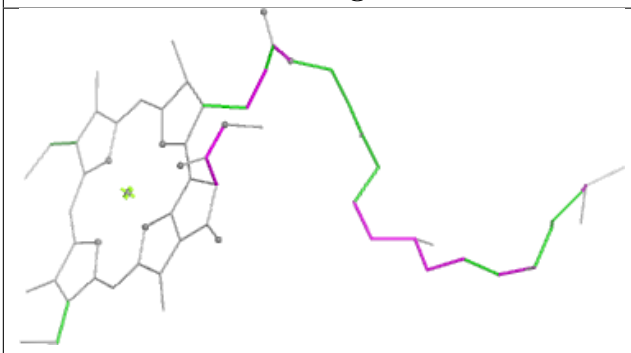


Bond angles



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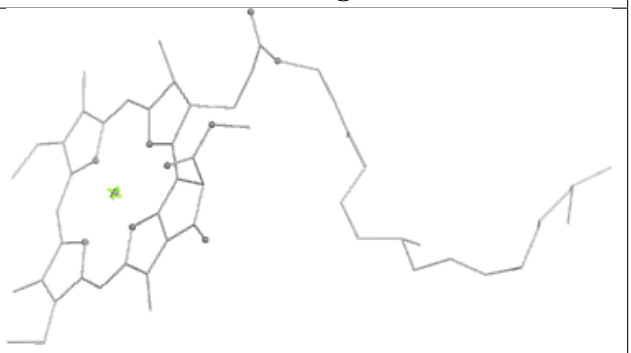
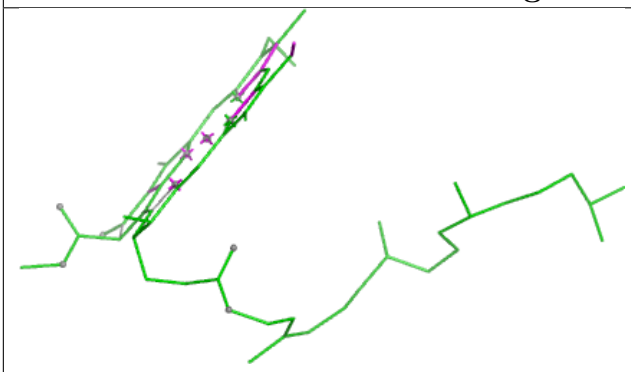


Rings

Ligand CLA A 810



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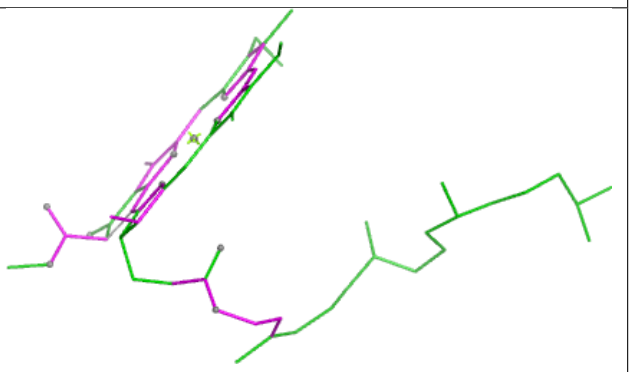

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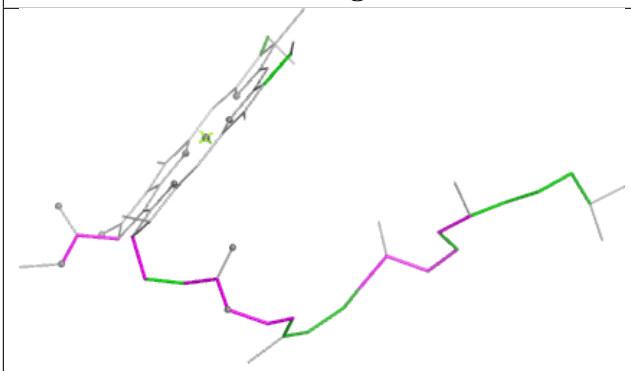
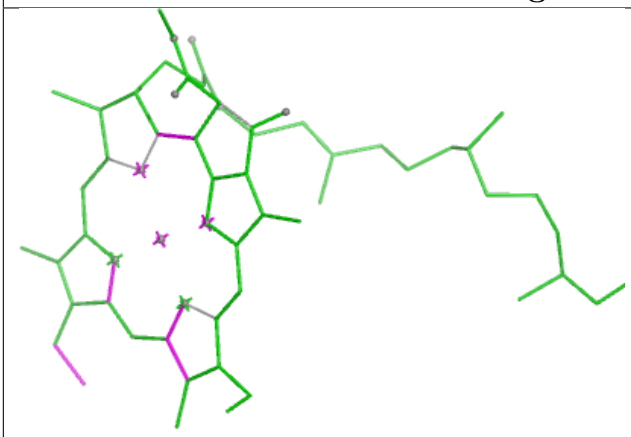
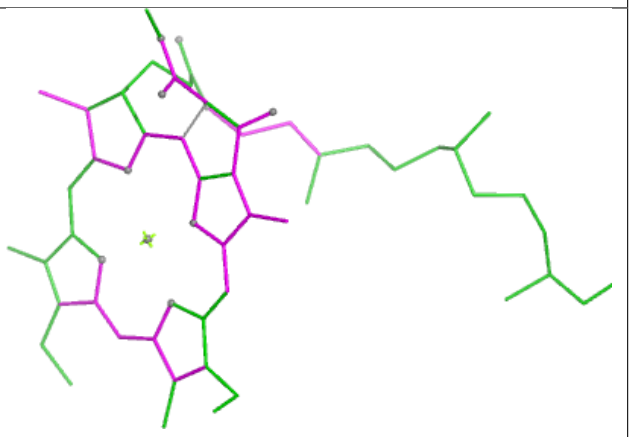
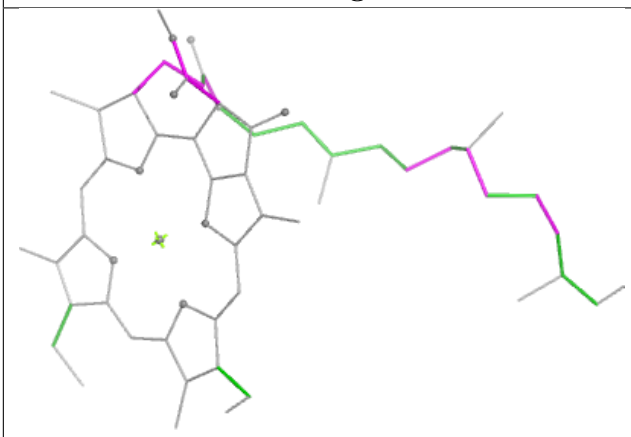
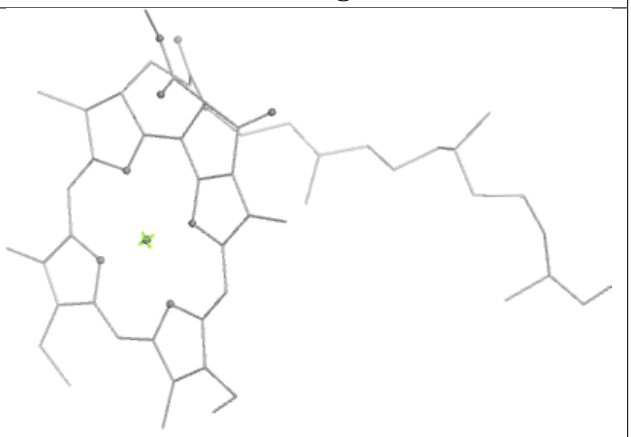
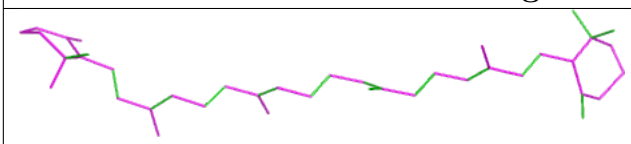
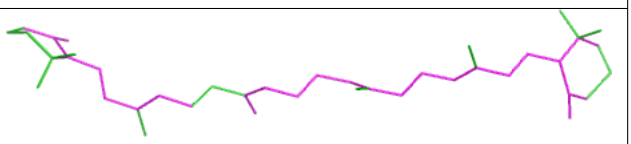
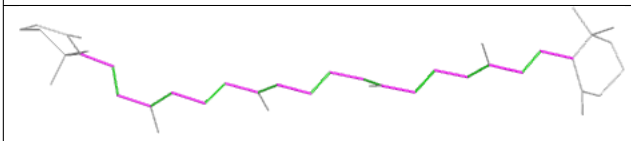
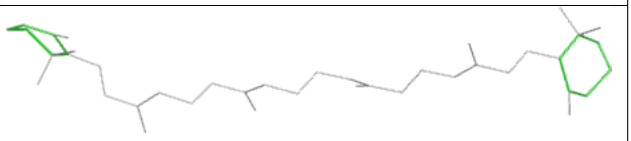


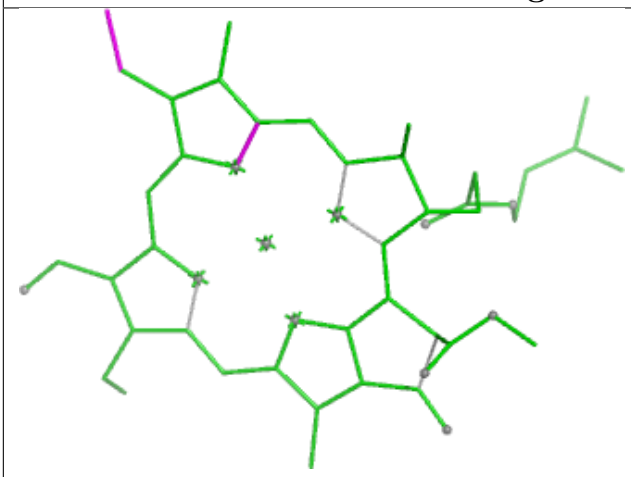
Torsions

Rings

Ligand CLA 5 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 4 814



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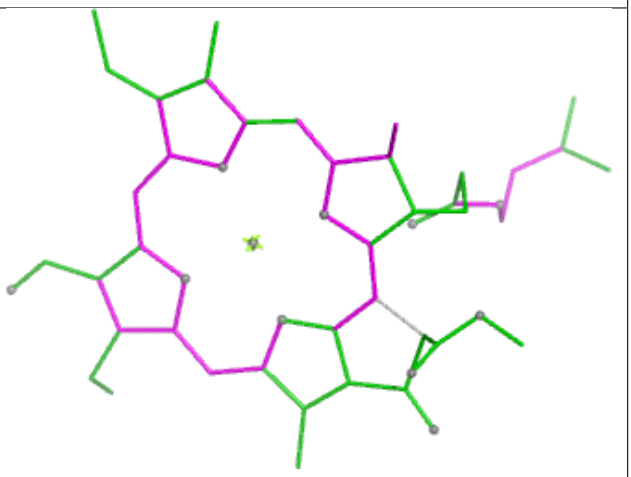
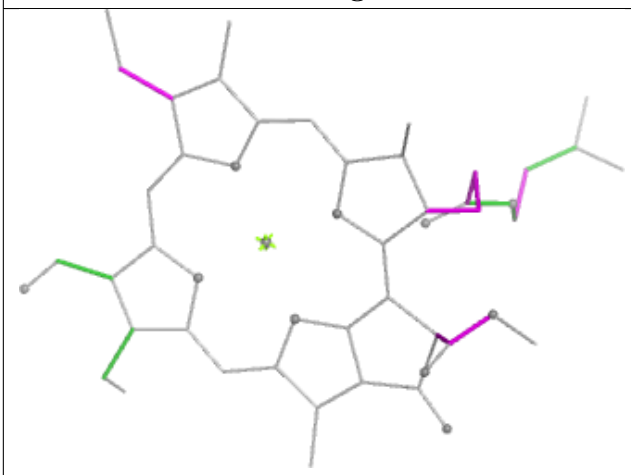


Bond angles



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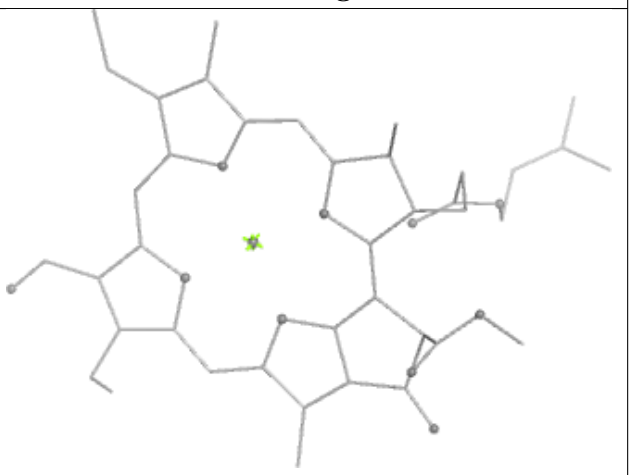
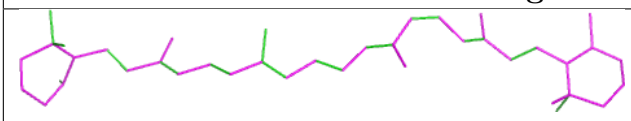


Rings

Ligand BCR 3 307



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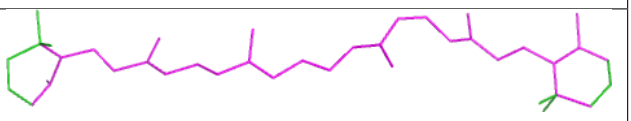
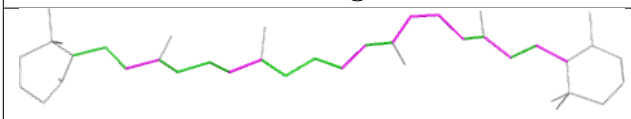
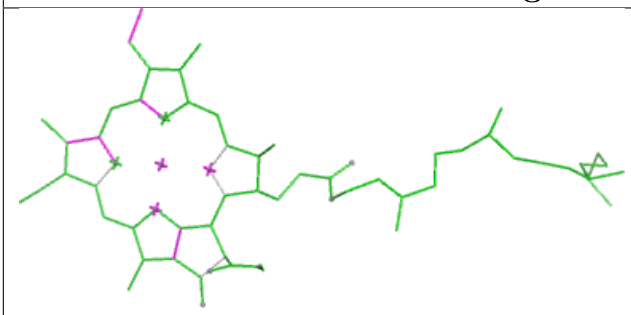
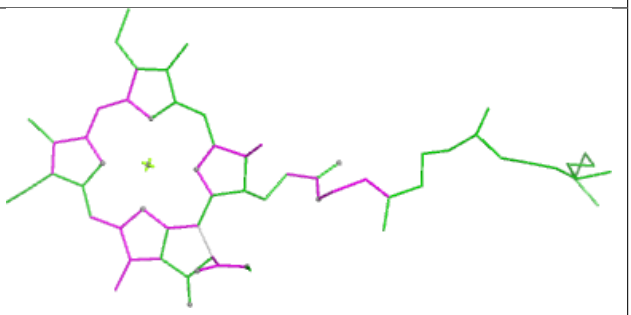


Bond angles



Torsions

Rings

Ligand CLA A 805	
	
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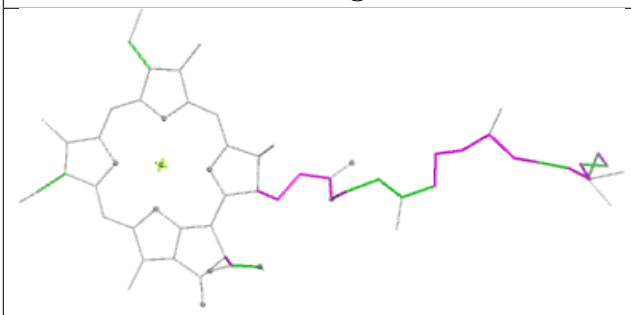
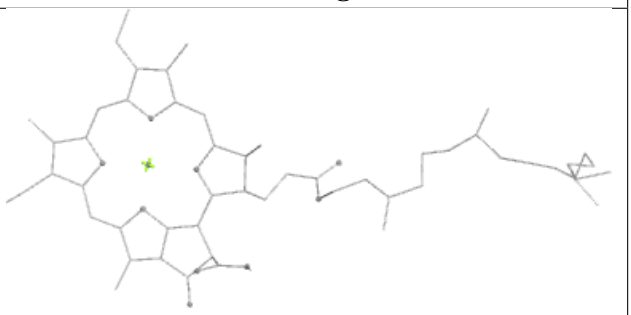
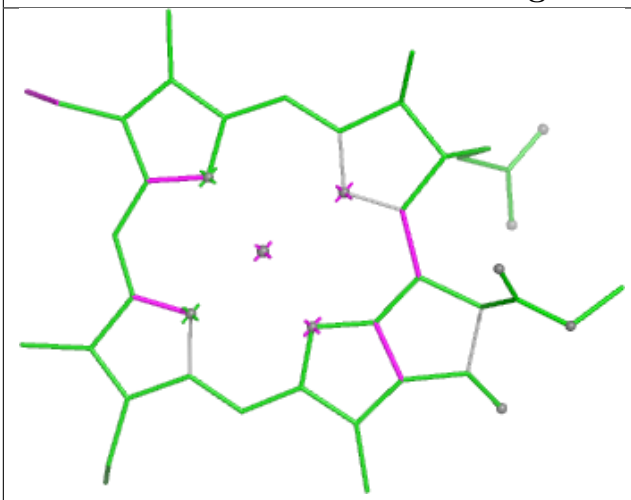
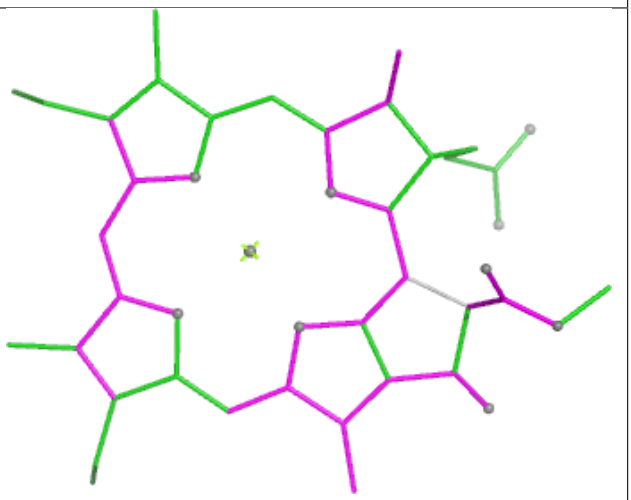
	
Torsions	**Rings**

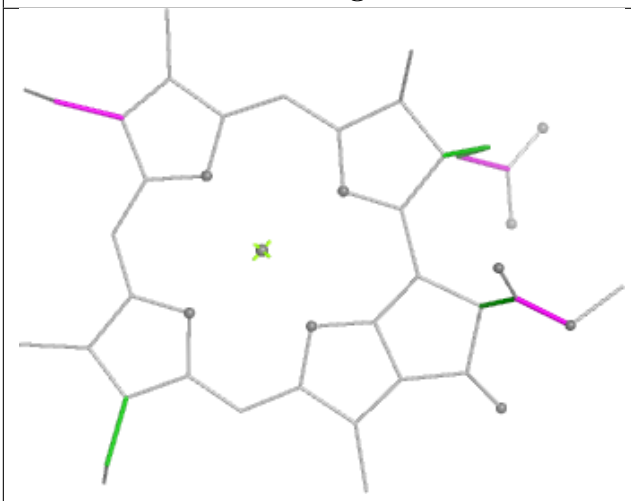
Ligand CLA 9 310



Bond lengths



Bond angles



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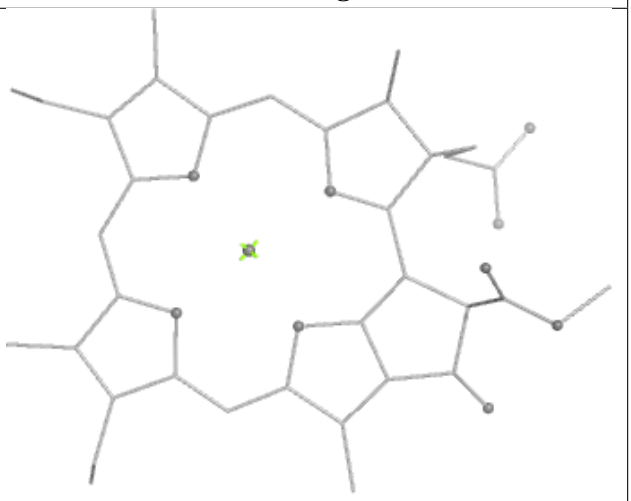
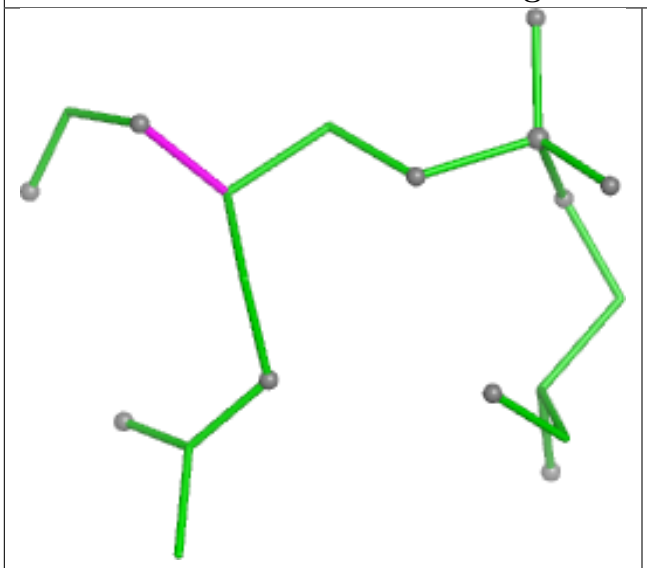


Rings

Ligand LHG B 851



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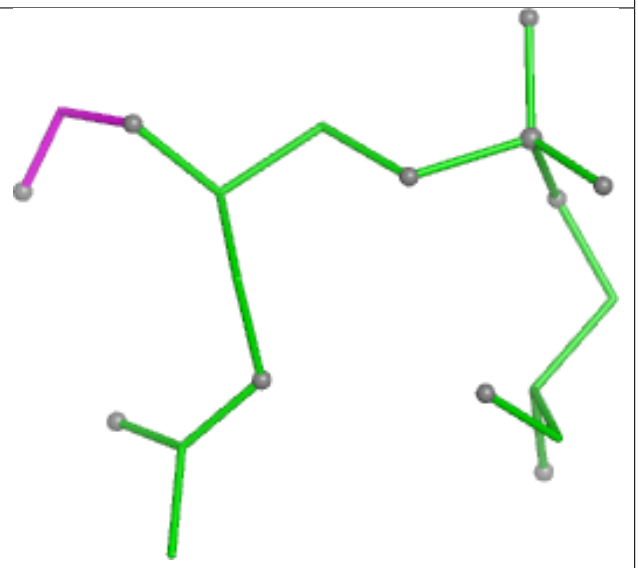
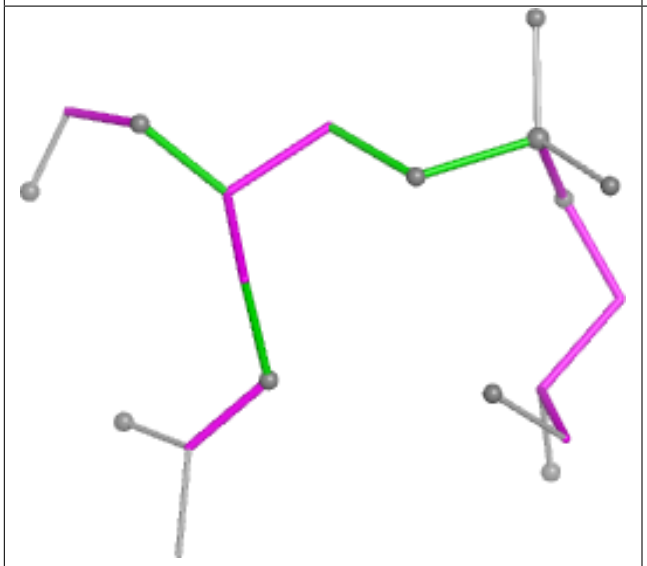


Bond angles



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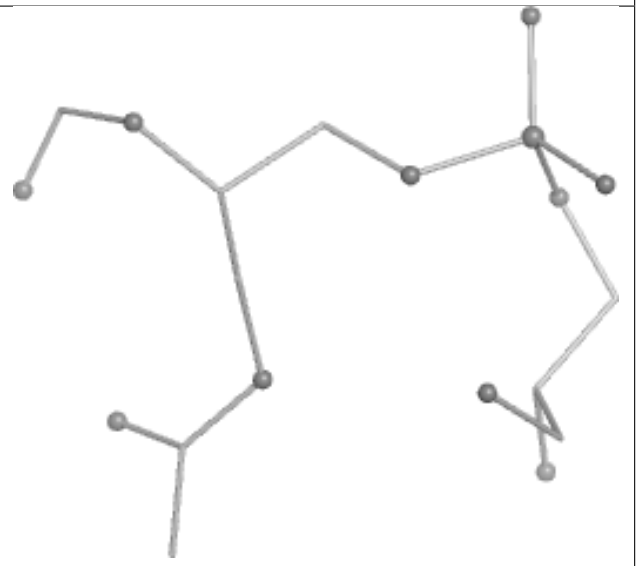
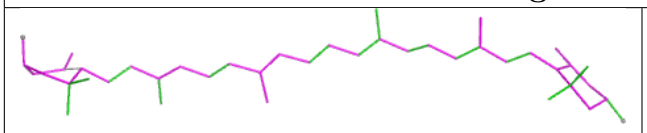


Rings

Ligand LUT 8 302



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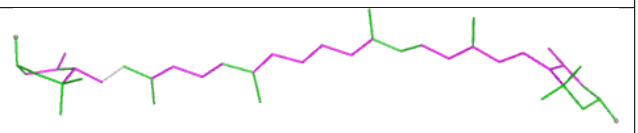
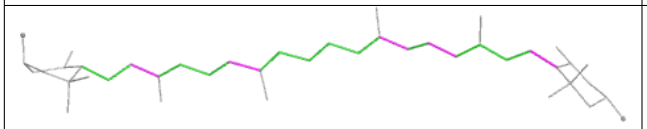


Bond angles



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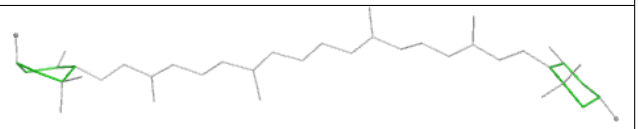
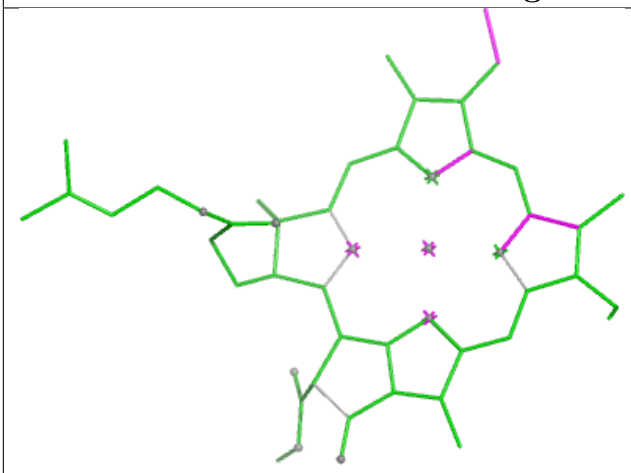
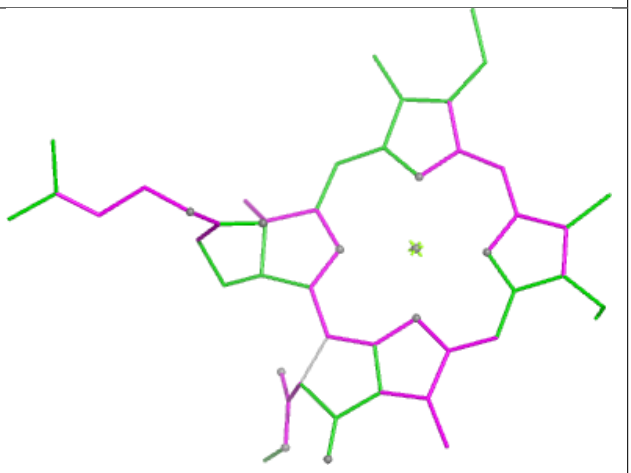


Rings

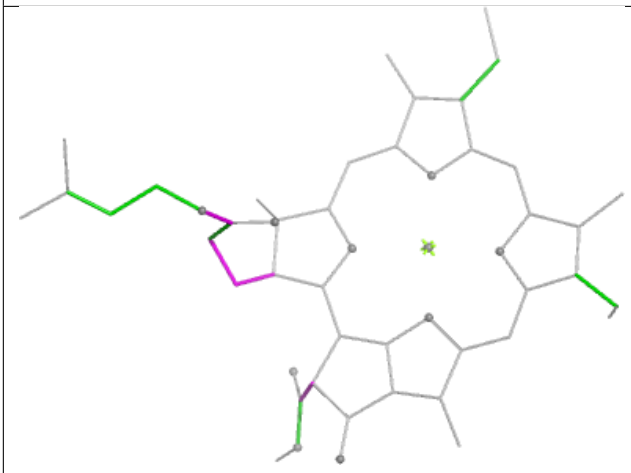
Ligand CLA A 826



Bond lengths



Bond angles



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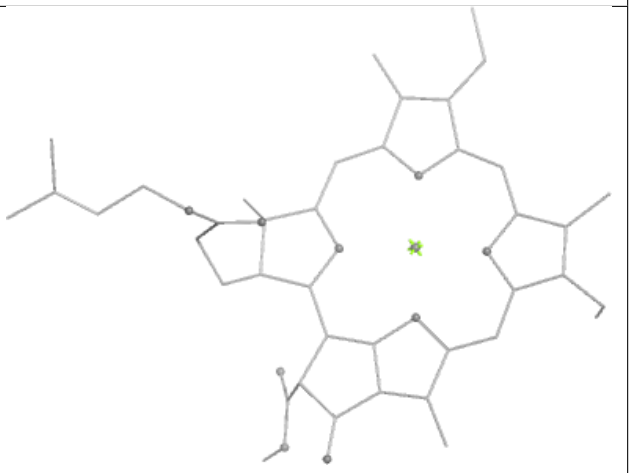
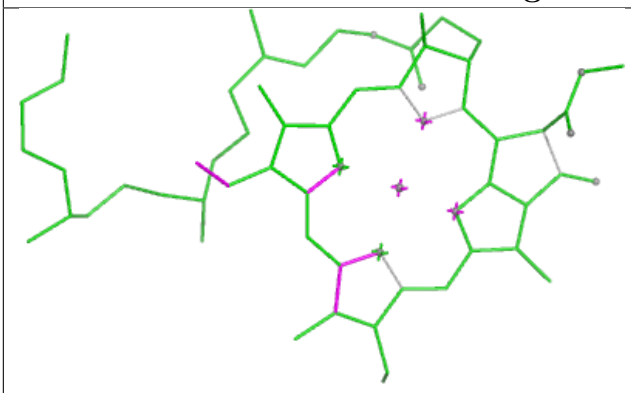
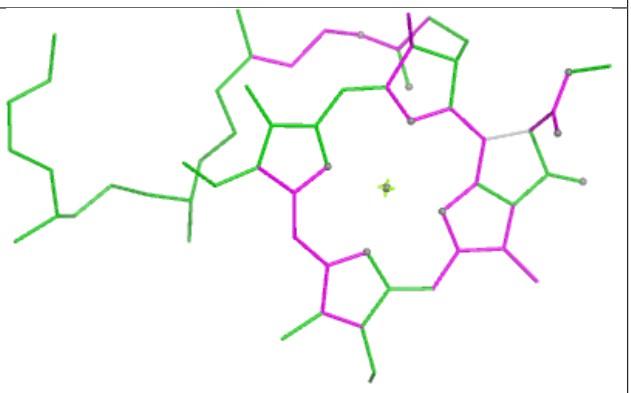
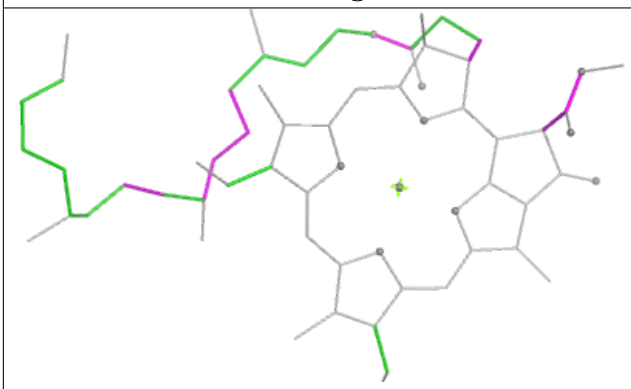
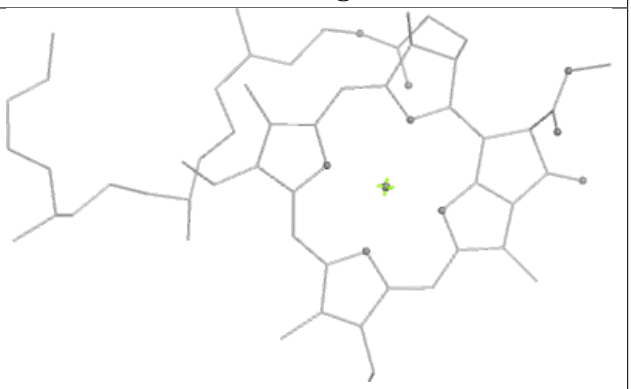
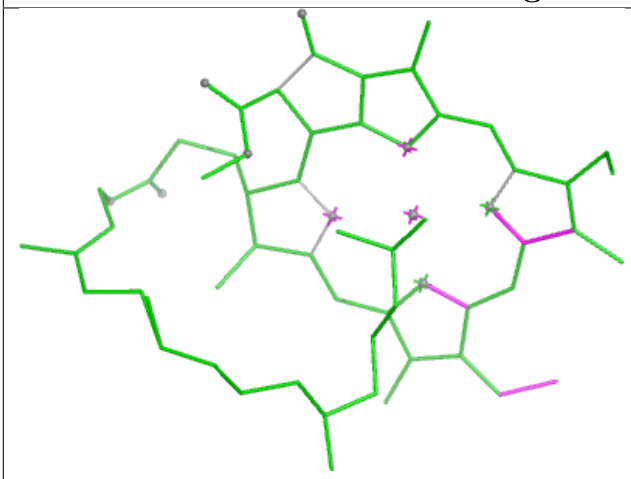


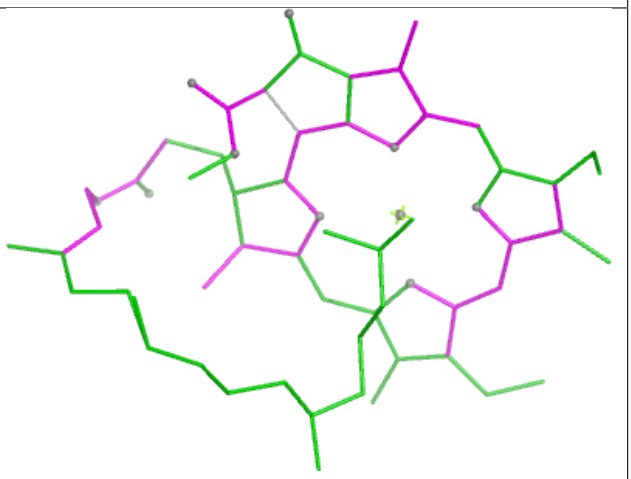
Rings

Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

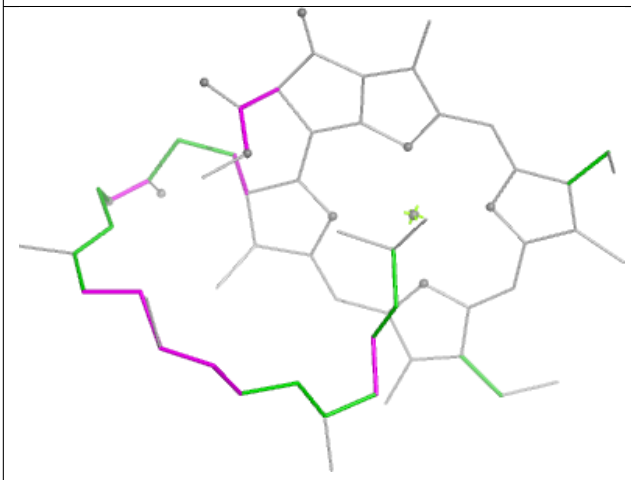
Ligand CLA A 806



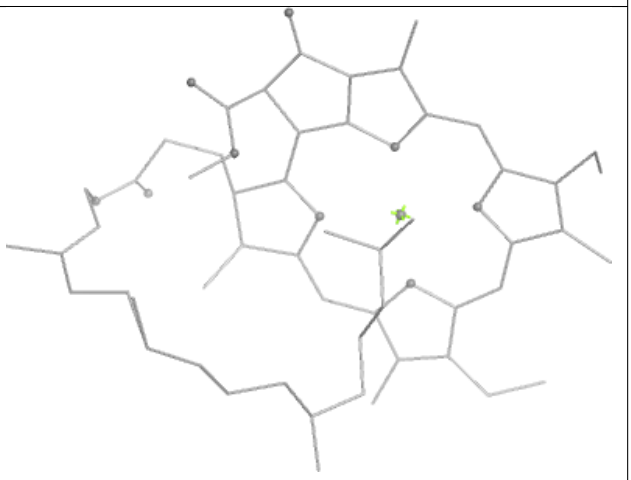
Bond lengths



Bond angles

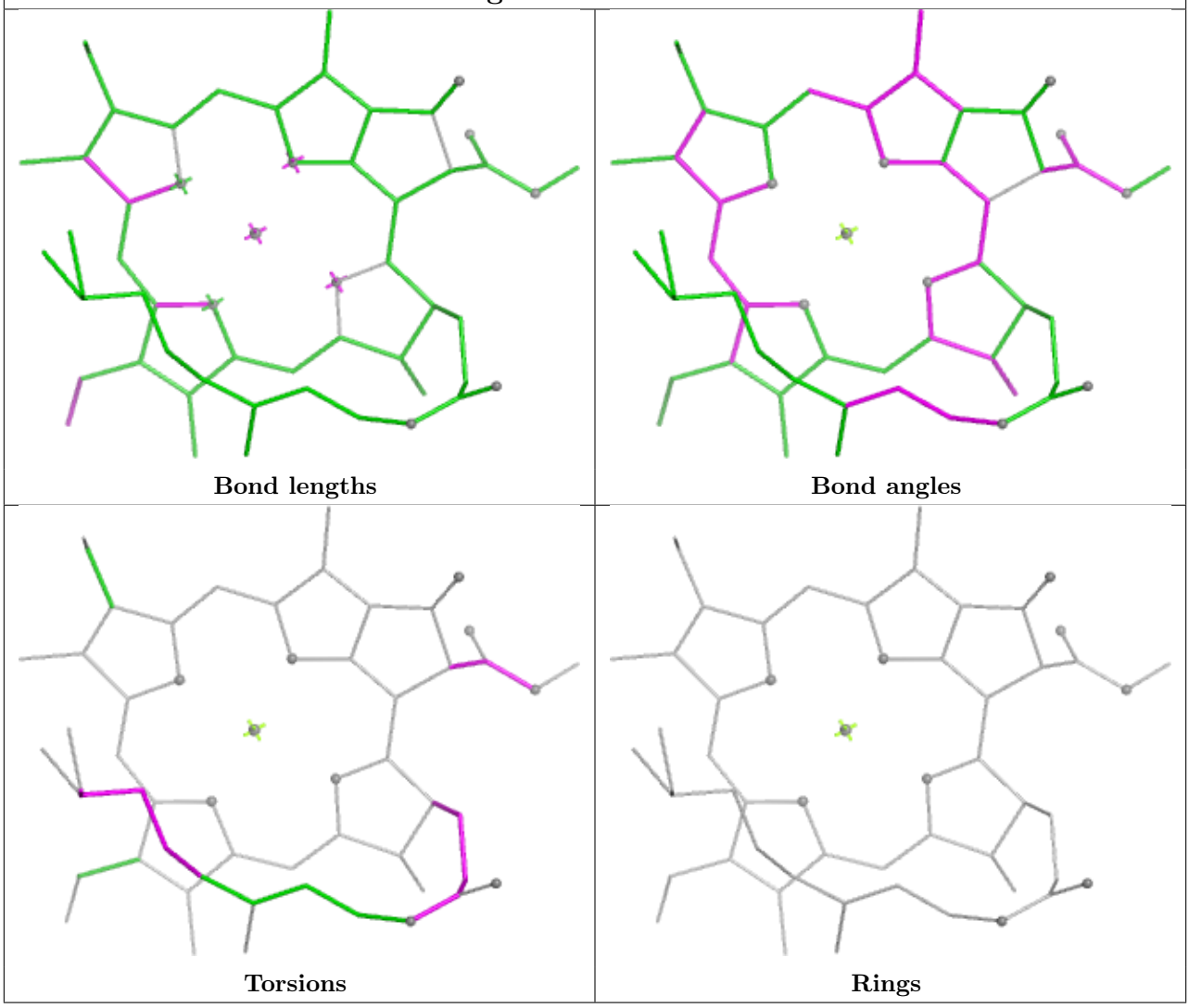


Torsions

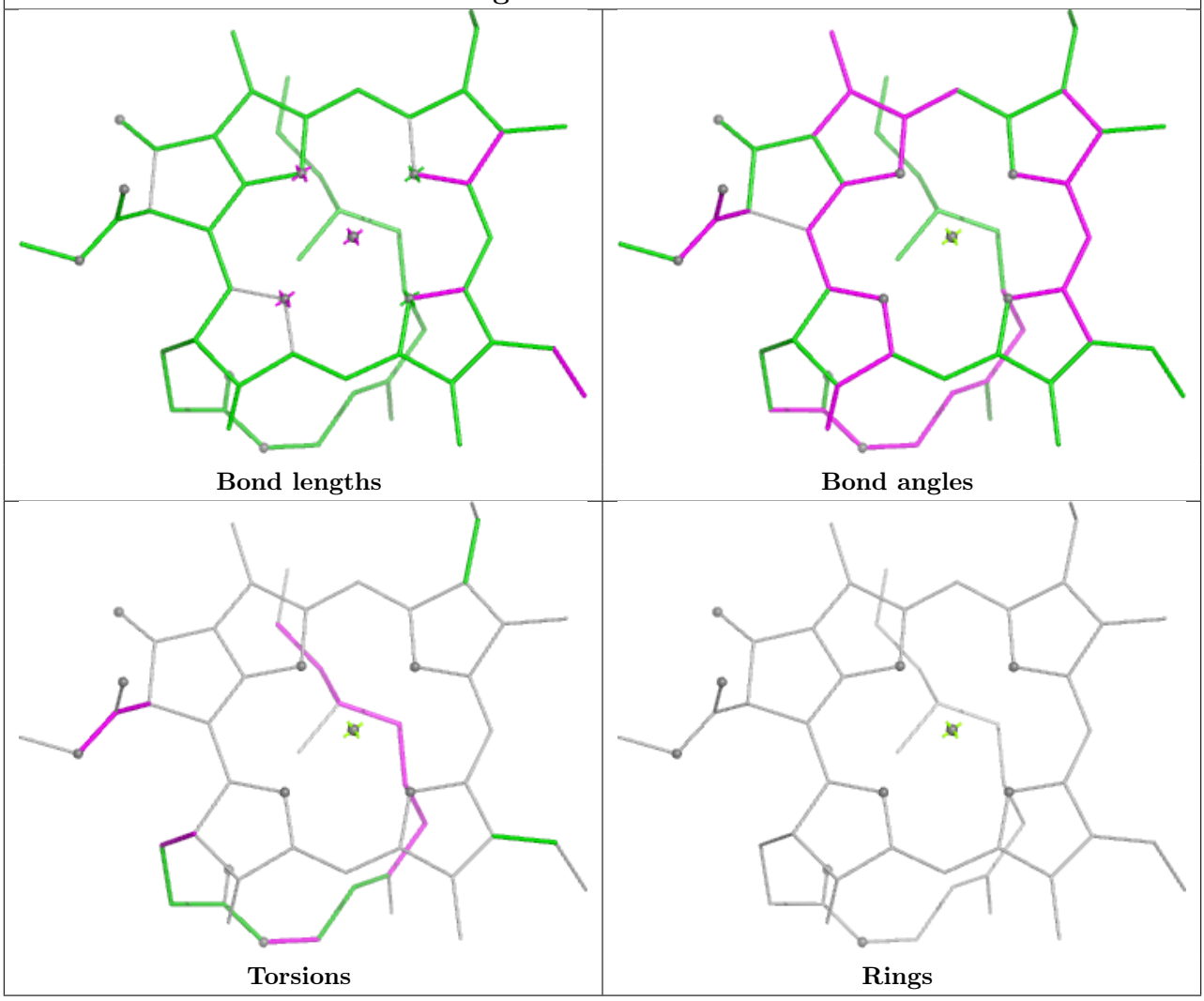


Rings

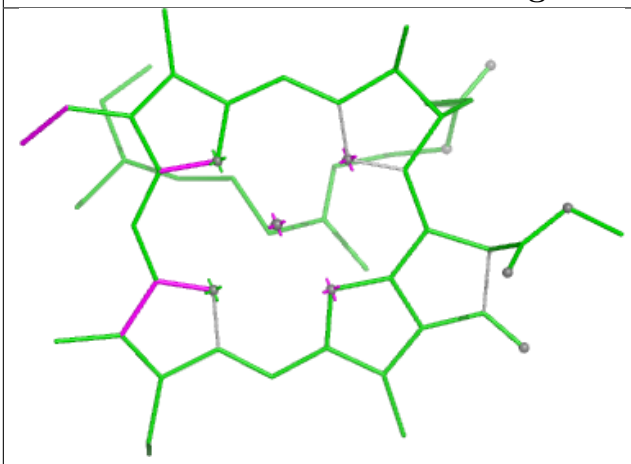
Ligand CLA B 822



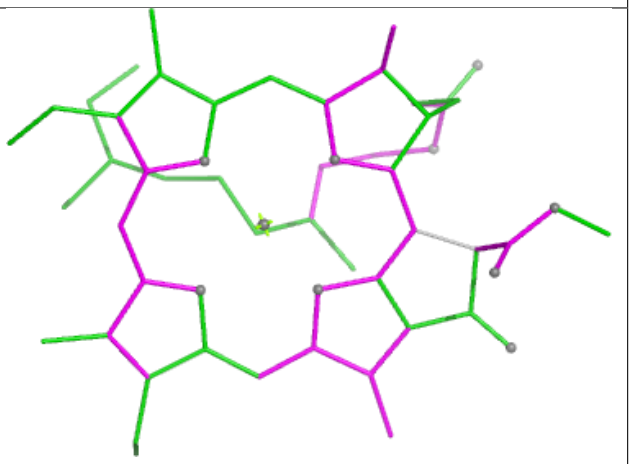
Ligand CLA B 829



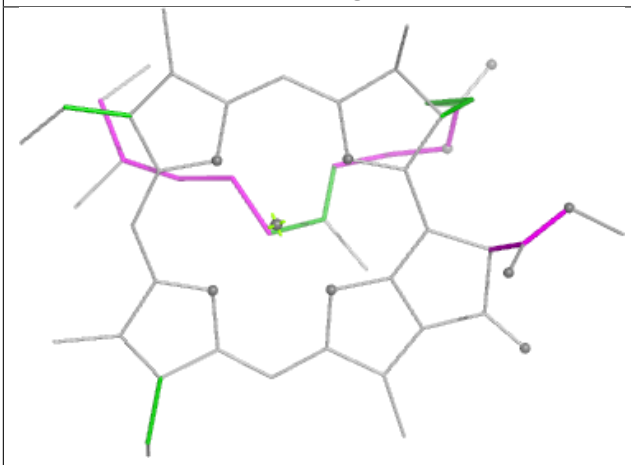
Ligand CLA 5 301



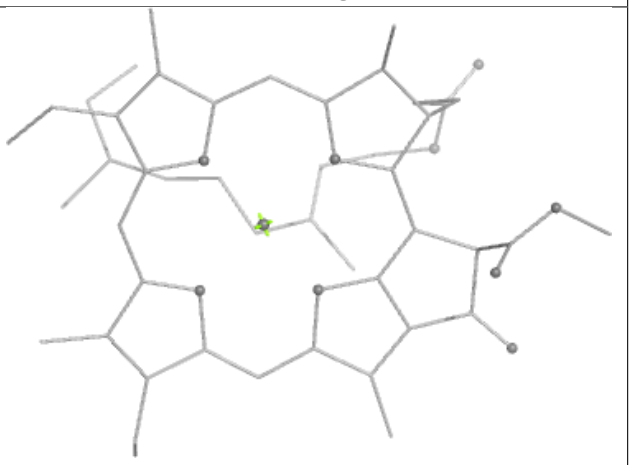
Bond lengths



Bond angles

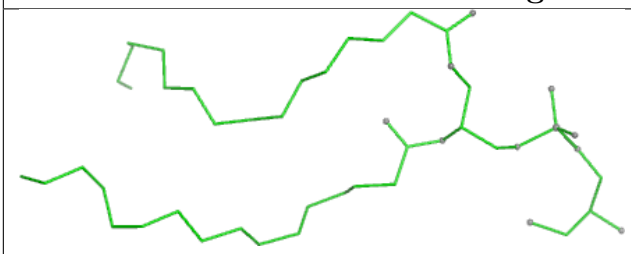


Torsions



Rings

Ligand LHG 4 820



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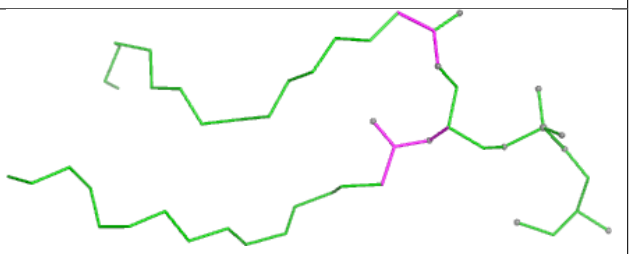
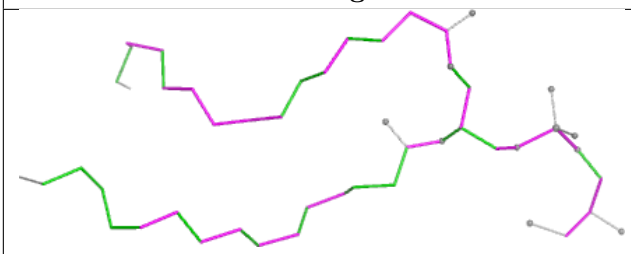


Bond angles



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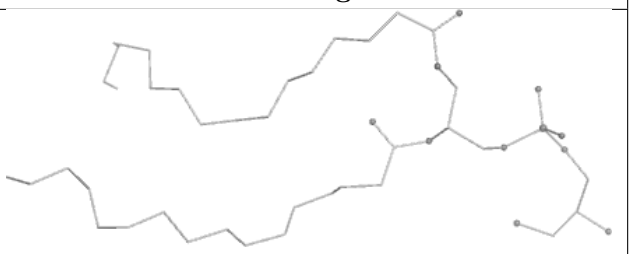

Rings

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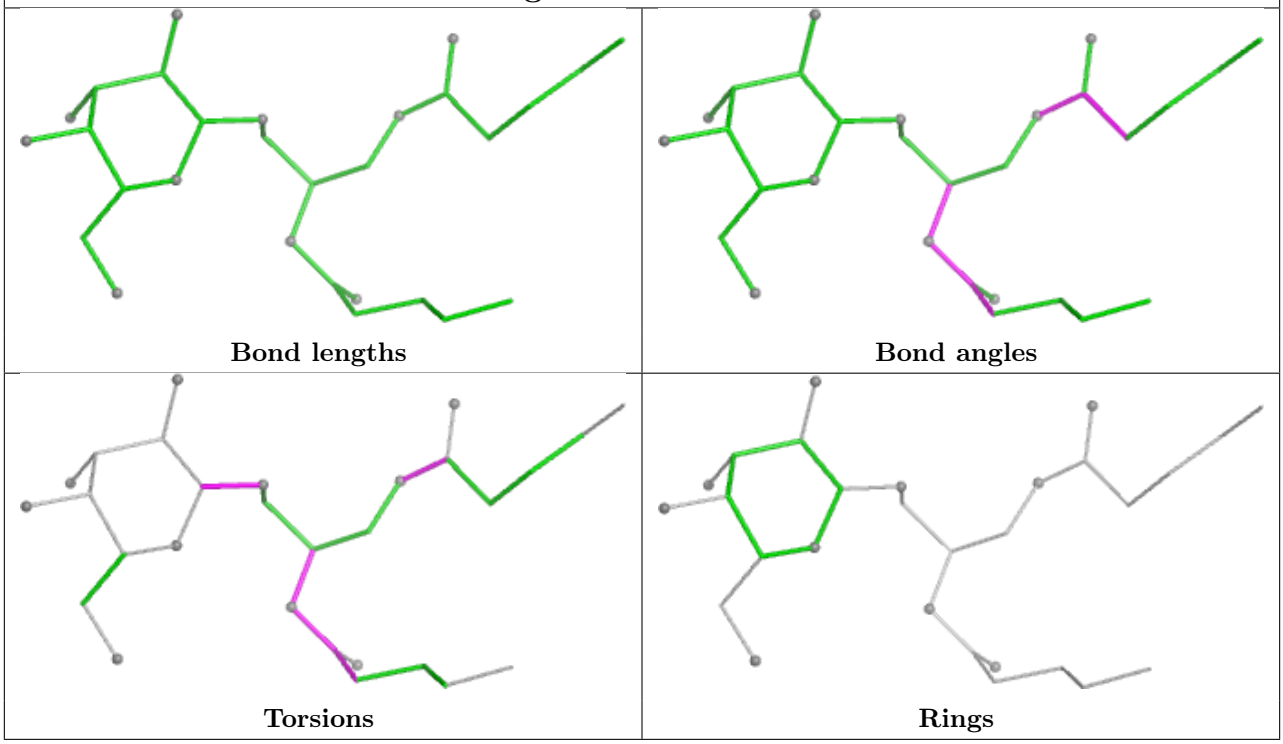
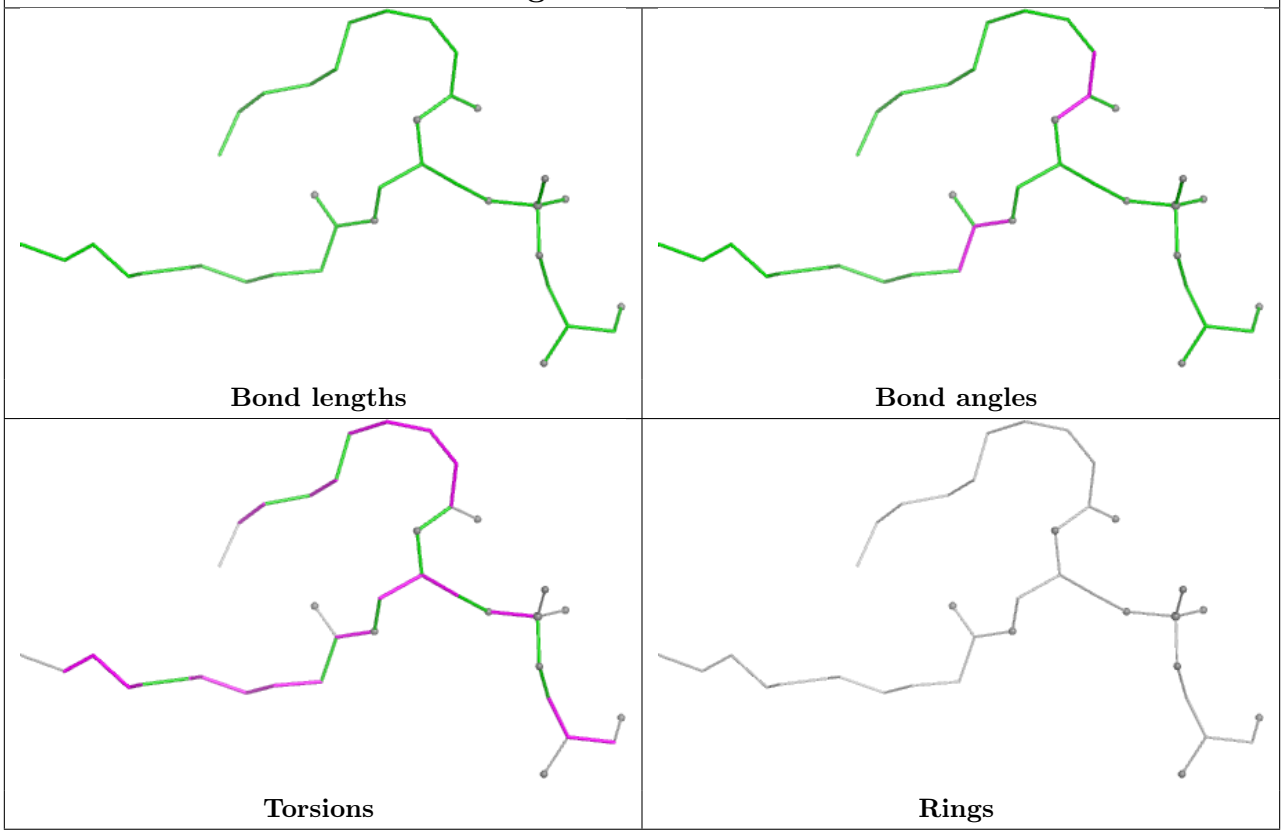
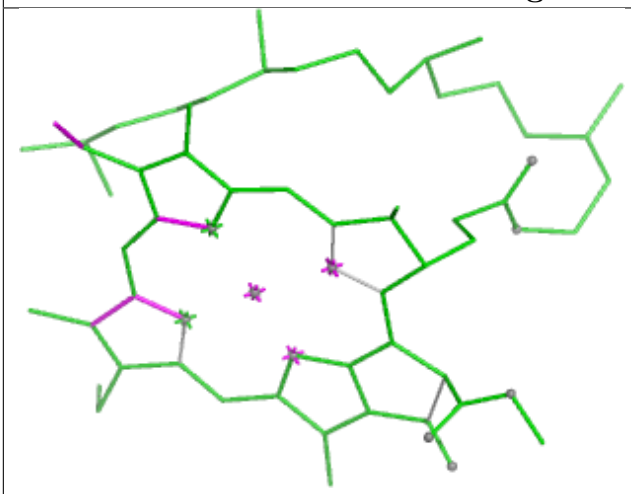


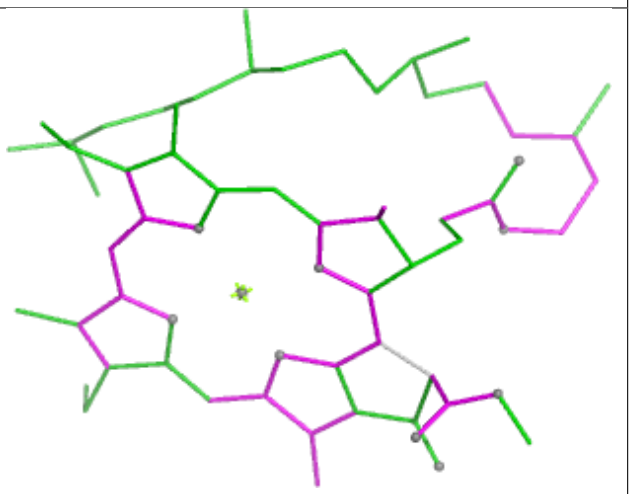
Ligand LHG 8 317



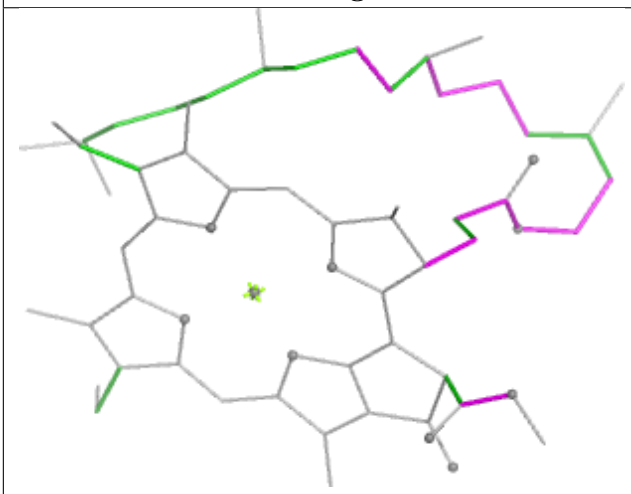
Ligand CLA Z 313



Bond lengths



Bond angles



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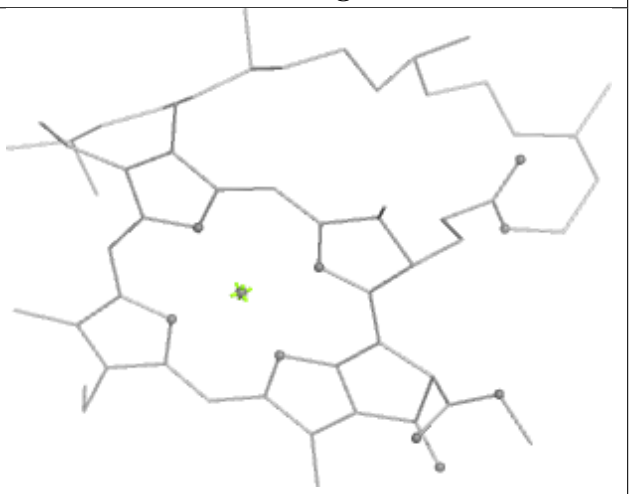
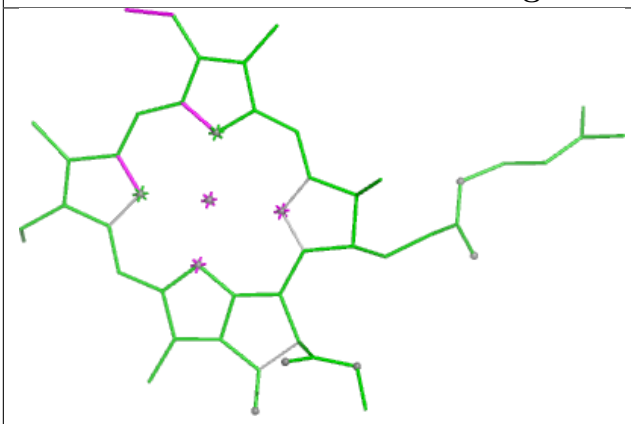
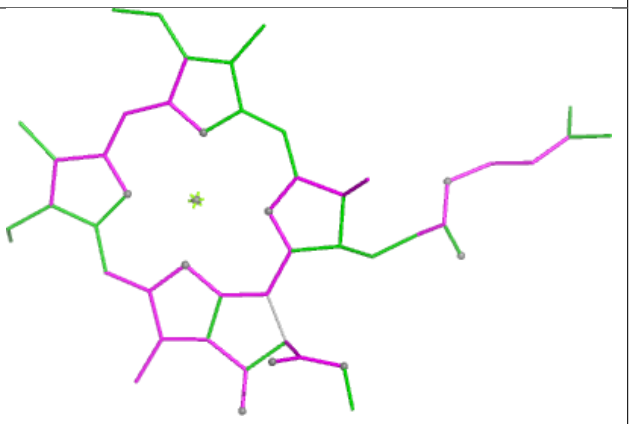
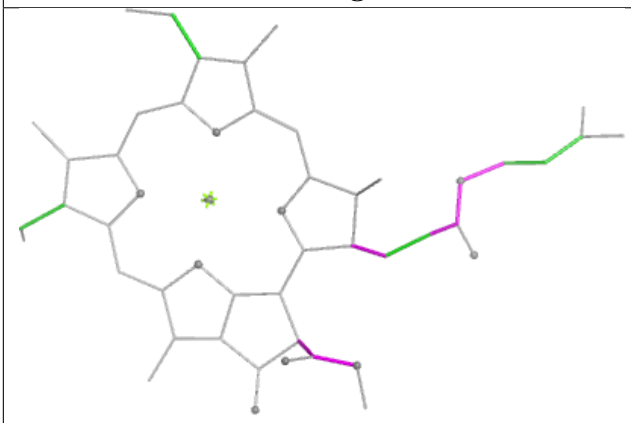
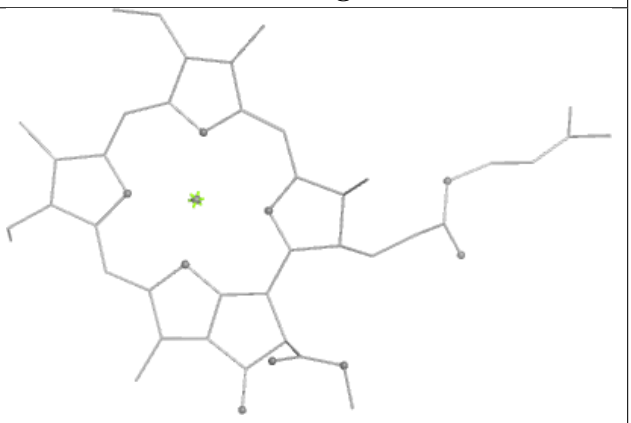
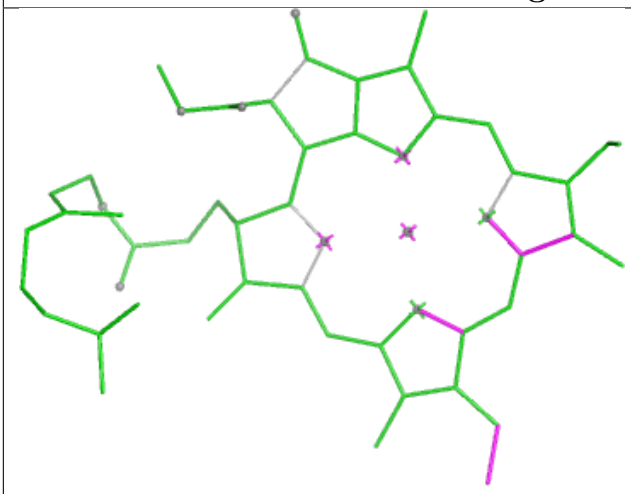


Rings

Ligand CLA G 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 6 311



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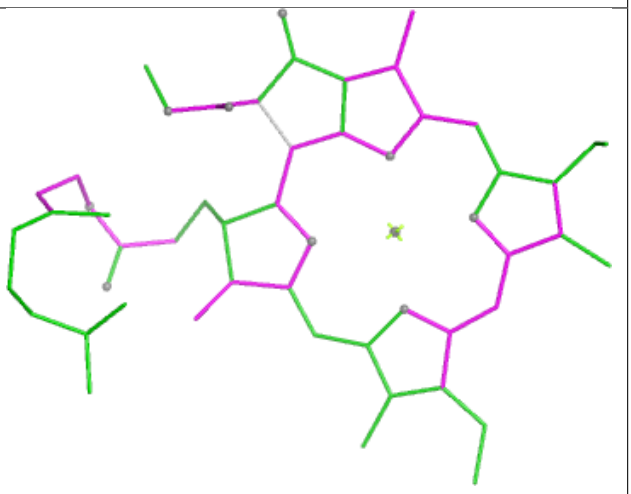
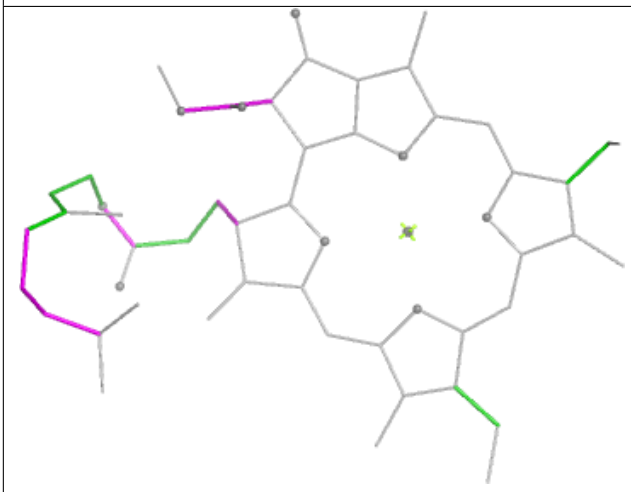


Bond angles



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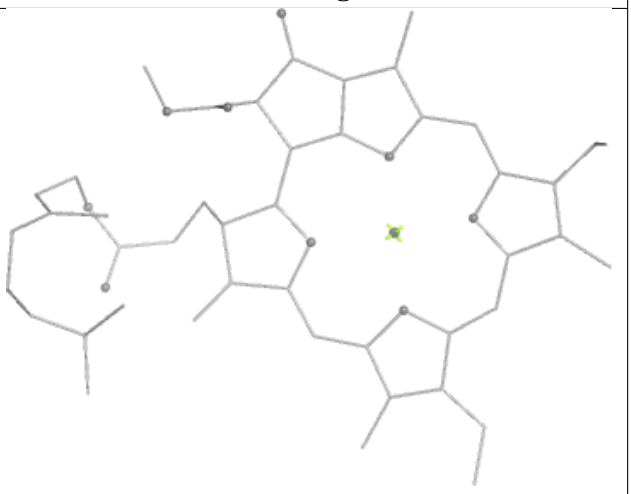
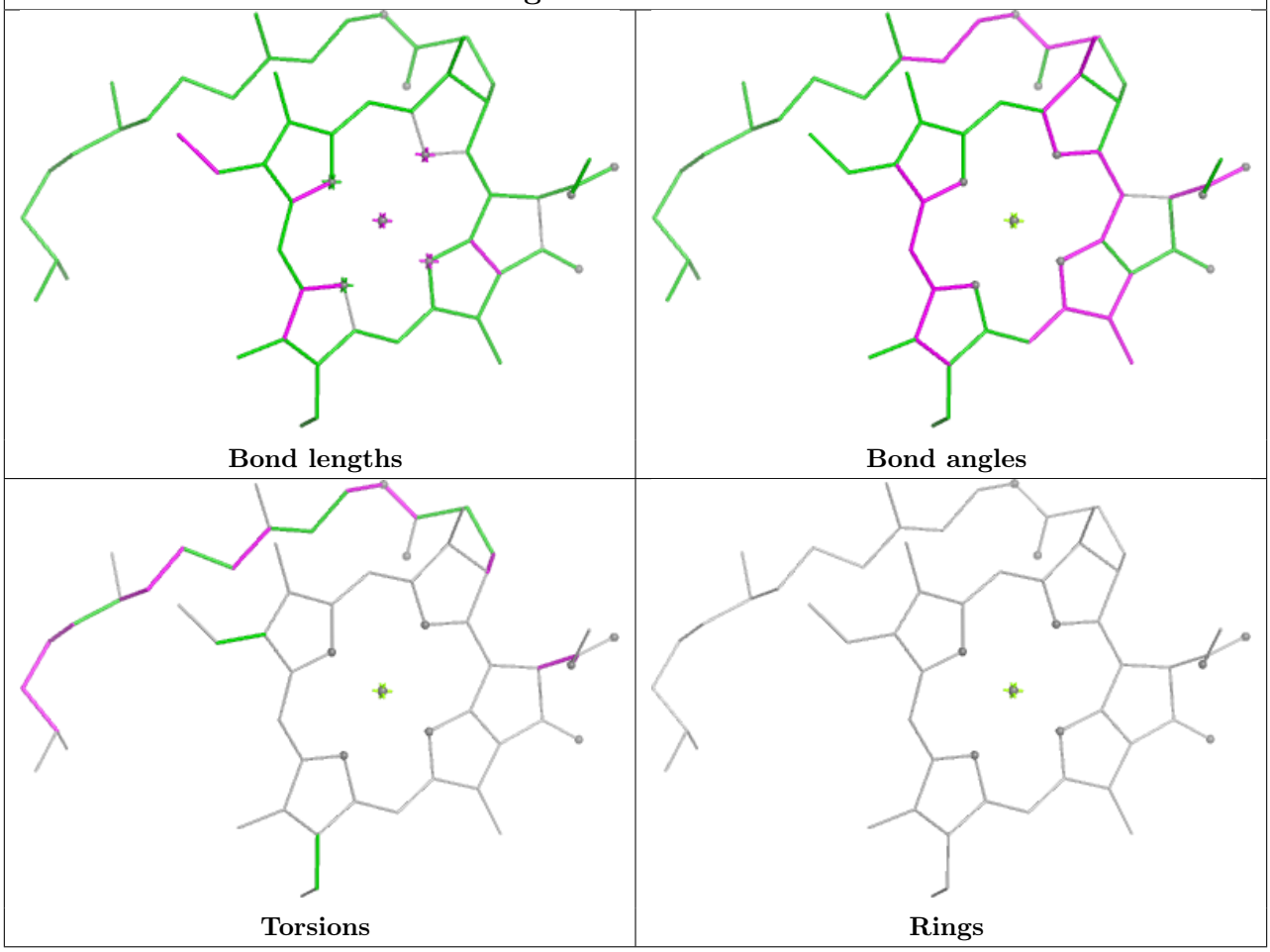
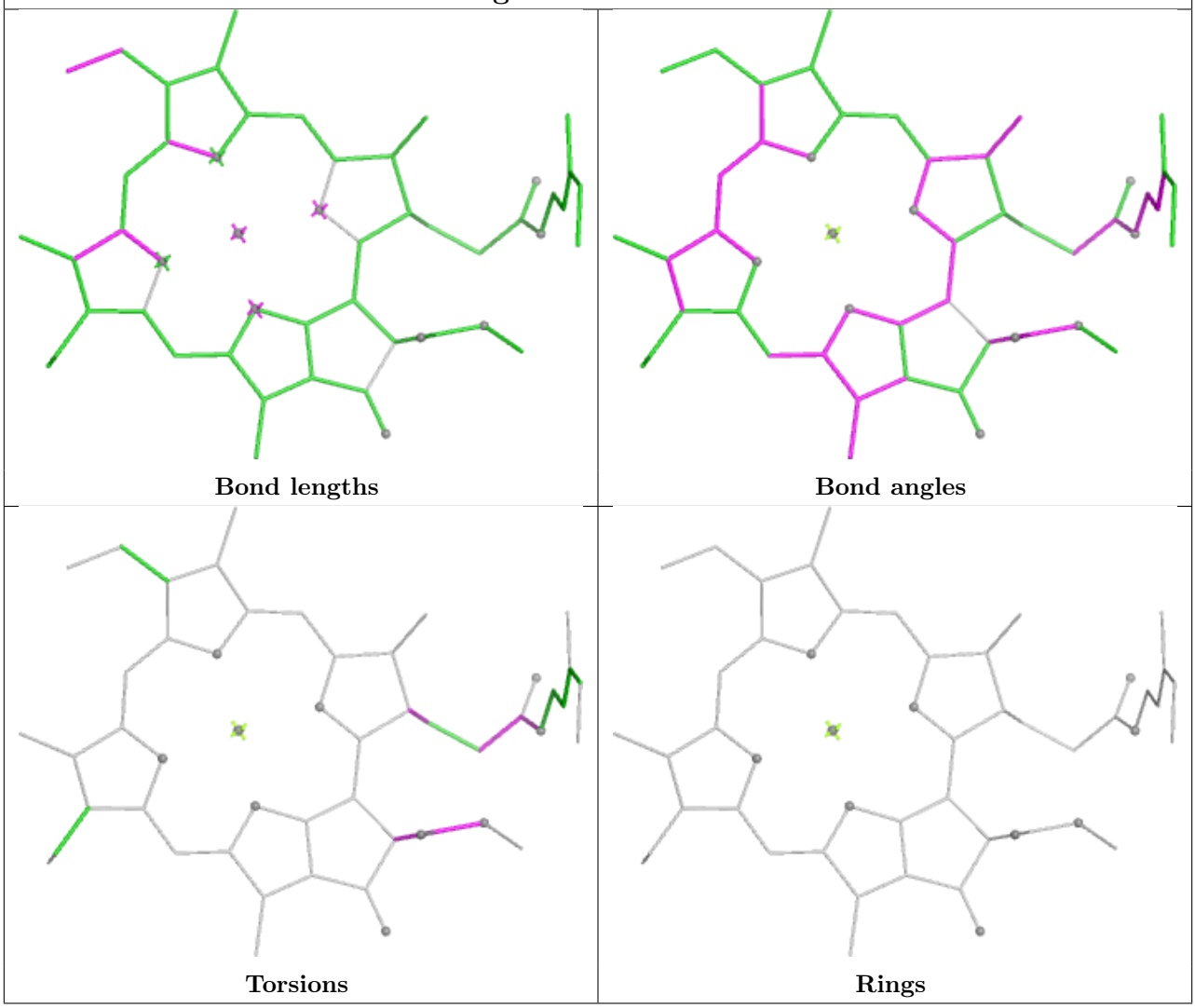


Rings

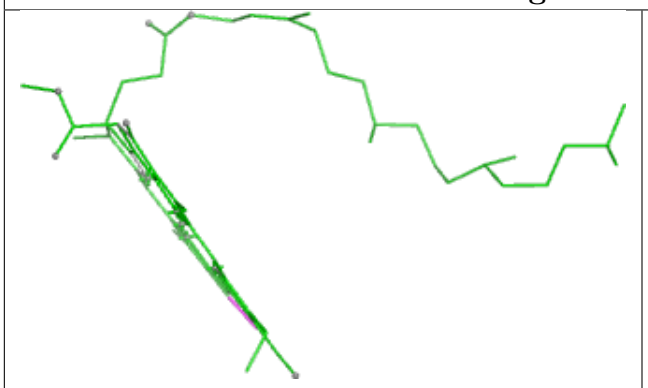
Ligand CLA 4 808



Ligand CLA 8 306



Ligand CHL 5 316



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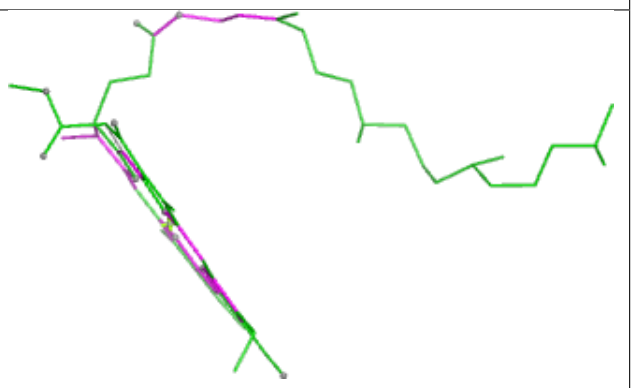
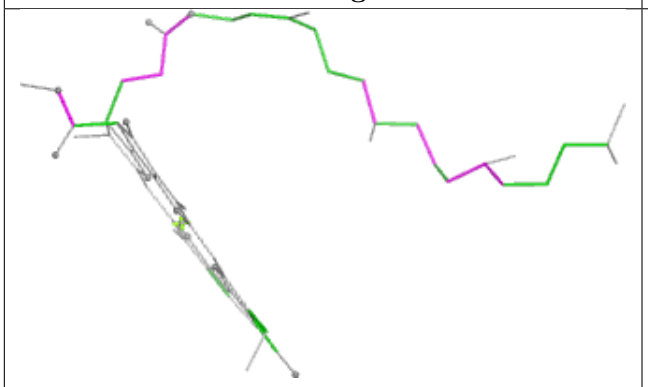


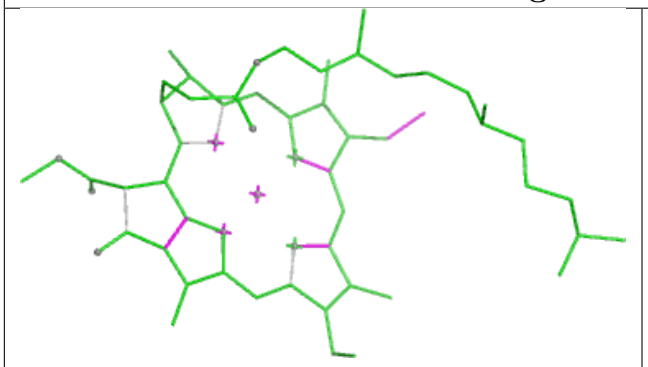
Bond angles



Torsions

Rings

Ligand CLA 9 303



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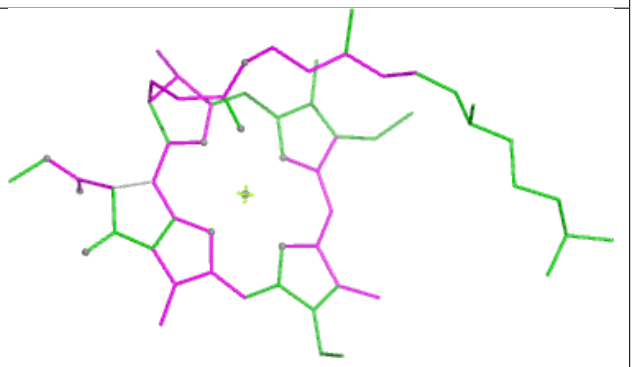
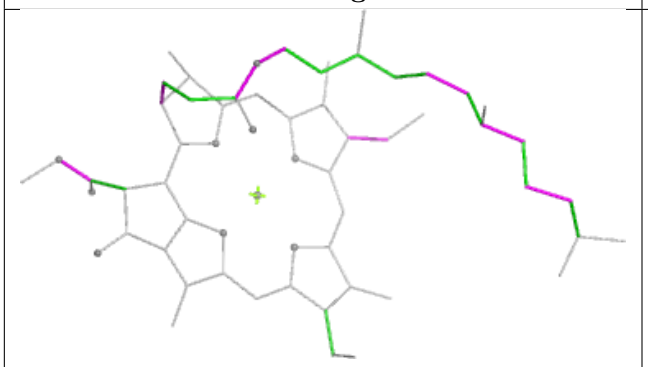


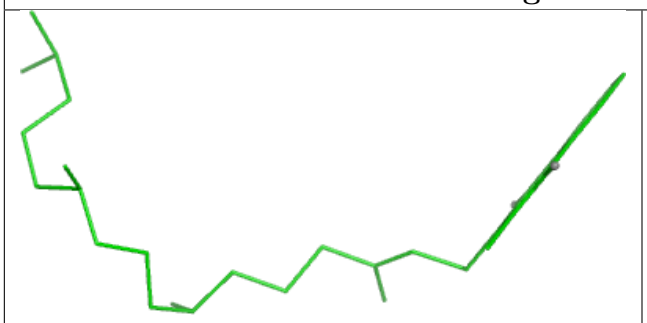
Bond angles



Torsions

Rings

Ligand PQN B 843



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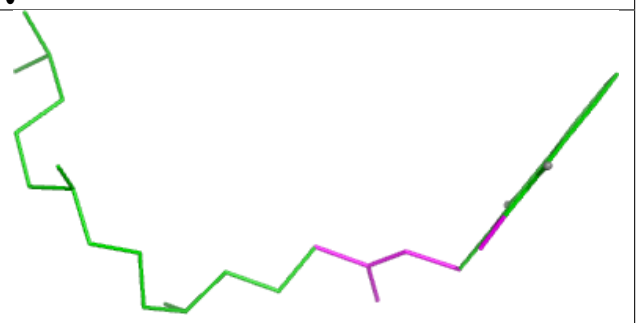
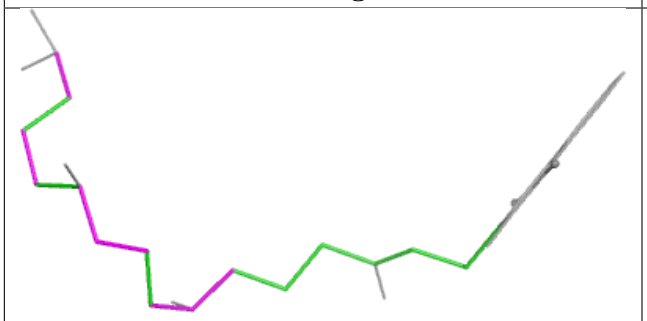
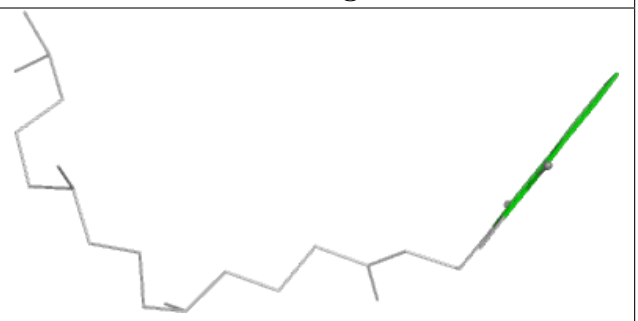


Bond angles

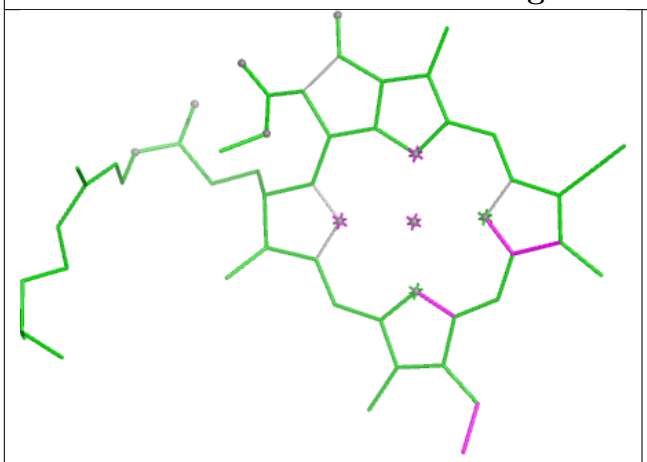


Torsions

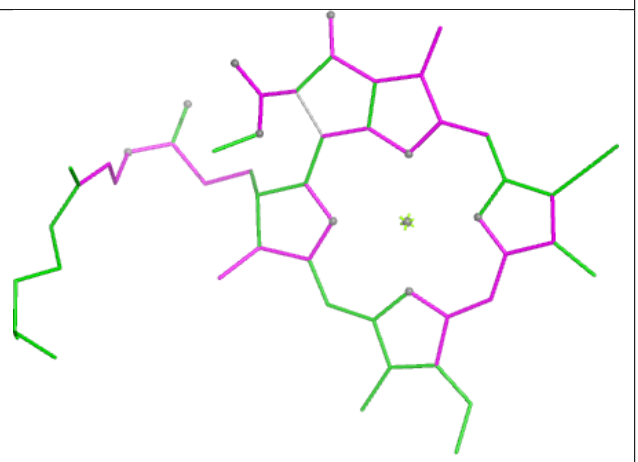


Rings

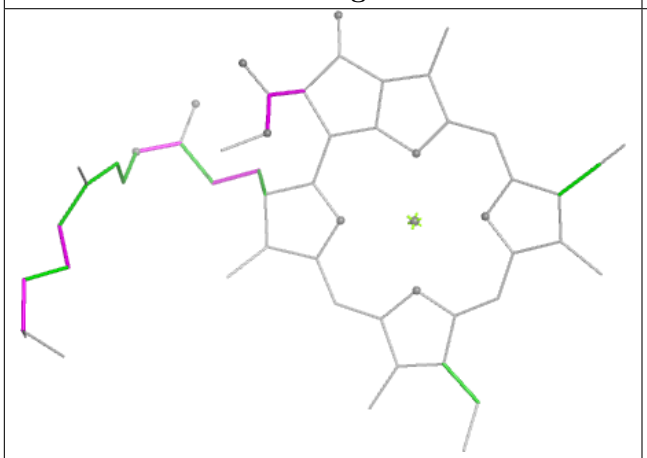
Ligand CLA Z 307



Bond lengths



Bond angles



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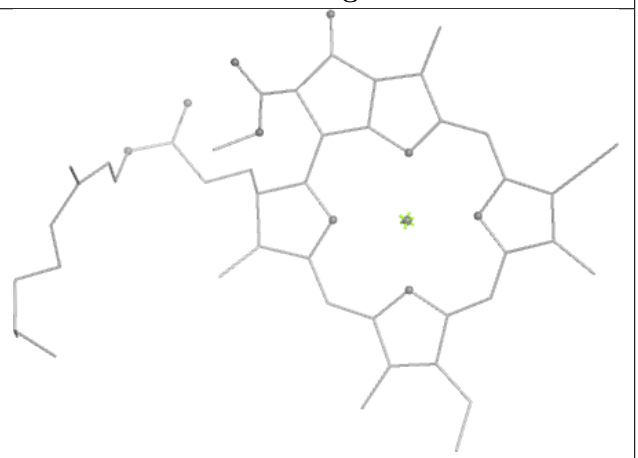
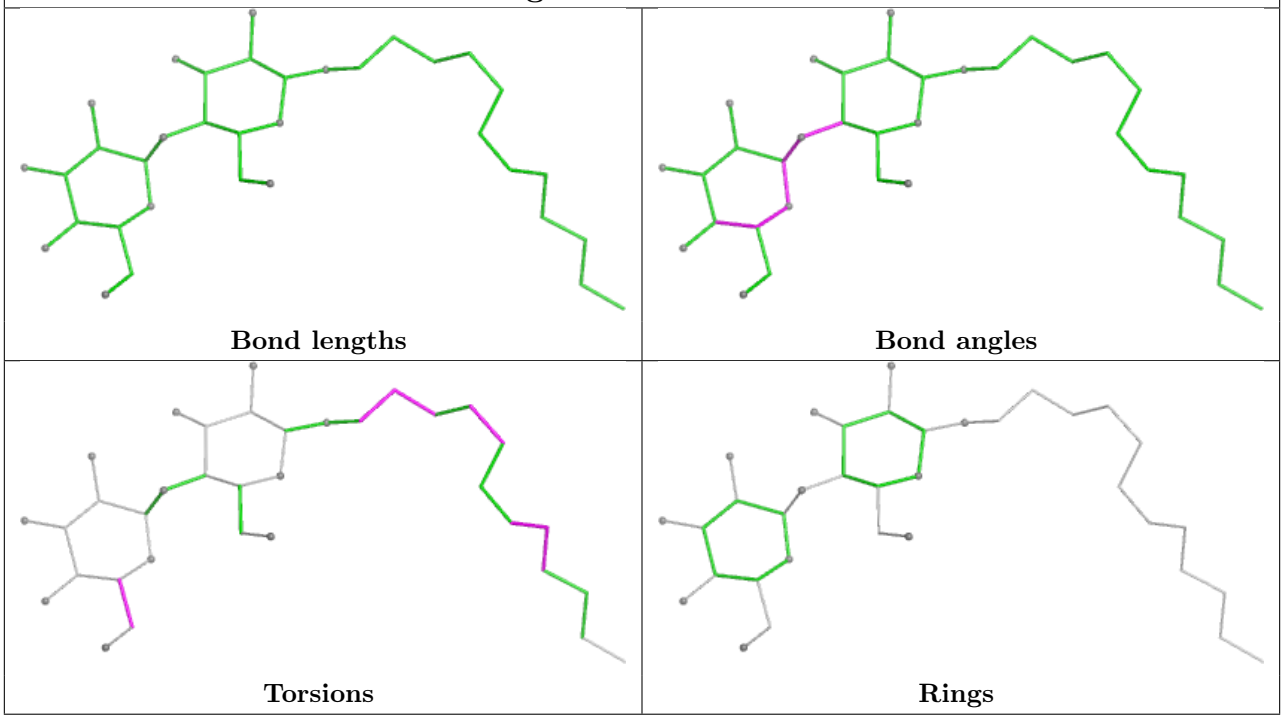
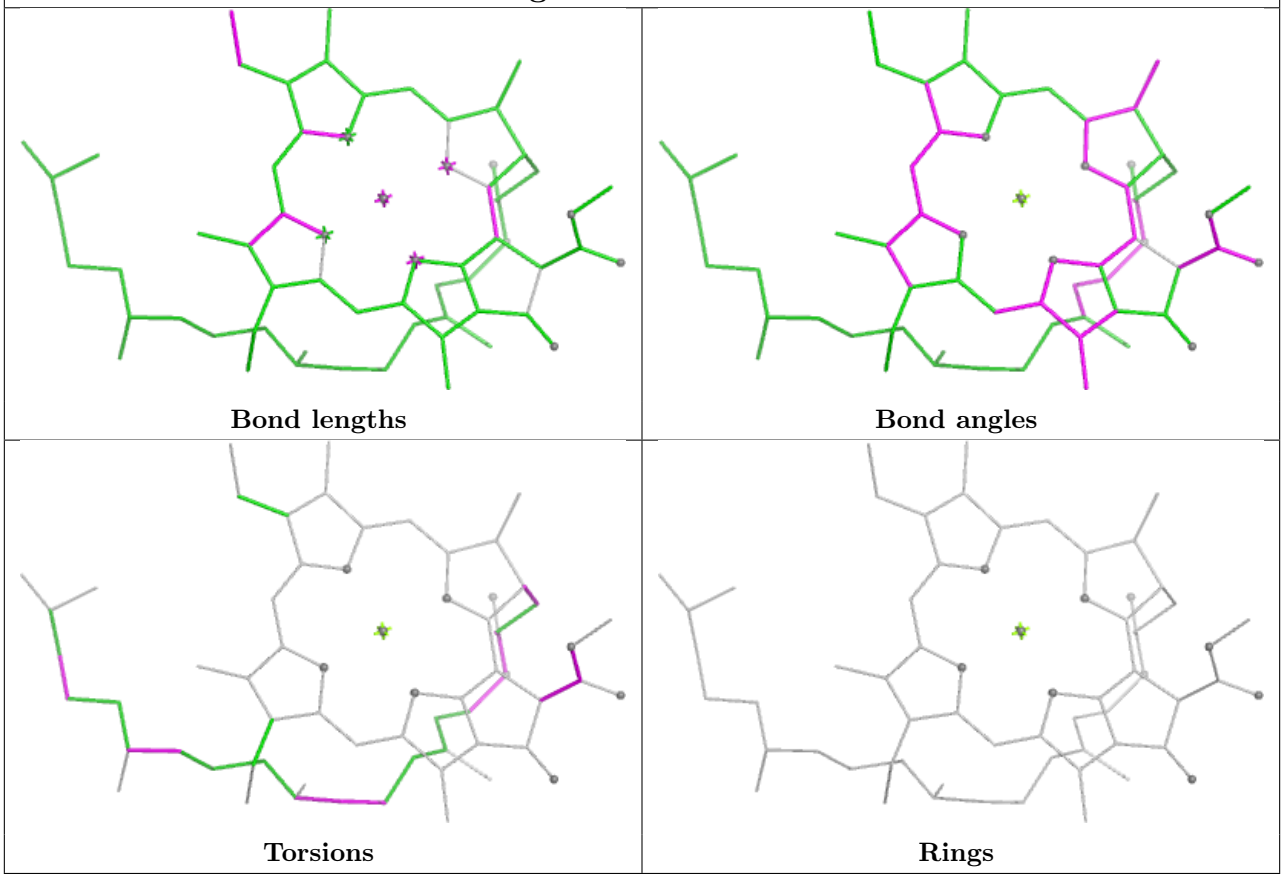


Rings

Ligand LMT 4 822



Ligand CLA 6 312



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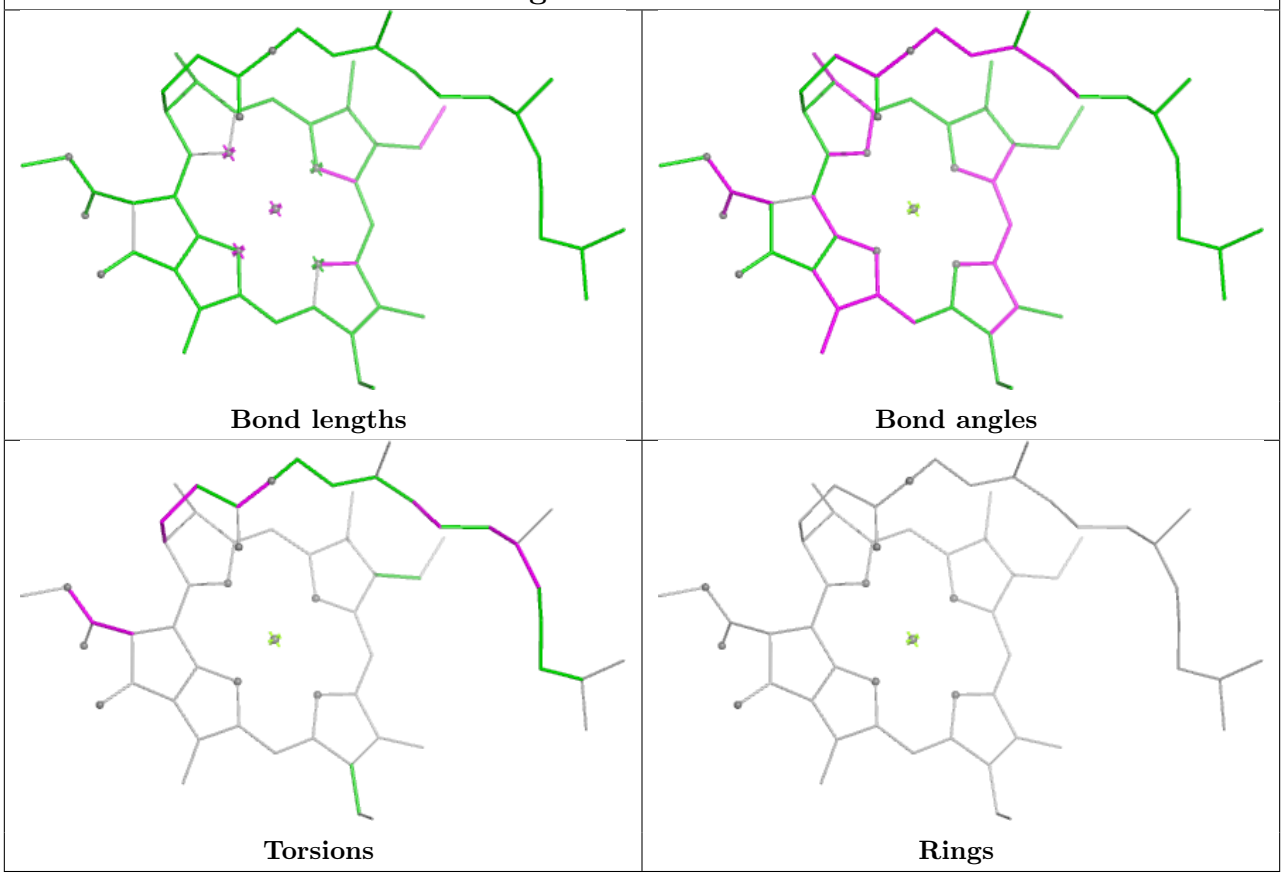

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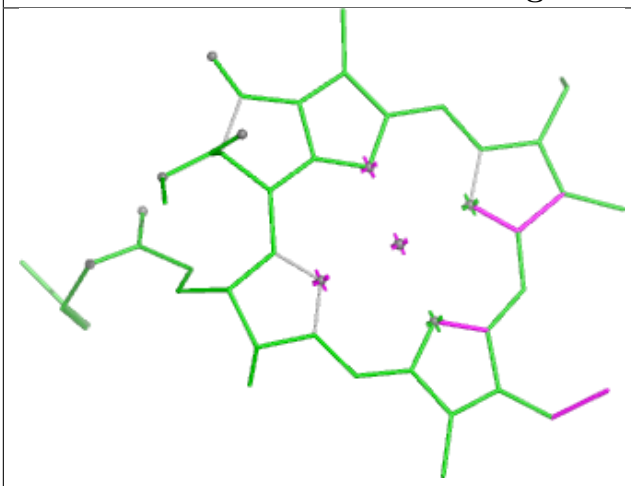
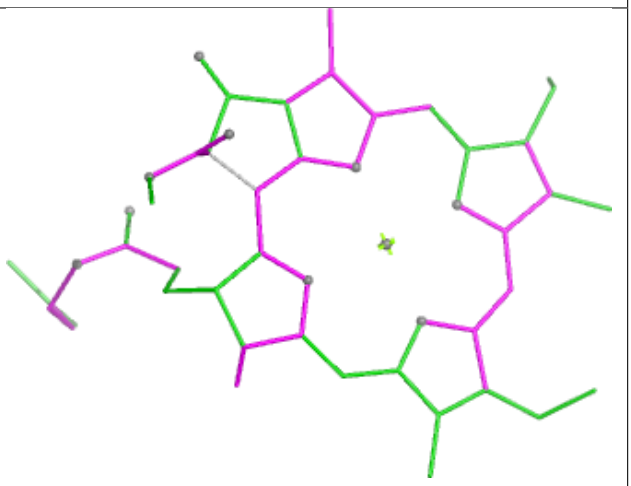
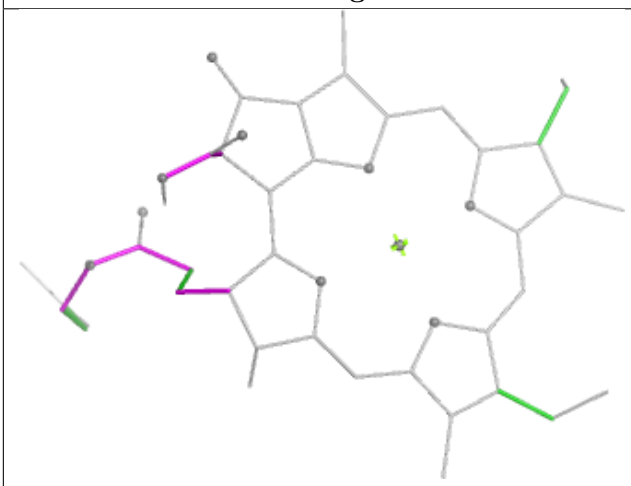
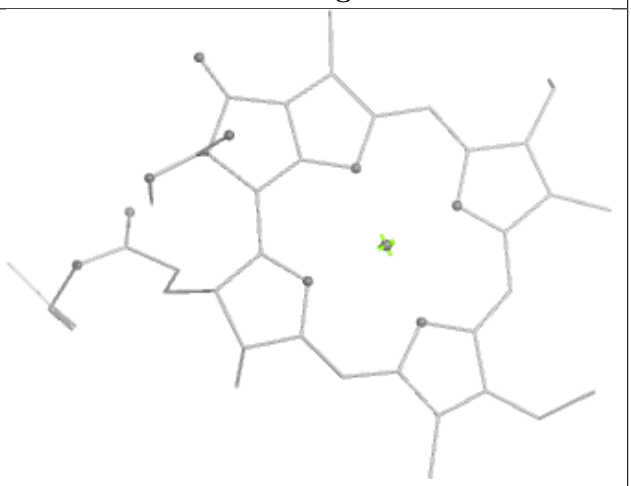
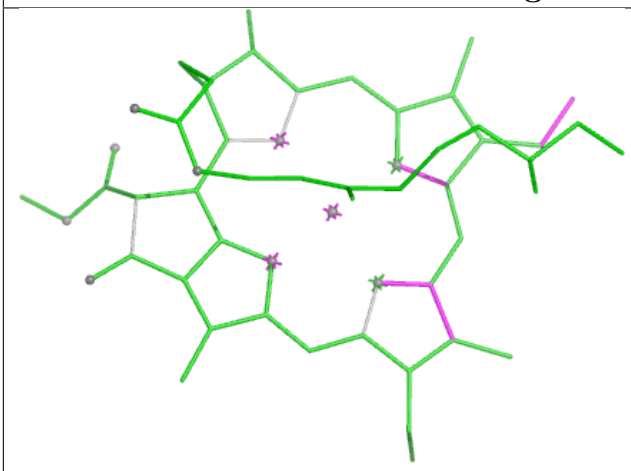
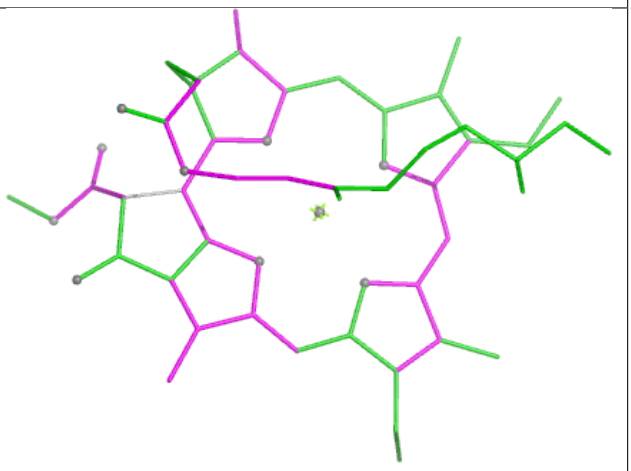
 Bond lengths	 Bond angles
 Torsions	 Rings

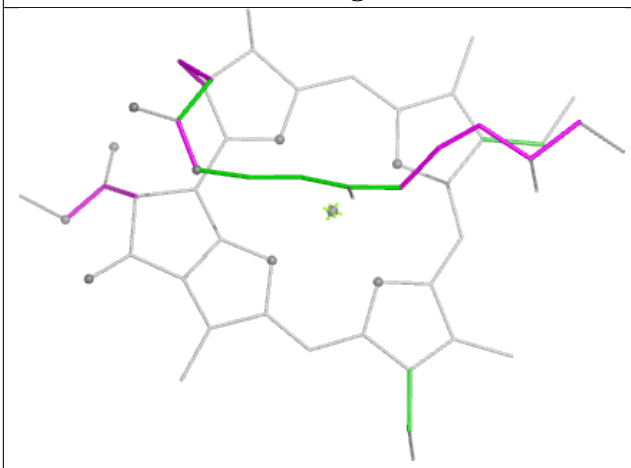
Ligand CLA B 813



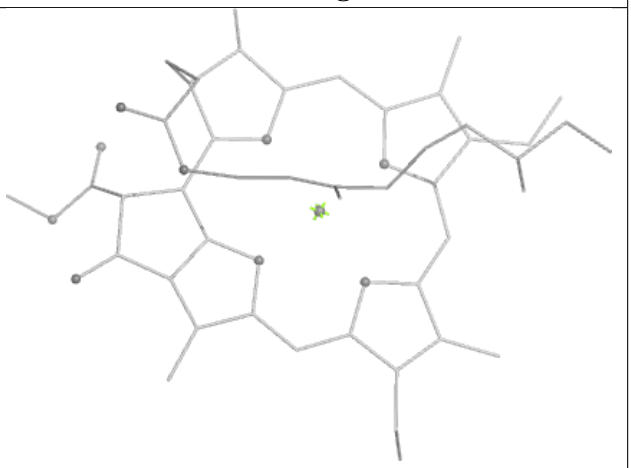
Bond lengths



Bond angles

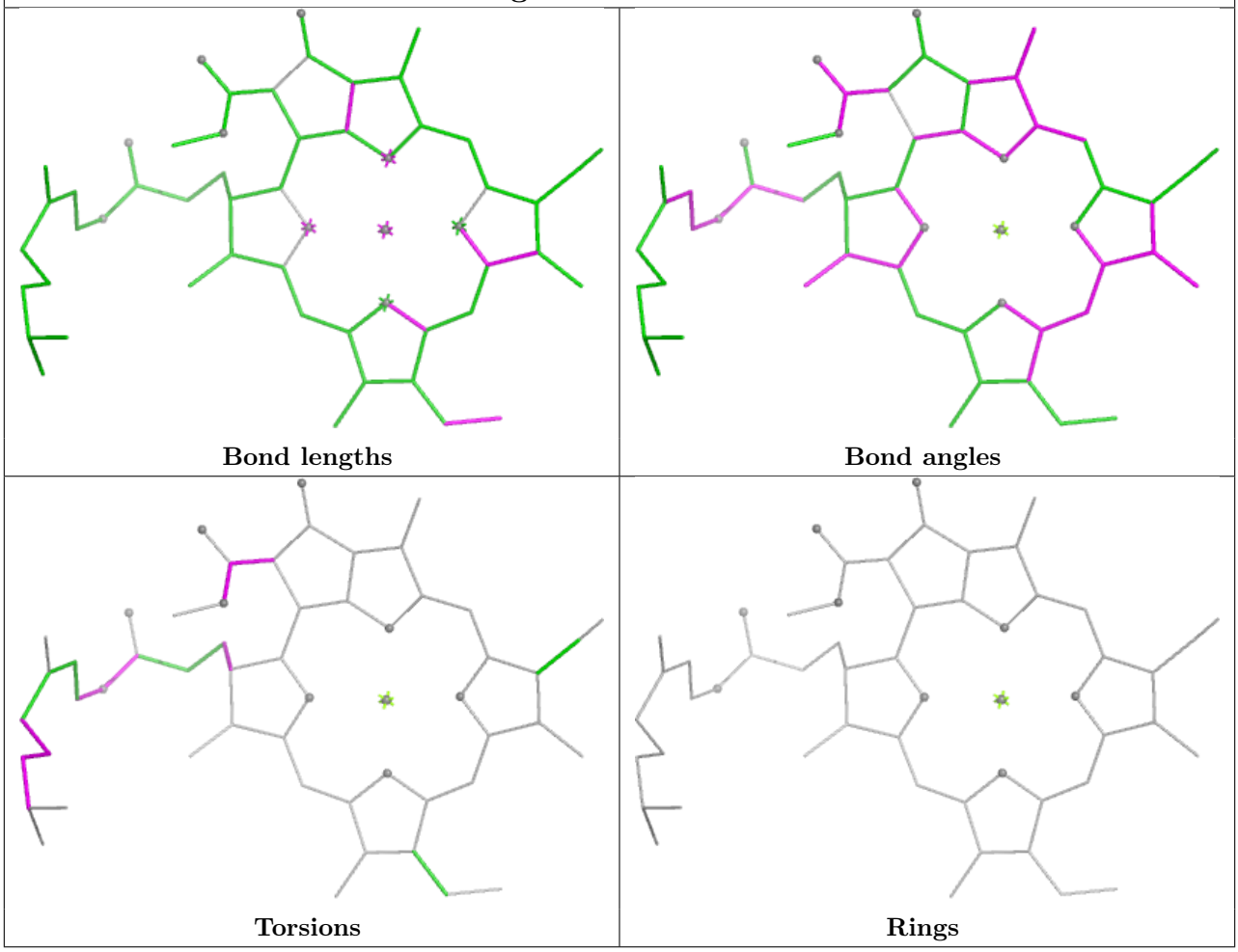


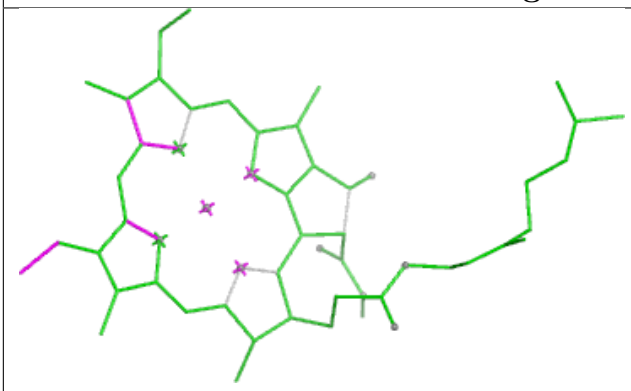
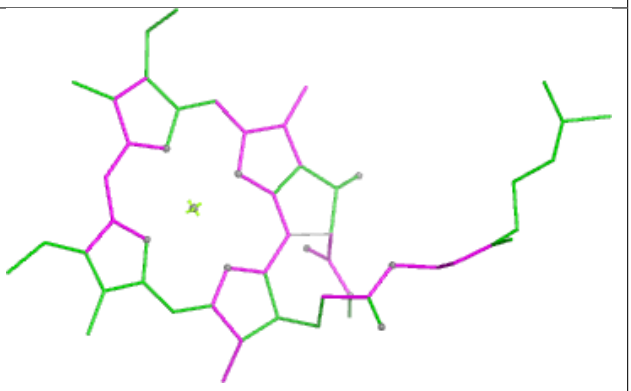
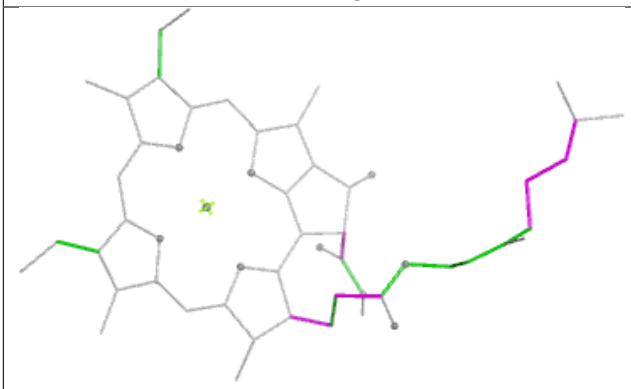
Torsions



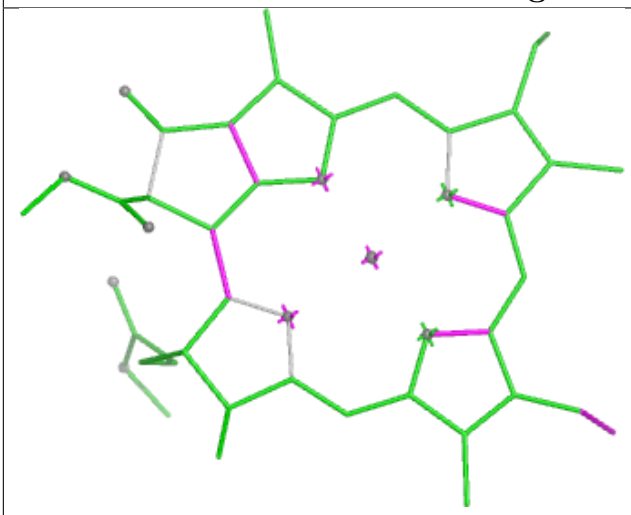
Rings

Ligand CLA 1 308

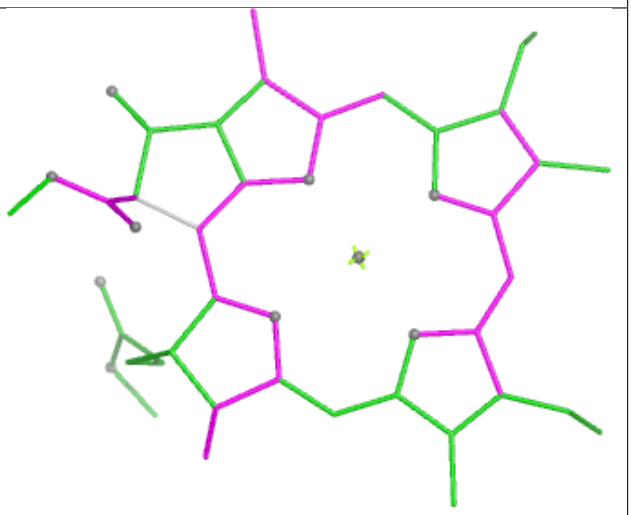


Ligand CLA K 203	
 Bond lengths	 Bond angles
 Torsions	Rings

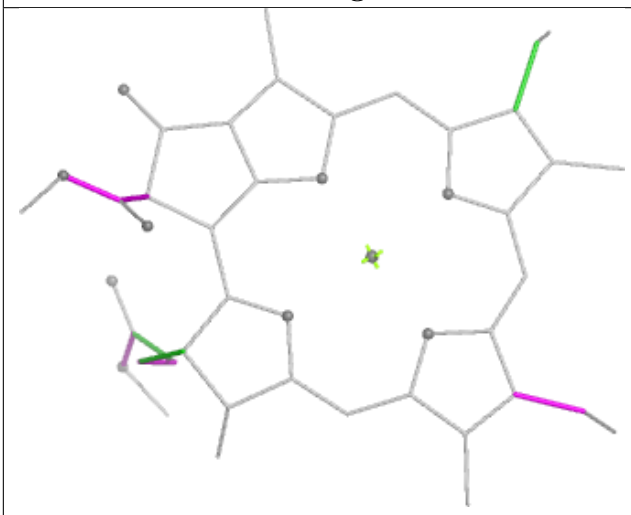
Ligand CLA 1 311



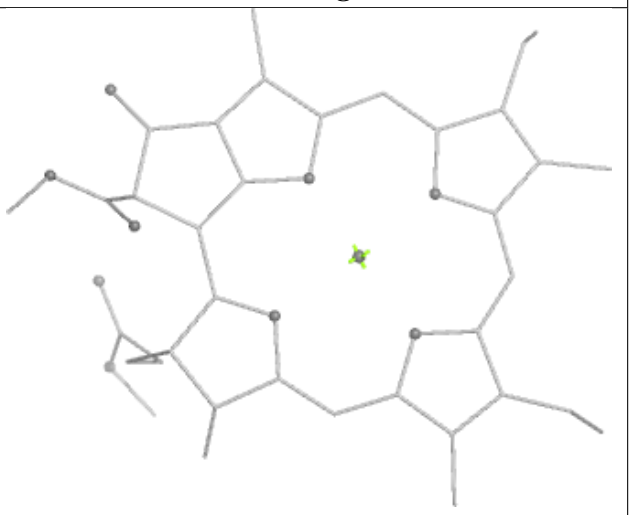
Bond lengths



Bond angles

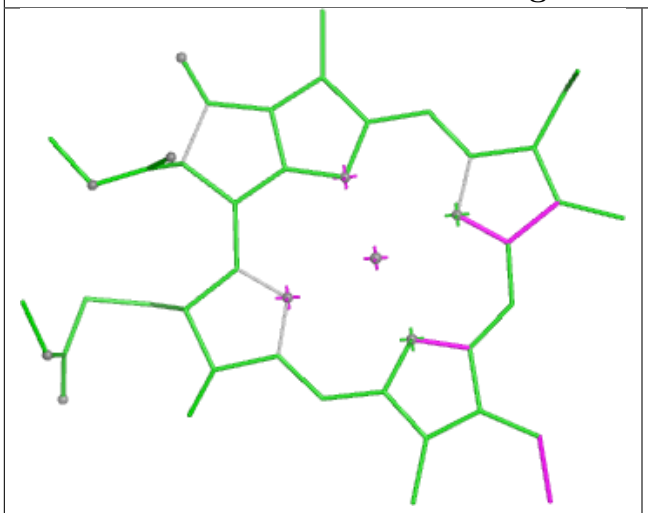


Torsions

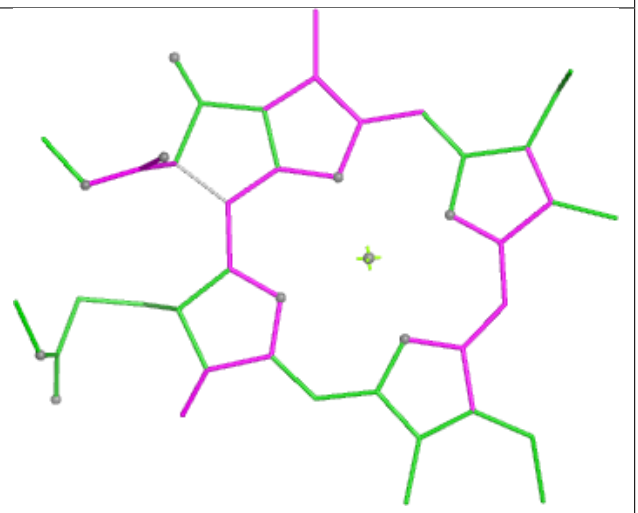


Rings

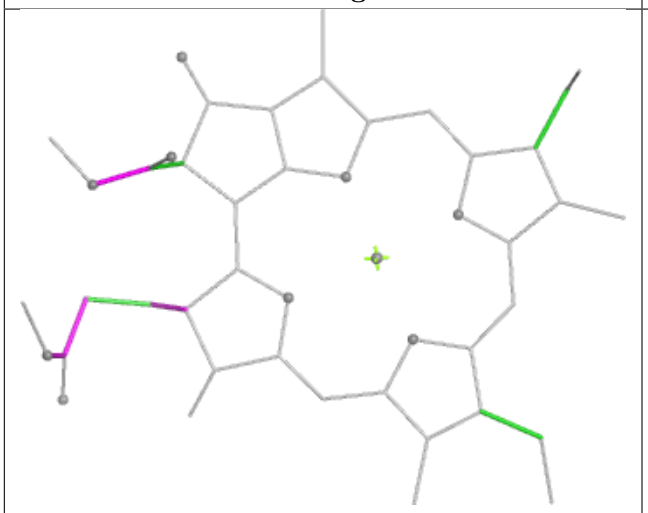
Ligand CLA 1 315



Bond lengths



Bond angles



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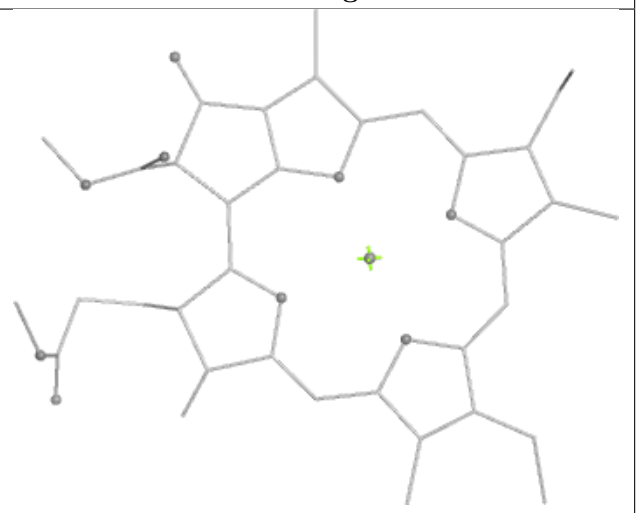

Rings

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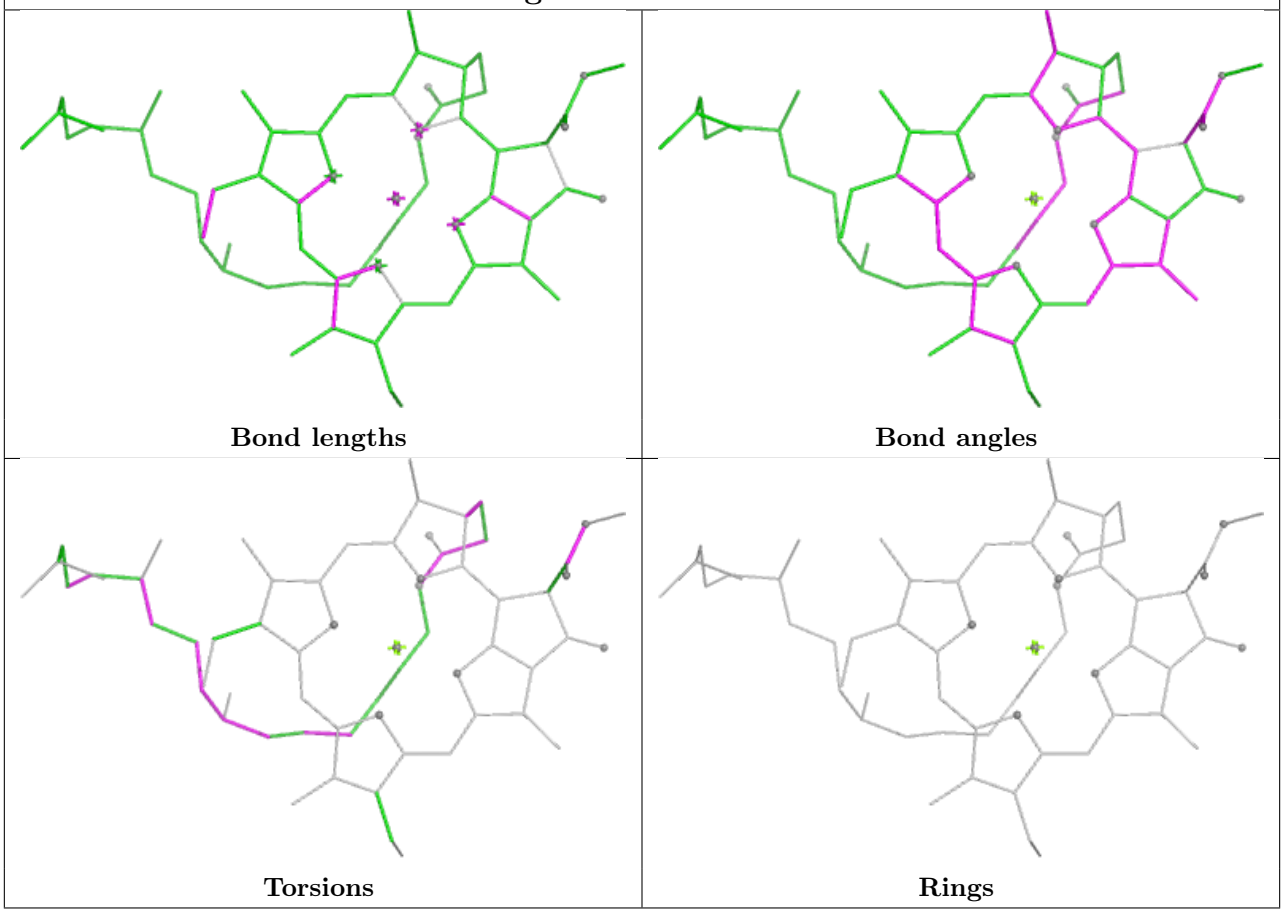

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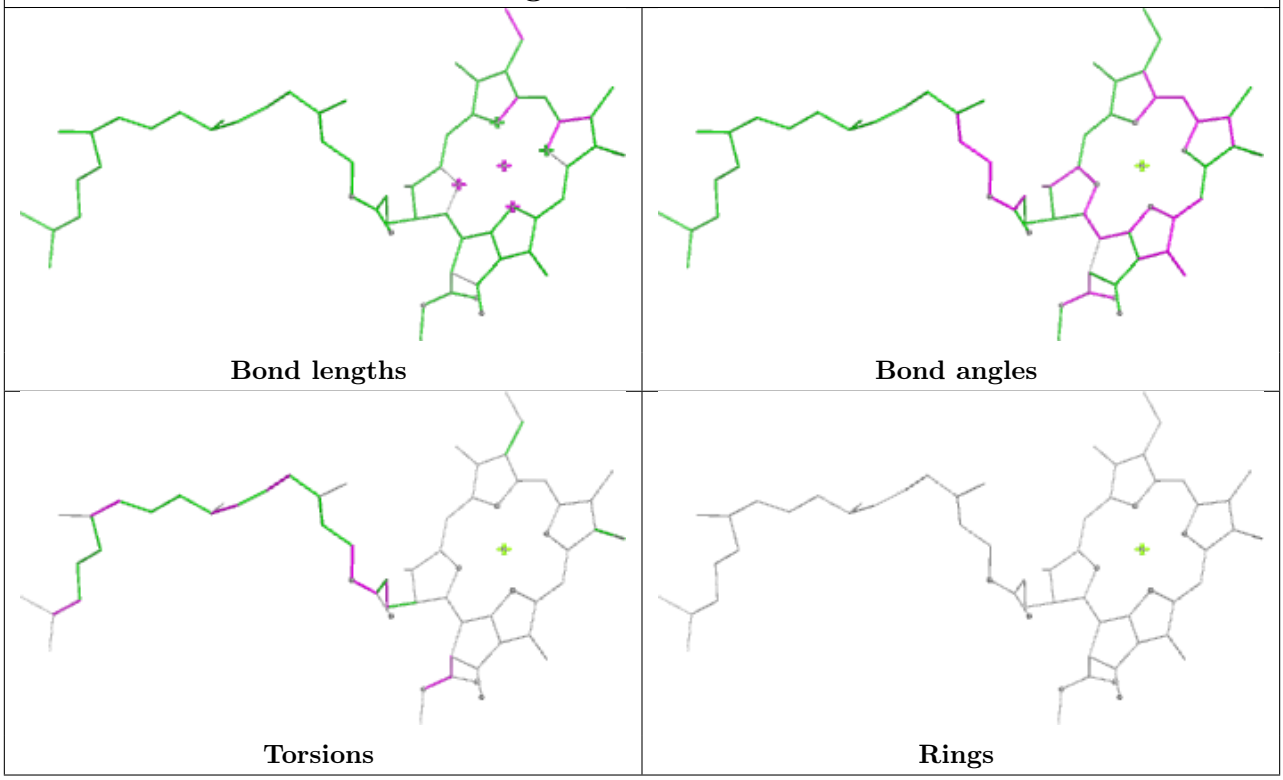
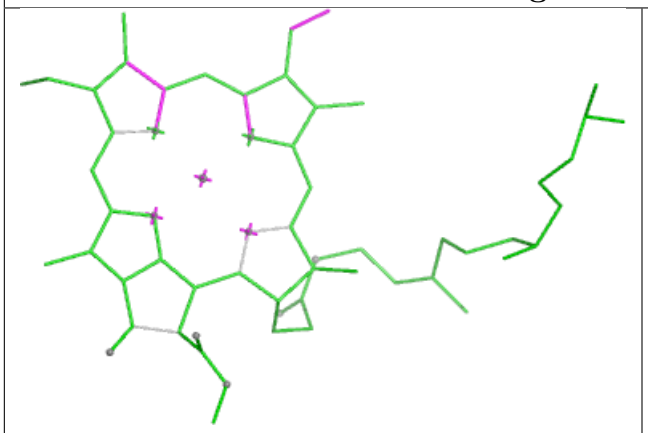


Ligand CLA 7 324



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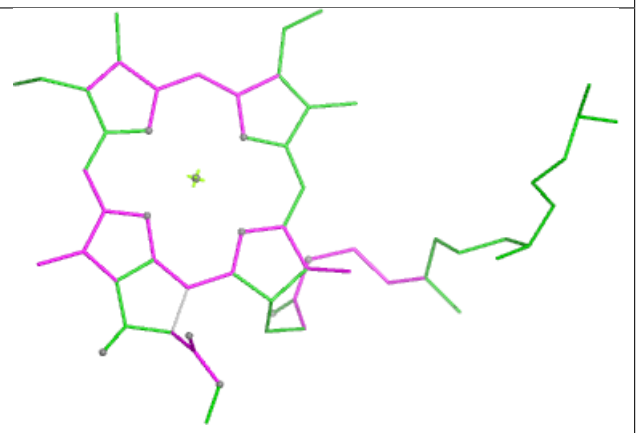

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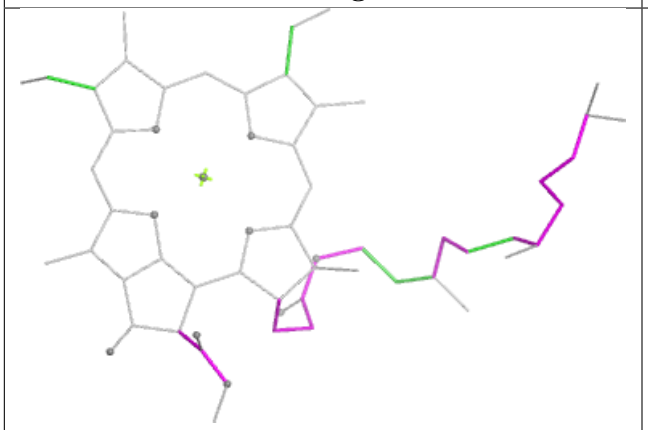

Torsions

Rings

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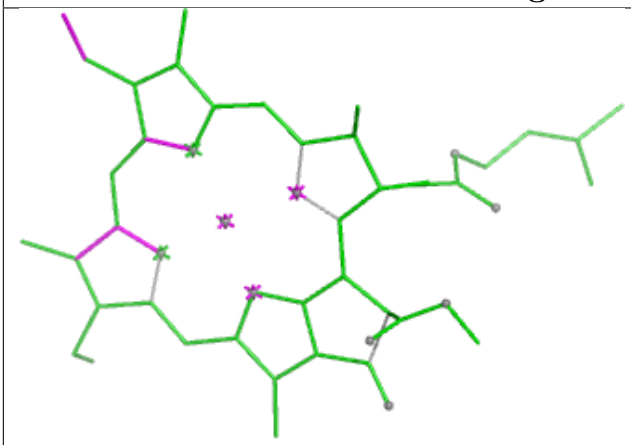	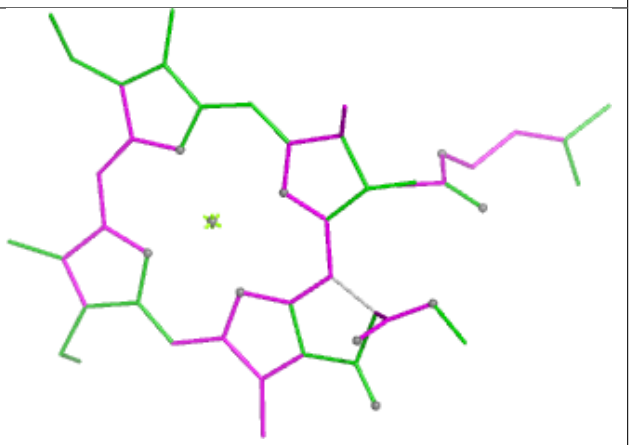
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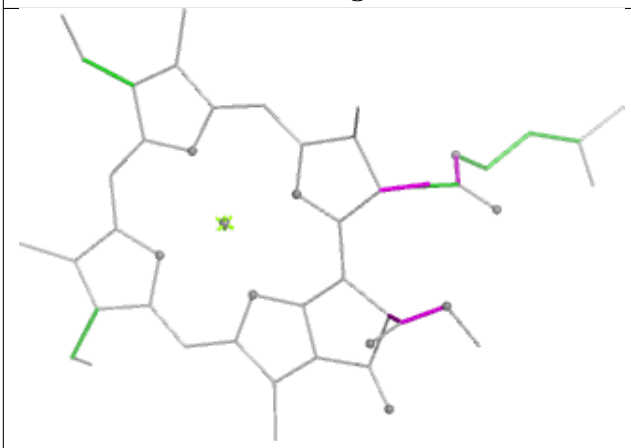
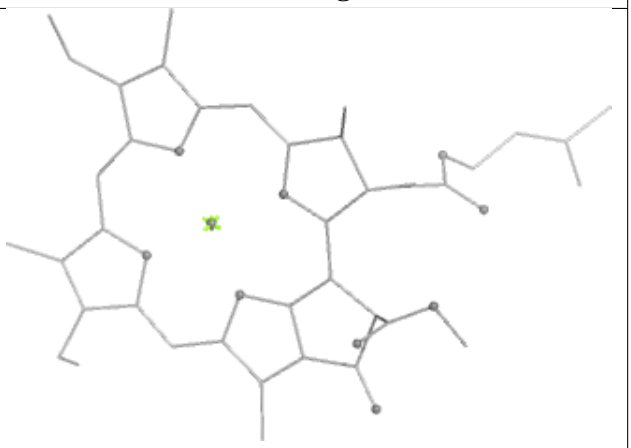
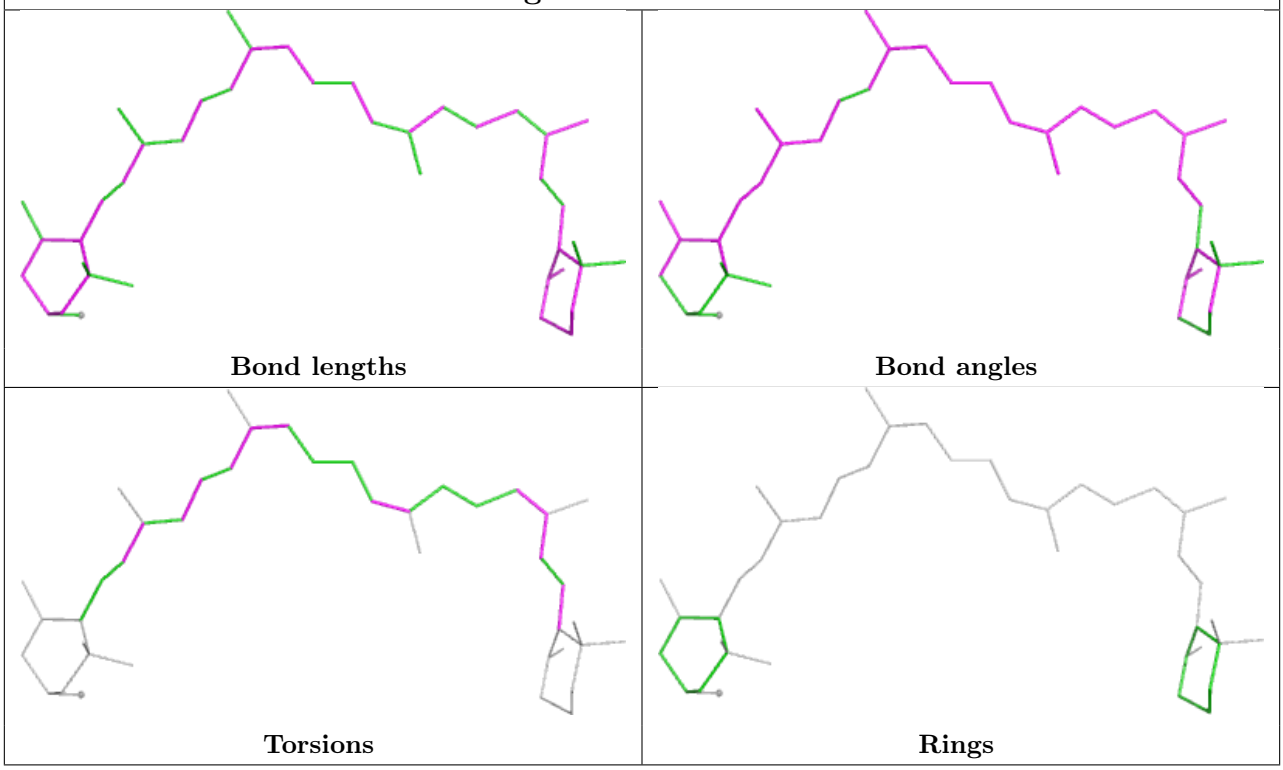
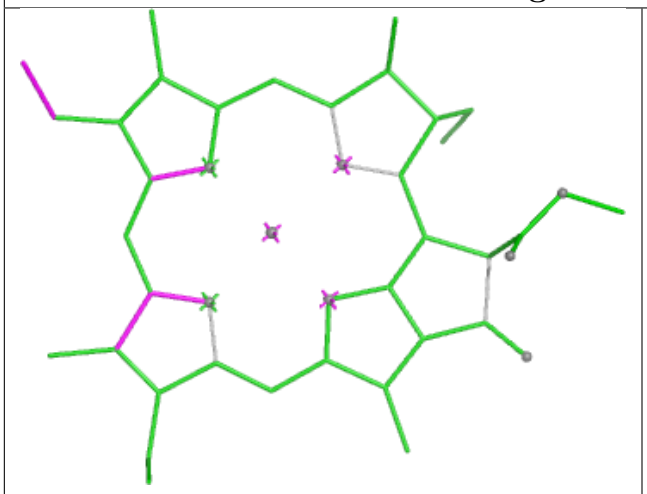
	
Torsions	**Rings**

Ligand RRX F 306



Ligand CLA J 103



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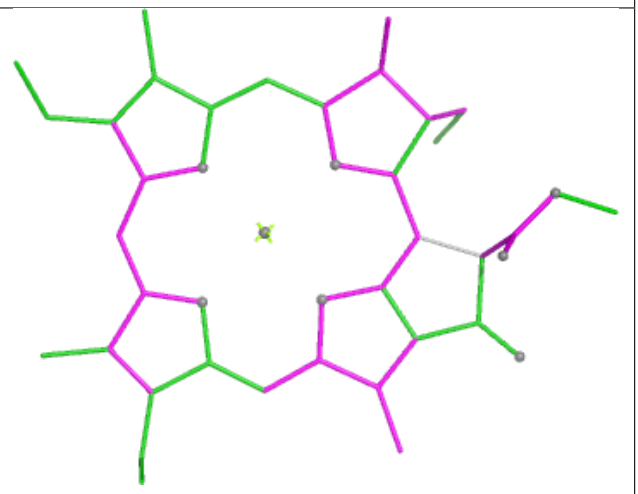
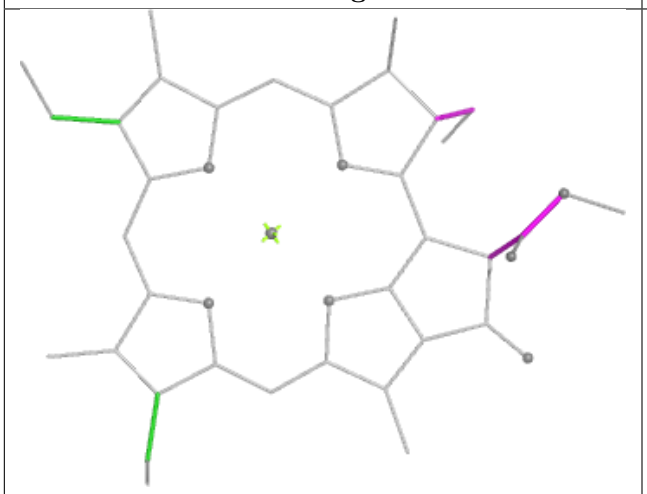


Bond angles



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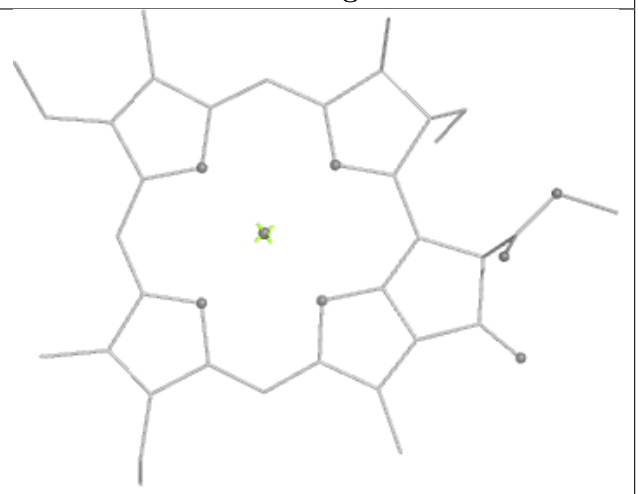
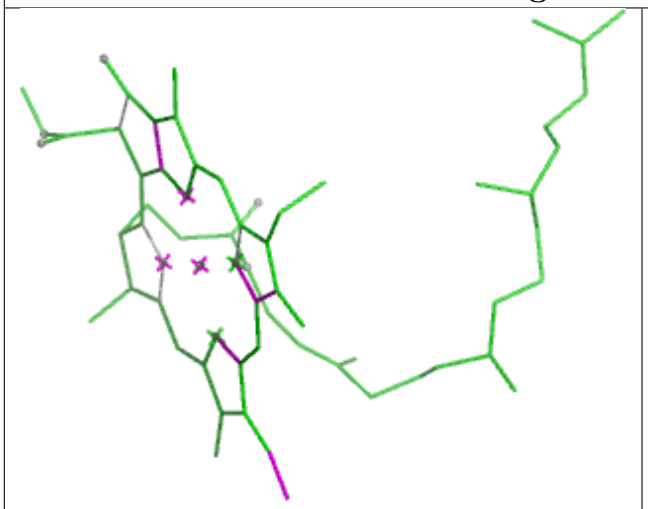


Rings

Ligand CLA 3 308



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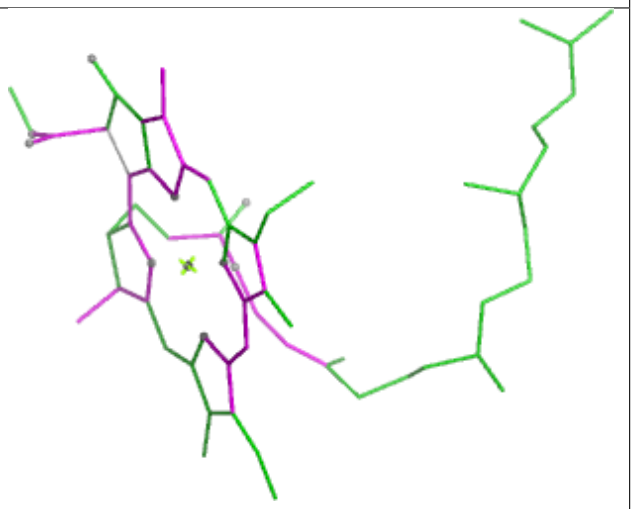
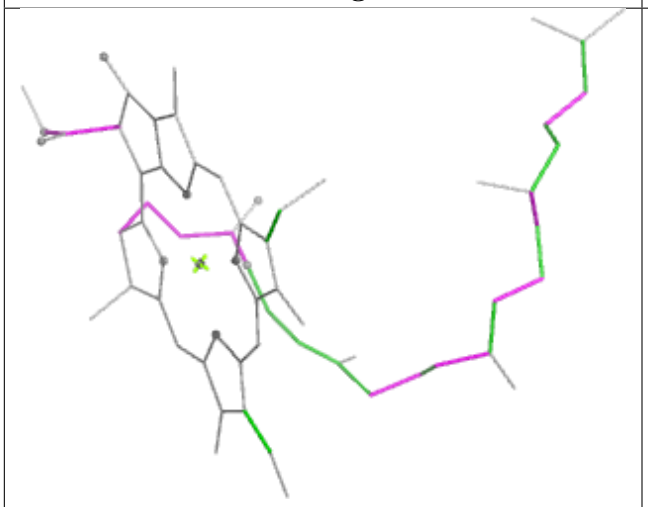


Bond angles



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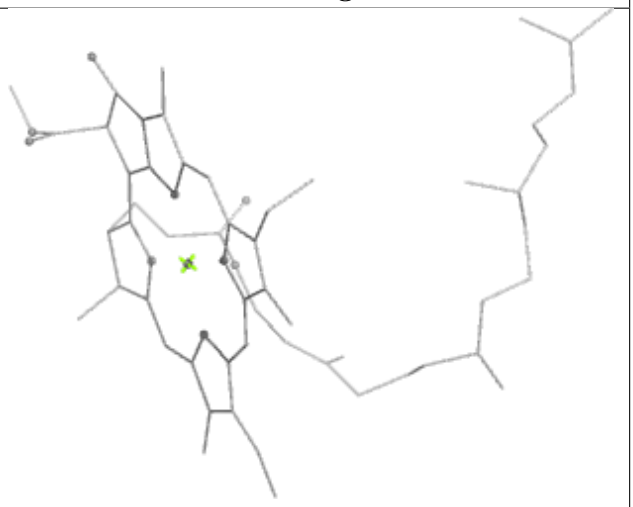
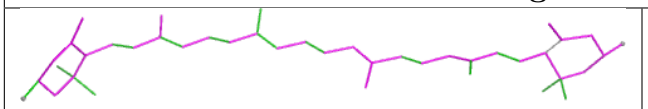


Rings

Ligand LUT 3 302



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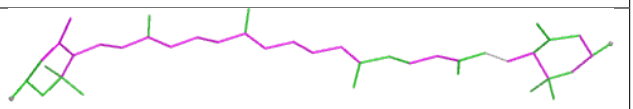
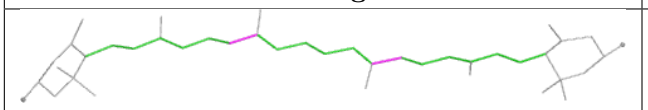


Bond angles



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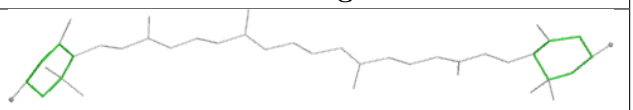

Rings

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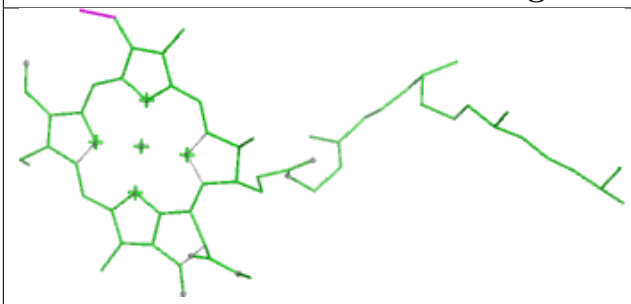
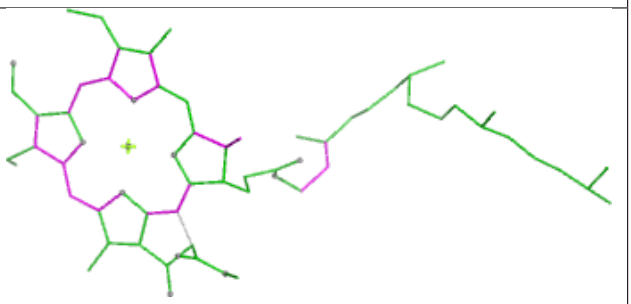
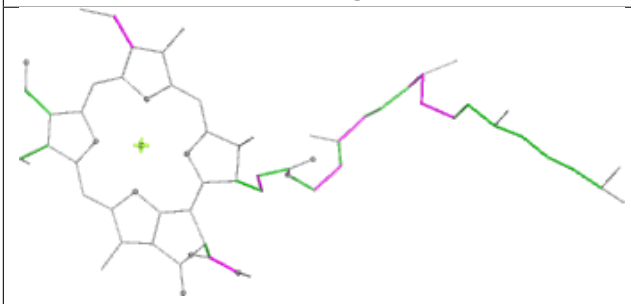
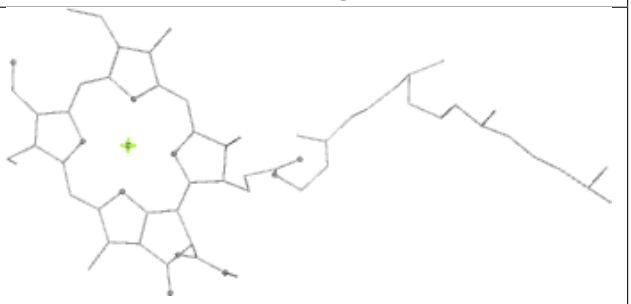
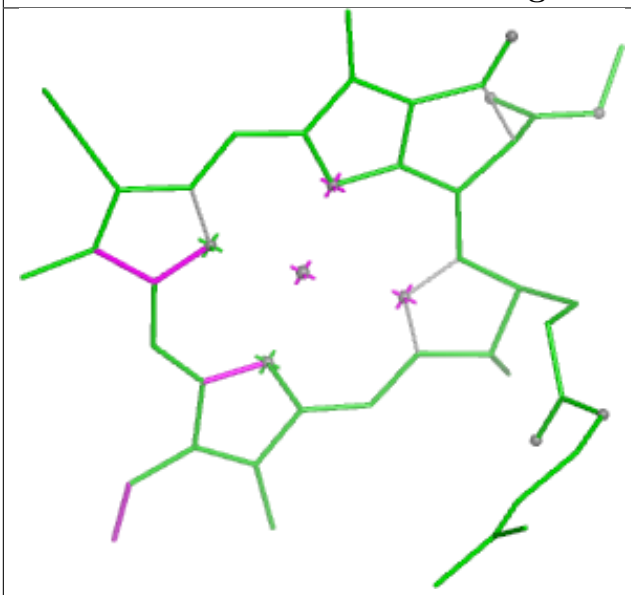
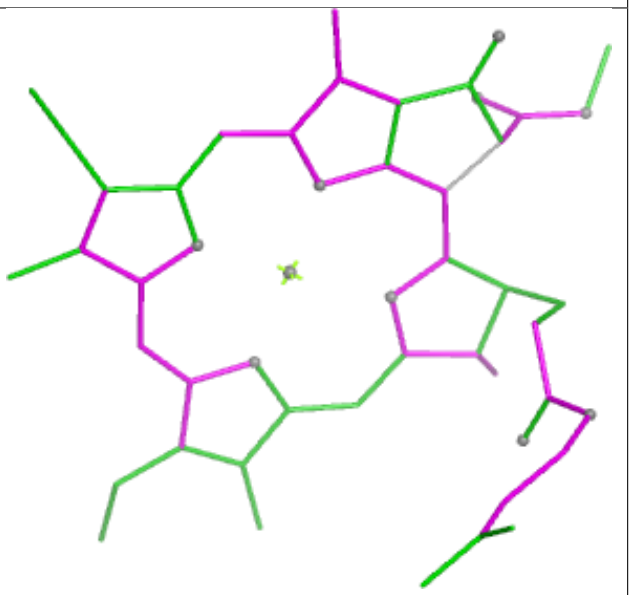
 Bond lengths	 Bond angles
 Torsions	 Rings

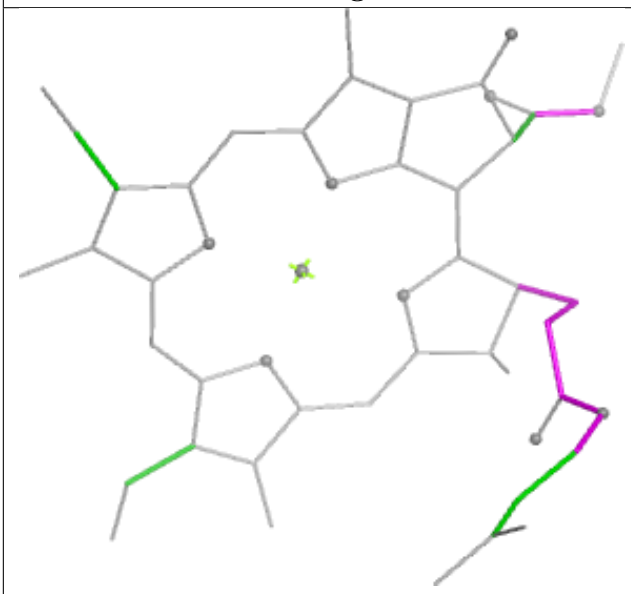
Ligand CLA 9 308



Bond lengths



Bond angles



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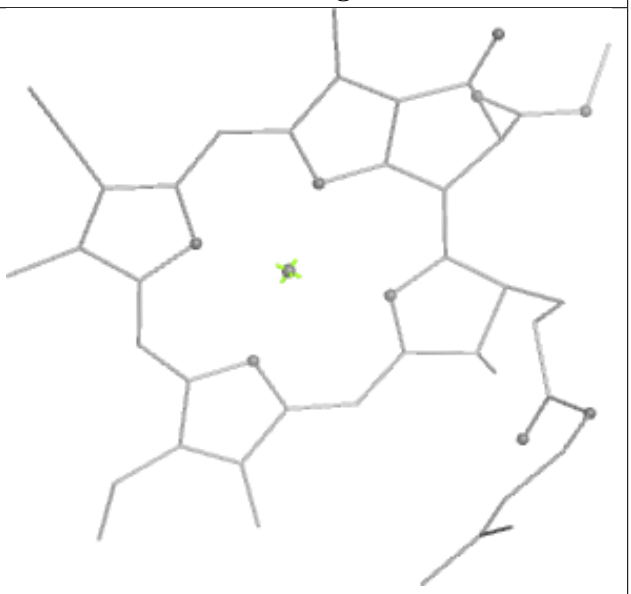
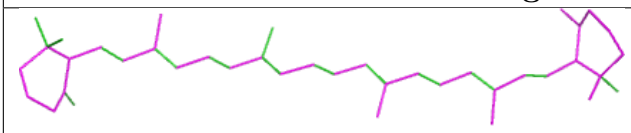


Rings

Ligand BCR B 845



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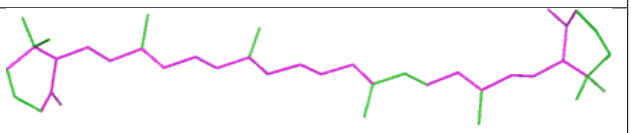
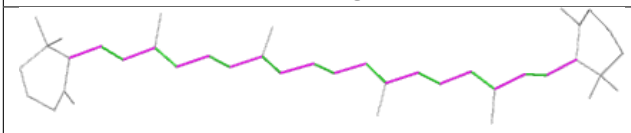


Bond angles



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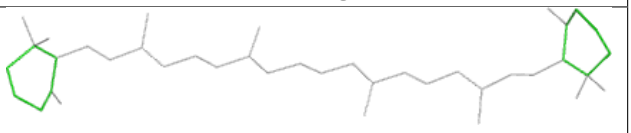
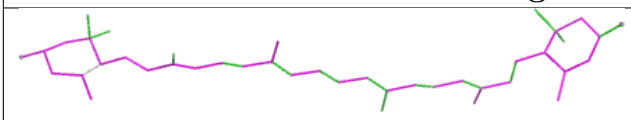


Rings

Ligand LUT 1 302



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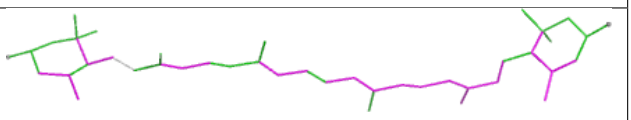

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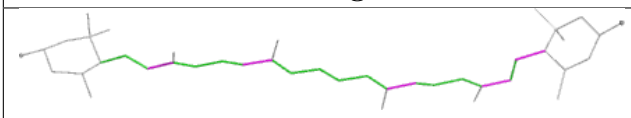

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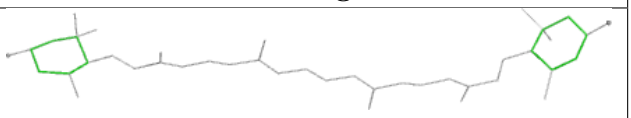
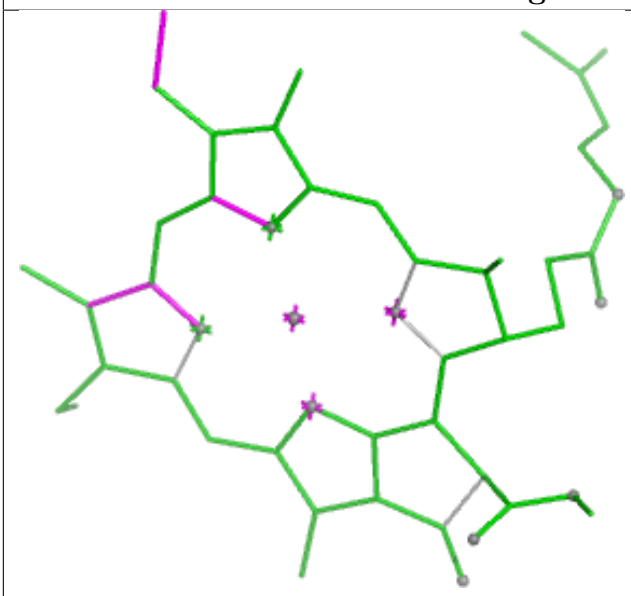


Rings

Ligand CLA 5 312



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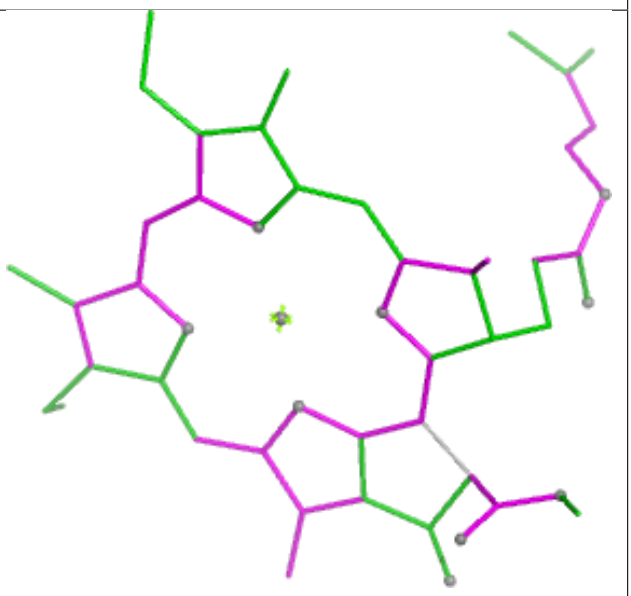
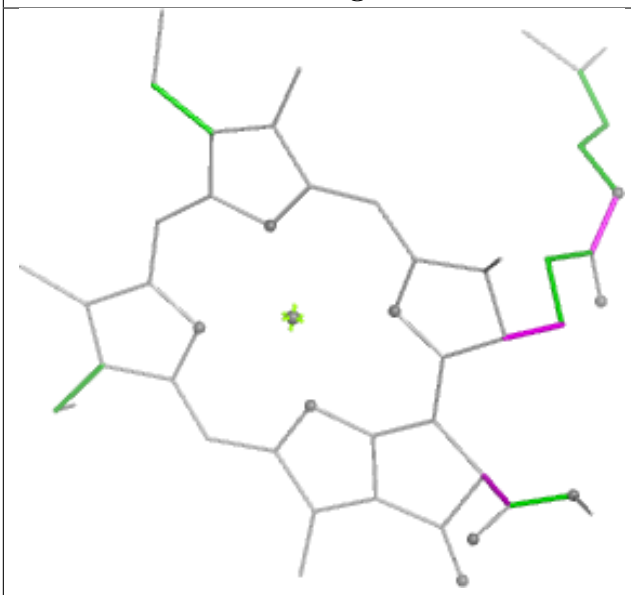


Bond angles



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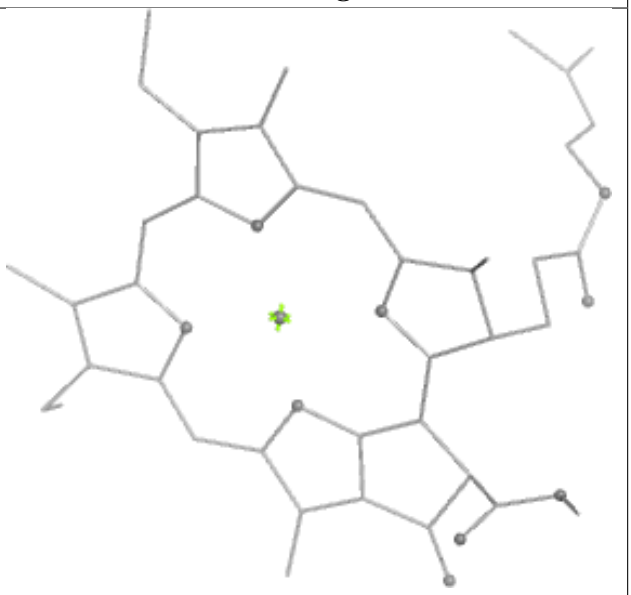
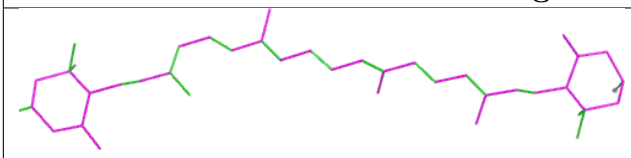


Rings

Ligand C7Z 5 306



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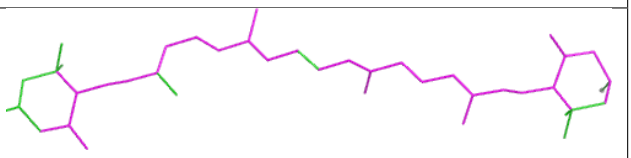
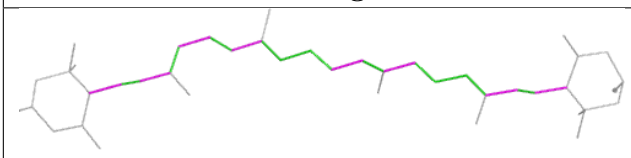


Bond angles



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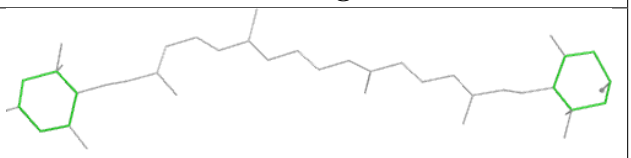
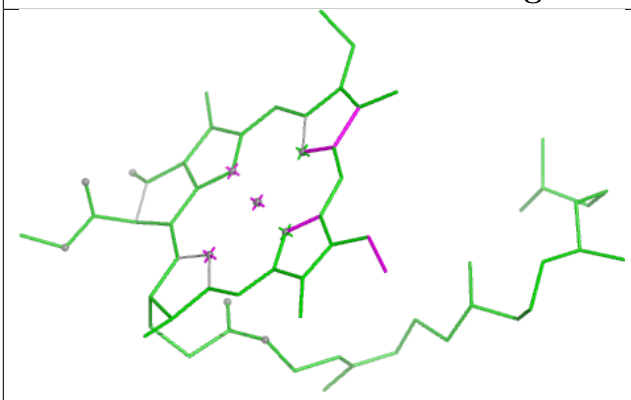


Rings

Ligand CLA B 833



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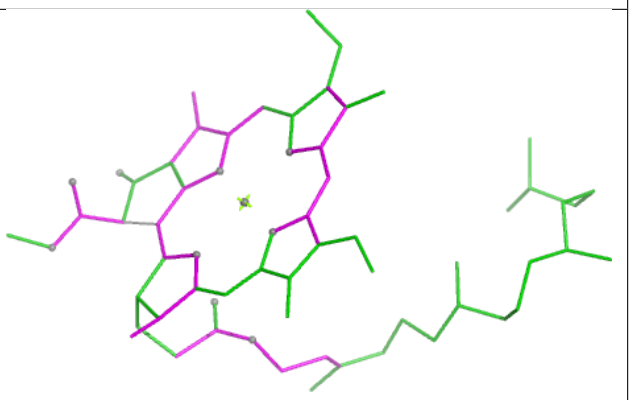
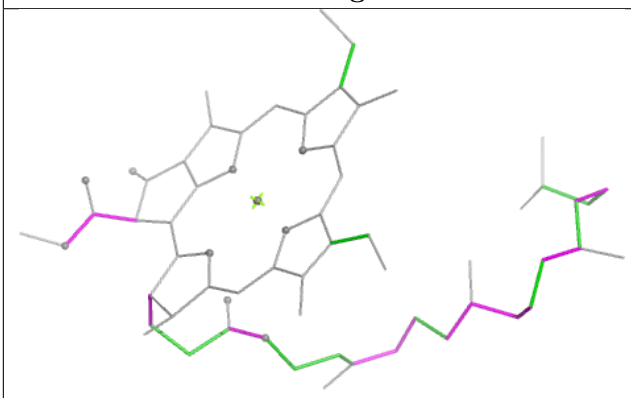


Bond angles



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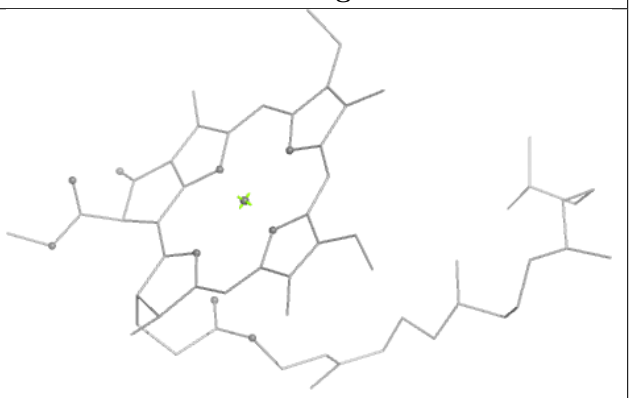
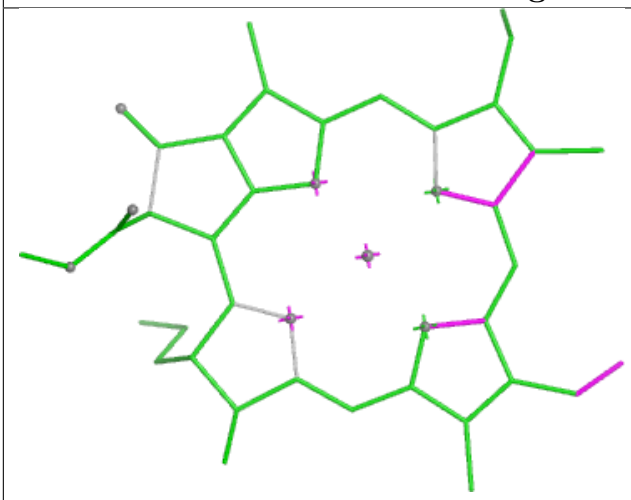


Rings

Ligand CLA 7 311



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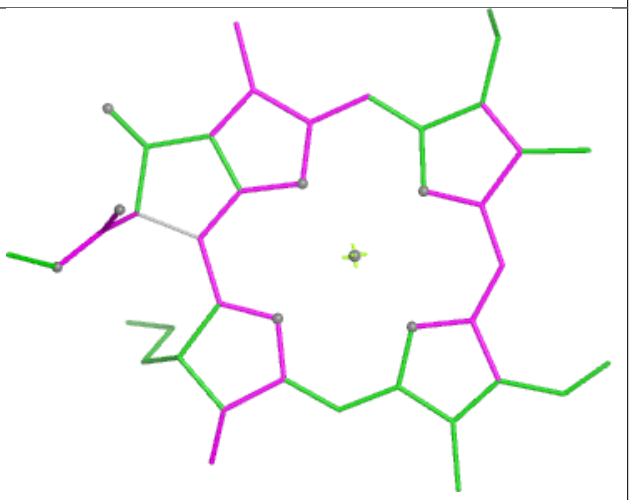
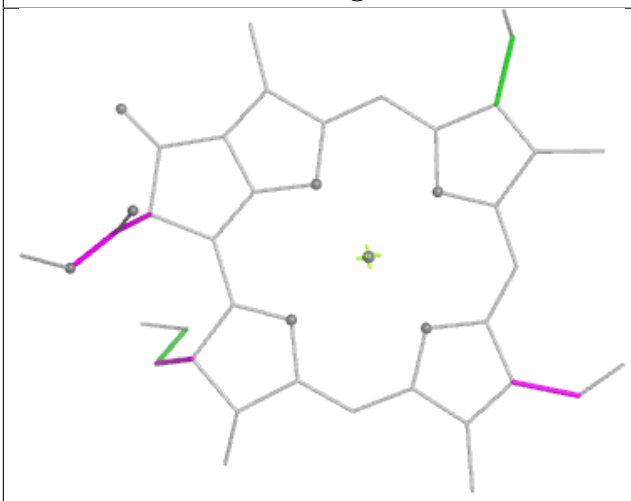
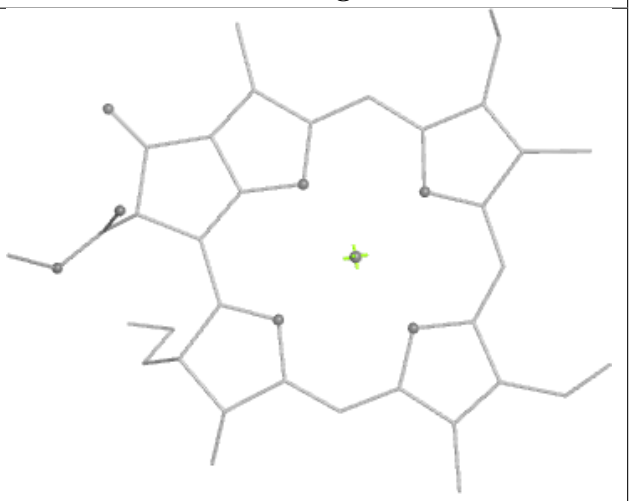


Bond angles

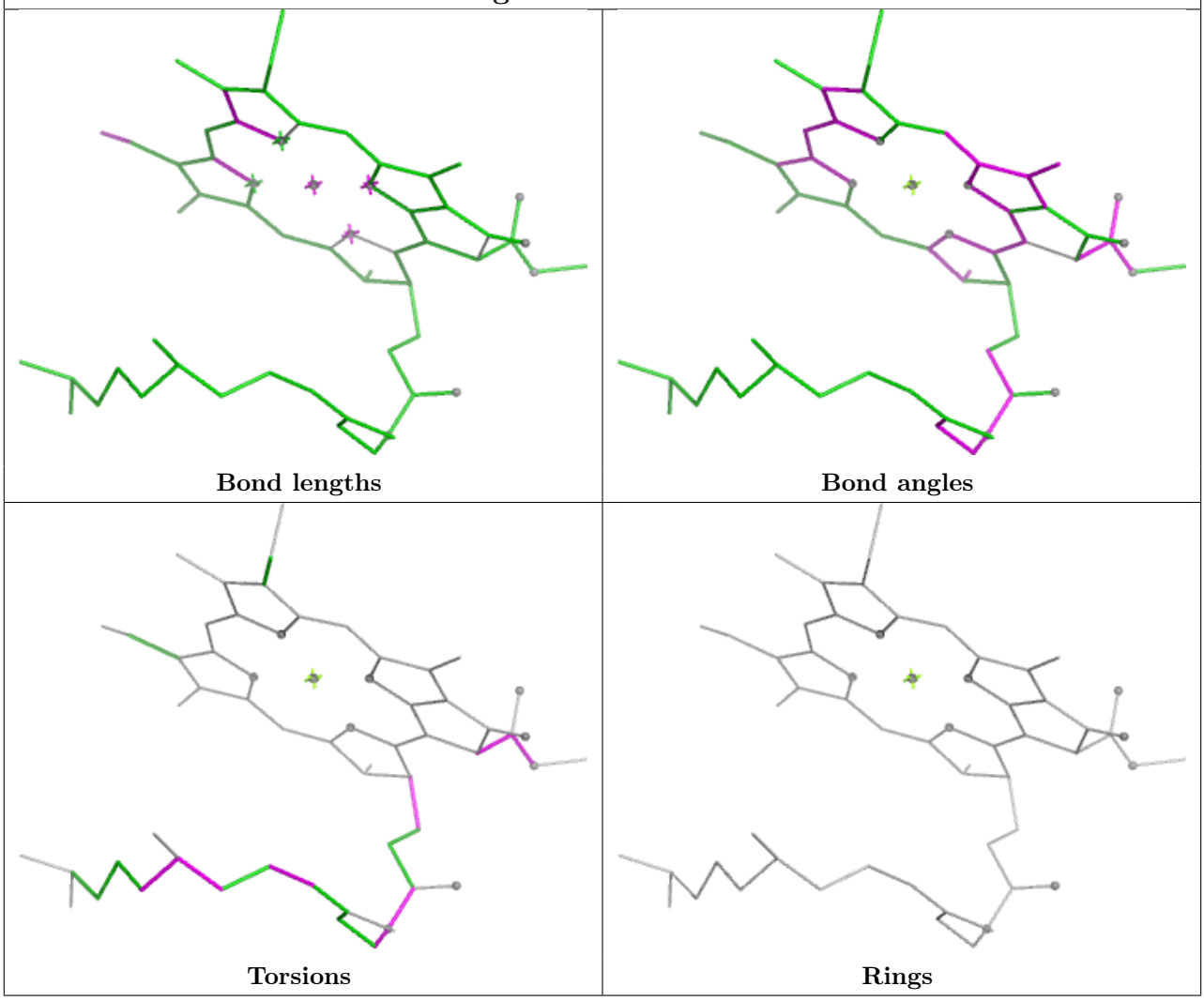


Torsions

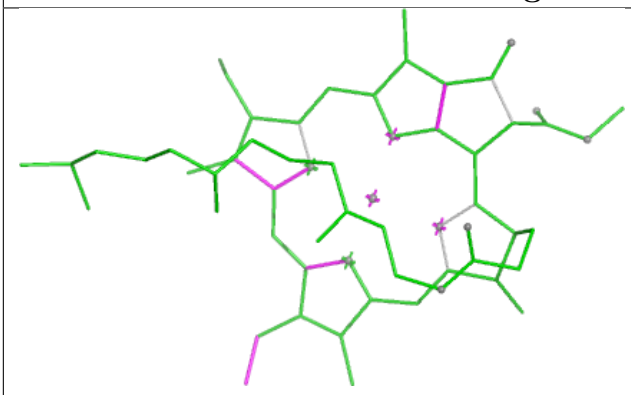


Rings

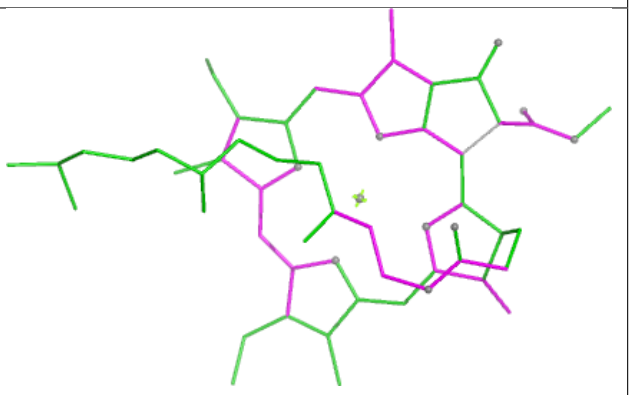
Ligand CLA B 816



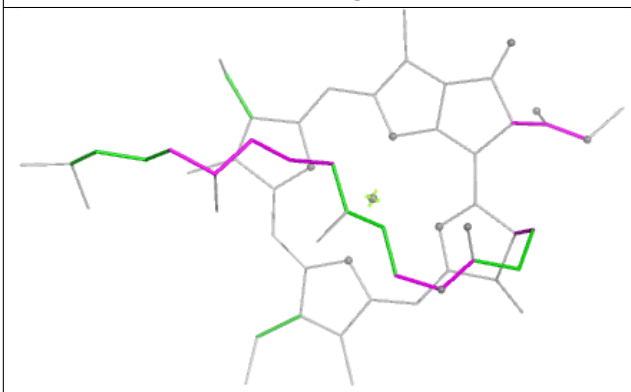
Ligand CLA A 818



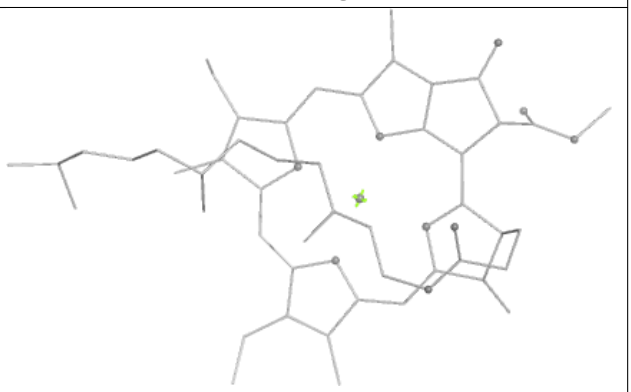
Bond lengths



Bond angles

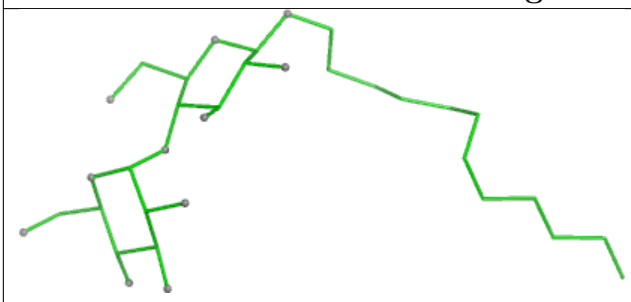


Torsions

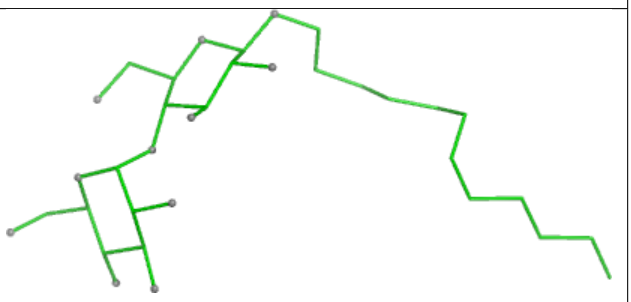


Rings

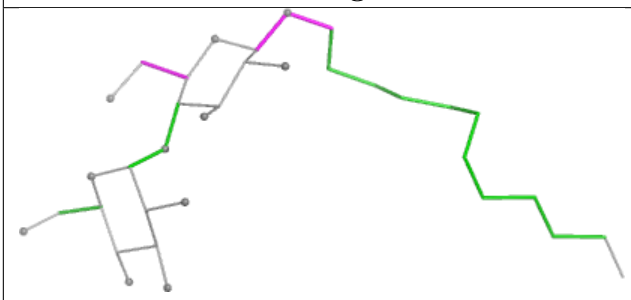
Ligand LMT 1 301



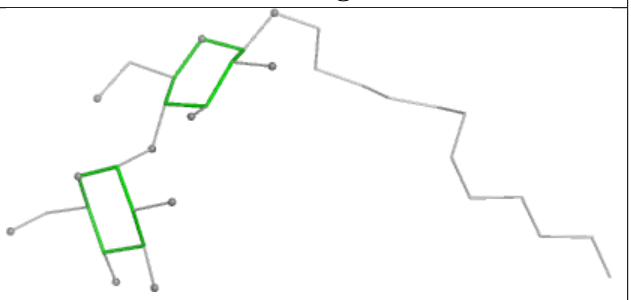
Bond lengths



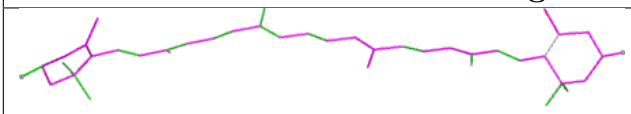
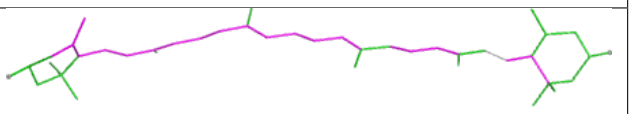
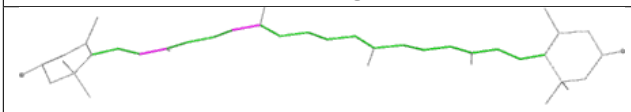
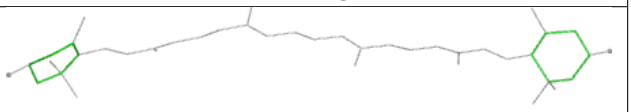
Bond angles

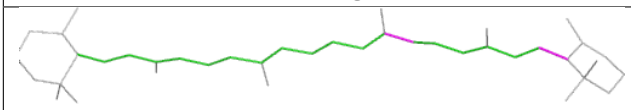
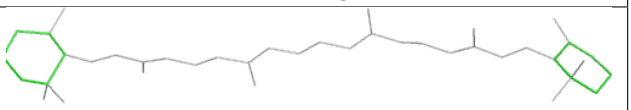


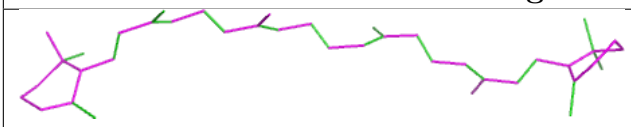
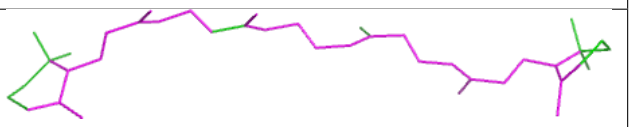
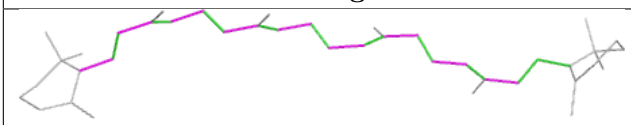
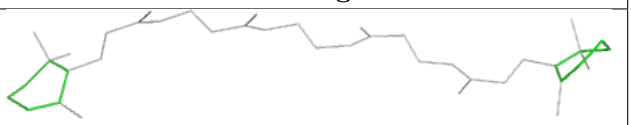
Torsions



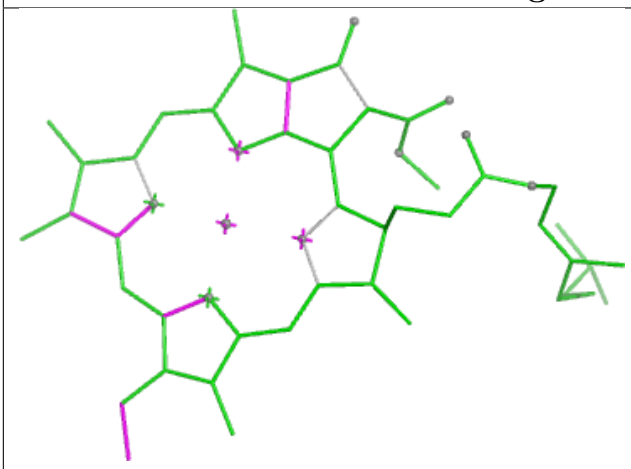
Rings

Ligand LUT 9 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

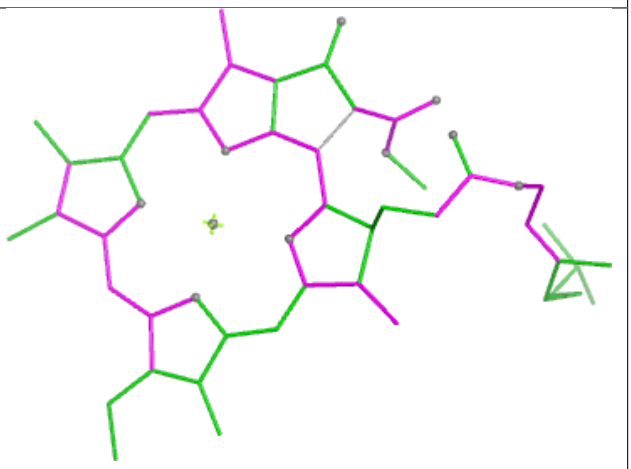
Ligand LUT 8 303	
Bond lengths	Bond angles
 Torsions	 Rings

Ligand BCR 5 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

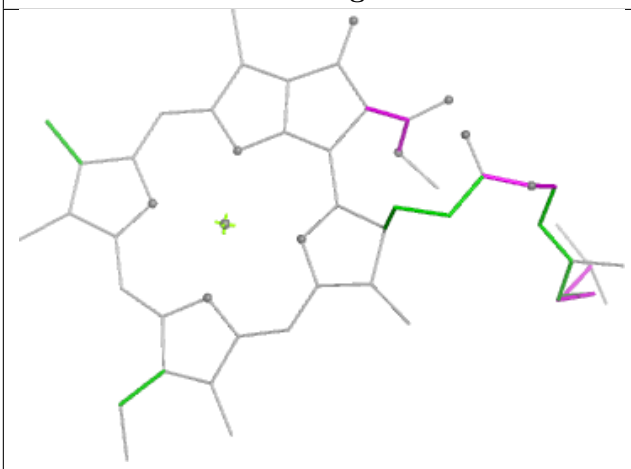
Ligand CLA 9 307



Bond lengths



Bond angles



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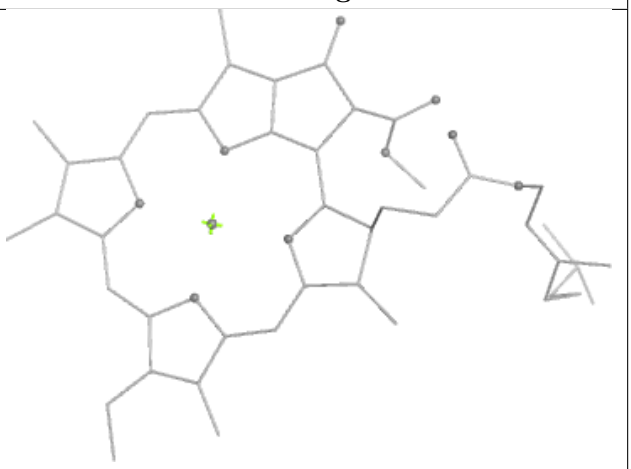
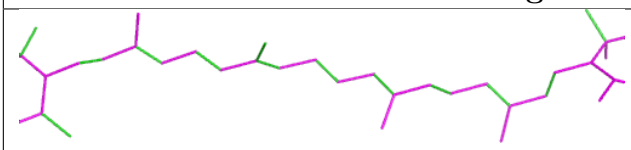
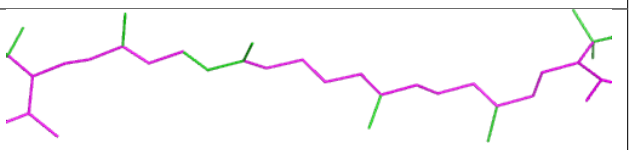


Rings

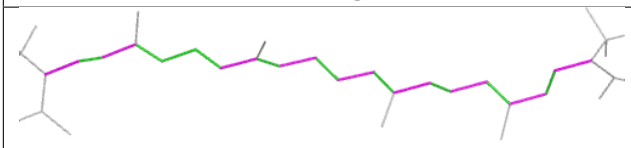
Ligand BCR J 104



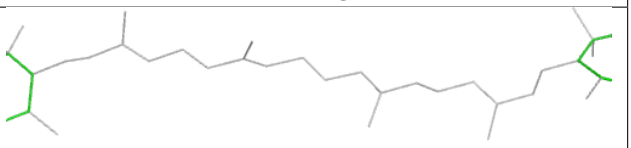
Bond lengths



Bond angles

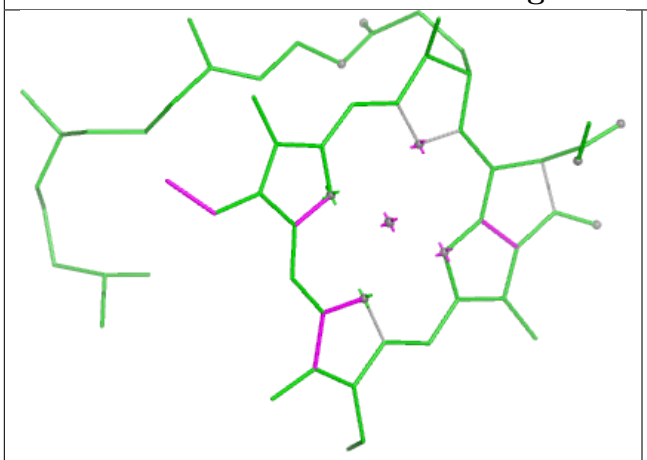


Torsions

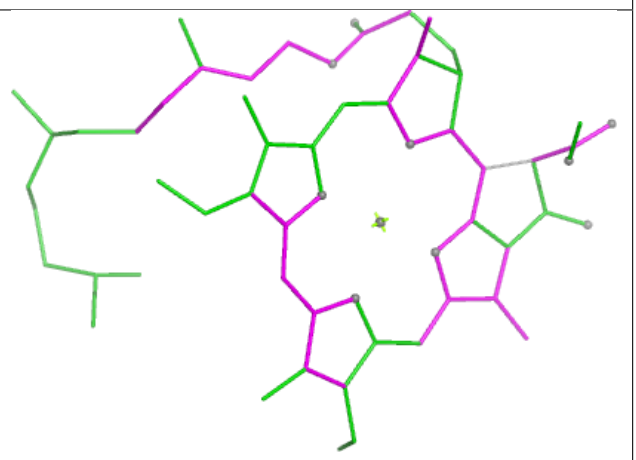


Rings

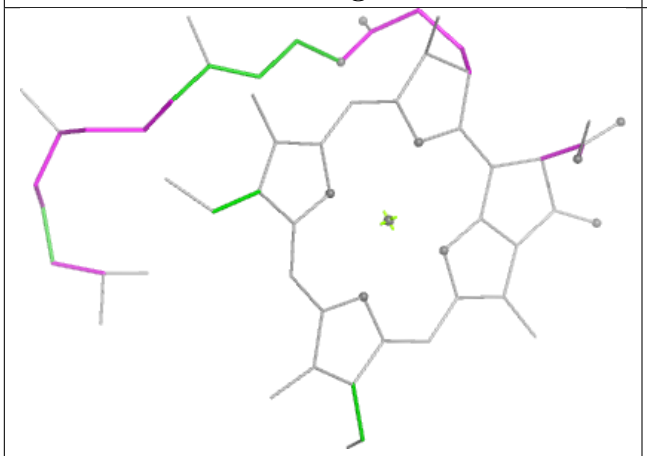
Ligand CLA Z 306



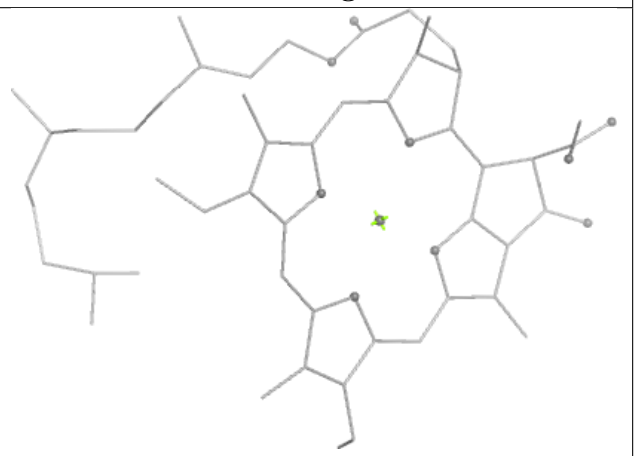
Bond lengths



Bond angles

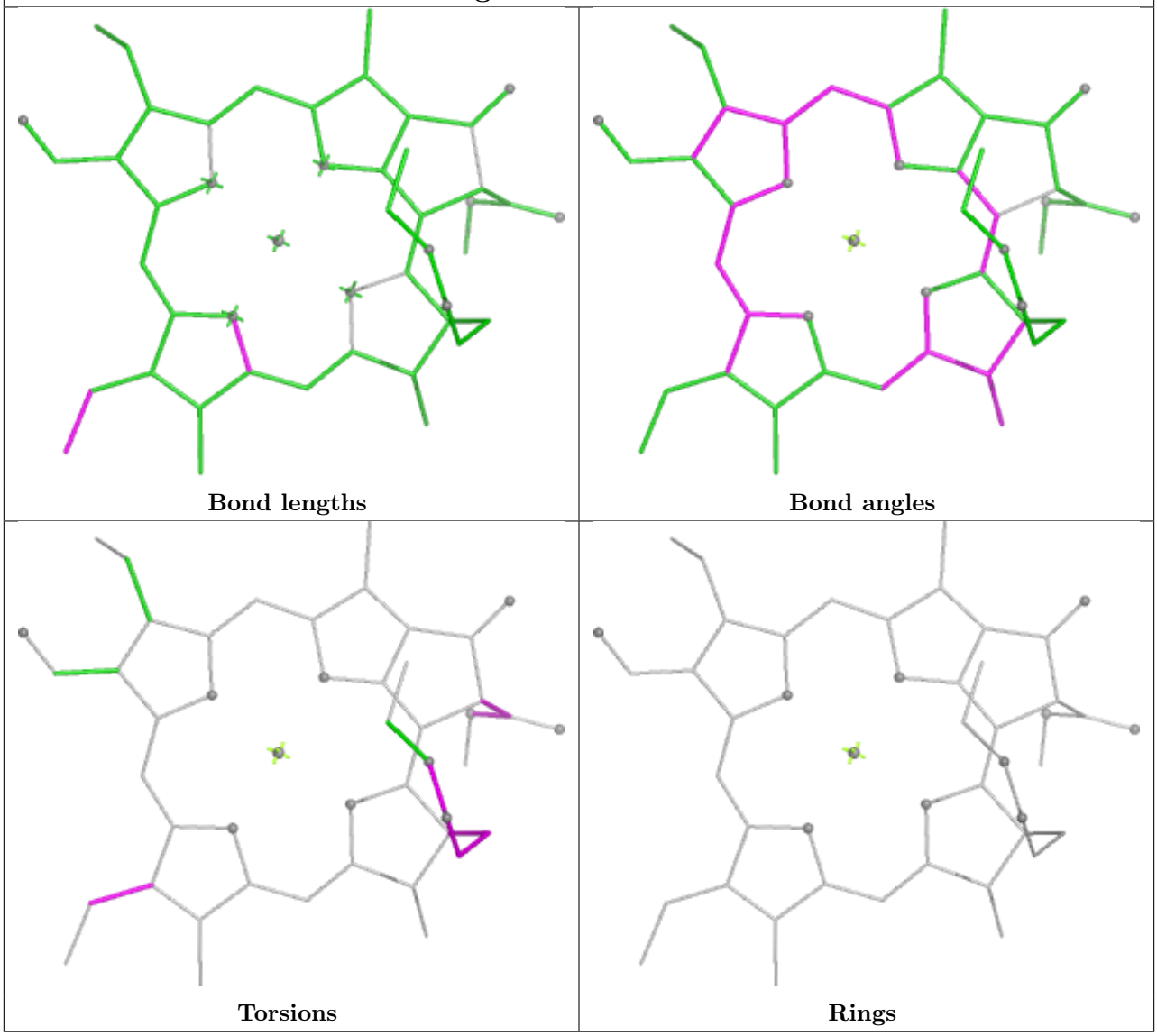


Torsions

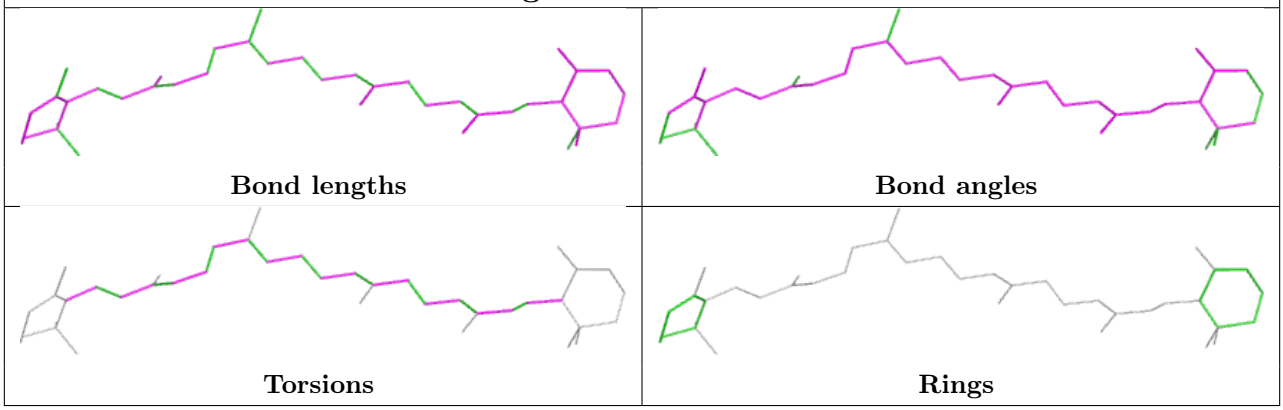


Rings

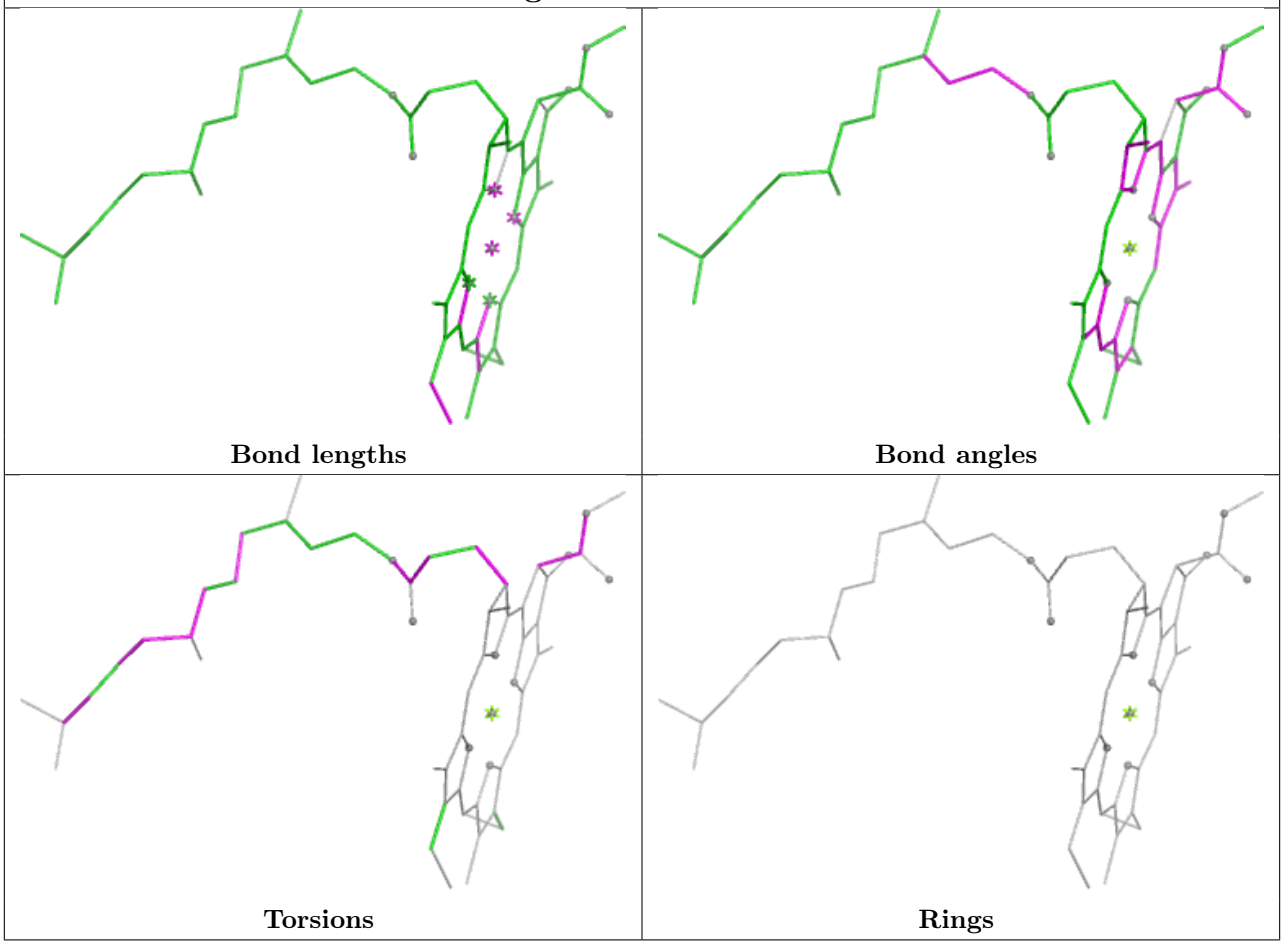
Ligand CHL Z 312



Ligand BCR G 203



Ligand CLA A 807



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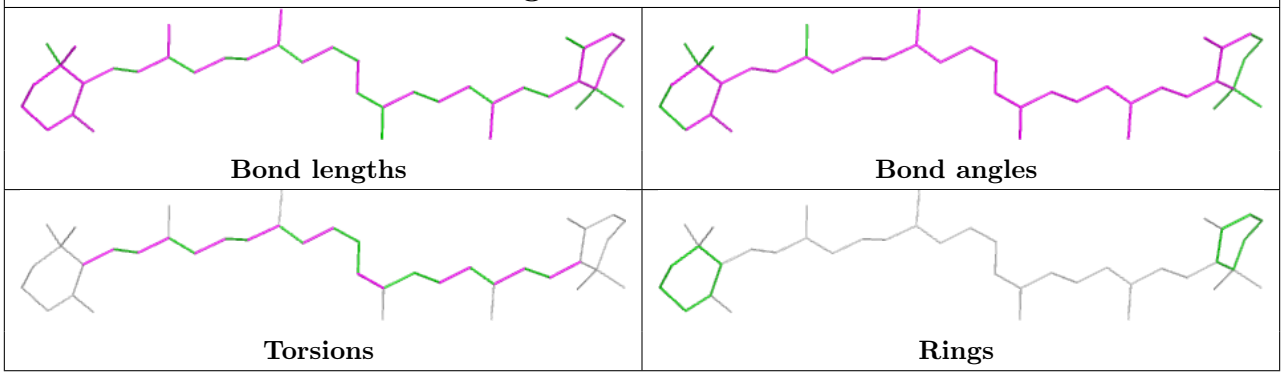
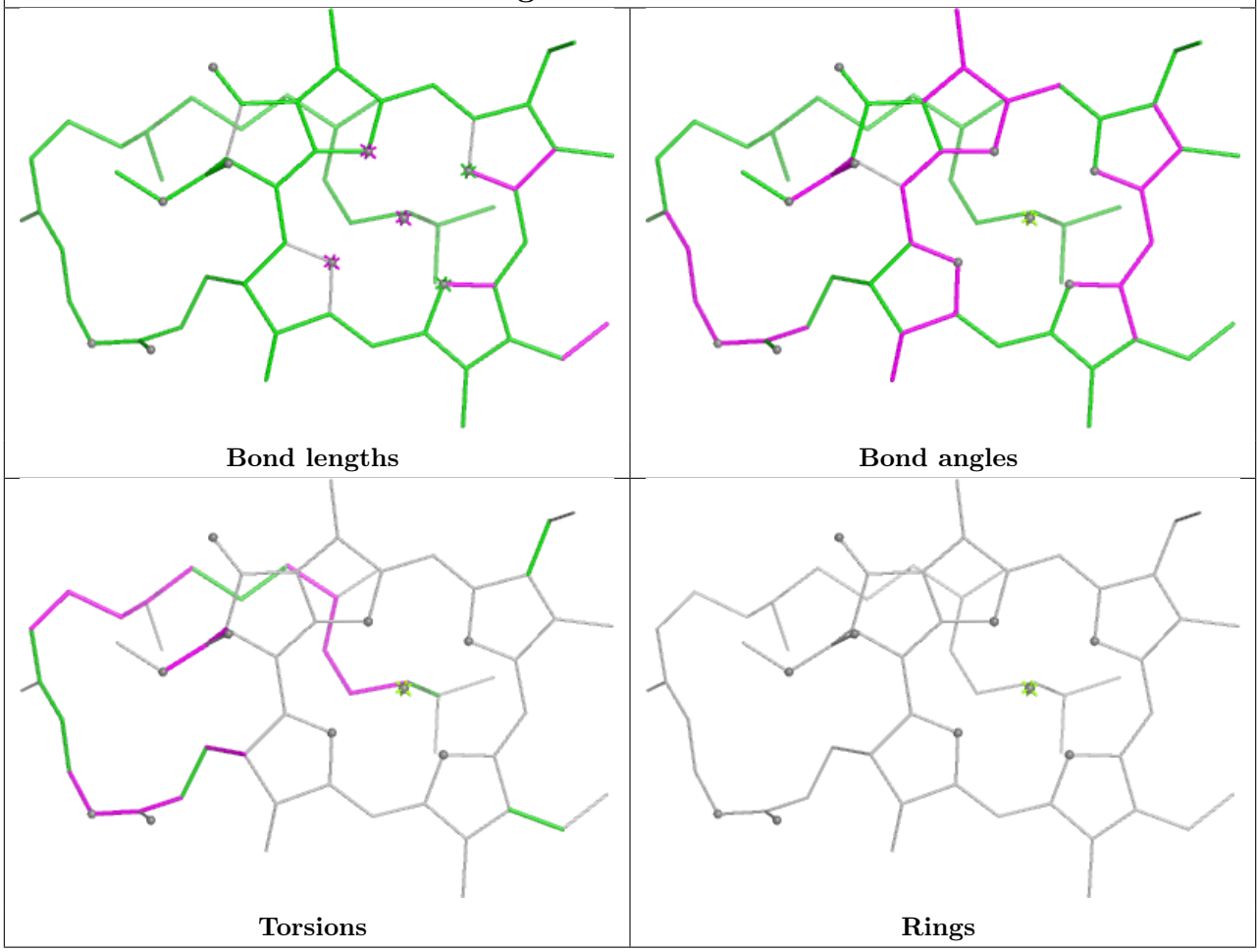
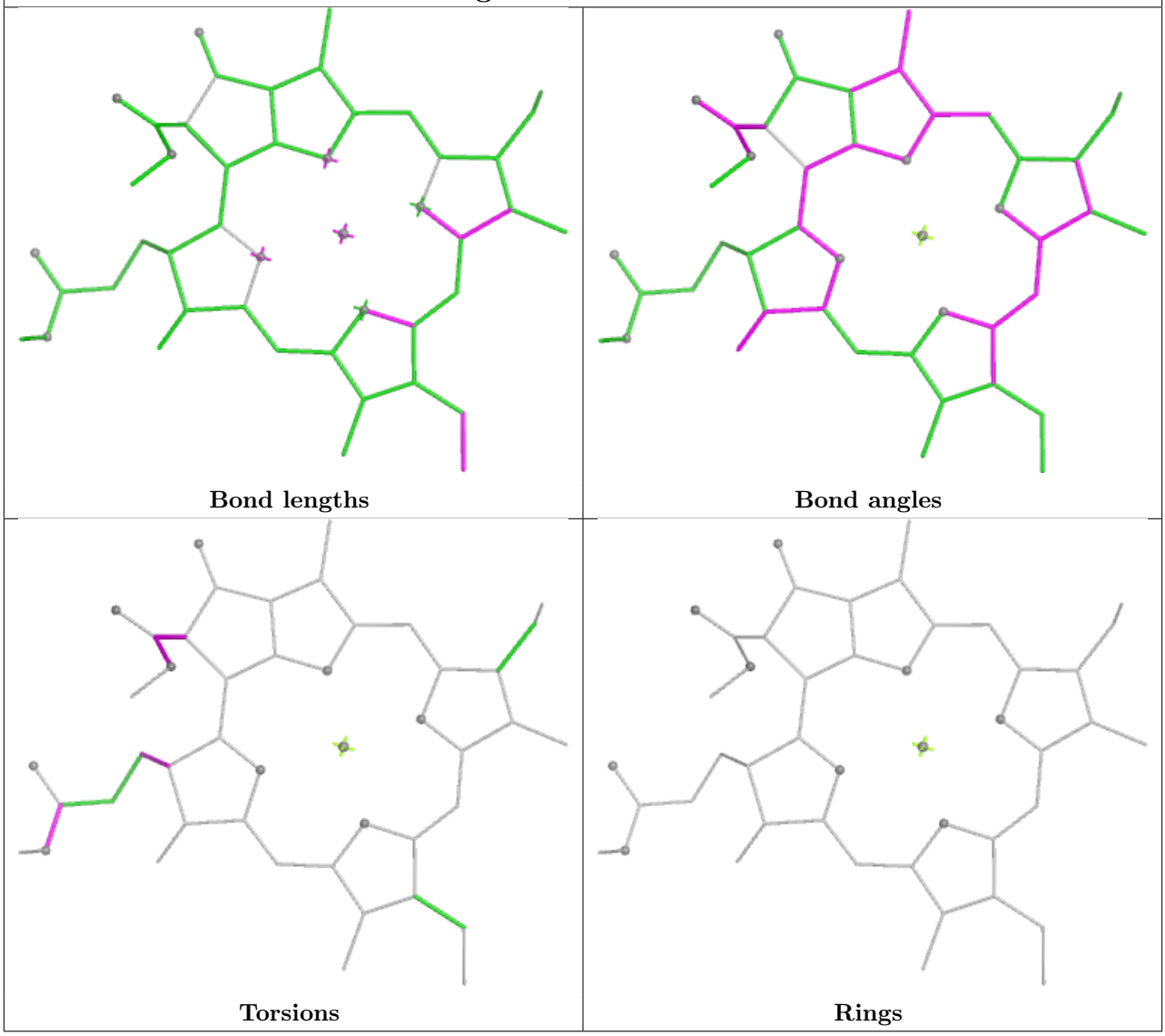


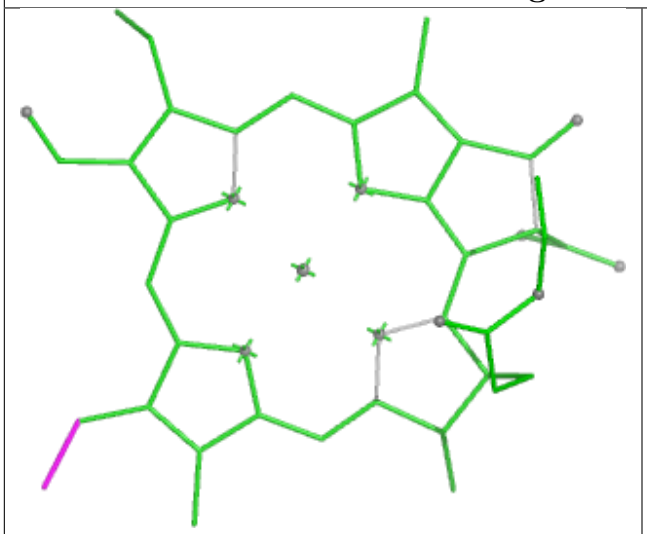
Ligand CLA Z 316



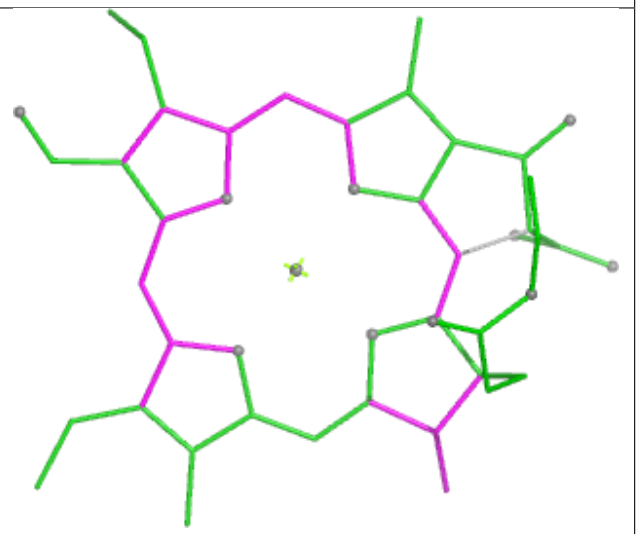
Ligand CLA G 202



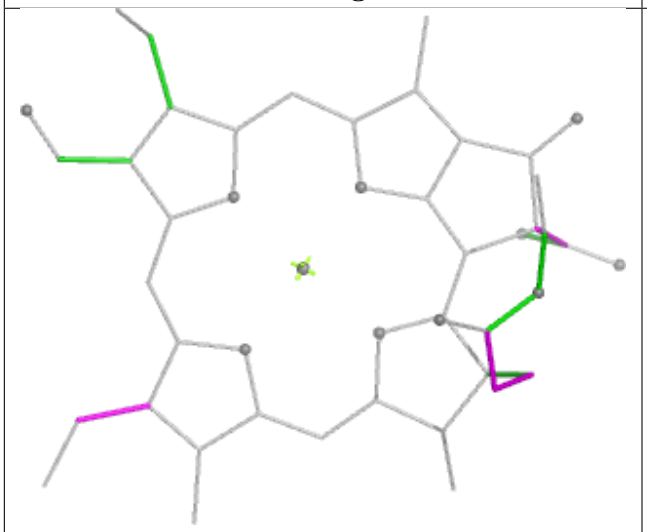
Ligand CHL 1 312



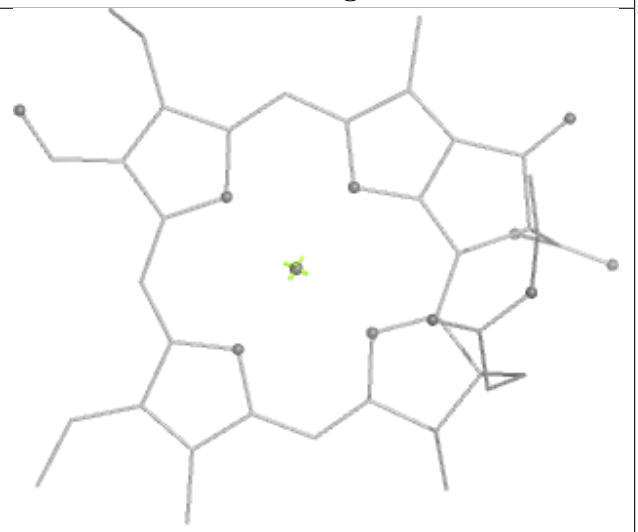
Bond lengths



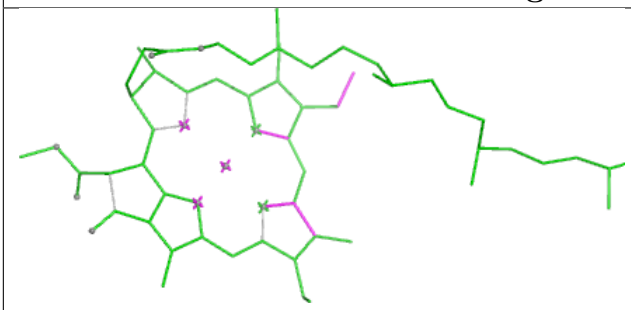
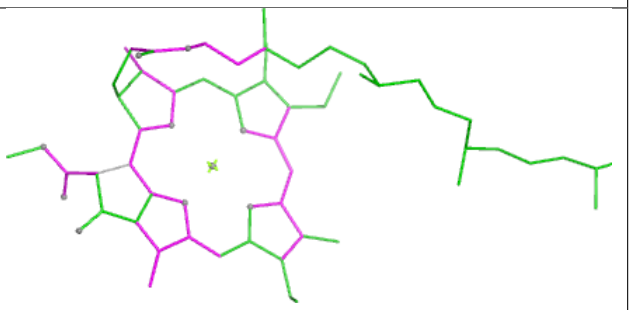
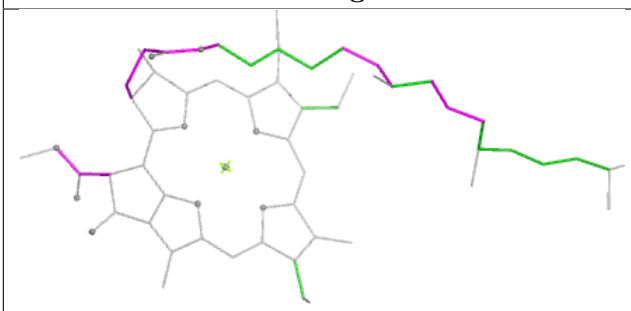
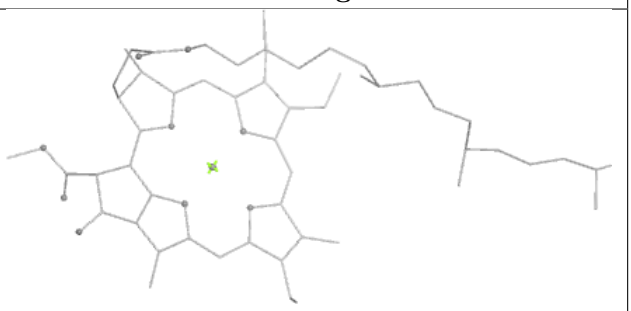
Bond angles

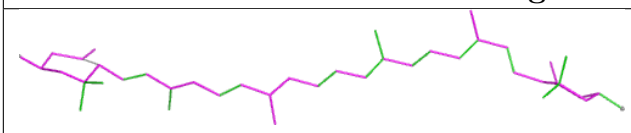
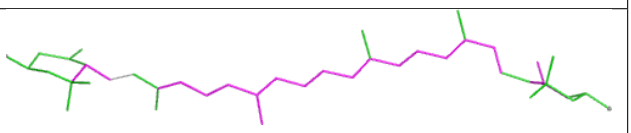
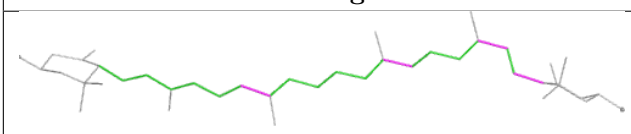
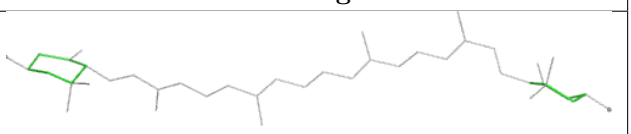


Torsions

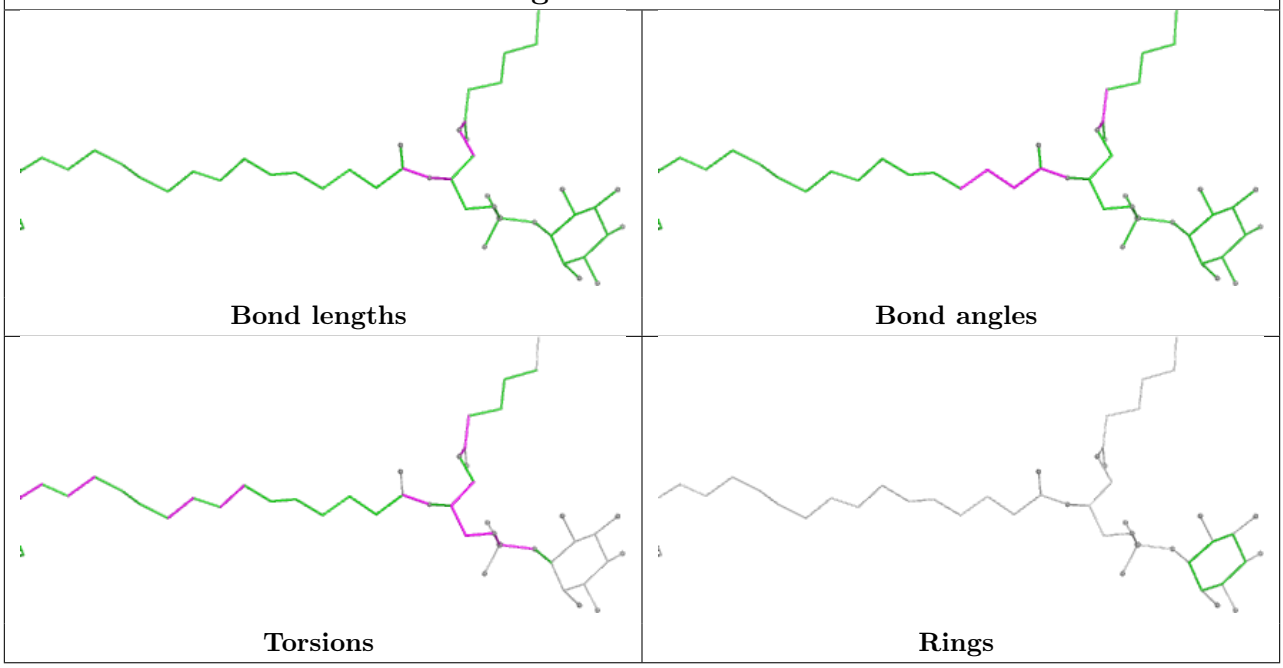


Rings

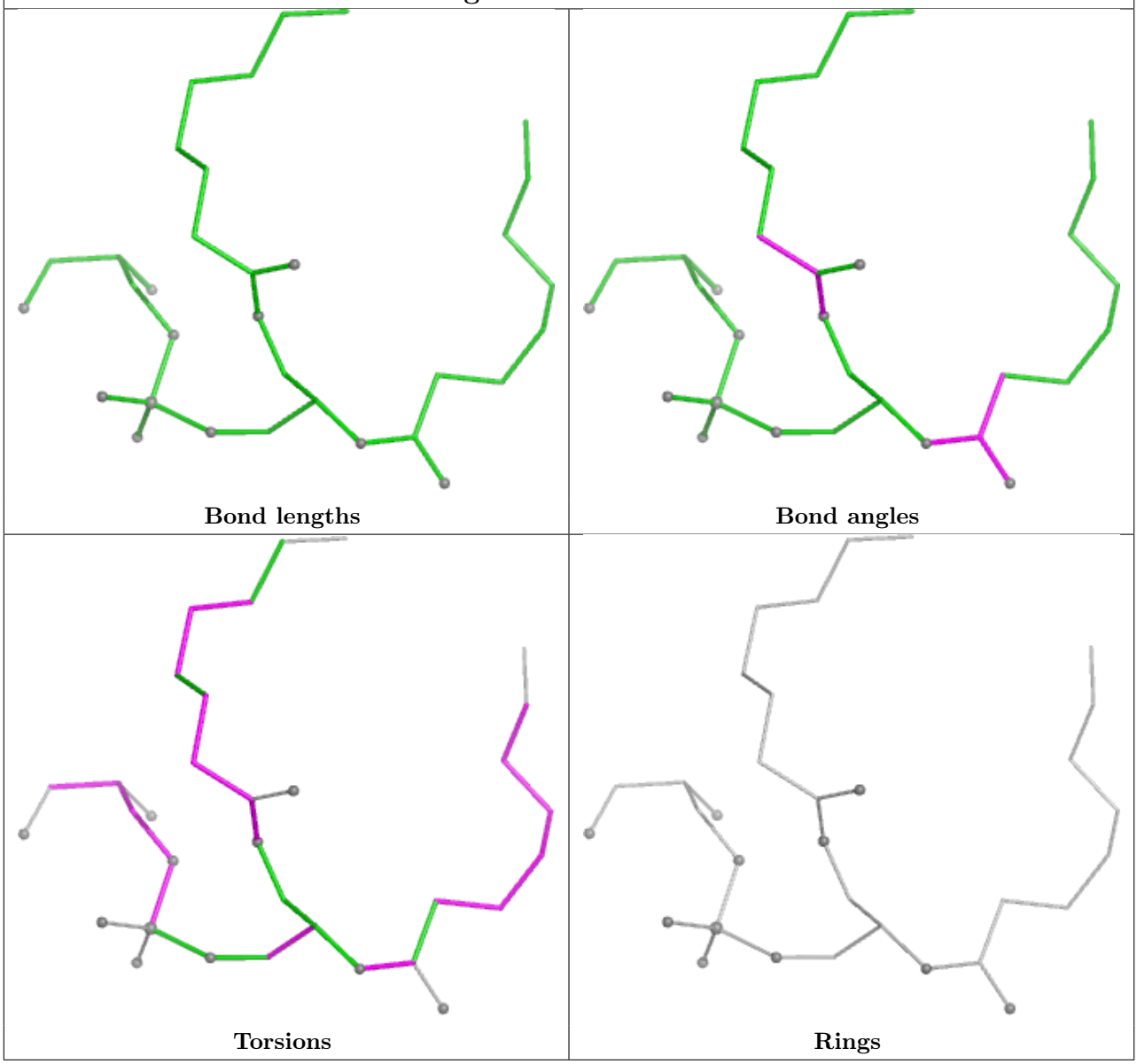
Ligand CLA Z 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 3 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand T7X J 102

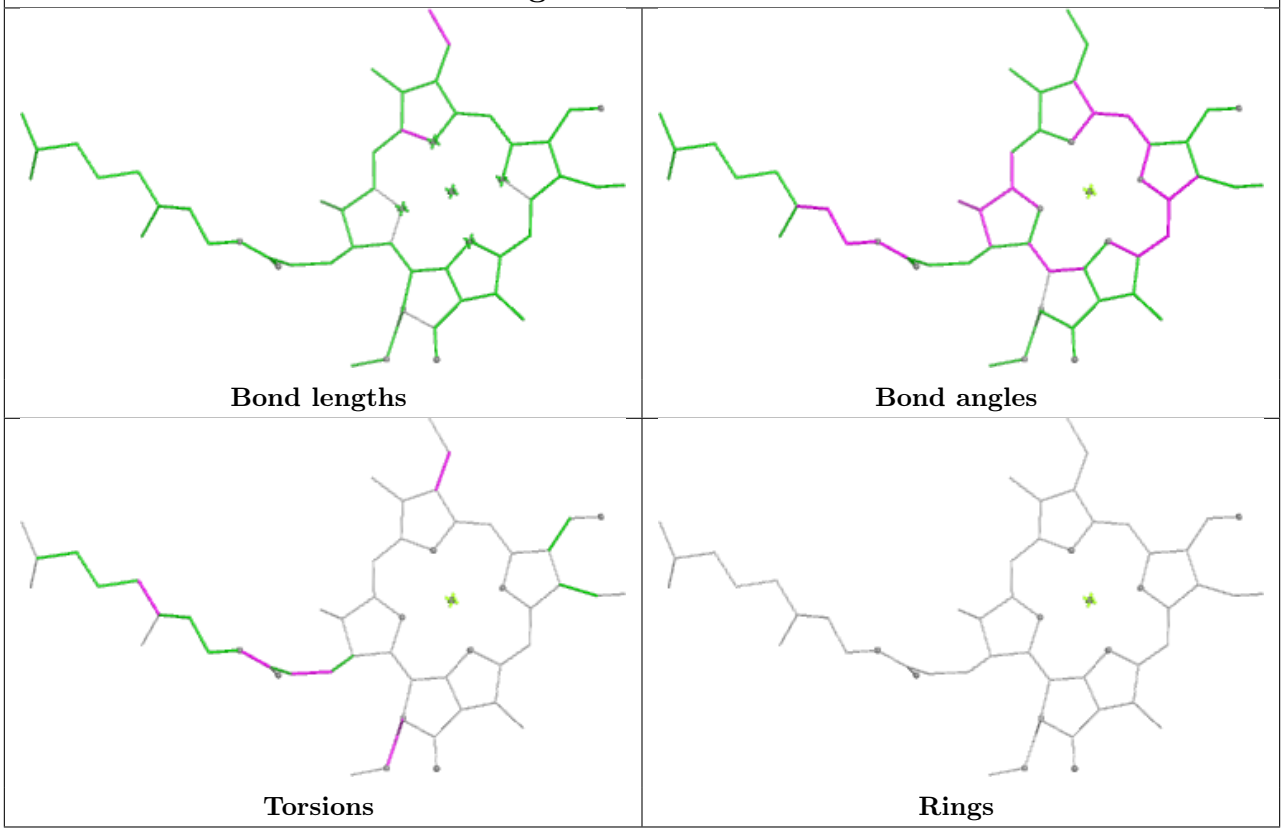


Ligand LHG B 803

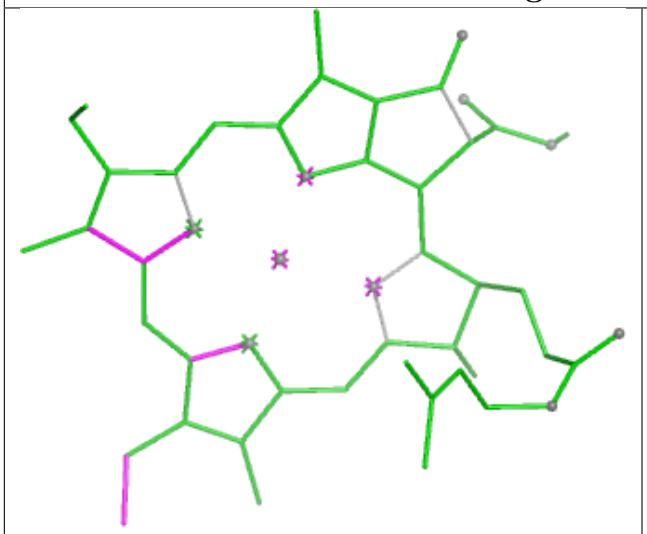


Ligand BCR 5 305

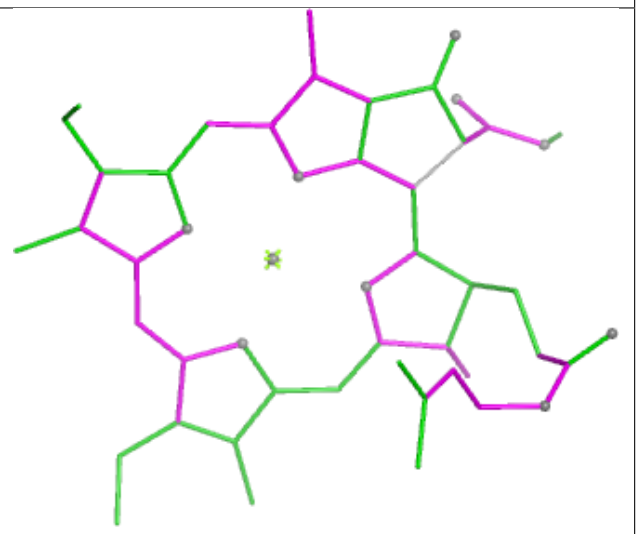
Ligand CHL 6 318



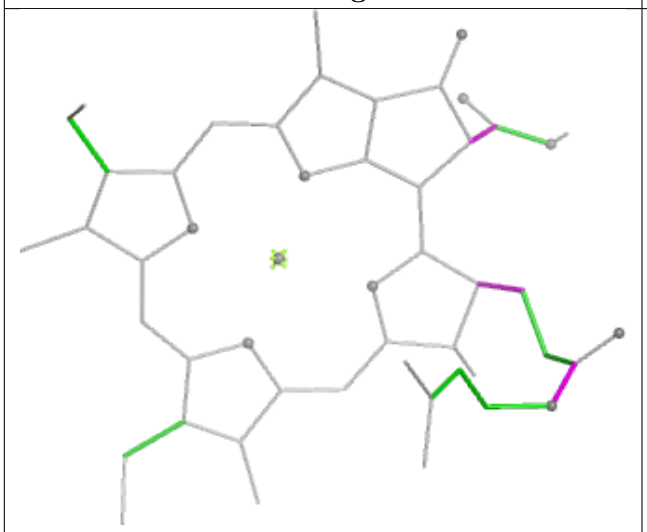
Ligand CLA B 832



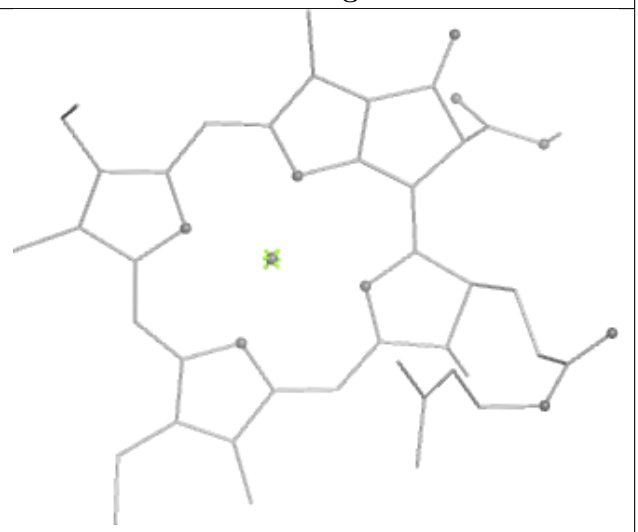
Bond lengths



Bond angles

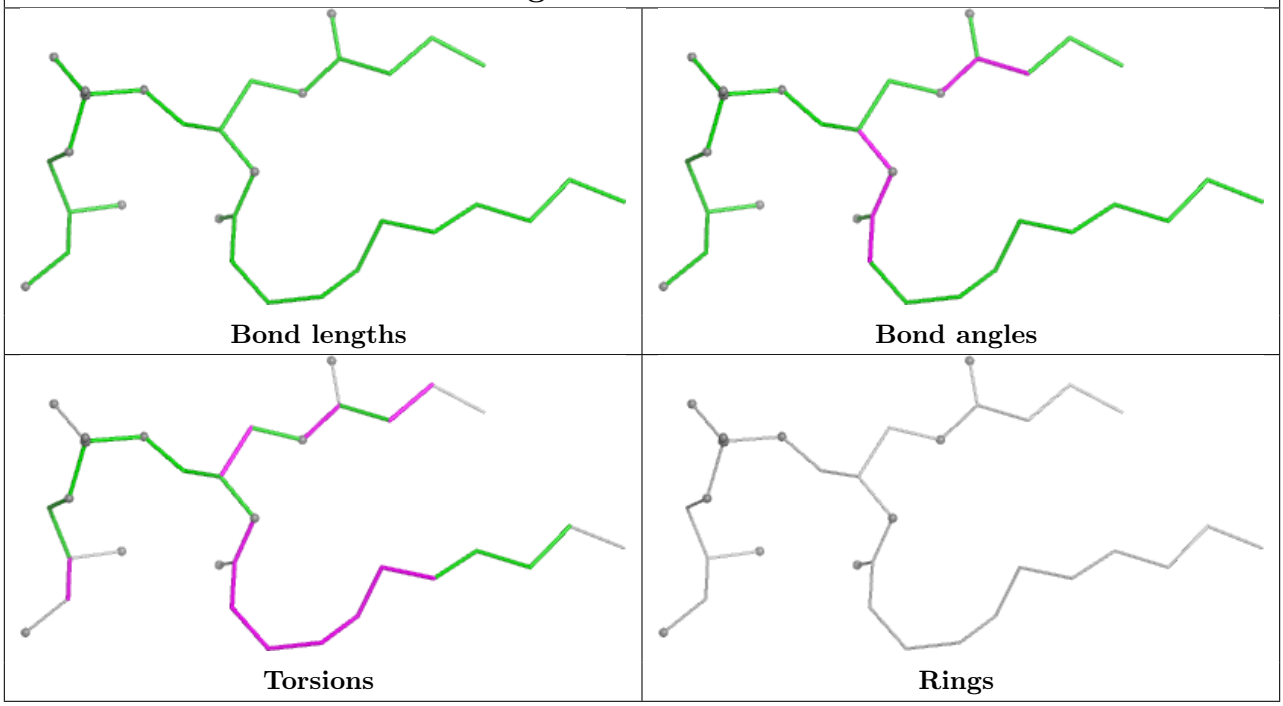


Torsions

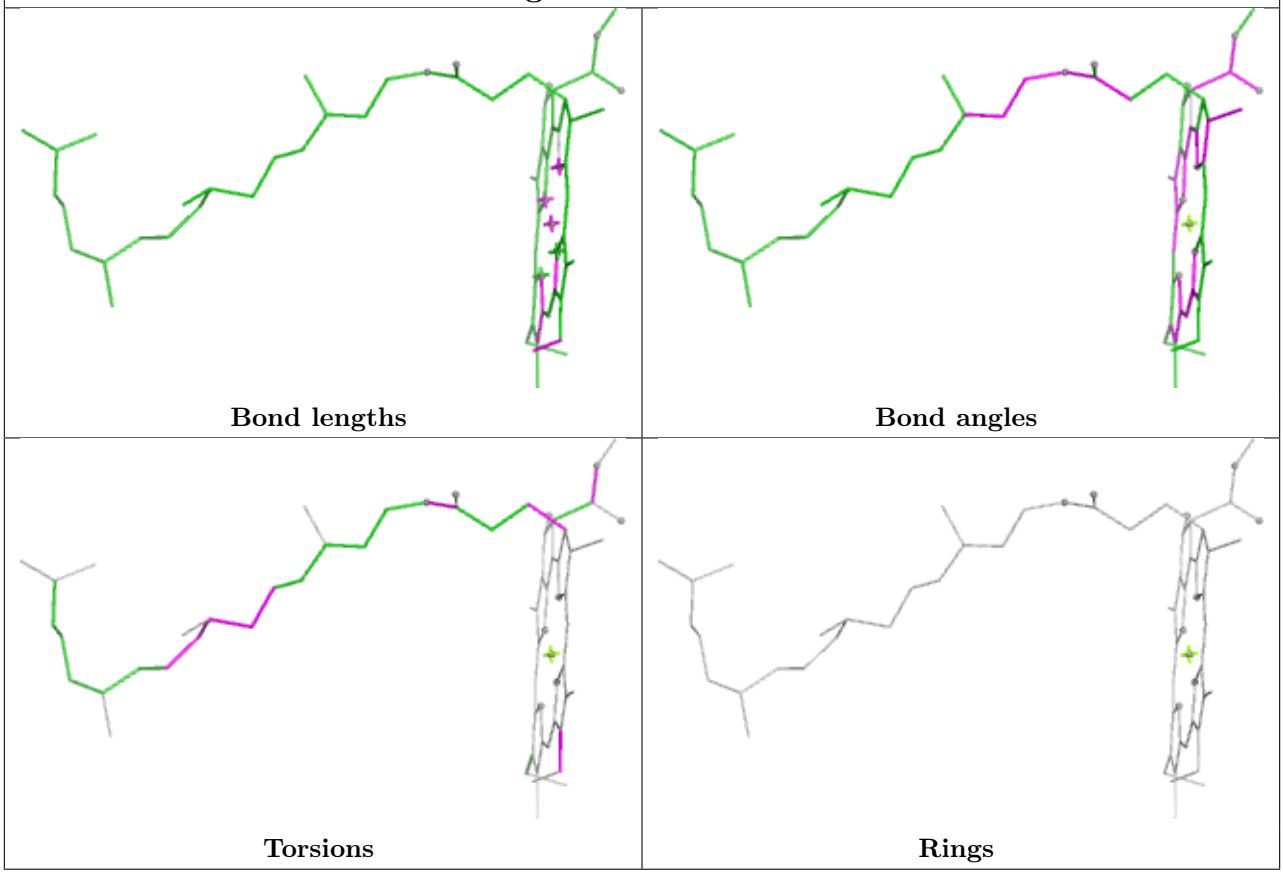


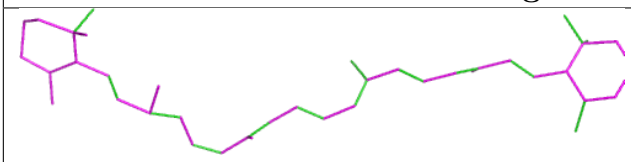
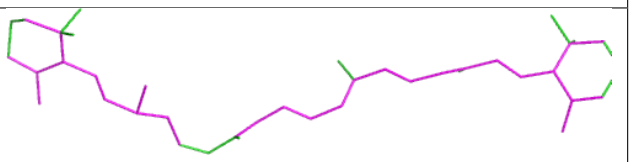
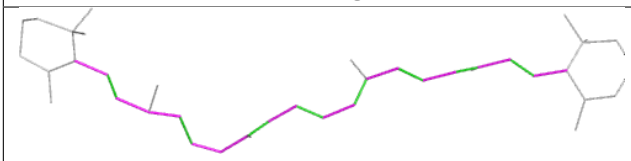
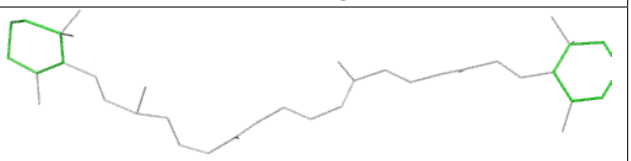
Rings

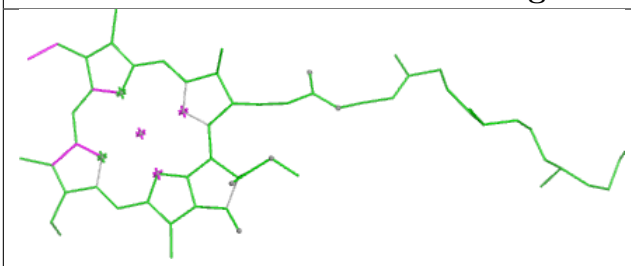
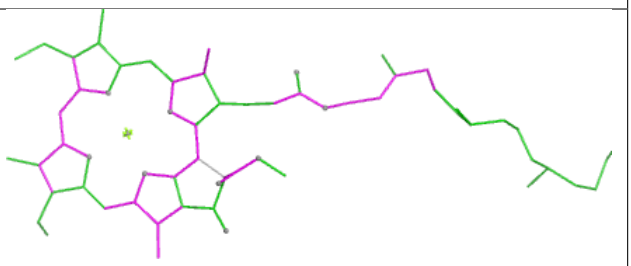
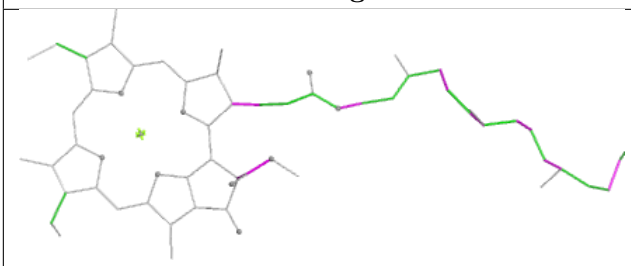
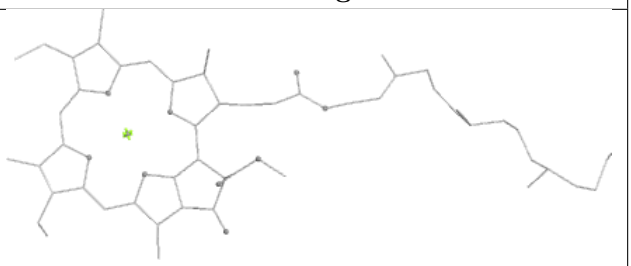
Ligand LHG 4 821



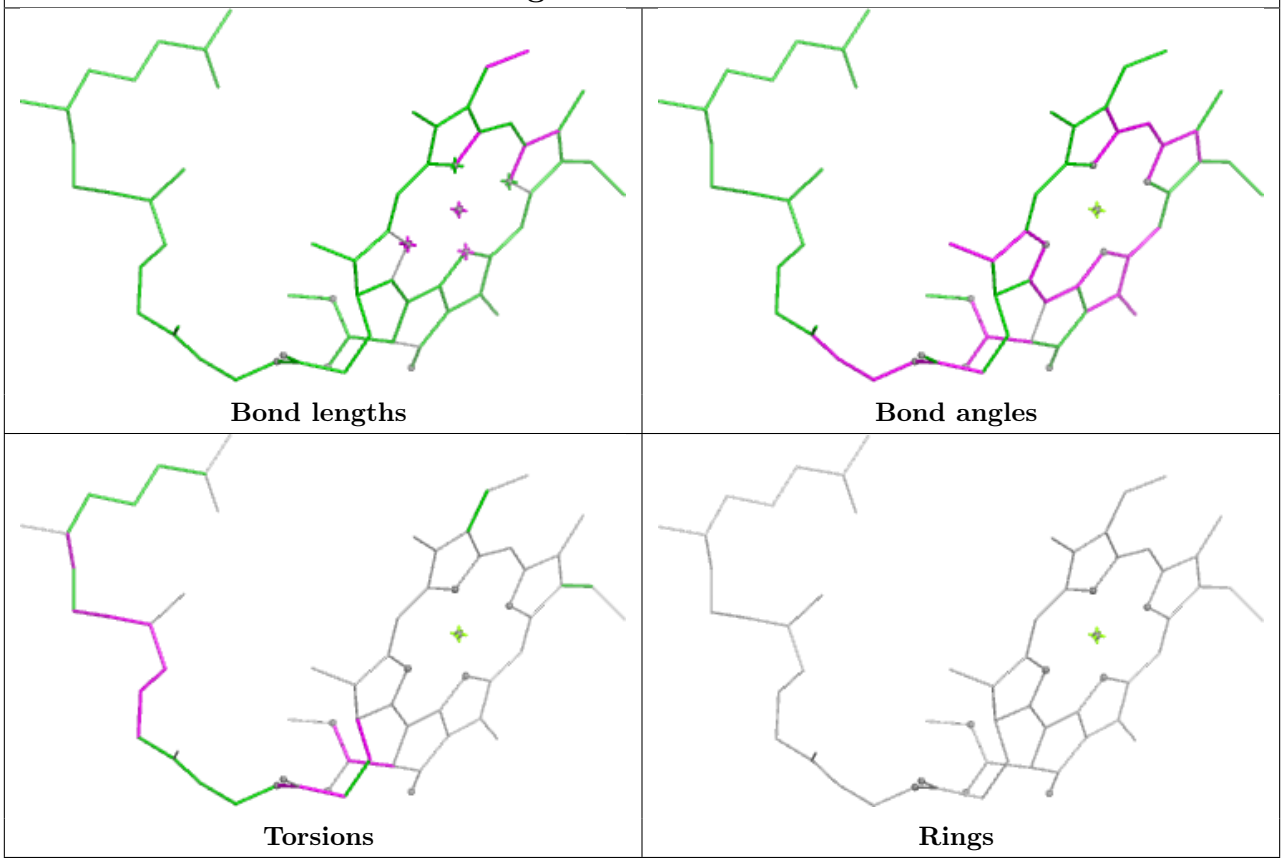
Ligand CLA B 841



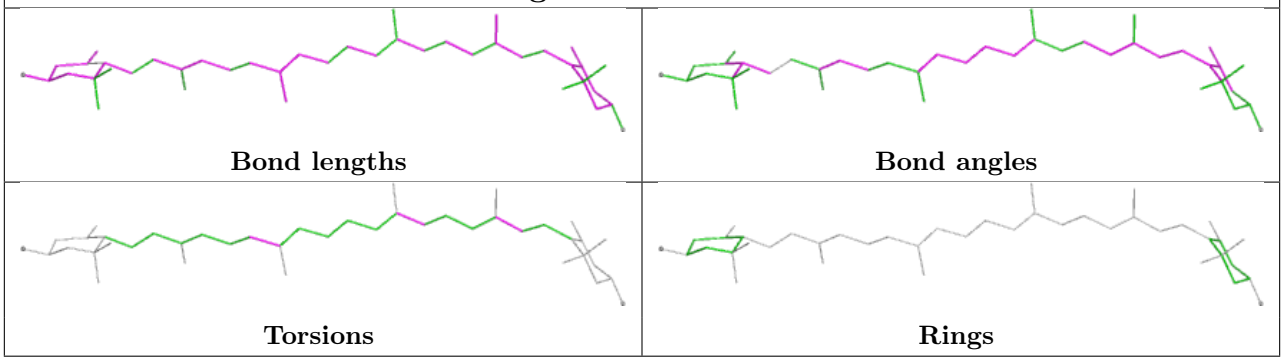
Ligand BCR B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

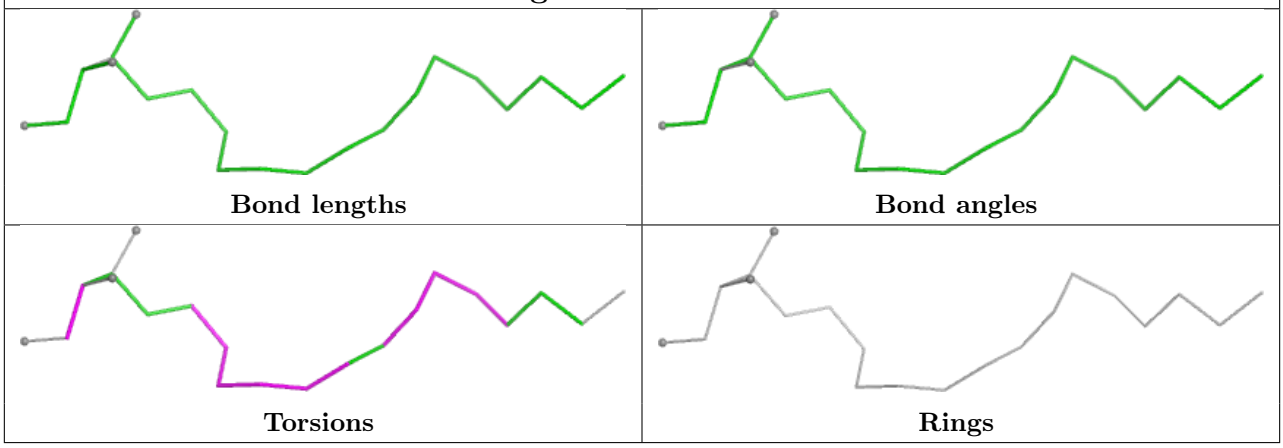
Ligand CLA L 201



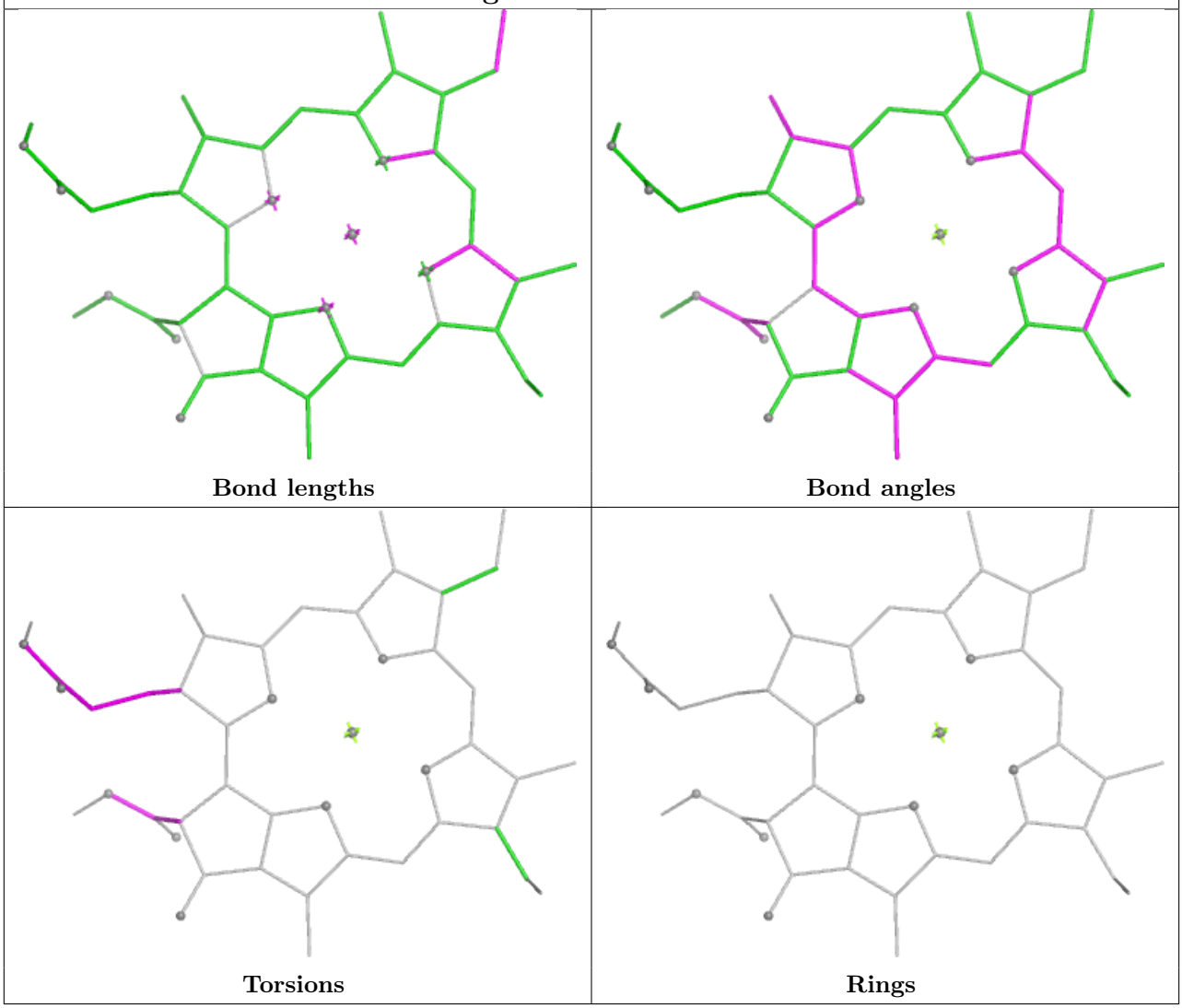
Ligand LUT 9 301



Ligand SPH 7 320



Ligand CLA K 202



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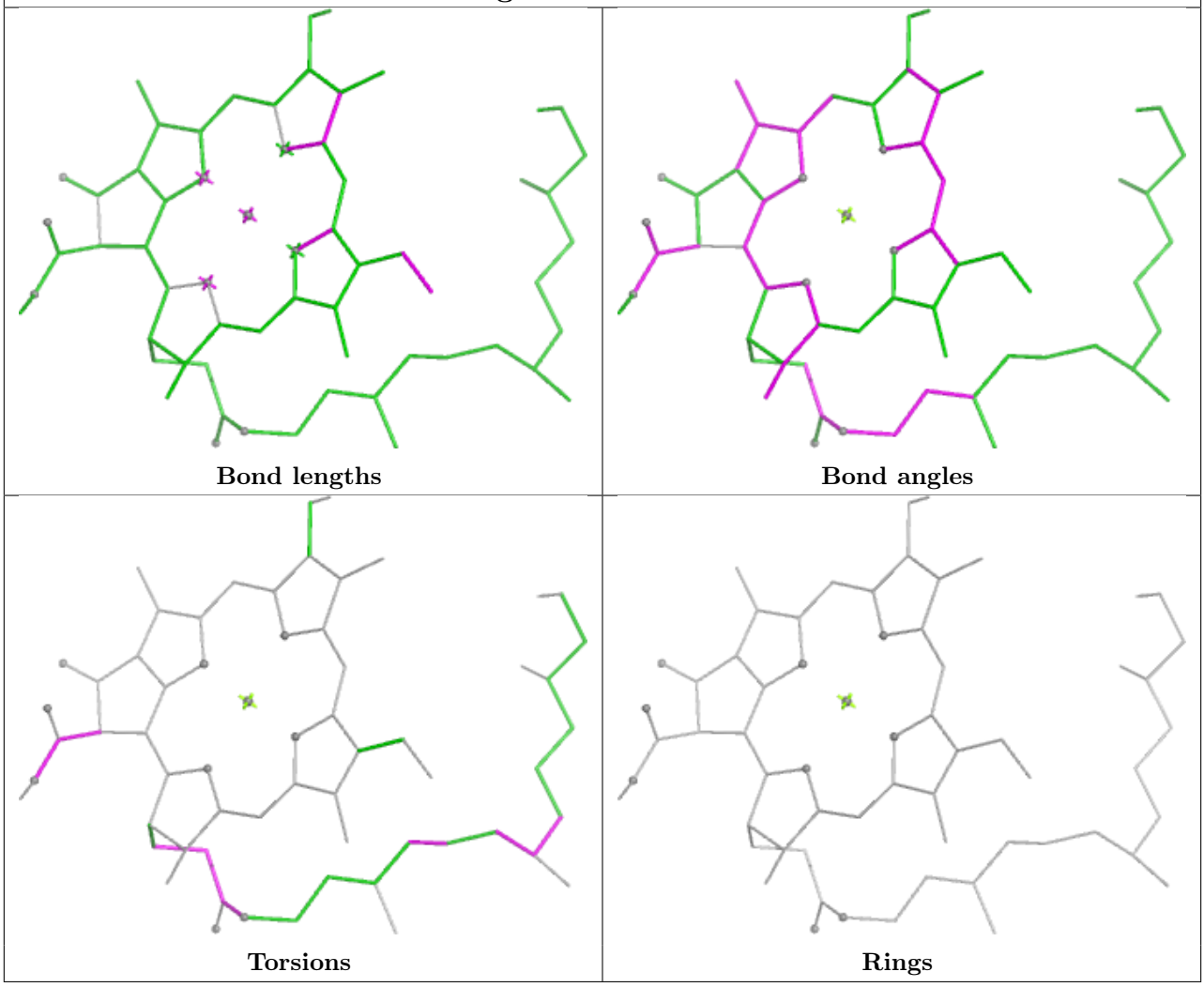
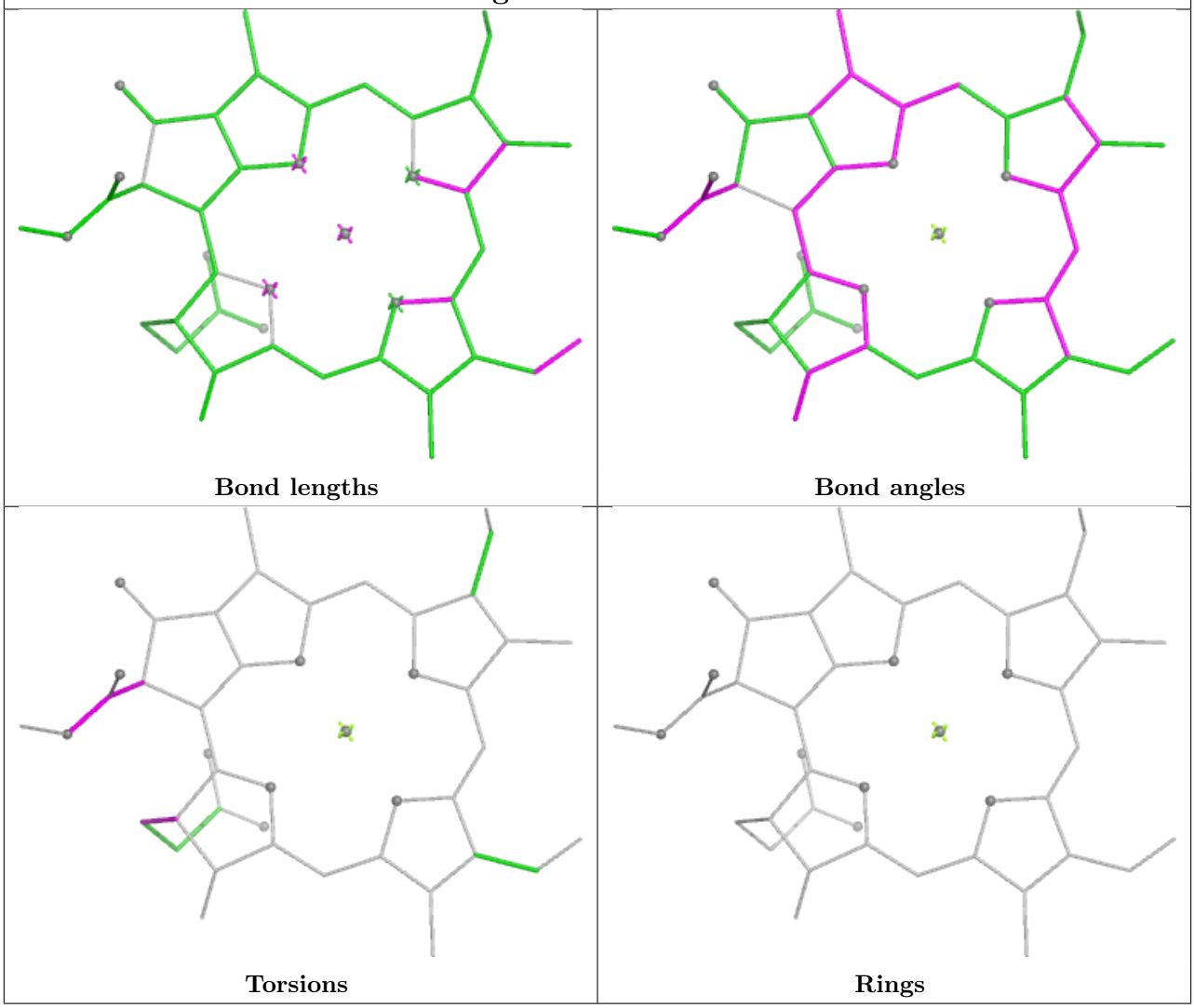


Ligand CLA 5 314



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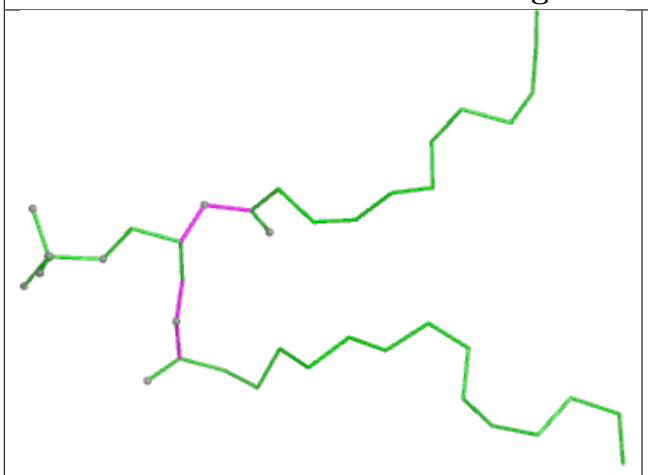
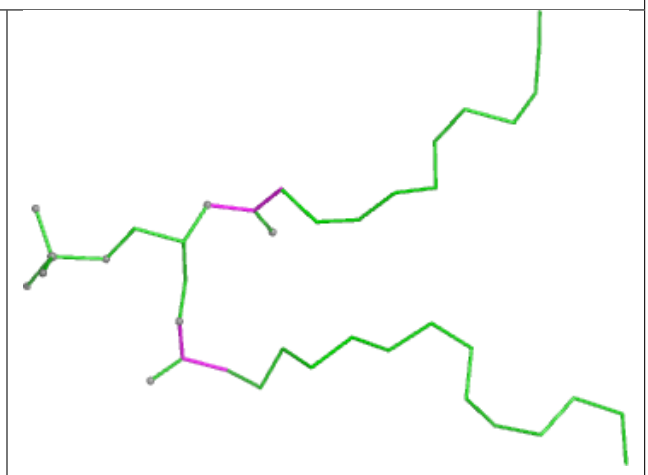
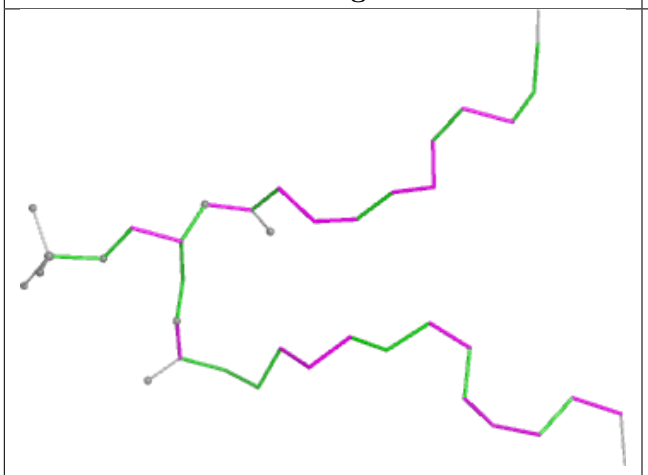


Bond lengths



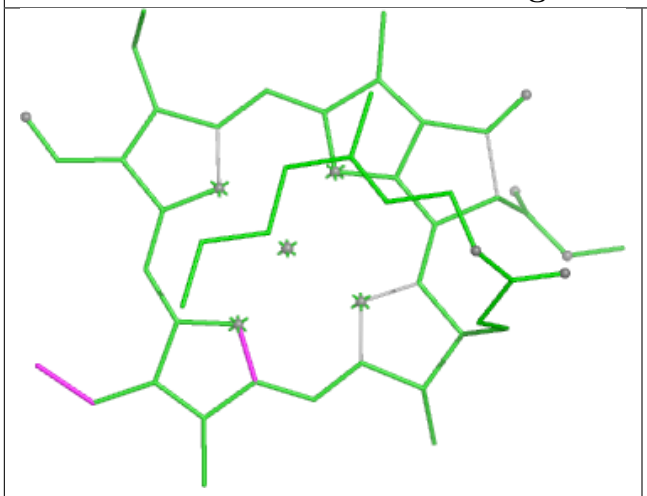
Bond angles



Torsions

Rings

Ligand CHL 7 313



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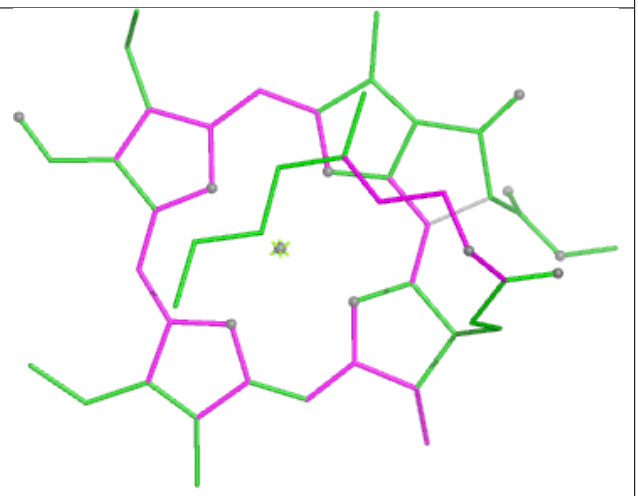
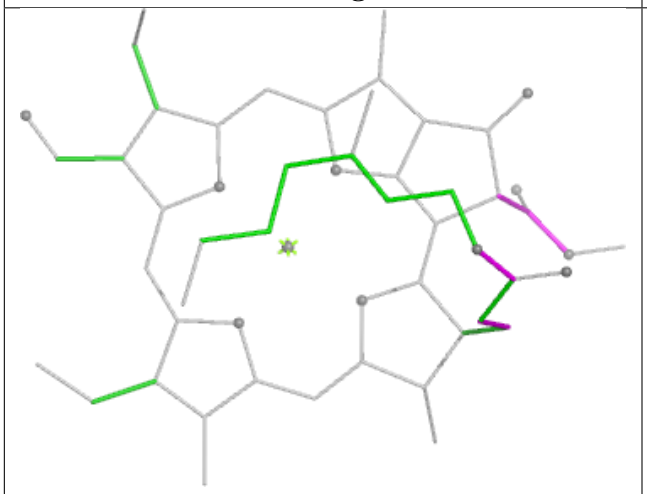
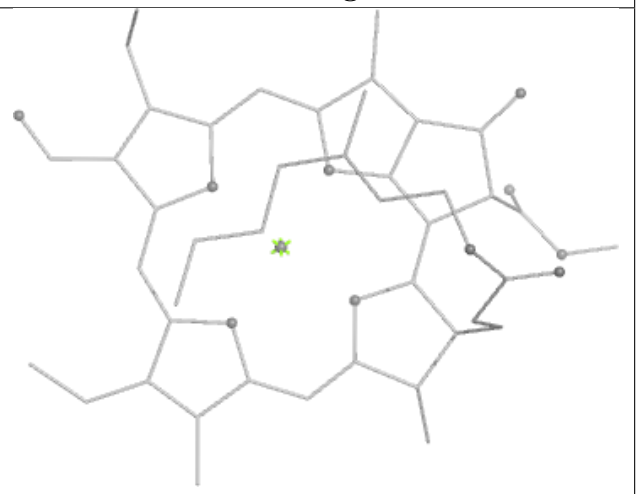


Bond angles

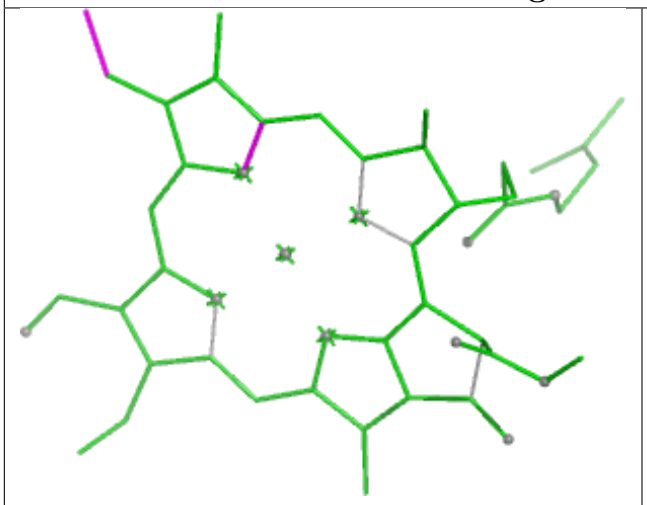


Torsions



Rings

Ligand CHL 4 813



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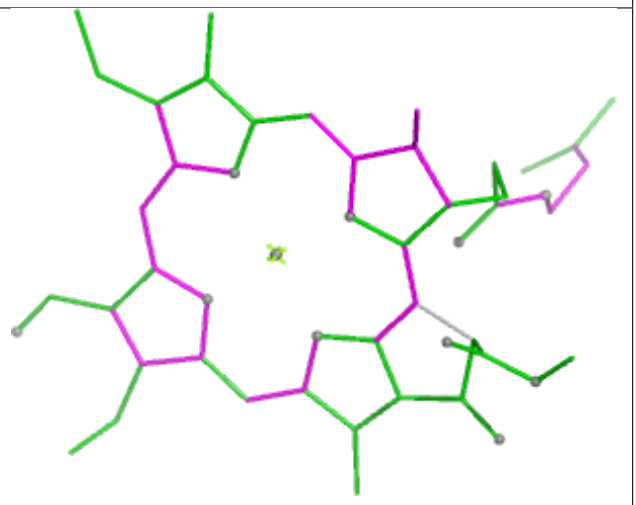
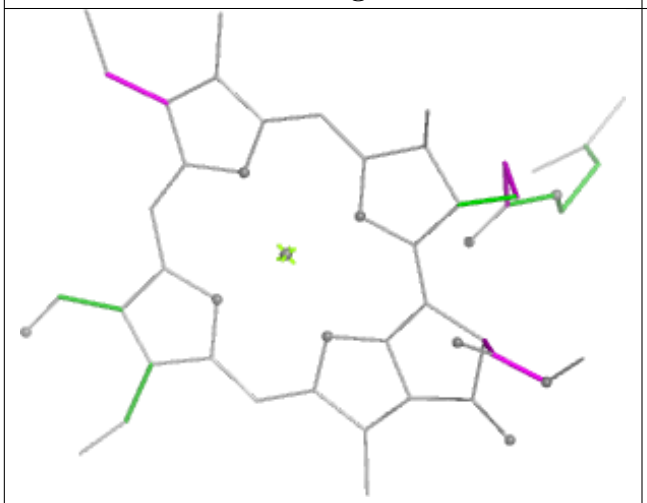


Bond angles



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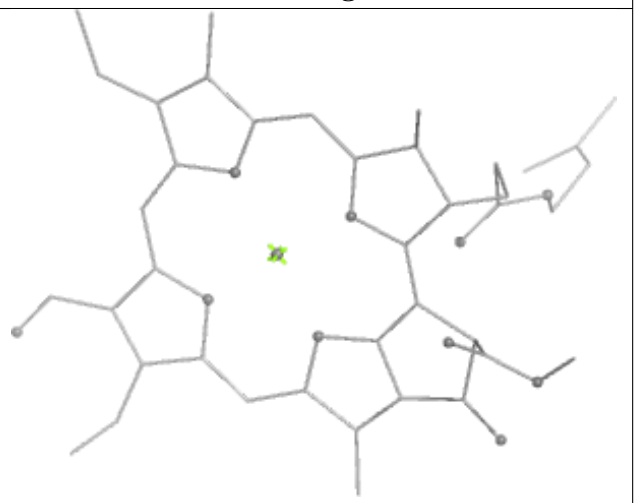
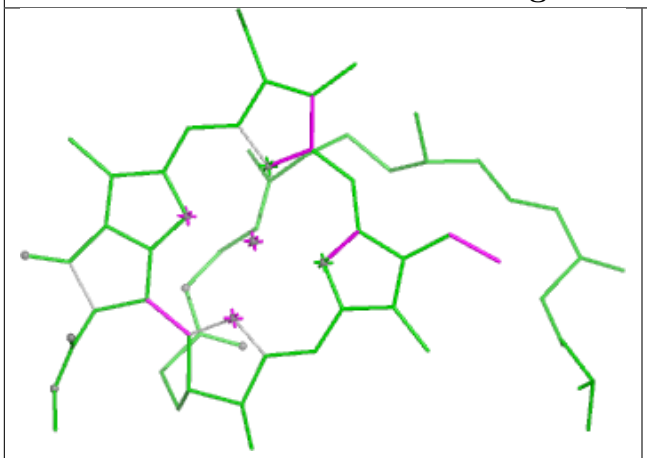
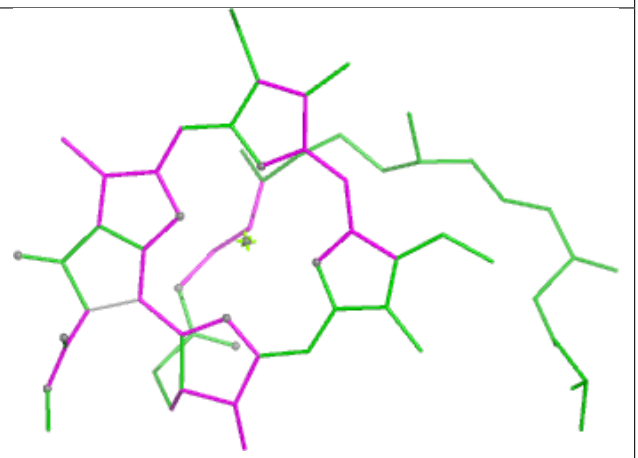


Rings

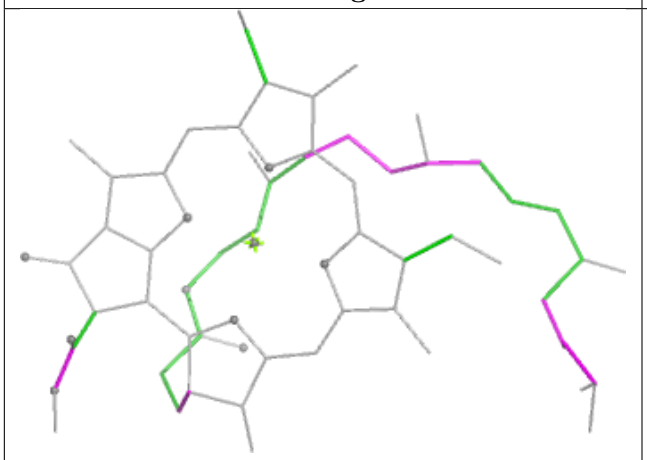
Ligand CLA 4 807



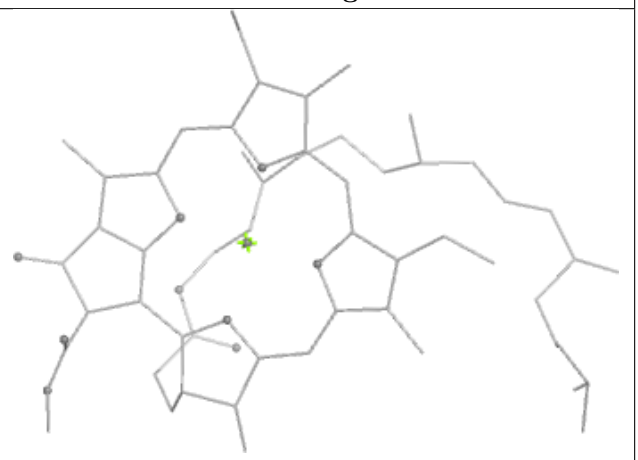
Bond lengths



Bond angles

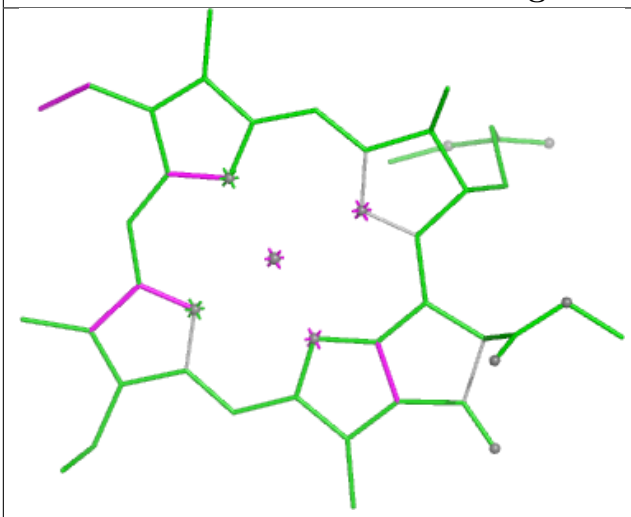


Torsions

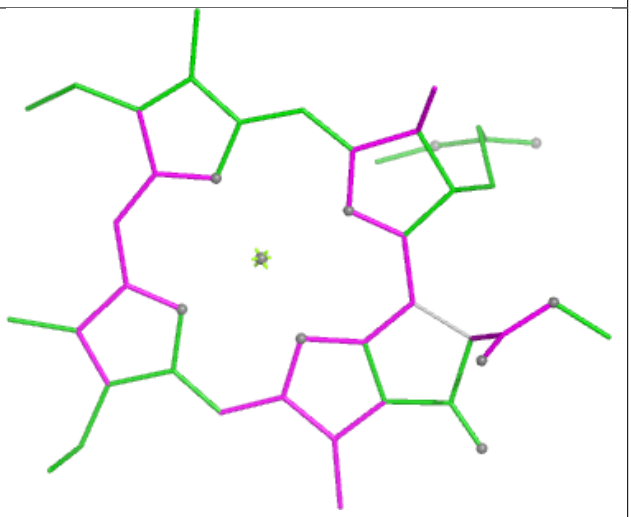


Rings

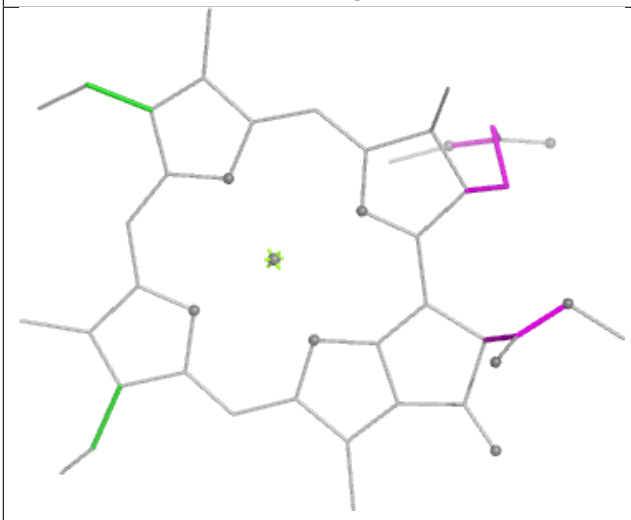
Ligand CLA 8 316



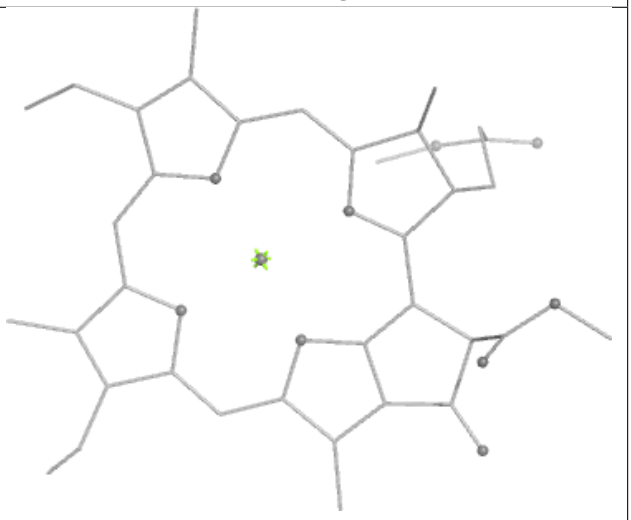
Bond lengths



Bond angles



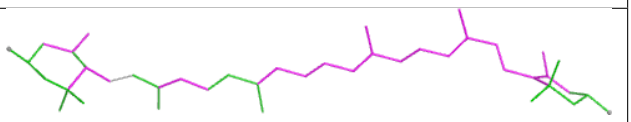
Torsions



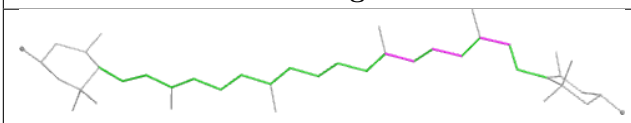
Rings

Ligand LUT 7 302

Bond lengths



Bond angles



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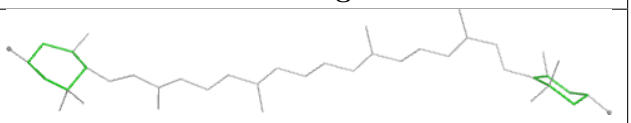
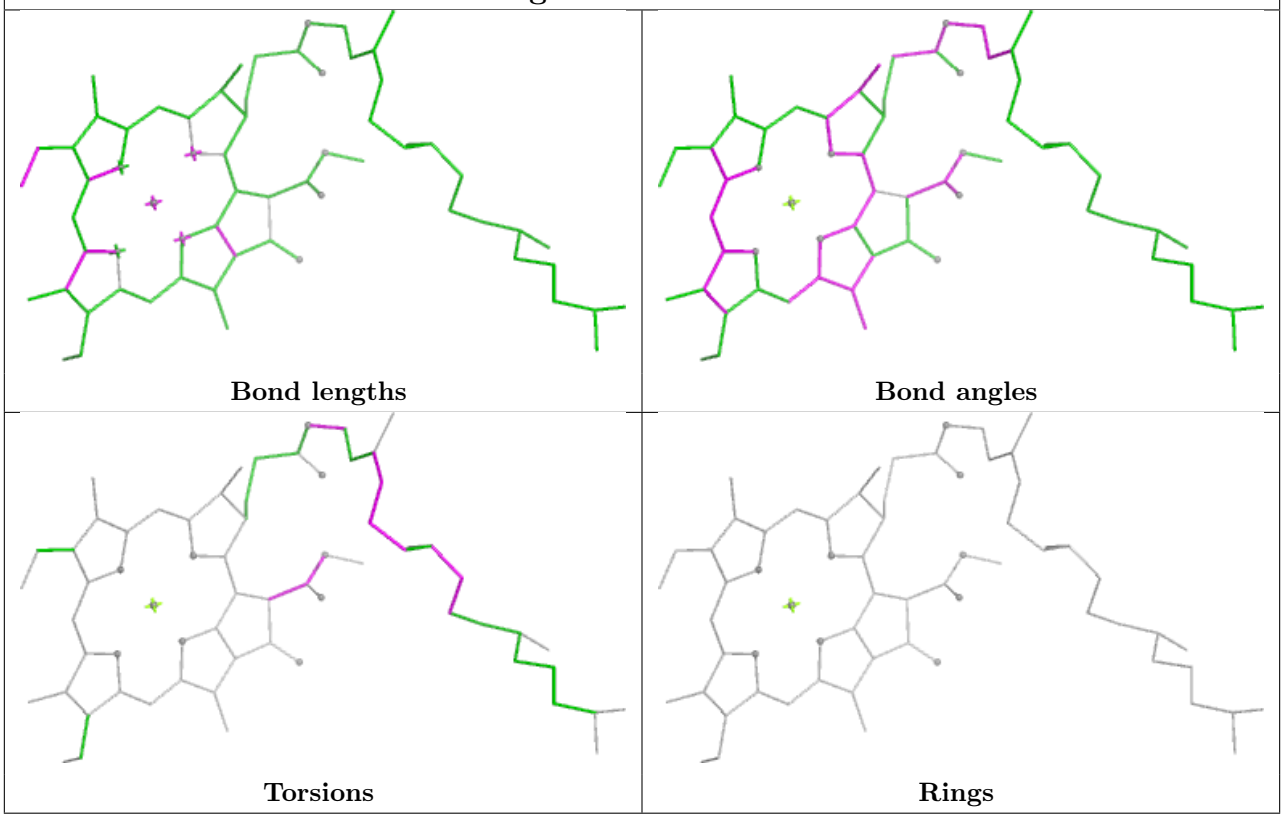
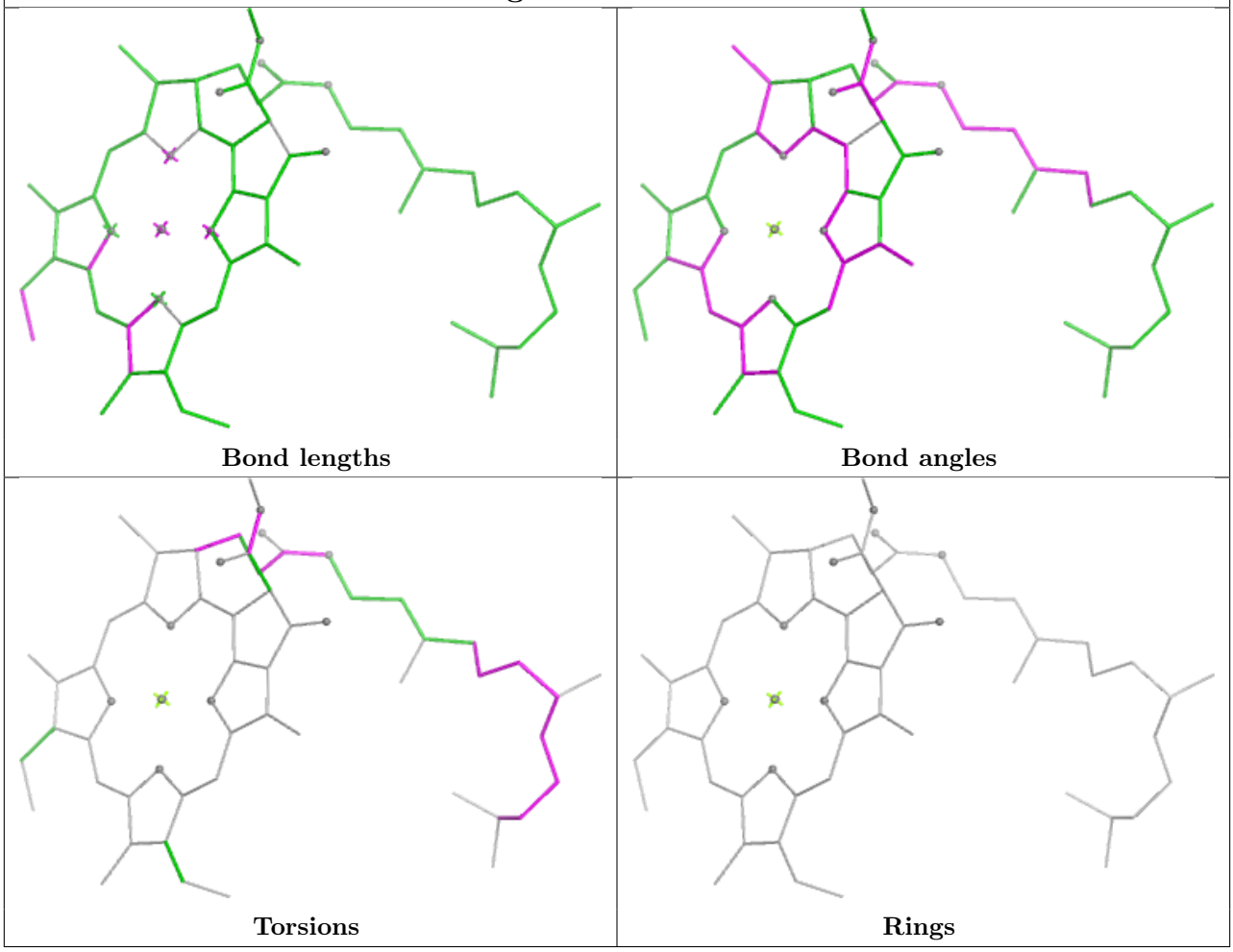


Rings

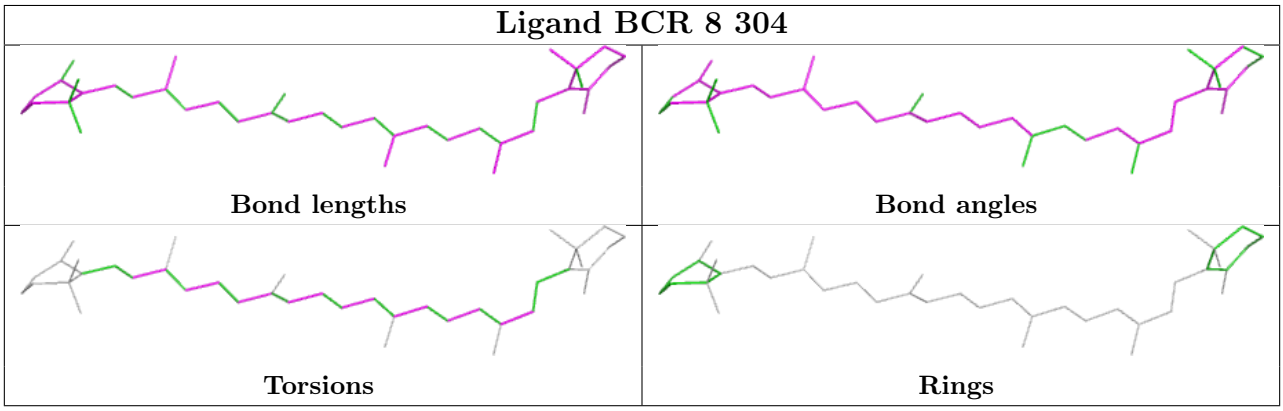
Ligand CLA 3 312



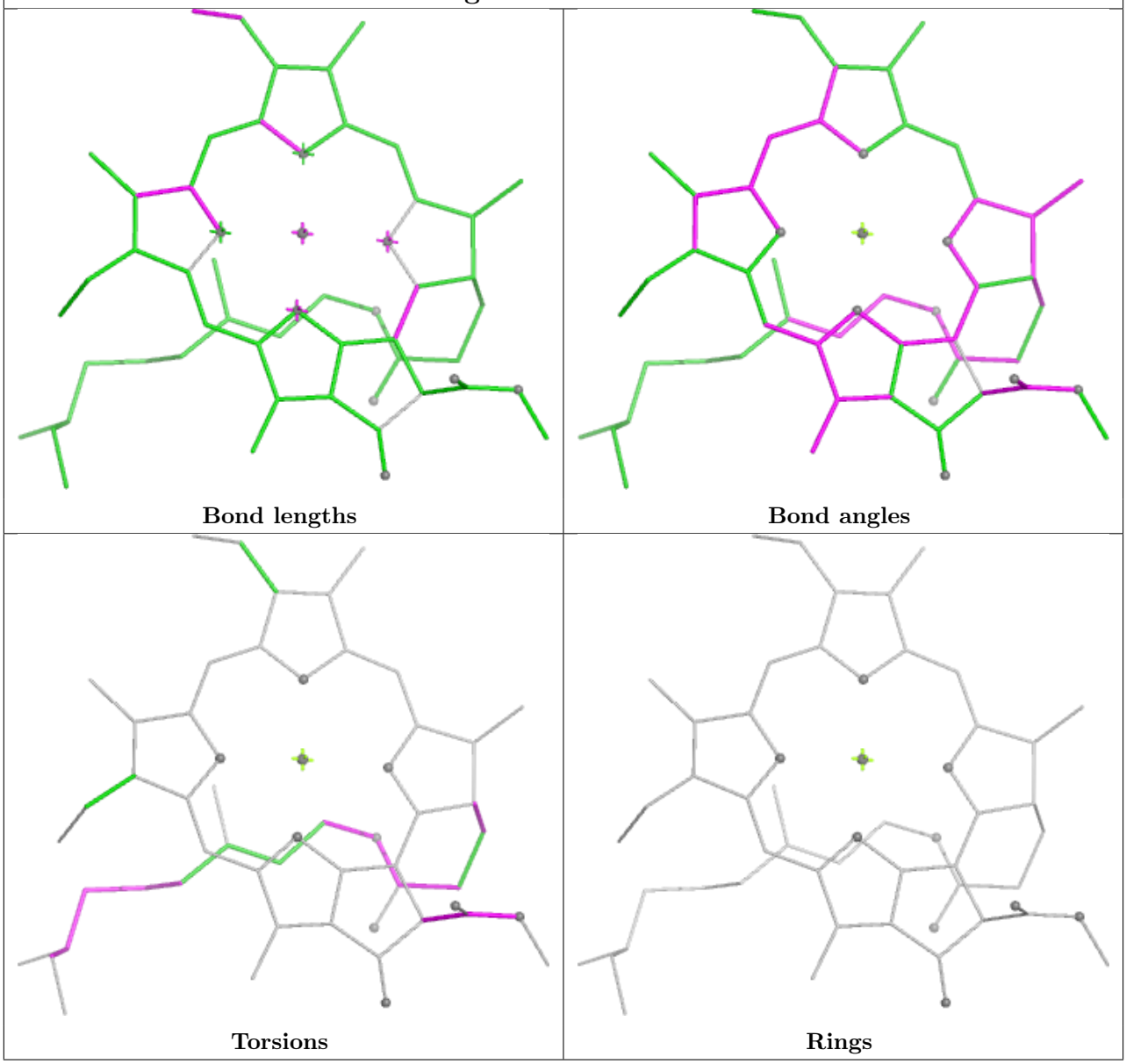
Ligand CLA Z 309



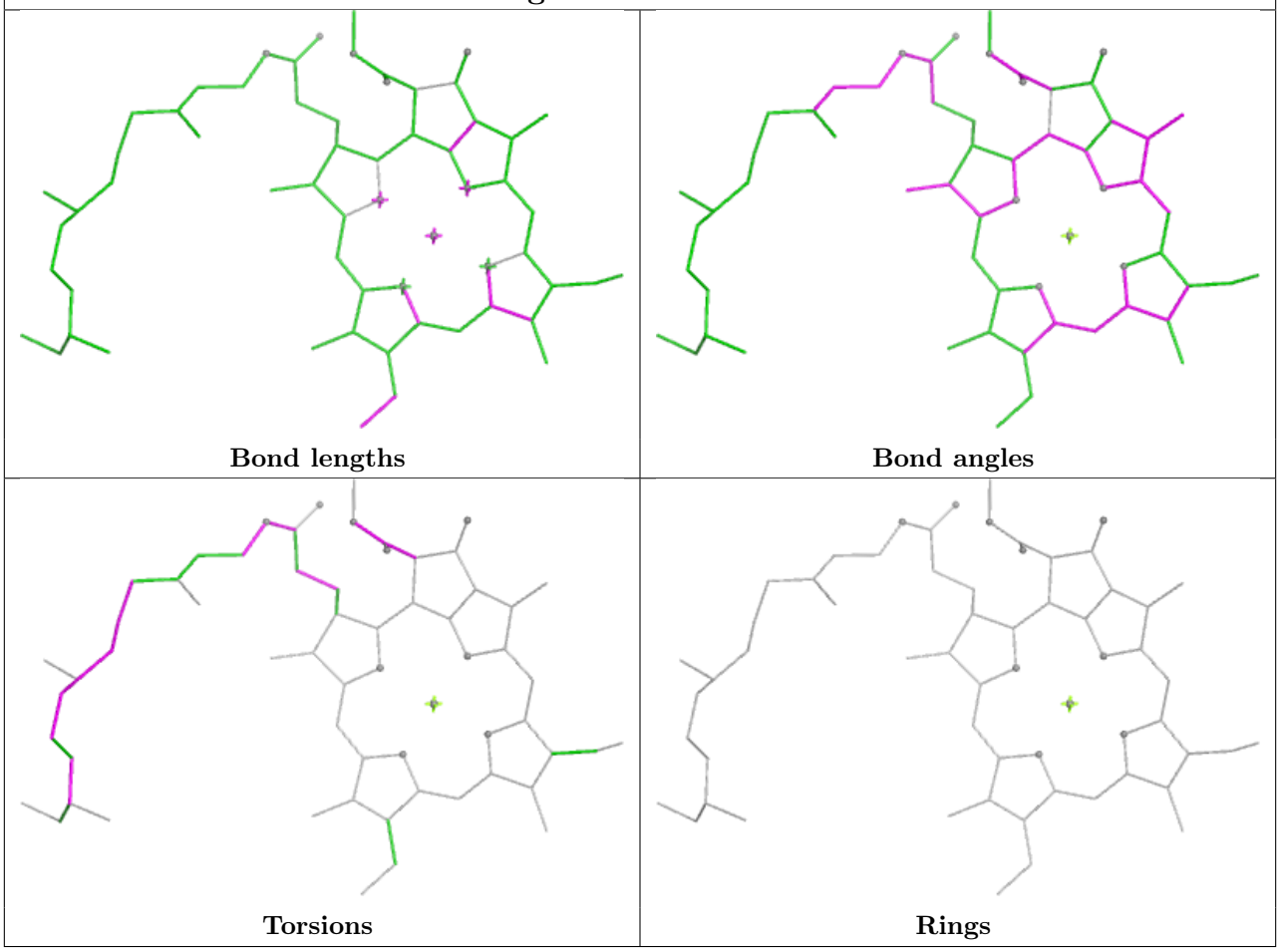
Ligand BCR 8 304



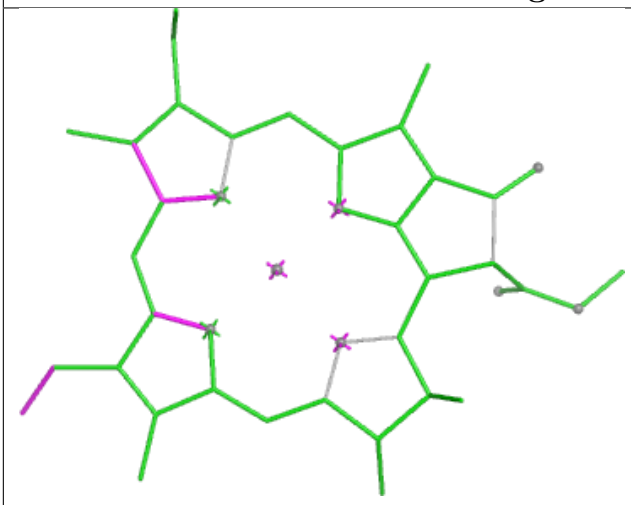
Ligand CLA 5 309



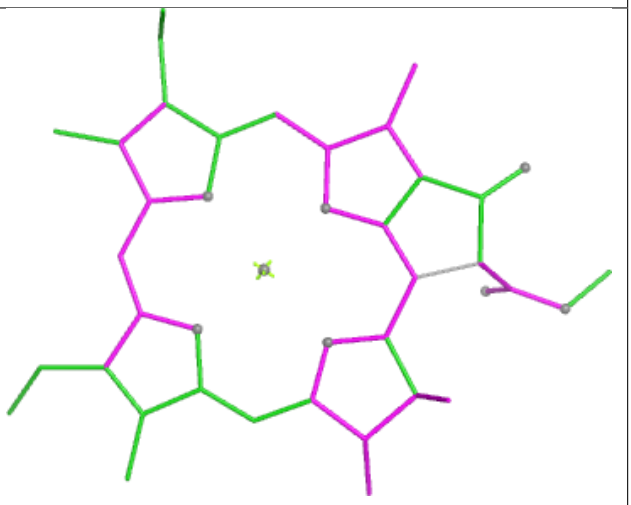
Ligand CLA 7 308



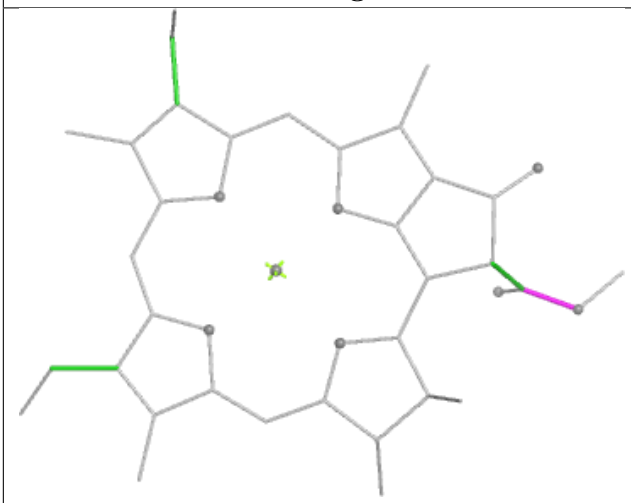
Ligand CLA 4 817



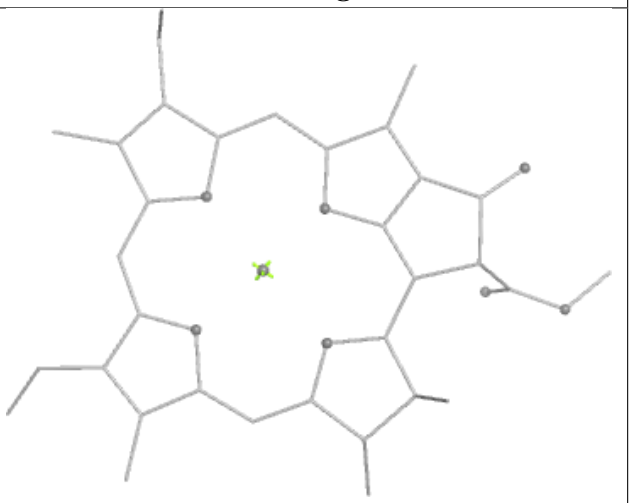
Bond lengths



Bond angles

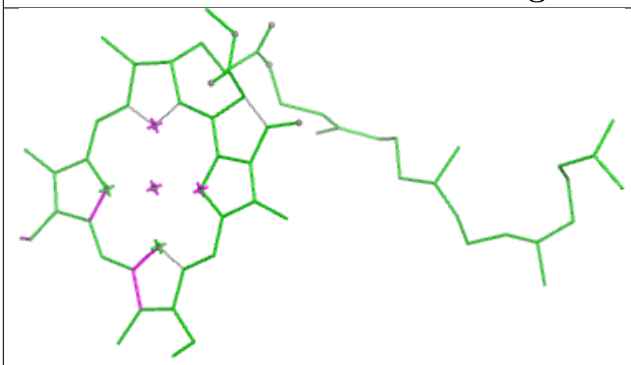


Torsions



Rings

Ligand CLA 7 310



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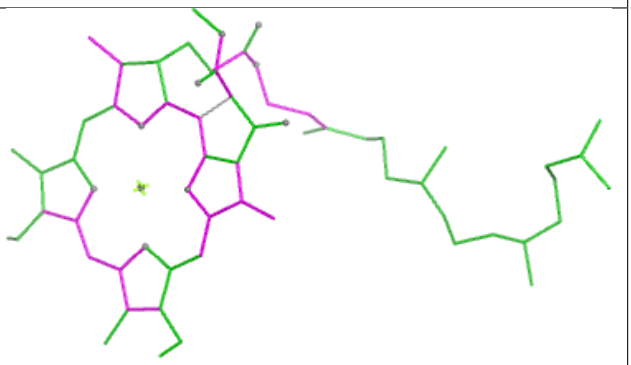
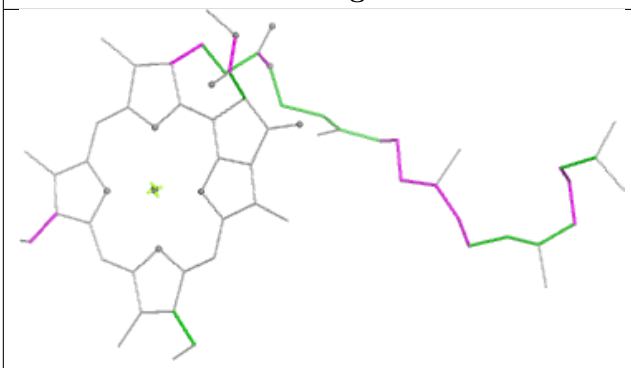


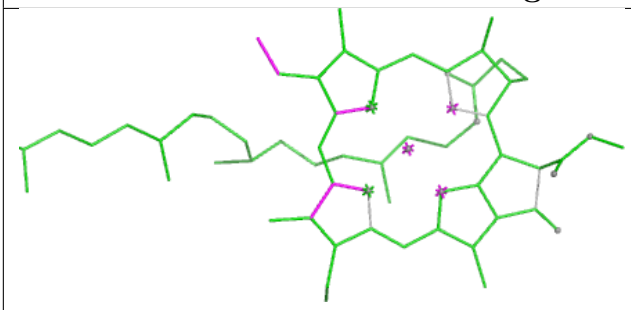
Bond angles



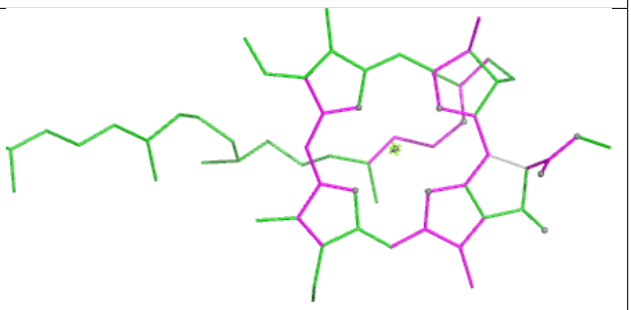
Torsions

Rings

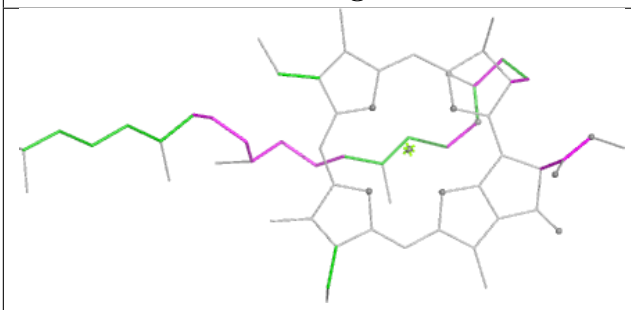
Ligand CLA A 838



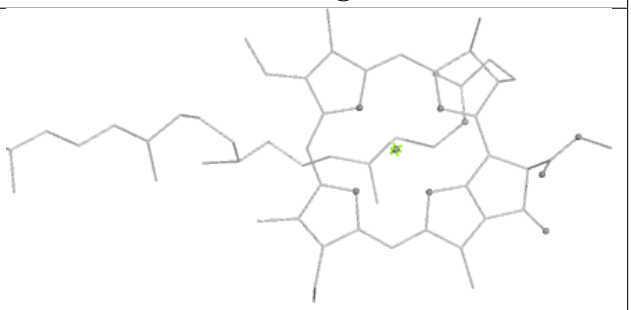
Bond lengths



Bond angles

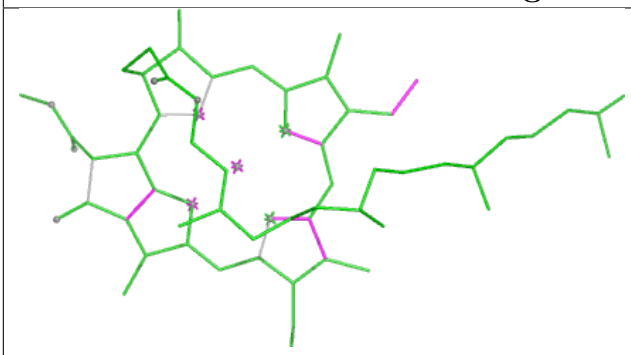


Torsions

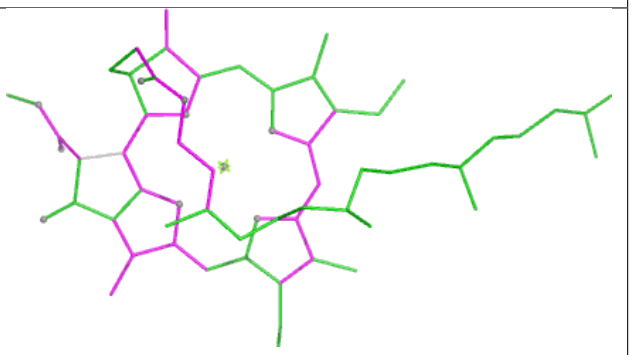


Rings

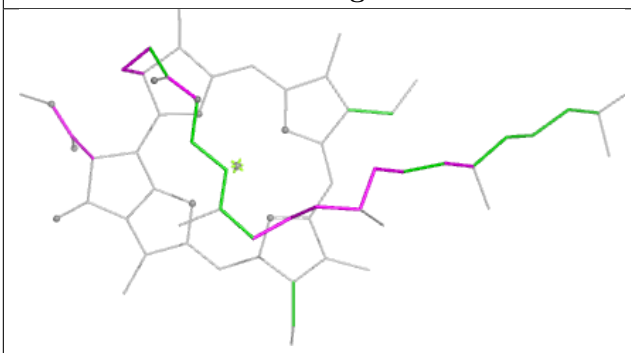
Ligand CLA A 840



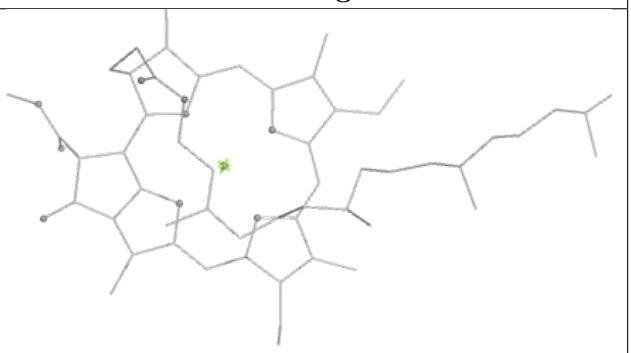
Bond lengths



Bond angles

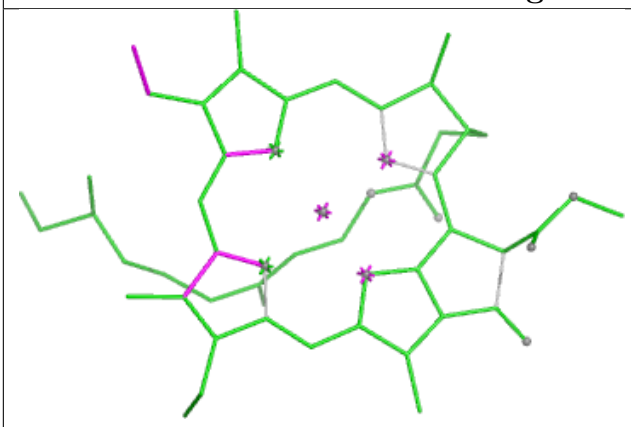


Torsions



Rings

Ligand CLA Z 305



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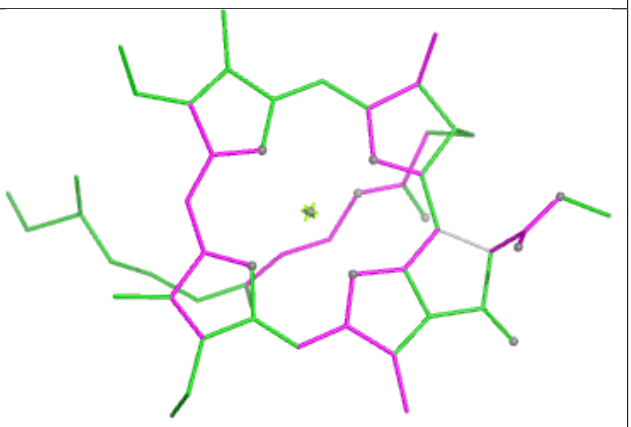
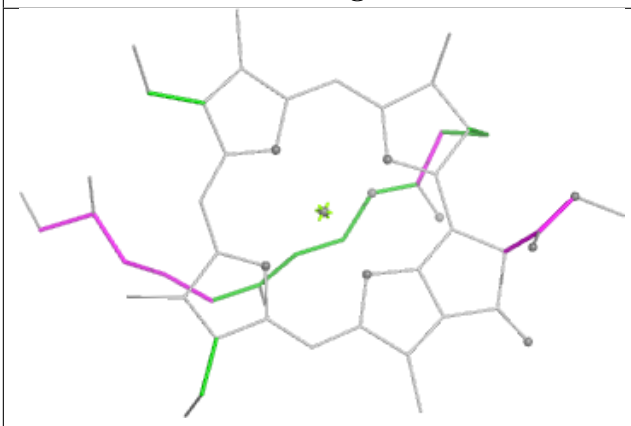


Bond angles



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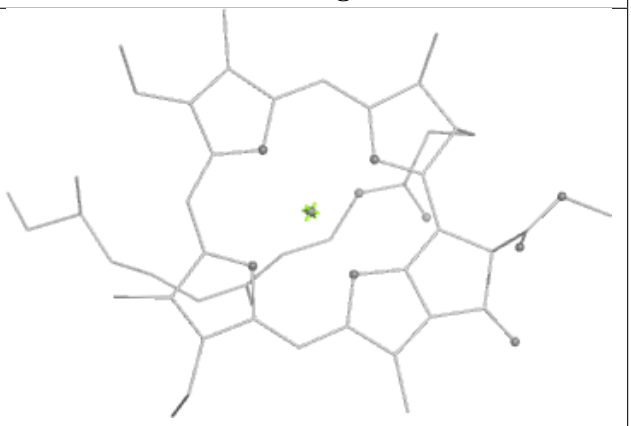
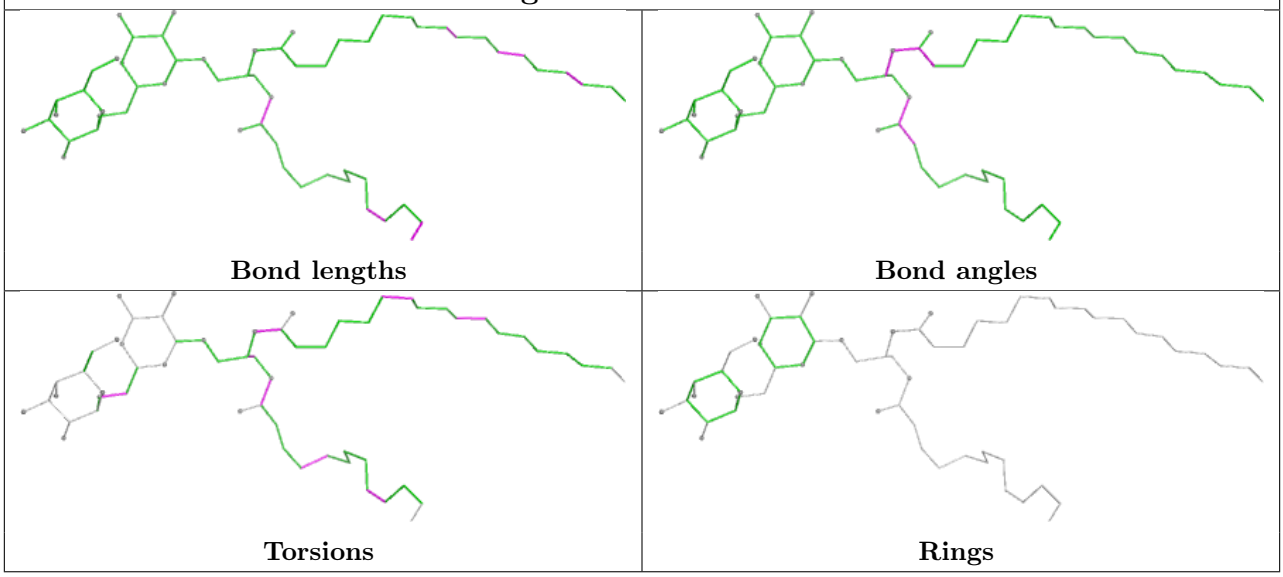


Rings

Ligand DGD B 852



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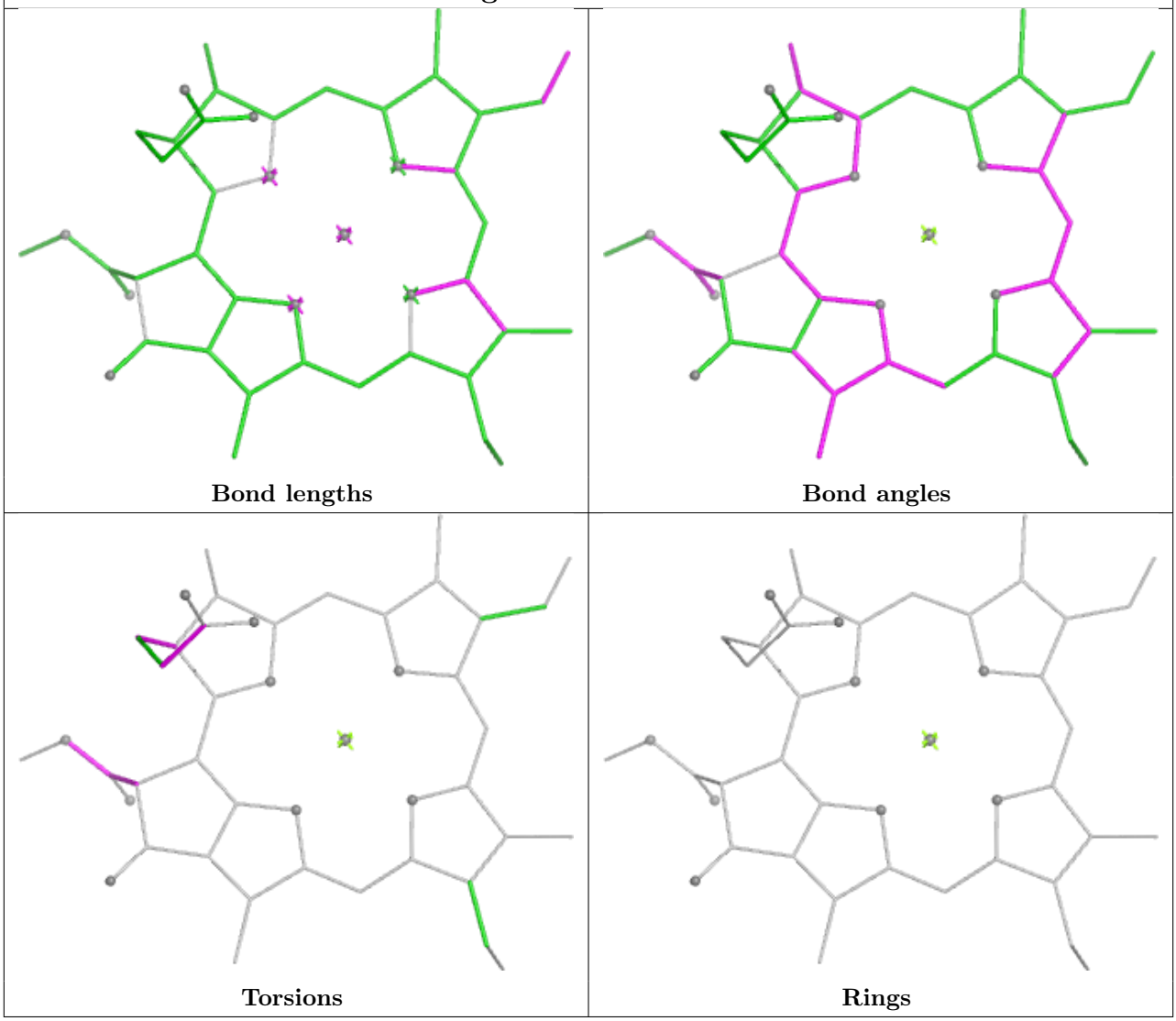
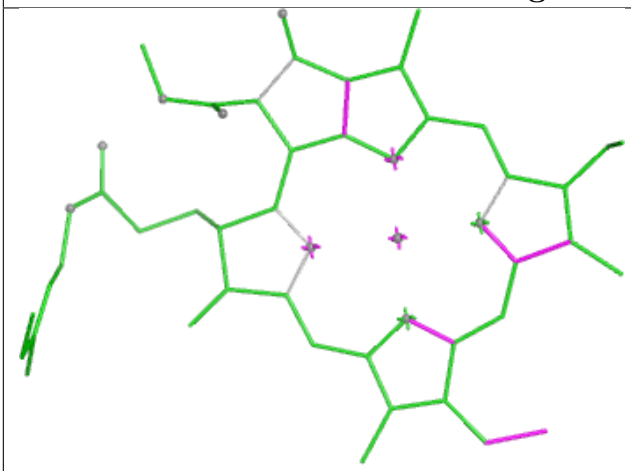


Ligand CLA 4 809



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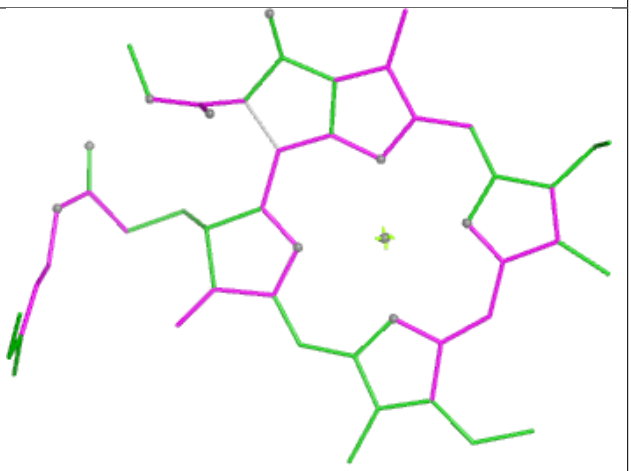

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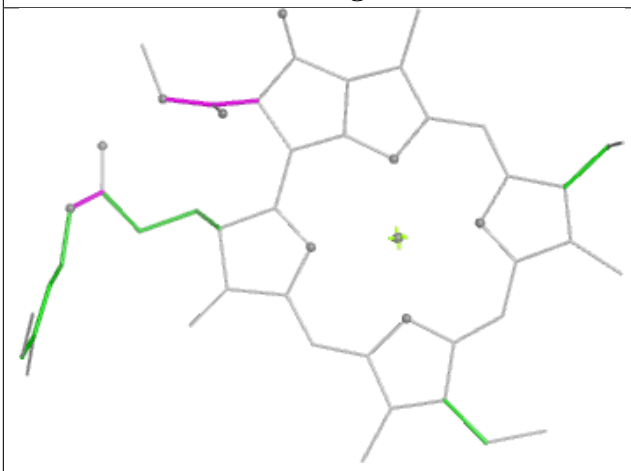

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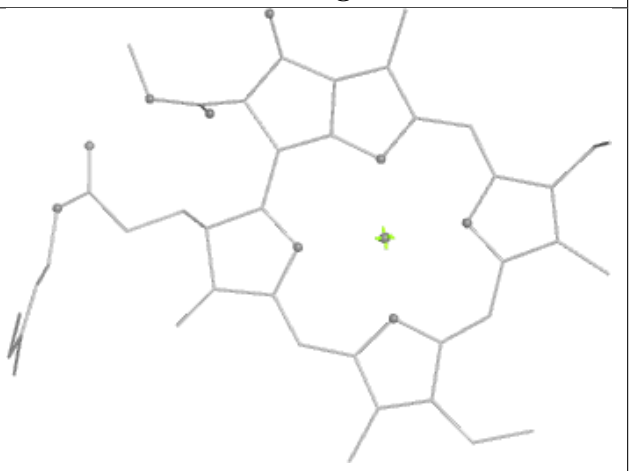
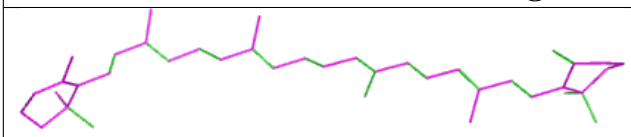


Rings

Ligand BCR 7 303



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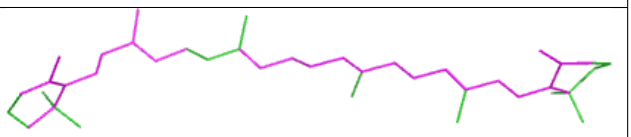
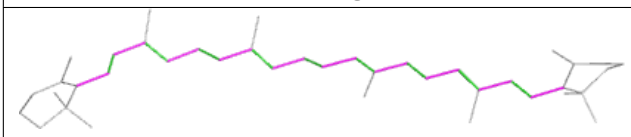


Bond angles



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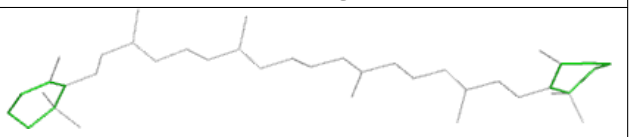
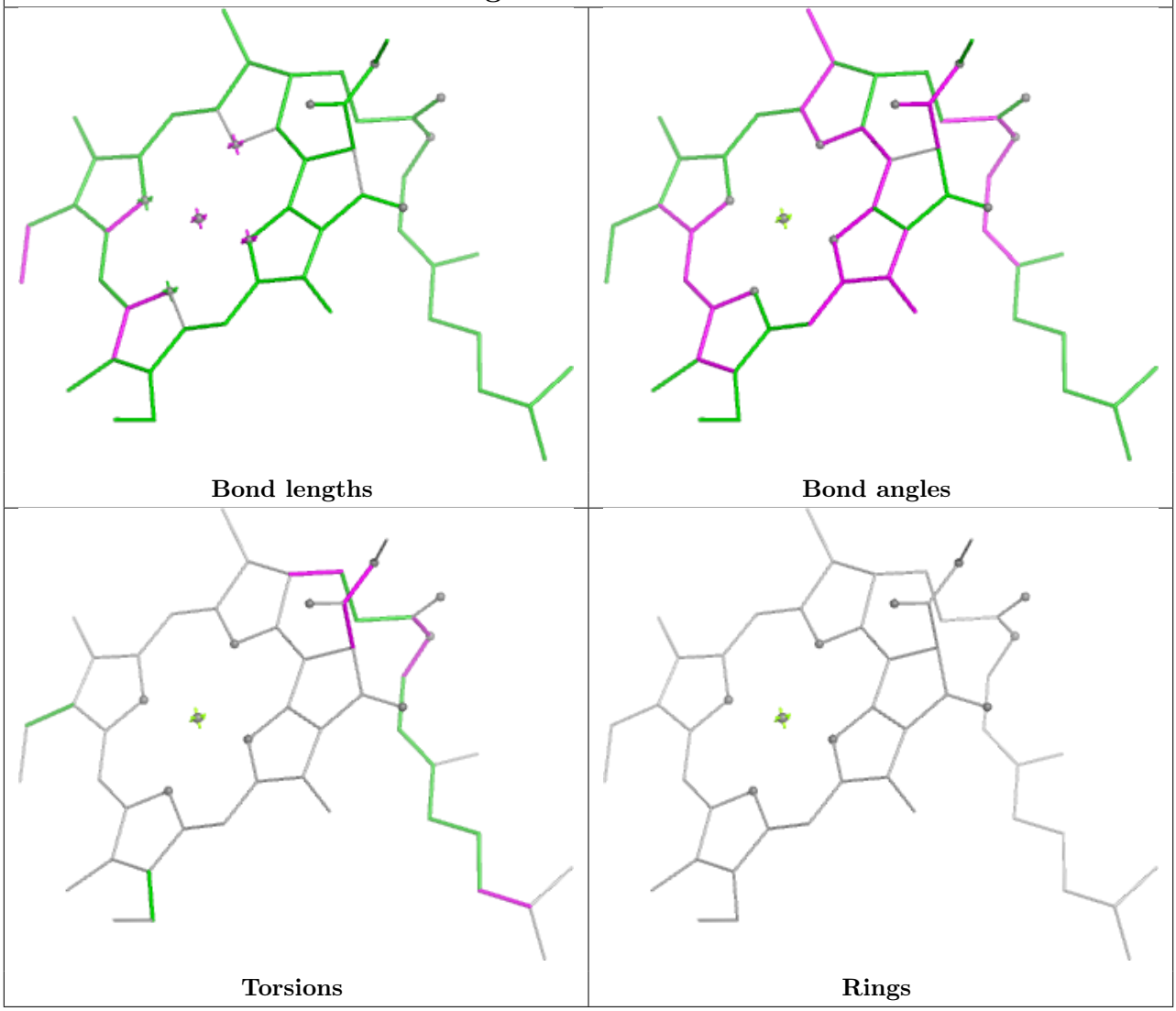
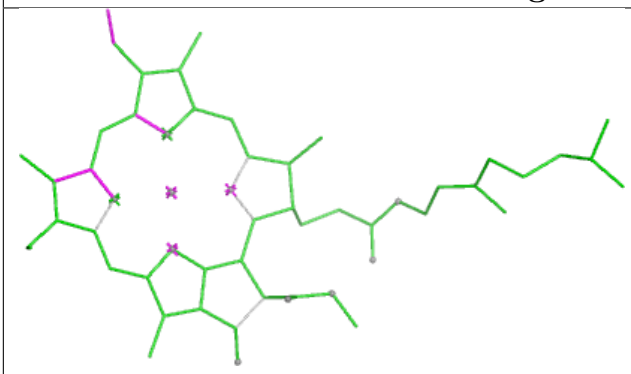
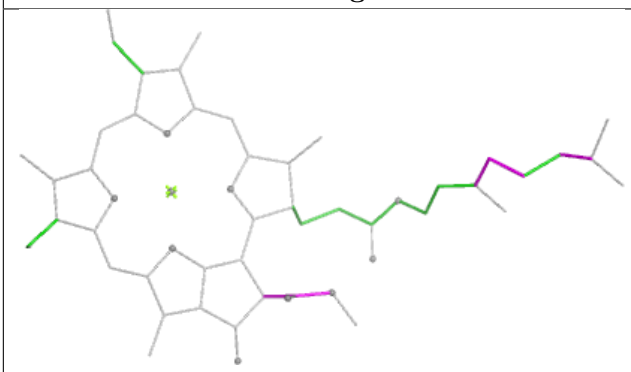
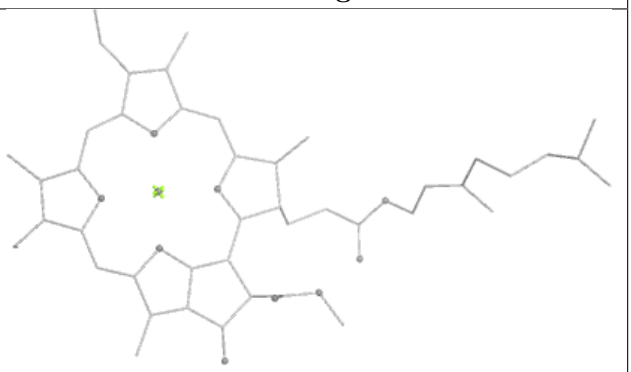


Rings

Ligand CLA 4 811



Ligand CLA 3 319	
 Bond lengths	Bond angles
 Torsions	 Rings

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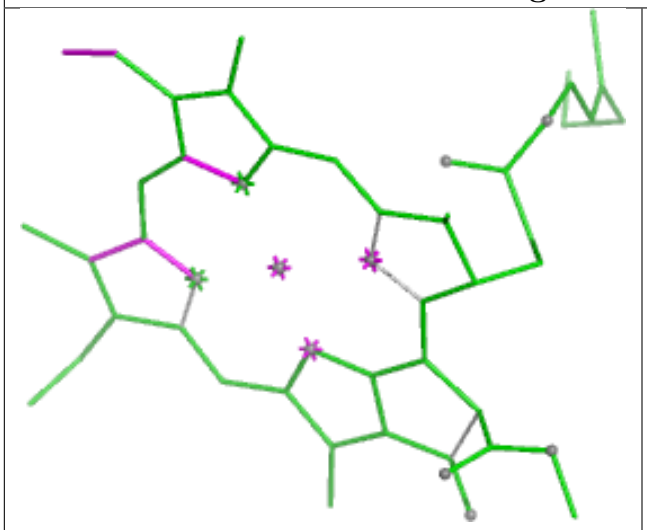

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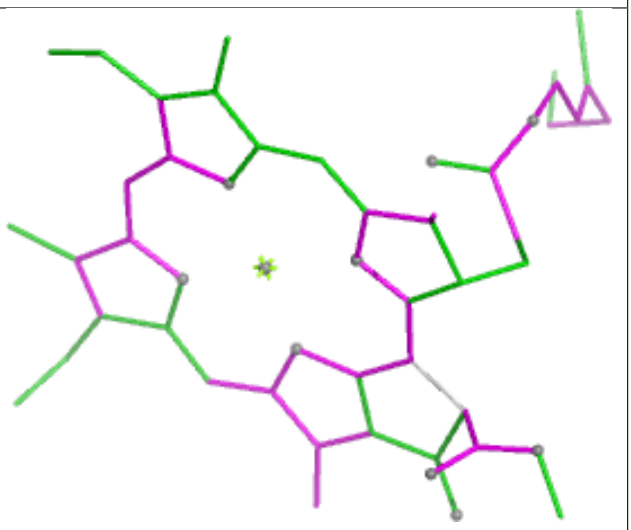
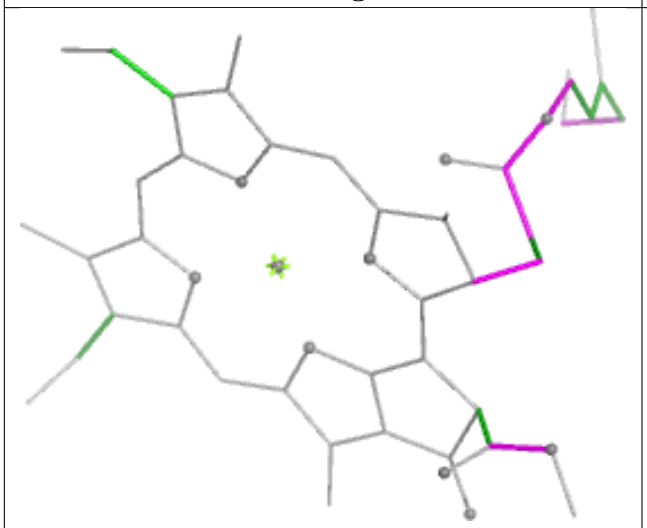


Bond angles



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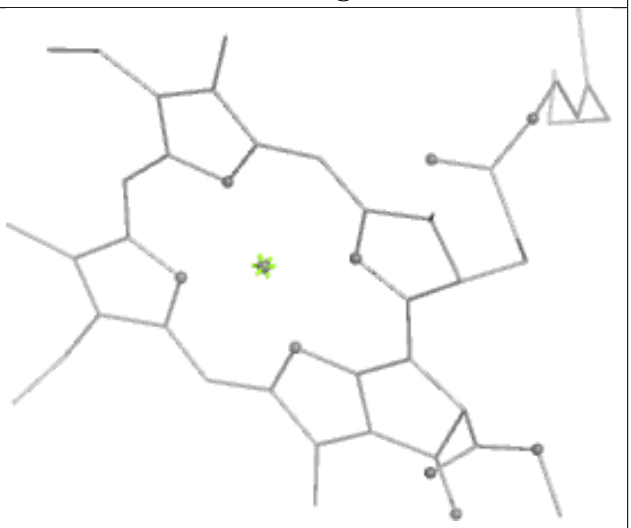
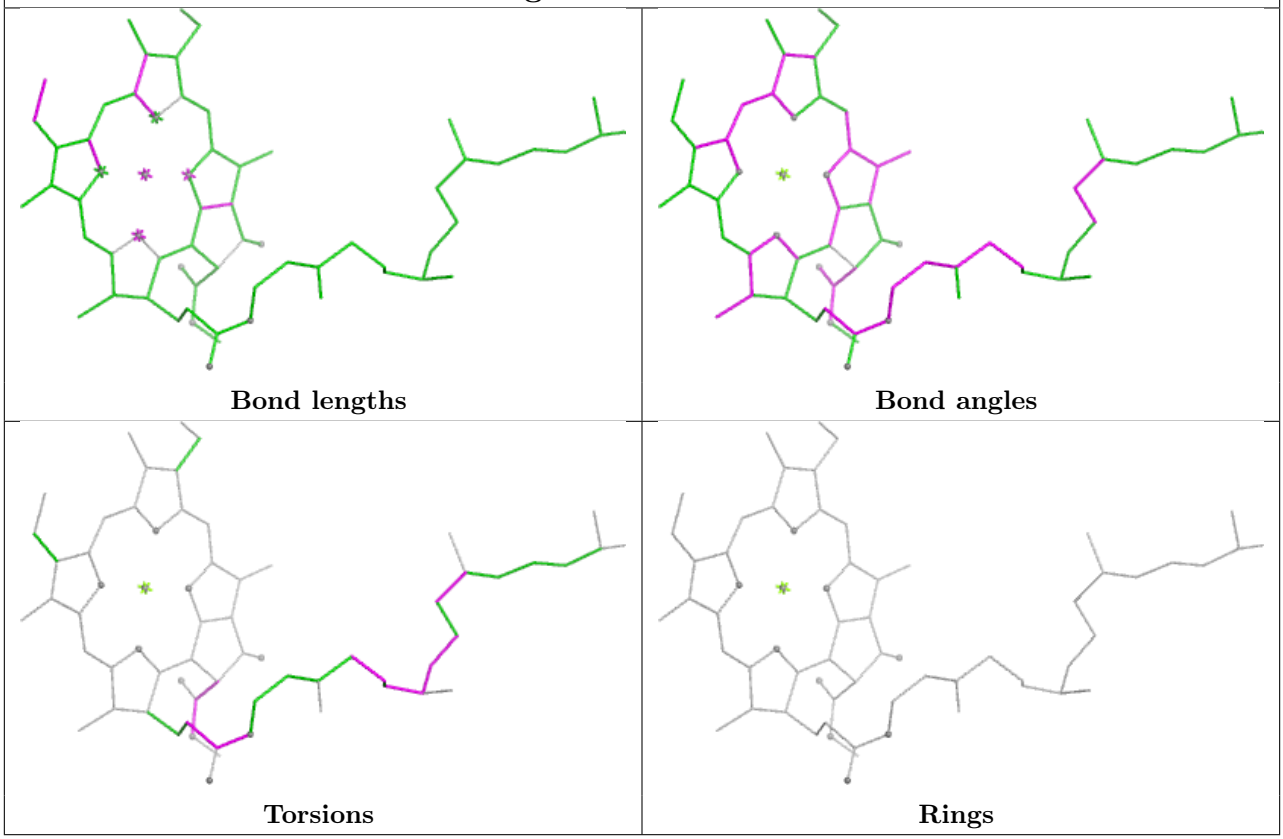
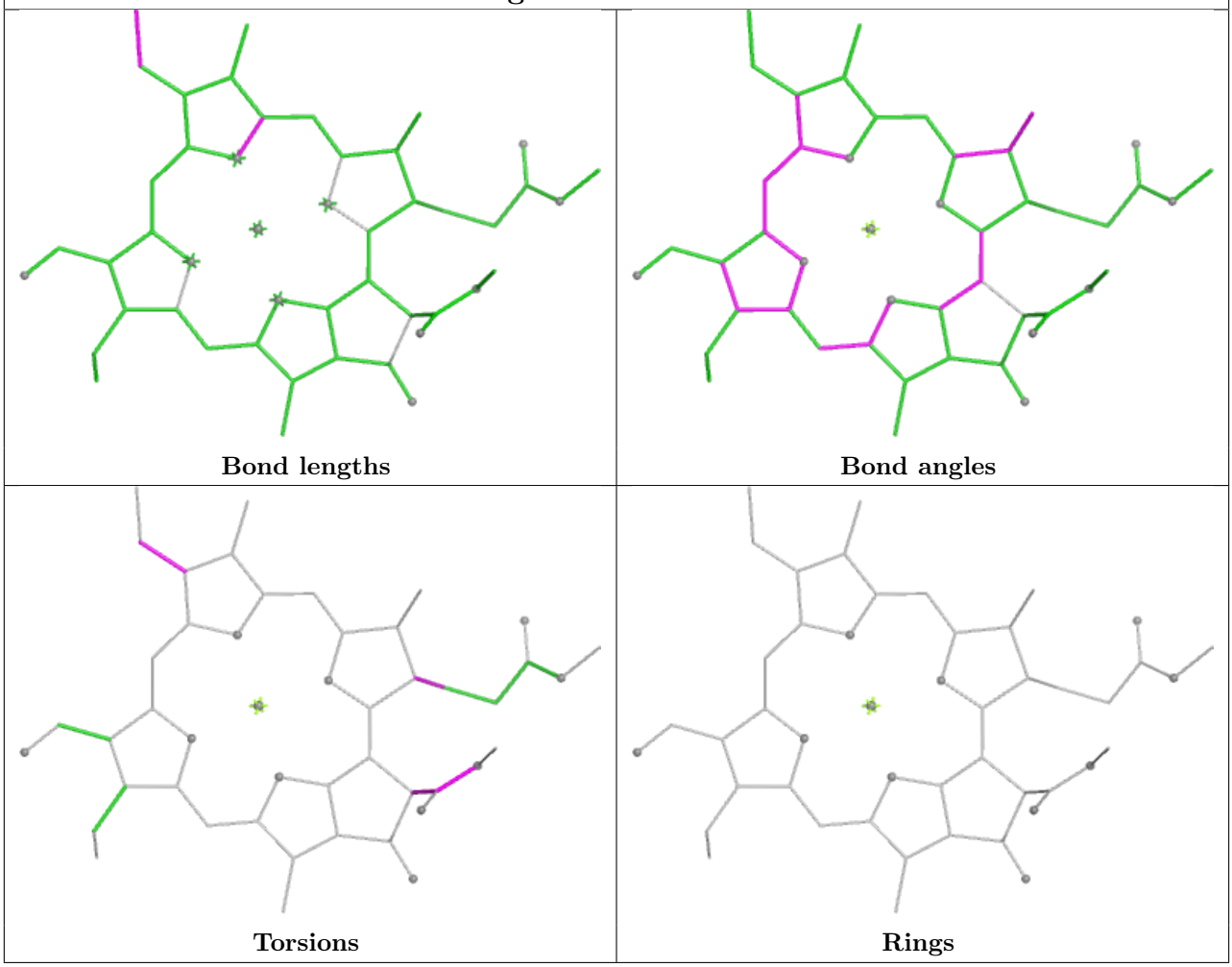


Rings

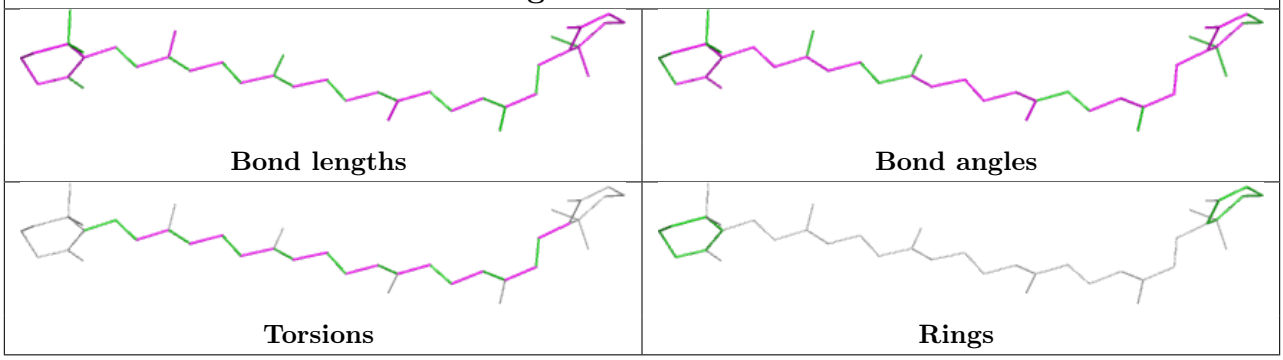
Ligand CLA A 823



Ligand CHL 4 816



Ligand BCR 4 804



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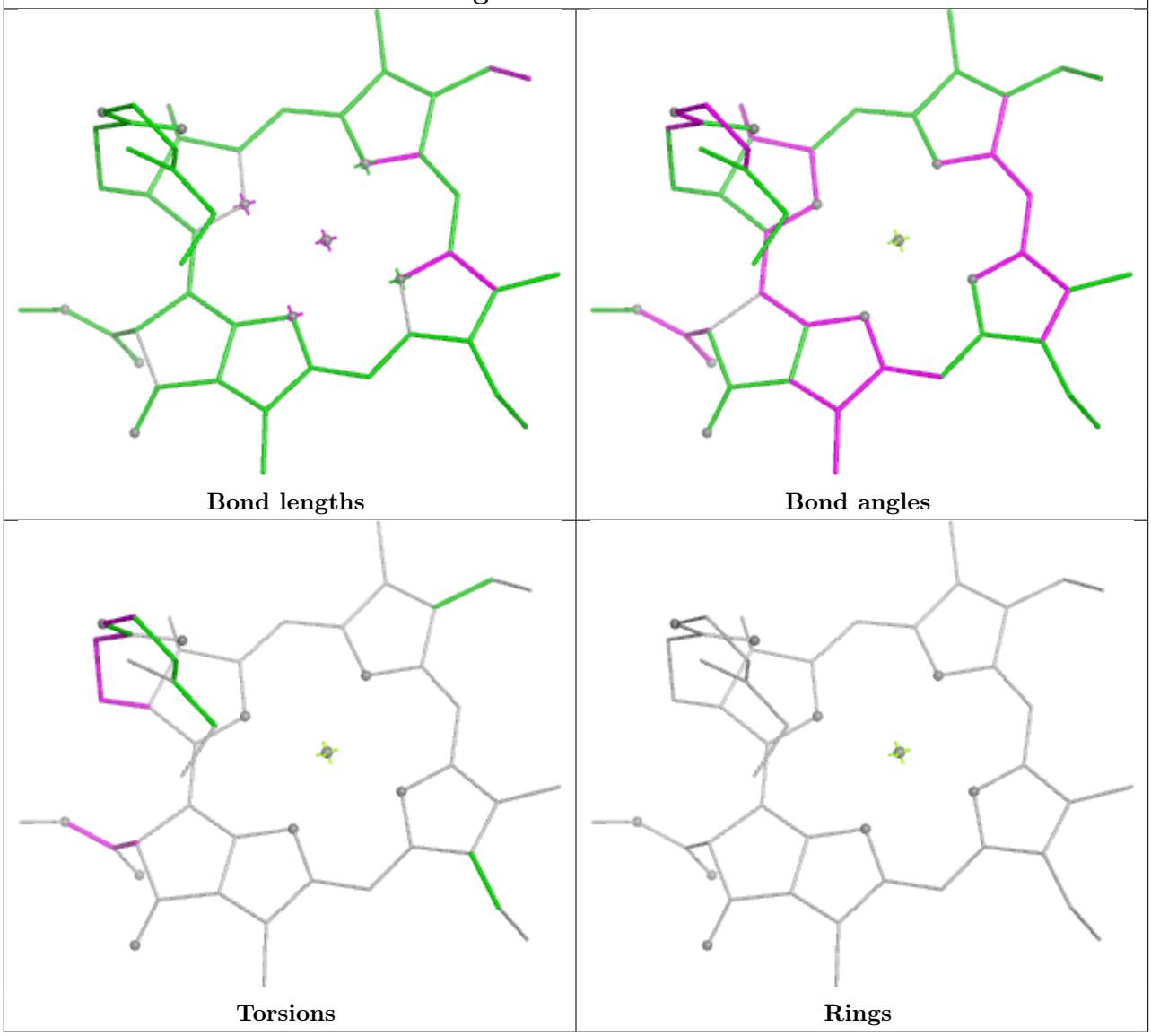
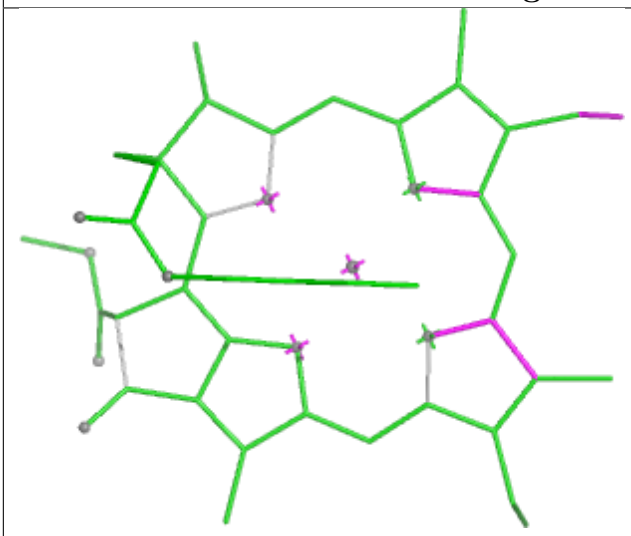
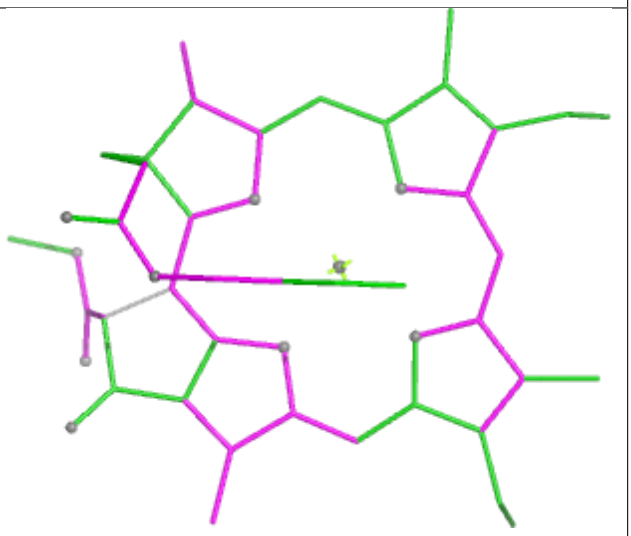


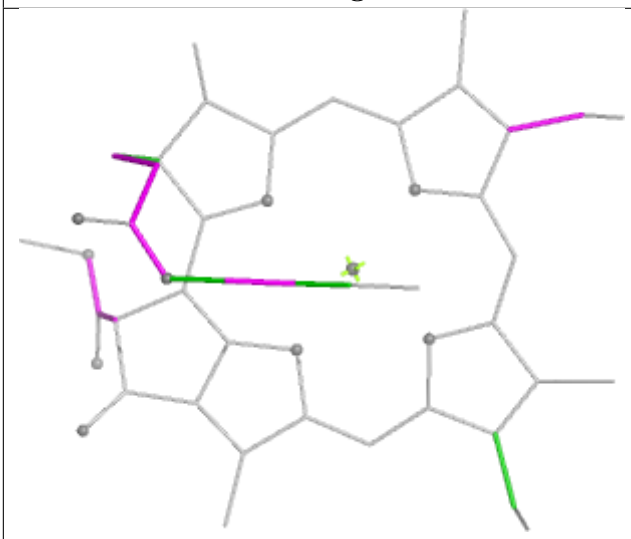
Ligand CLA K 204



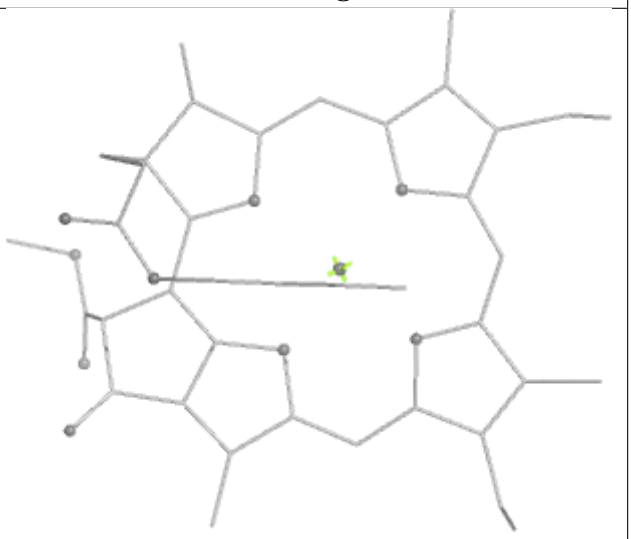
Bond lengths



Bond angles

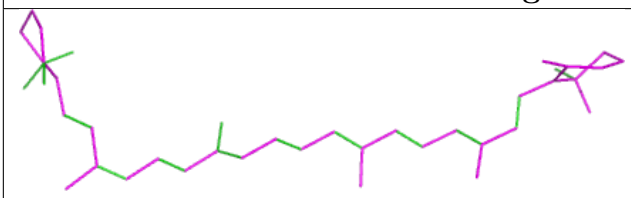


Torsions

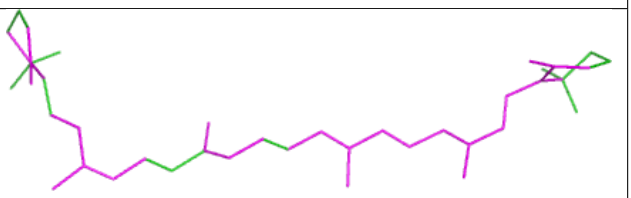


Rings

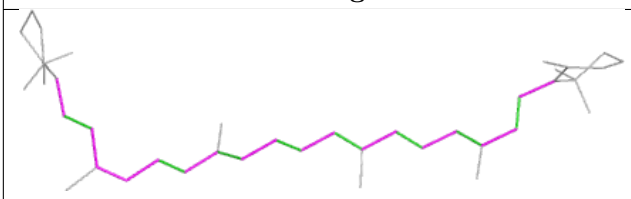
Ligand BCR B 853



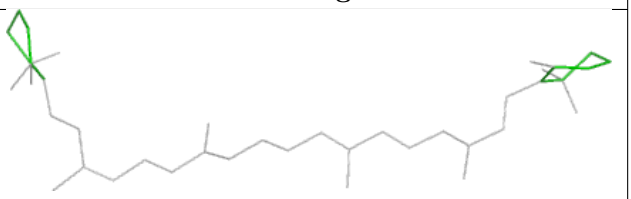
Bond lengths



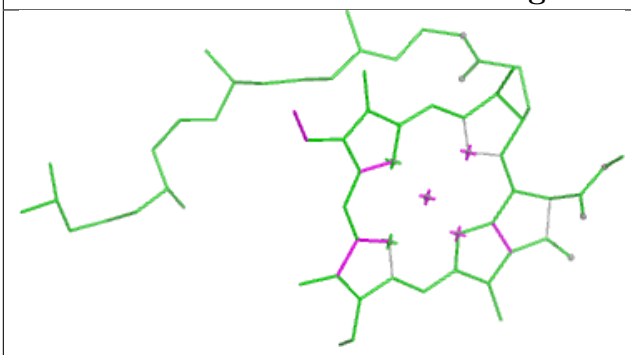
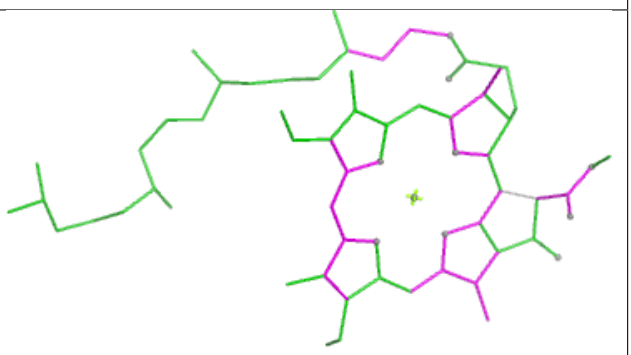
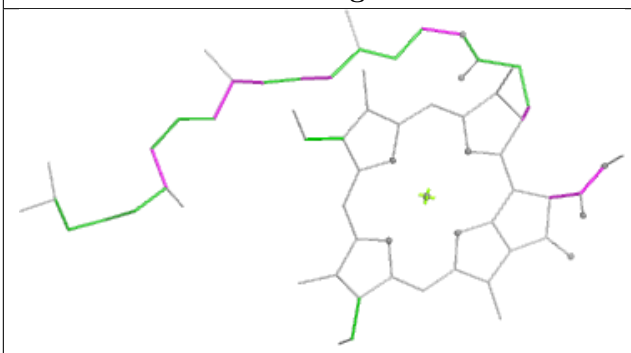
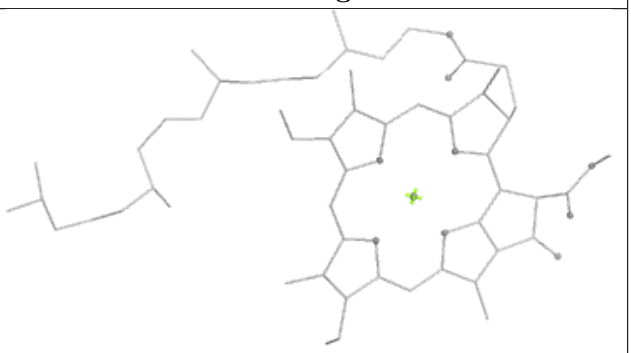
Bond angles

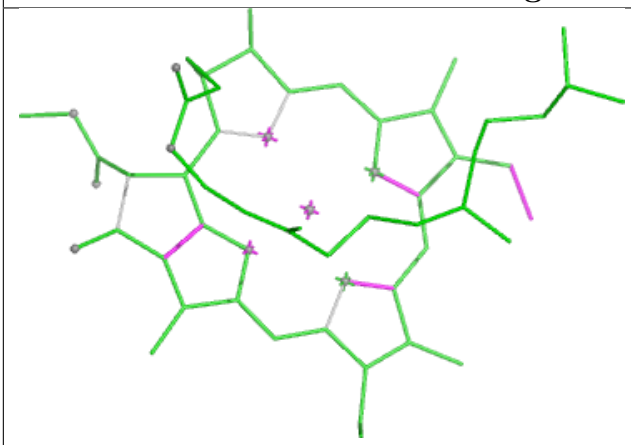
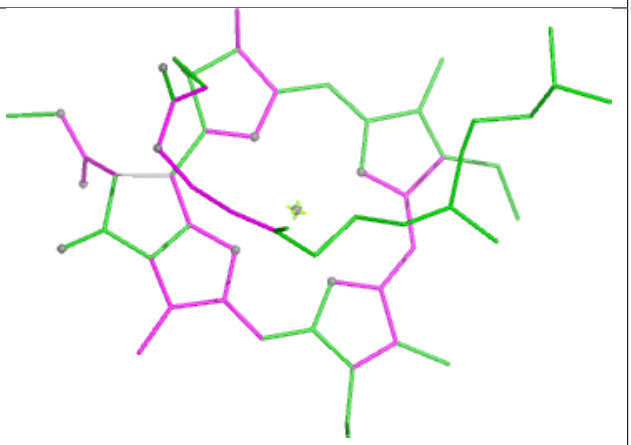
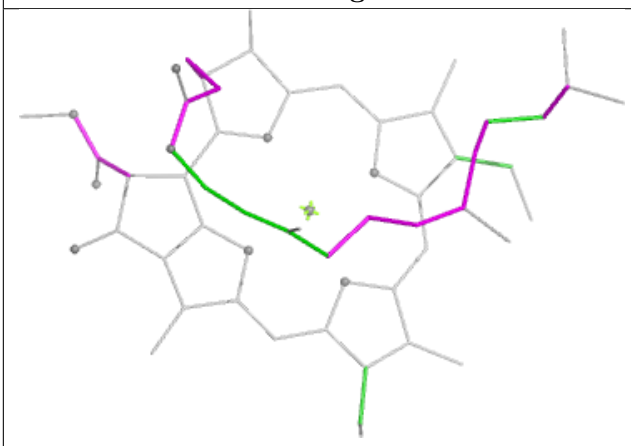
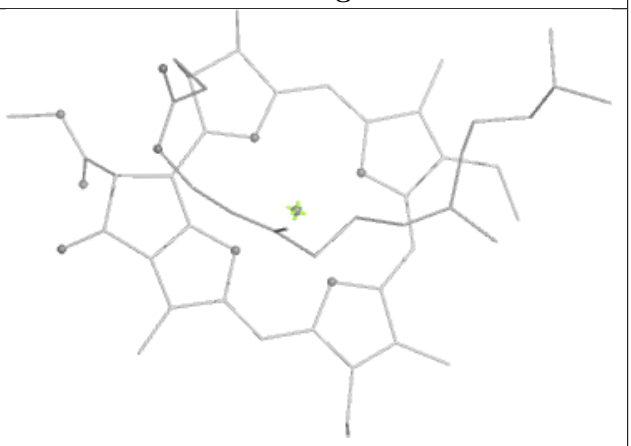


Torsions

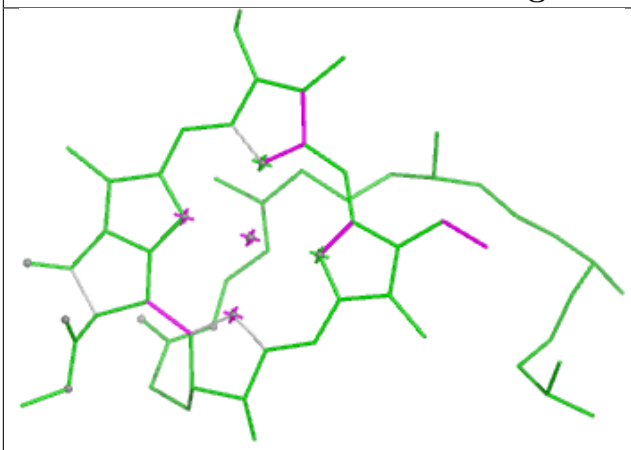


Rings

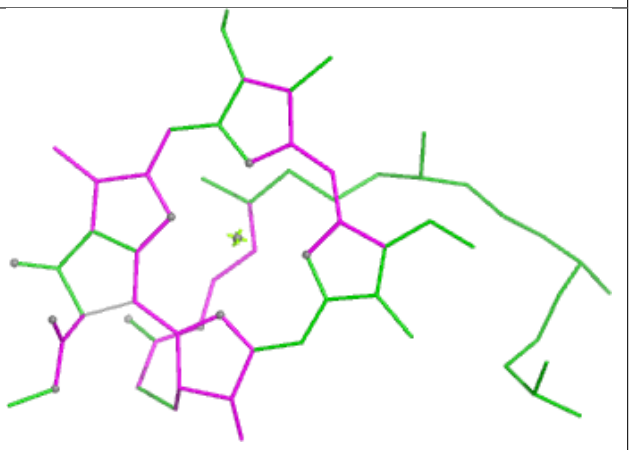
Ligand CLA 7 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 814	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

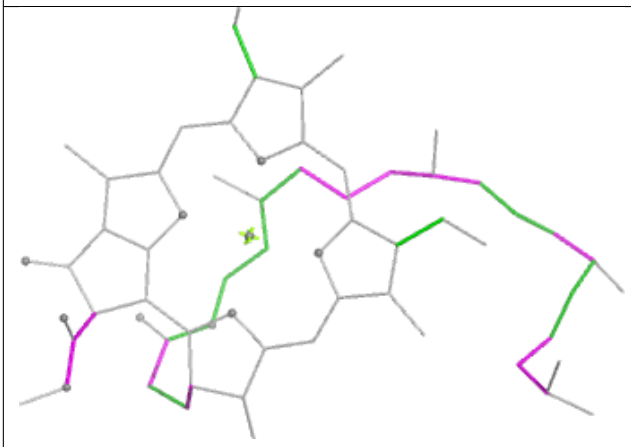
Ligand CLA 6 309



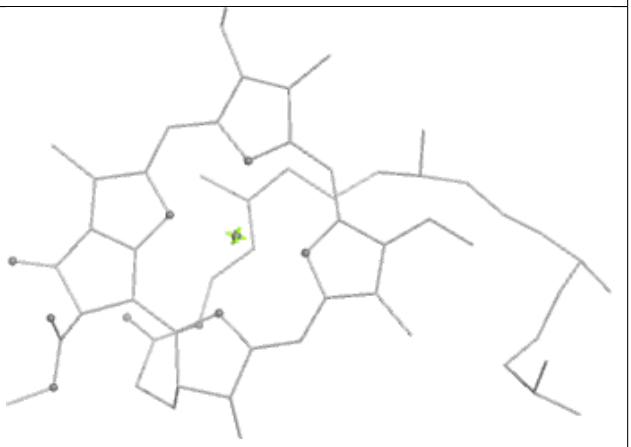
Bond lengths



Bond angles

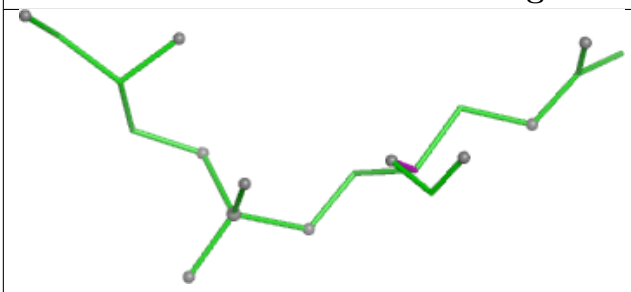


Torsions

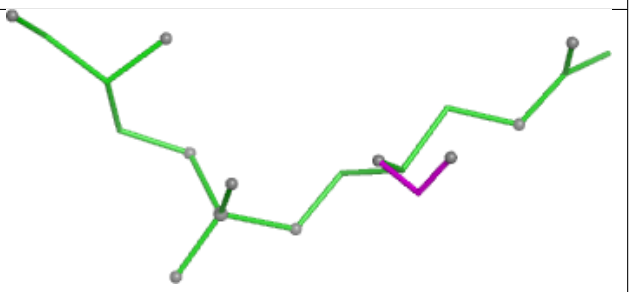


Rings

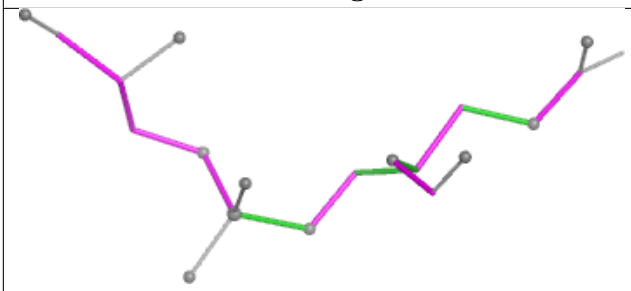
Ligand LHG 3 321



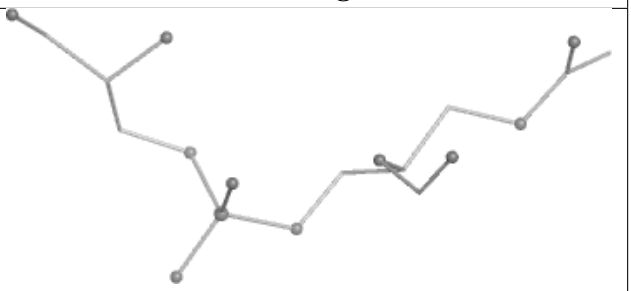
Bond lengths



Bond angles

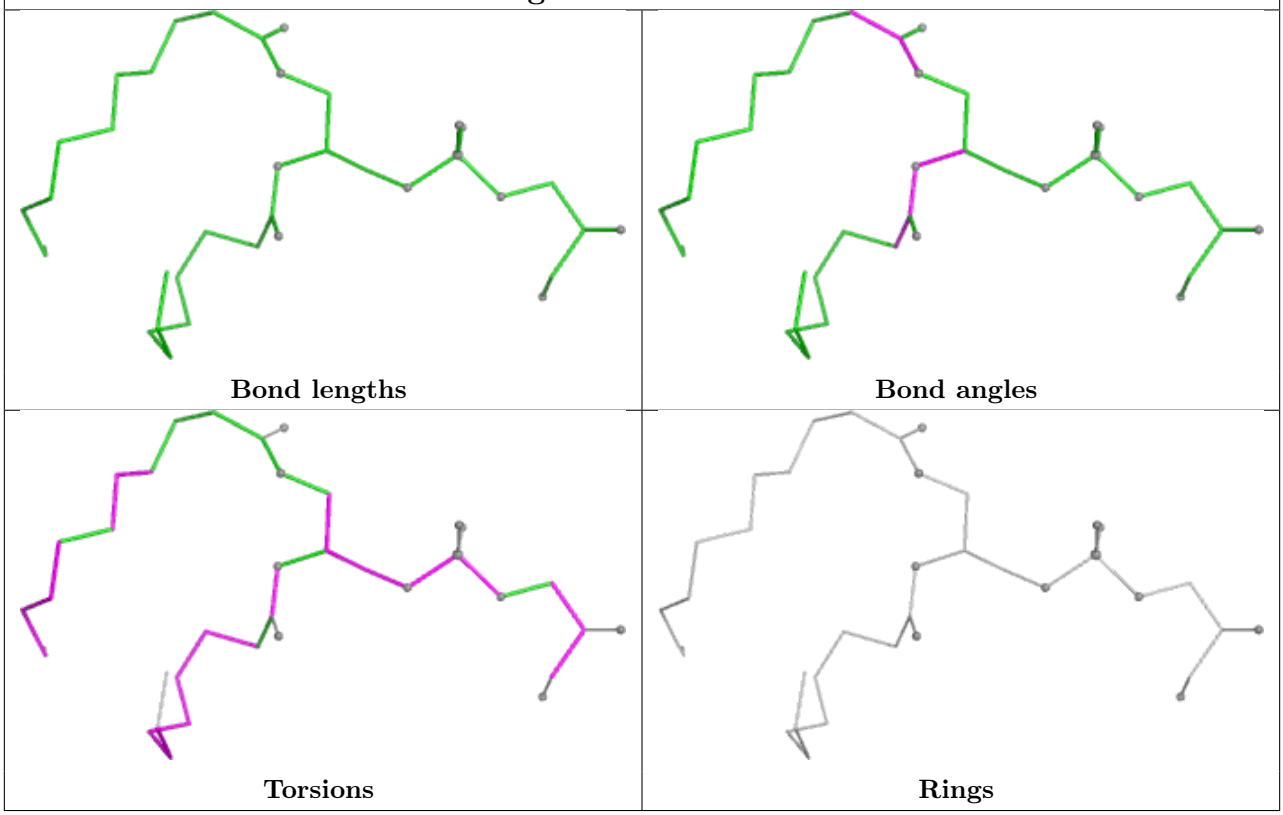


Torsions

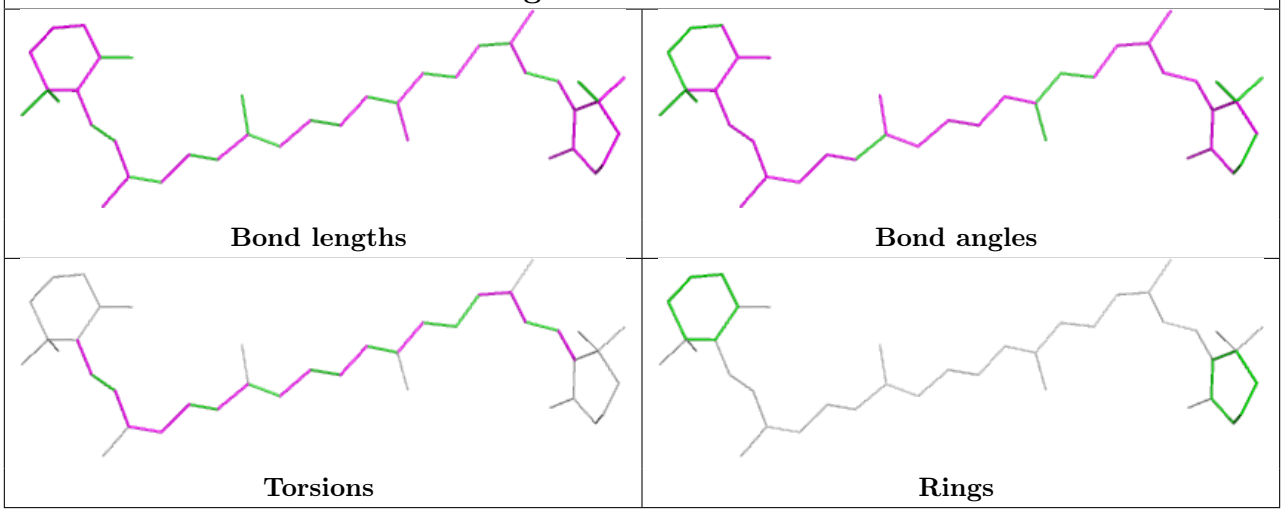


Rings

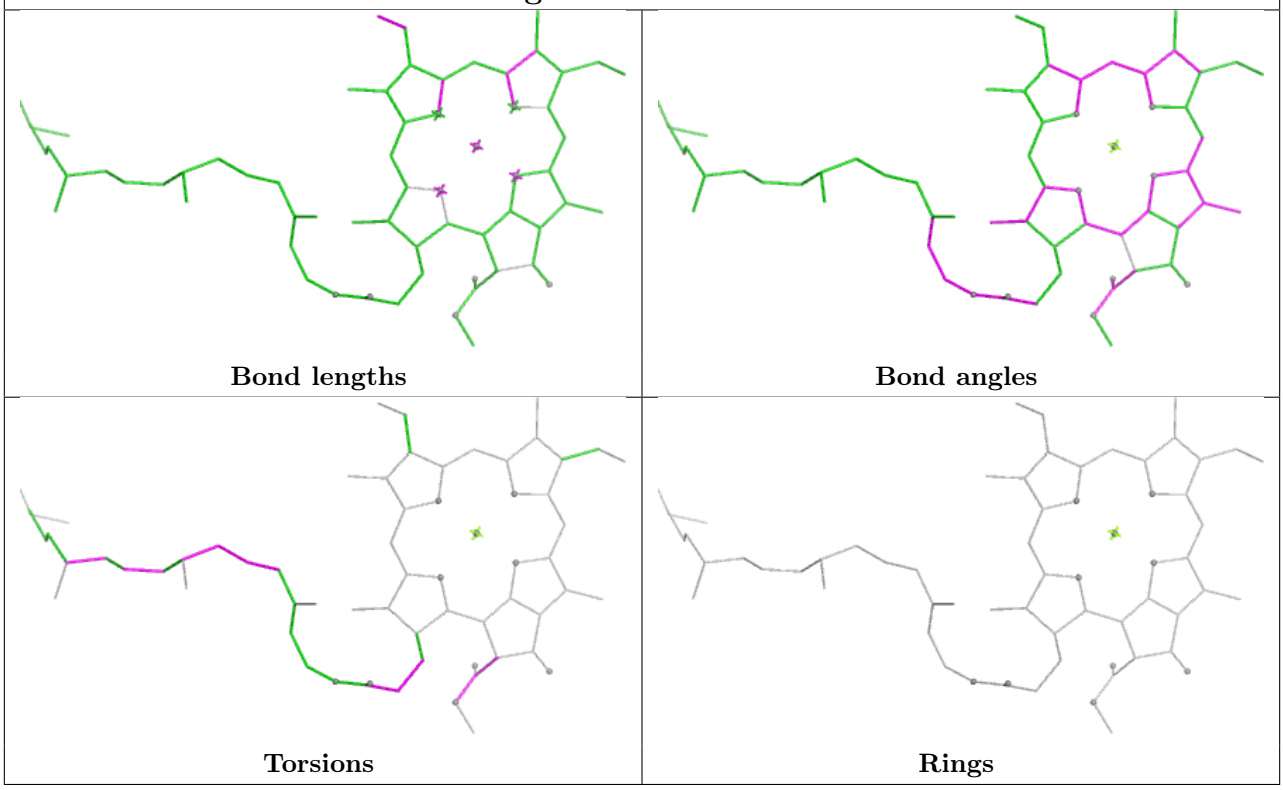
Ligand LHG 7 318



Ligand BCR B 846



Ligand CLA A 854



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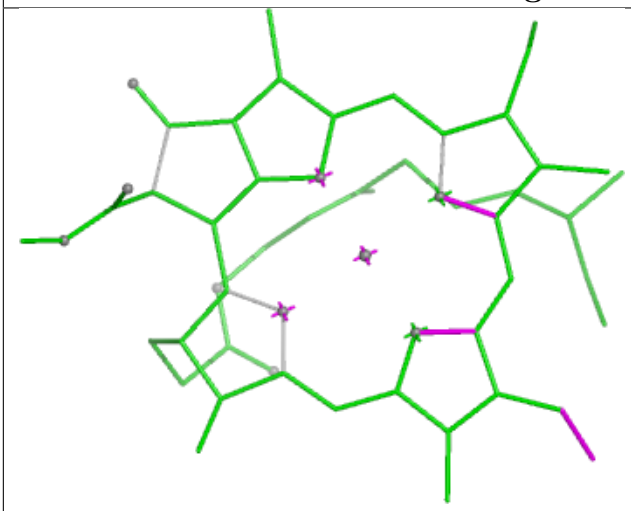
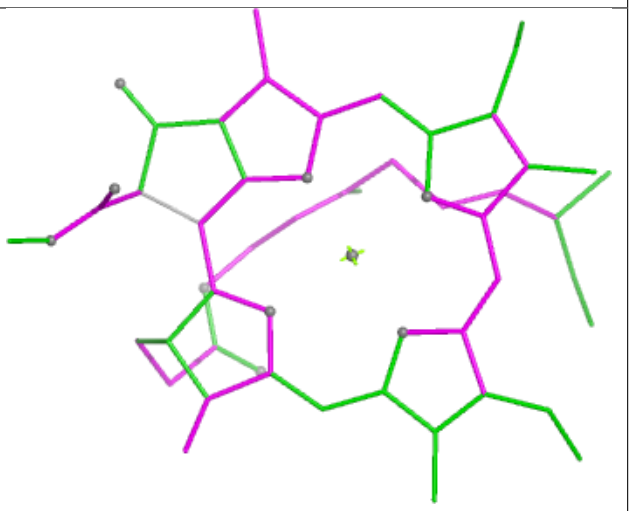
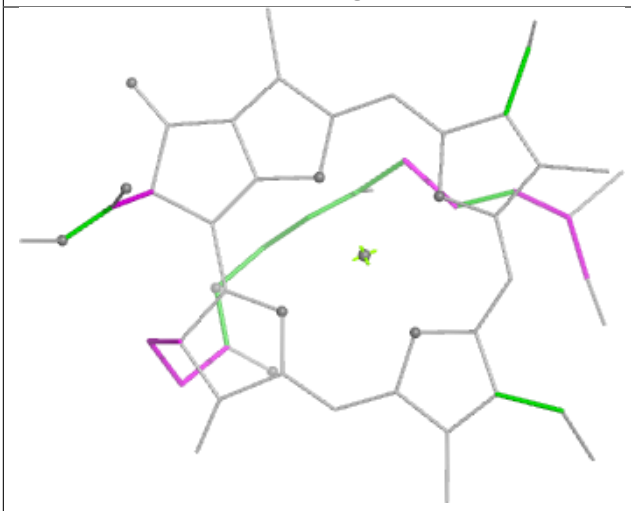


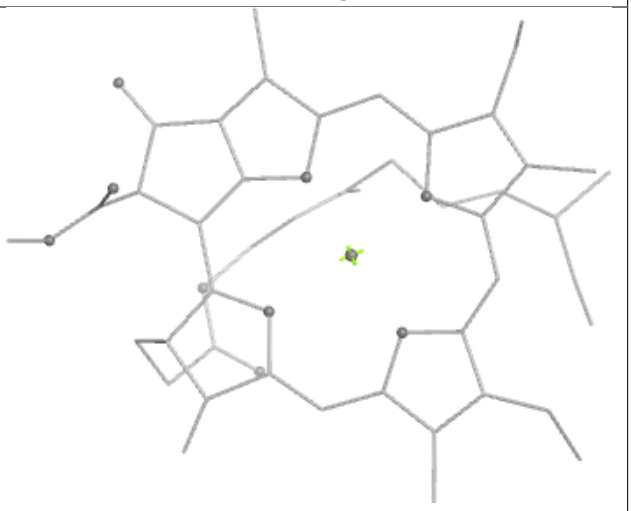
Bond lengths



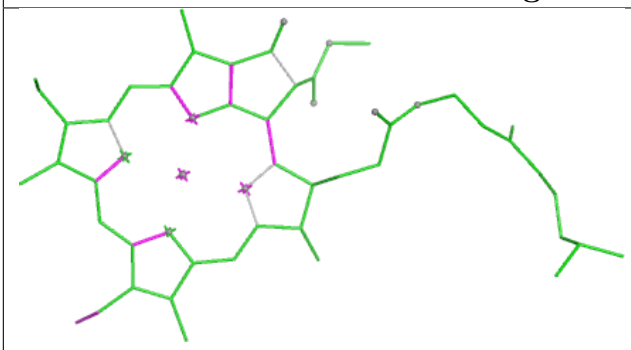
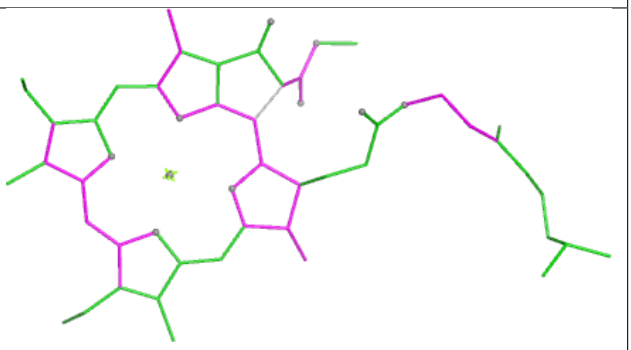
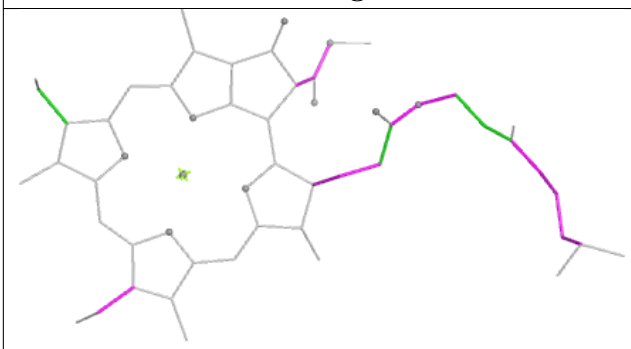
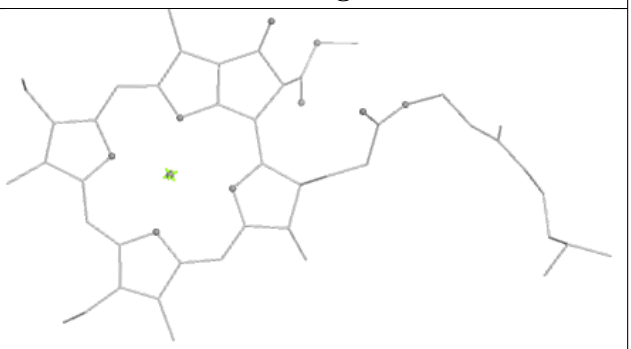
Bond angles



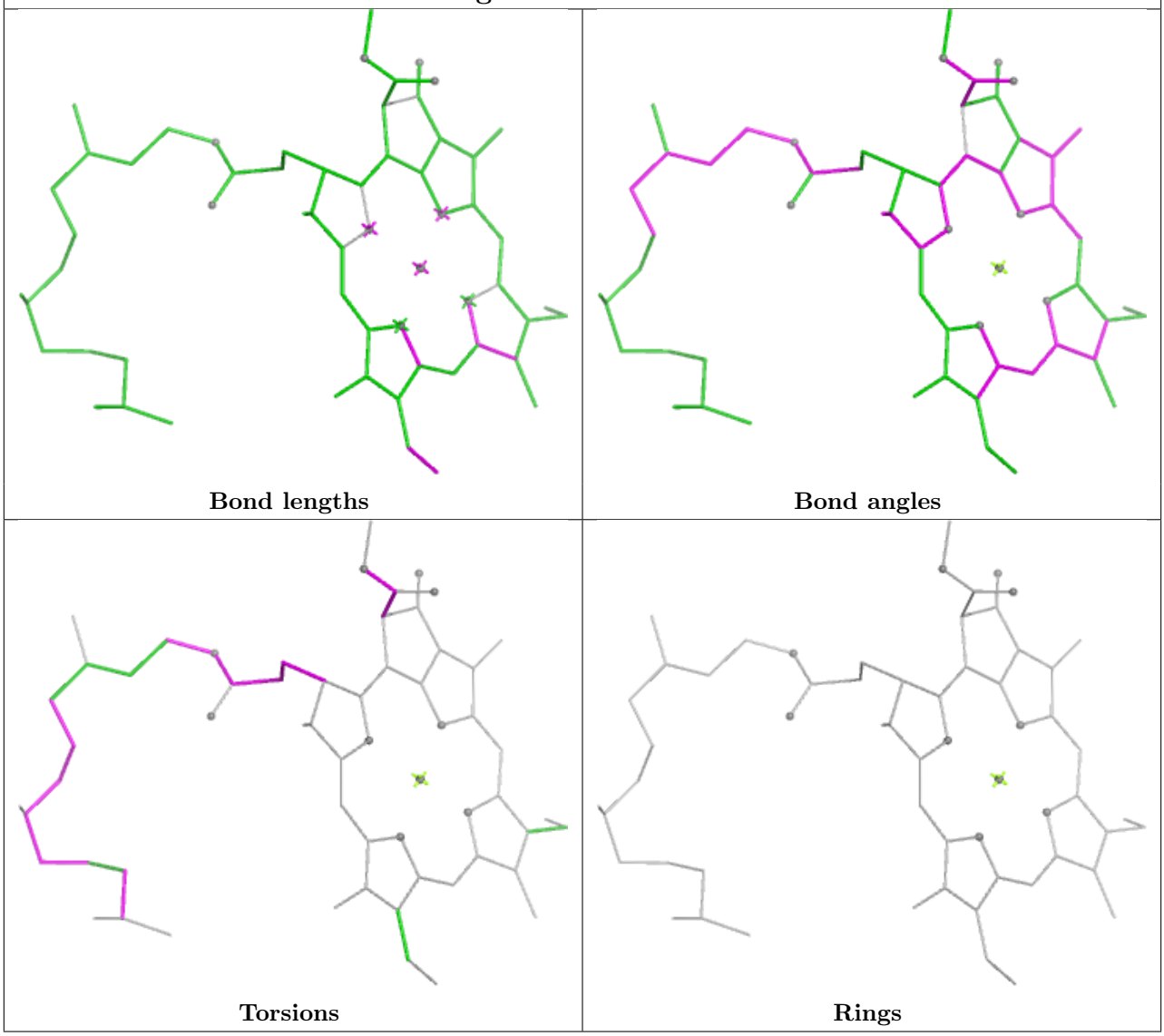
Torsions



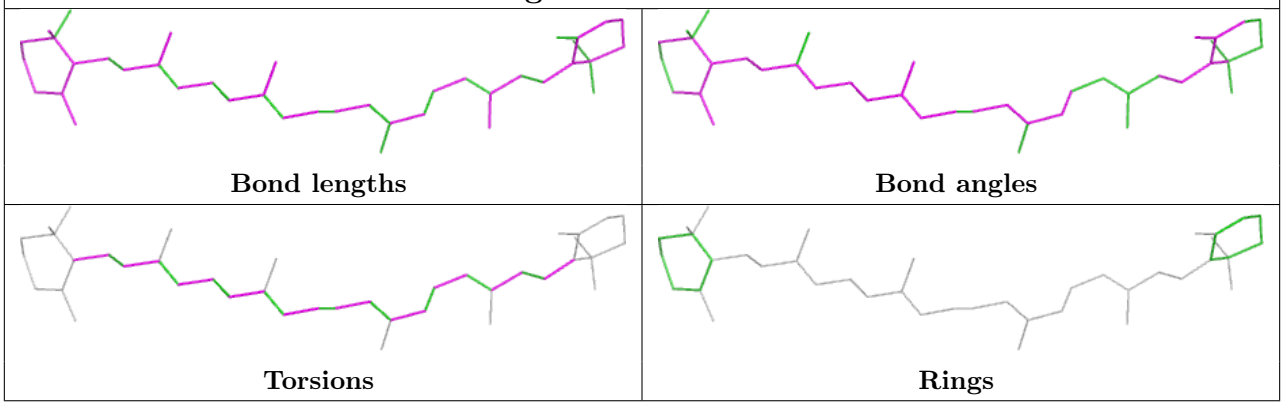
Rings

Ligand CLA K 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

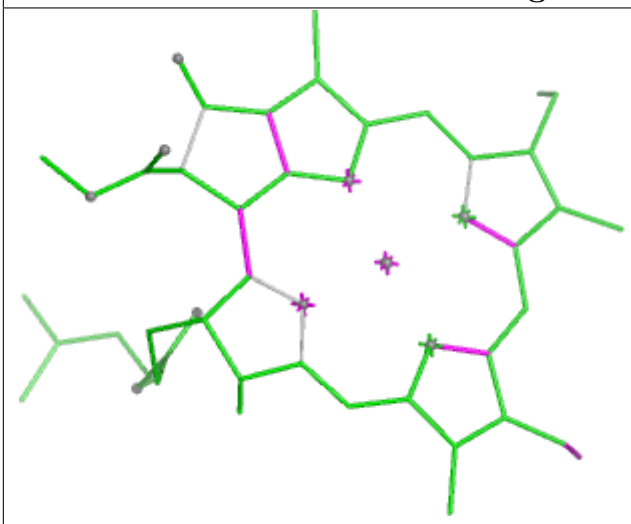
Ligand CLA A 820



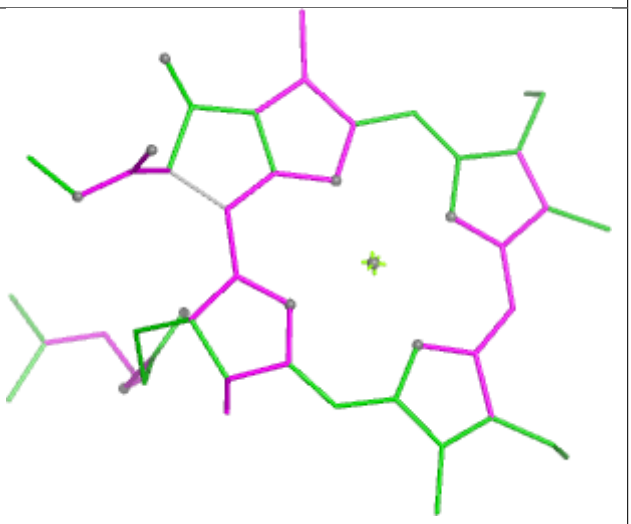
Ligand BCR F 303



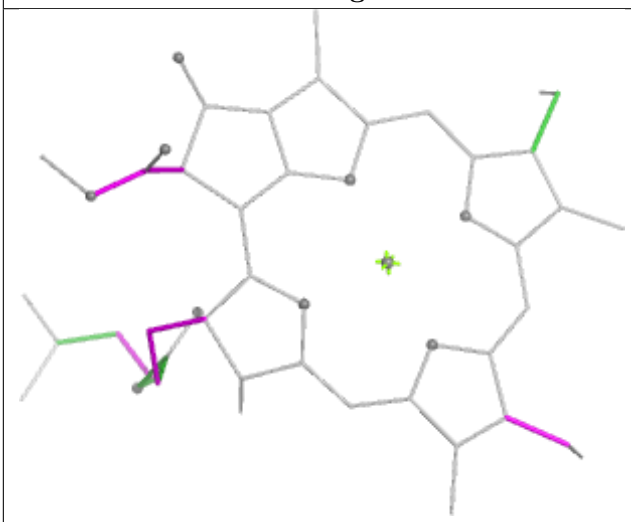
Ligand CLA 5 320



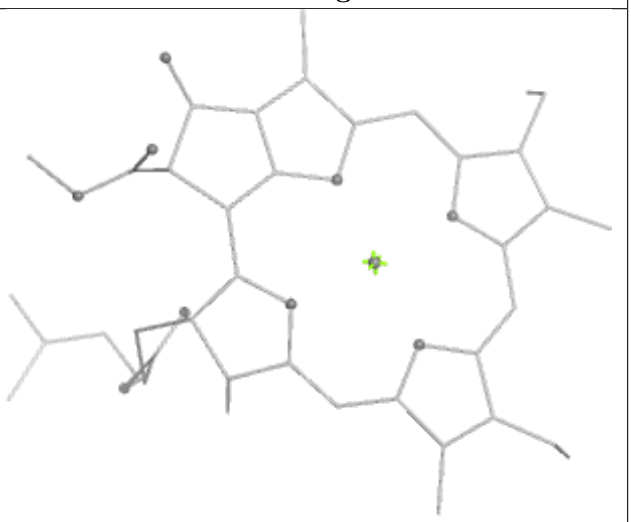
Bond lengths



Bond angles

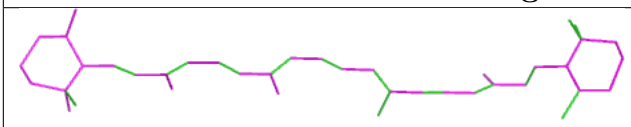


Torsions

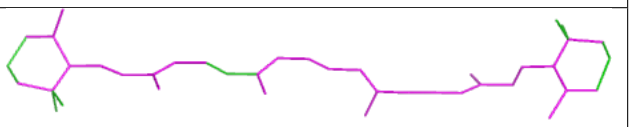


Rings

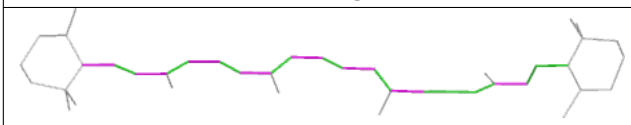
Ligand BCR K 206



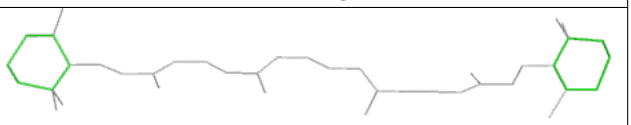
Bond lengths



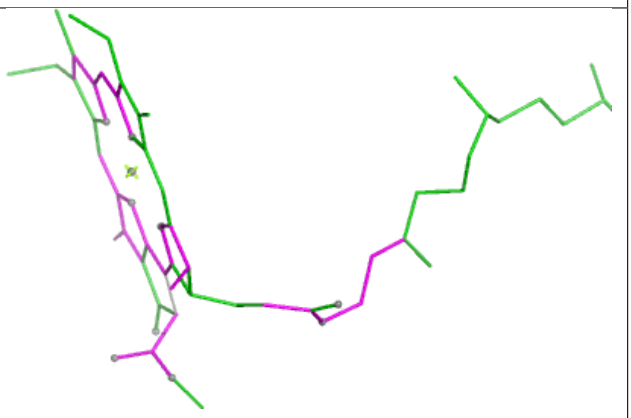
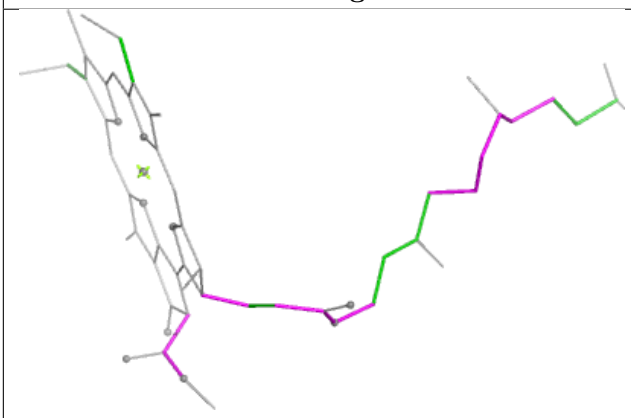
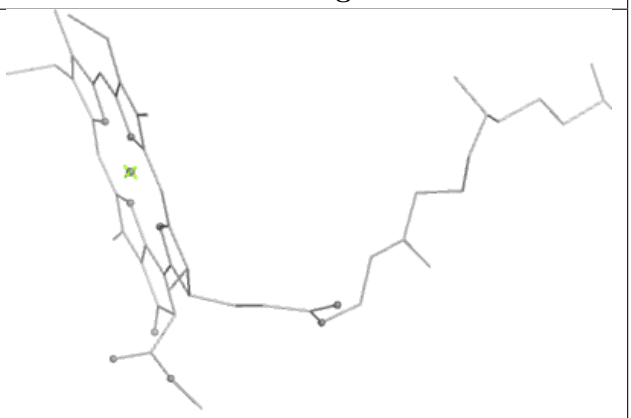
Bond angles



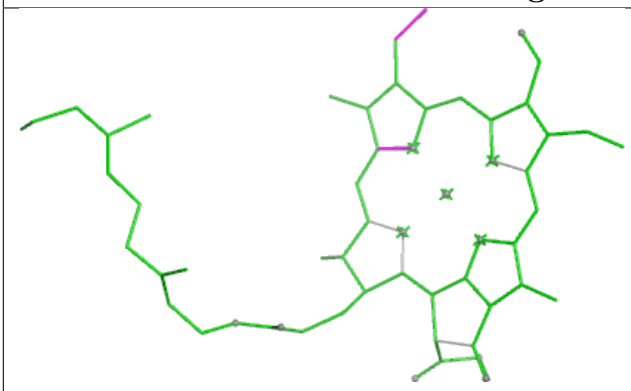
Torsions



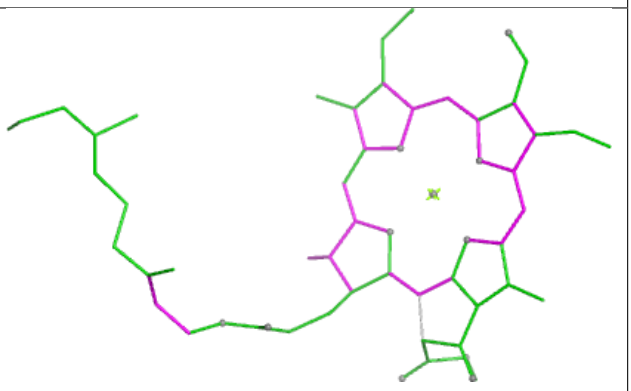
Rings

Ligand CLA 6 302	
Bond lengths	 Bond angles
 Torsions	 Rings

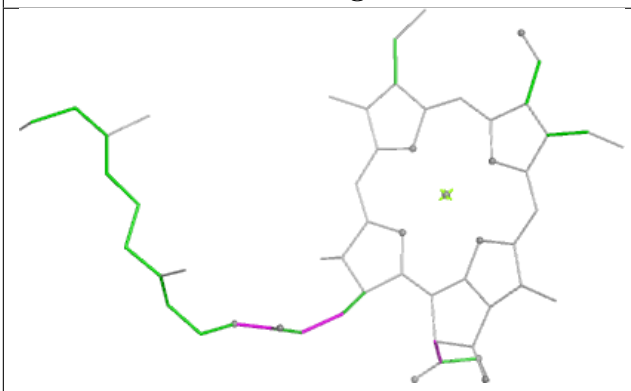
Ligand CHL 8 301



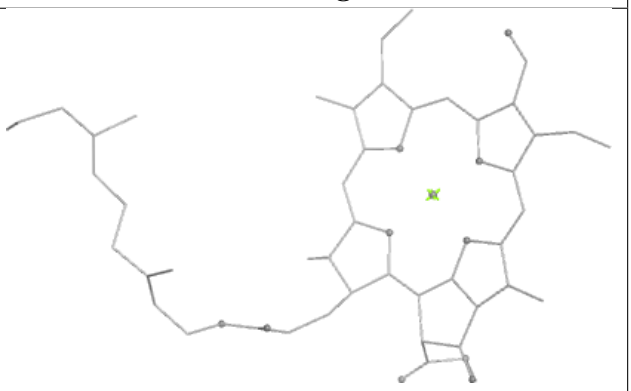
Bond lengths



Bond angles

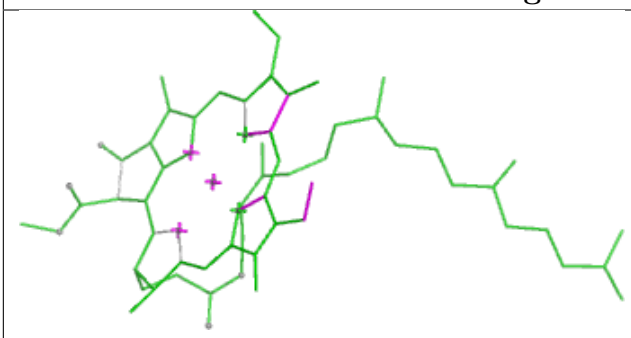


Torsions

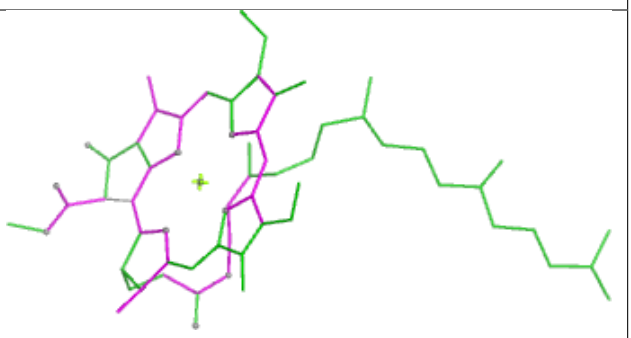


Rings

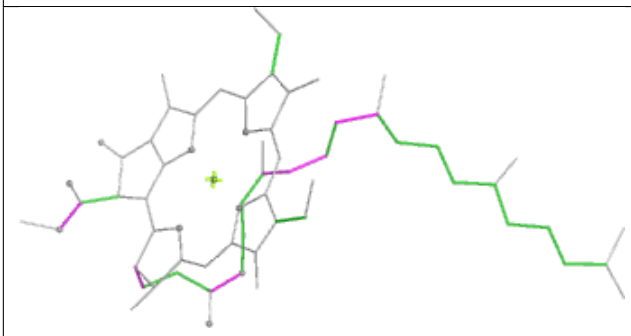
Ligand CLA A 841



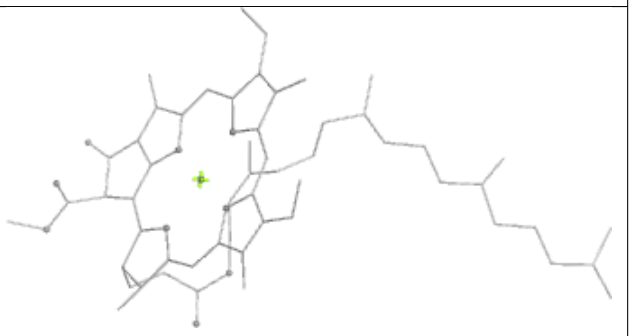
Bond lengths



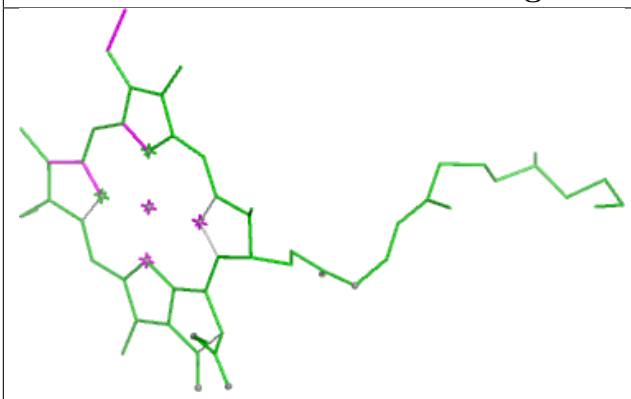
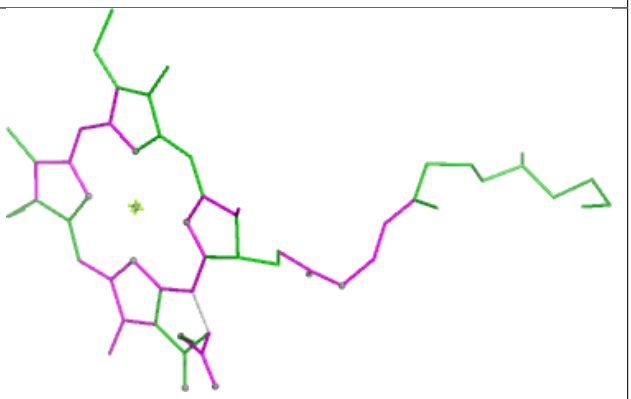
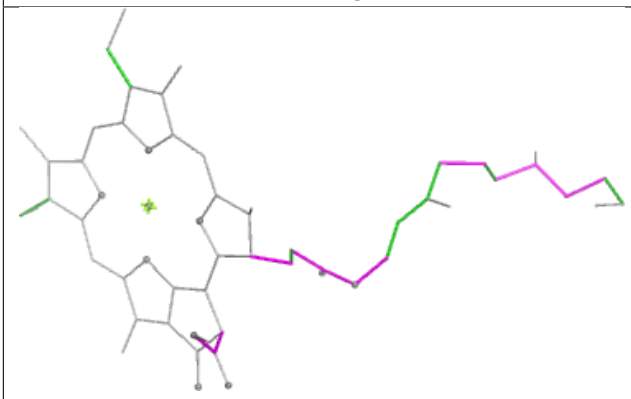
Bond angles



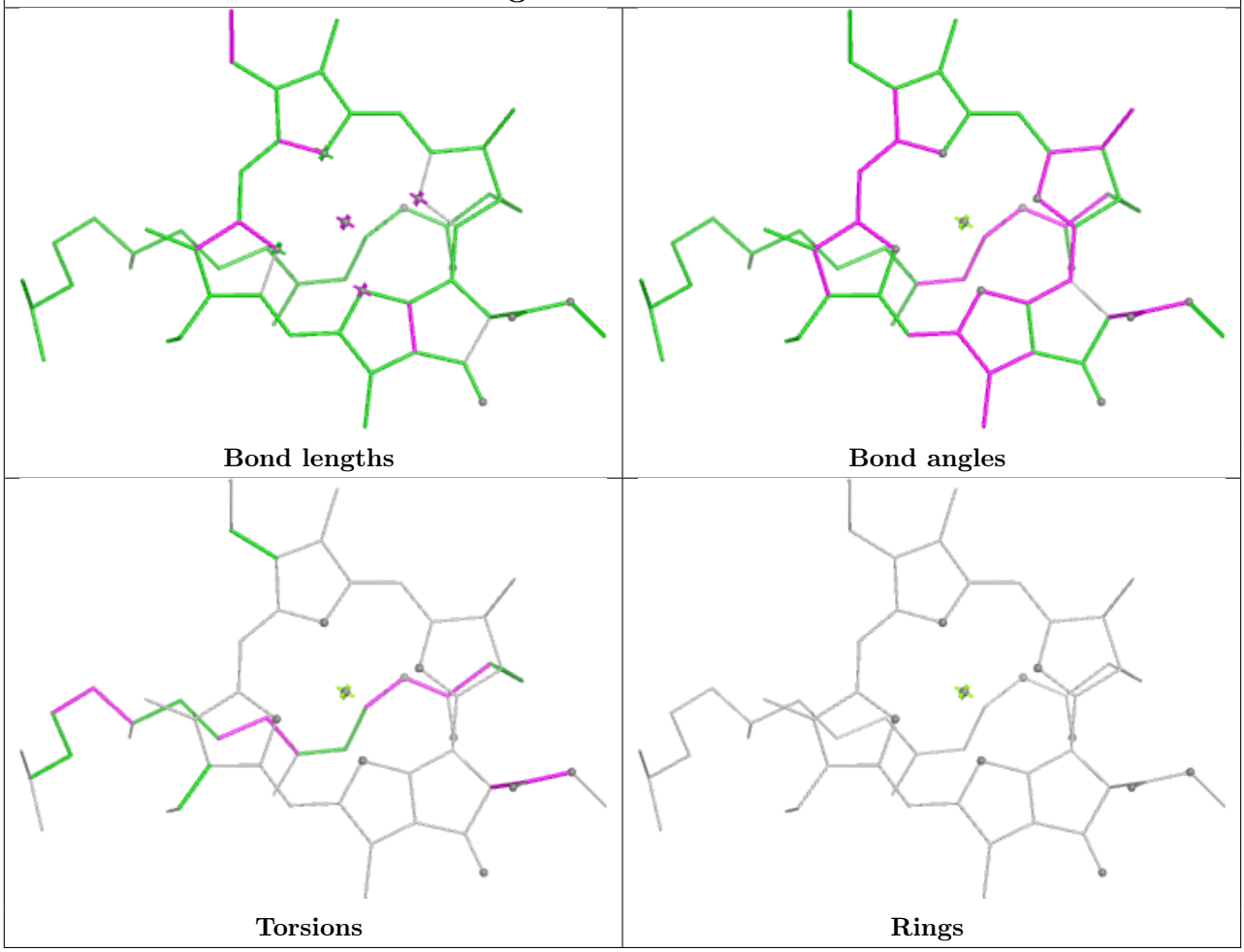
Torsions



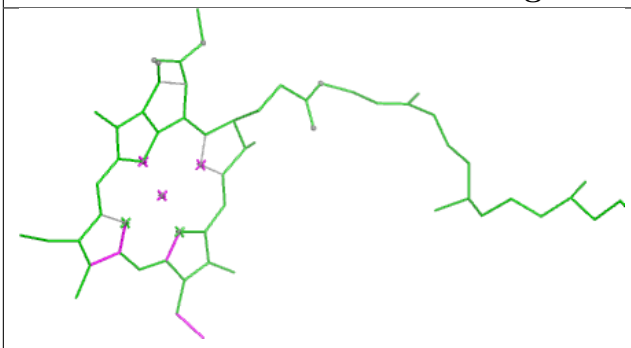
Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	Rings

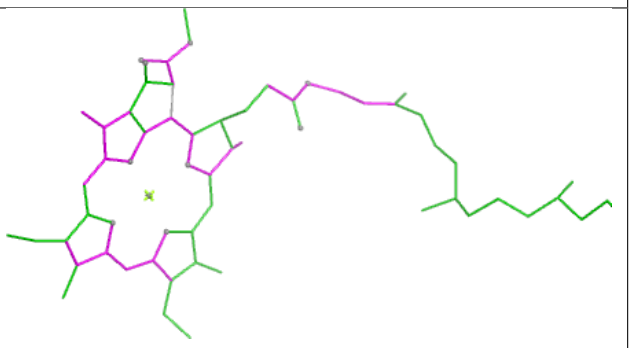
Ligand CLA A 817



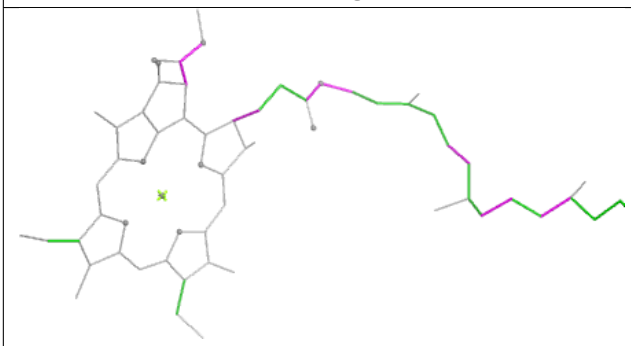
Ligand CLA B 806



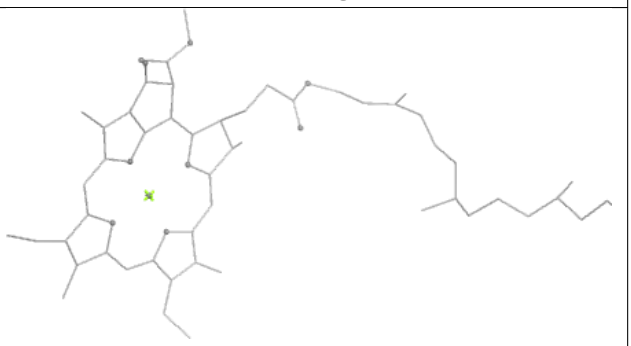
Bond lengths



Bond angles

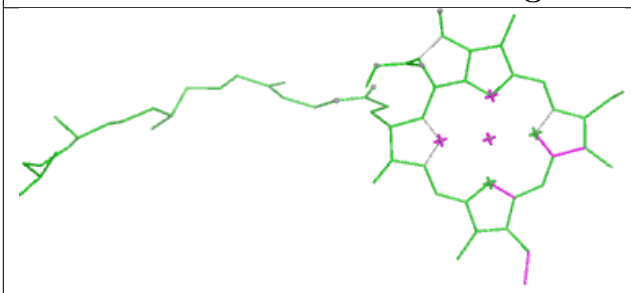


Torsions

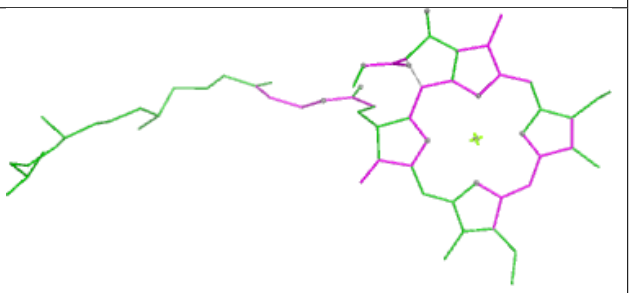


Rings

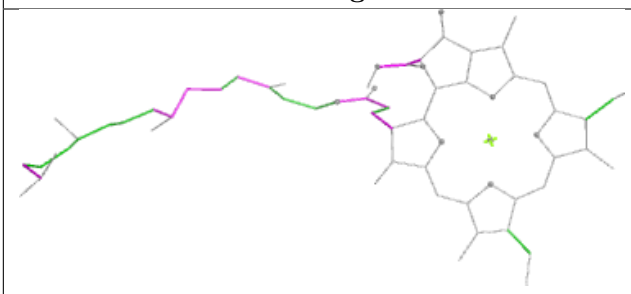
Ligand CLA B 842



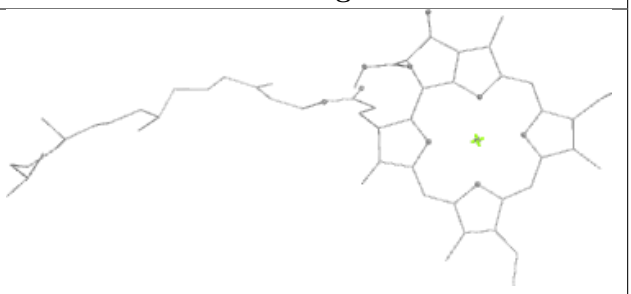
Bond lengths



Bond angles

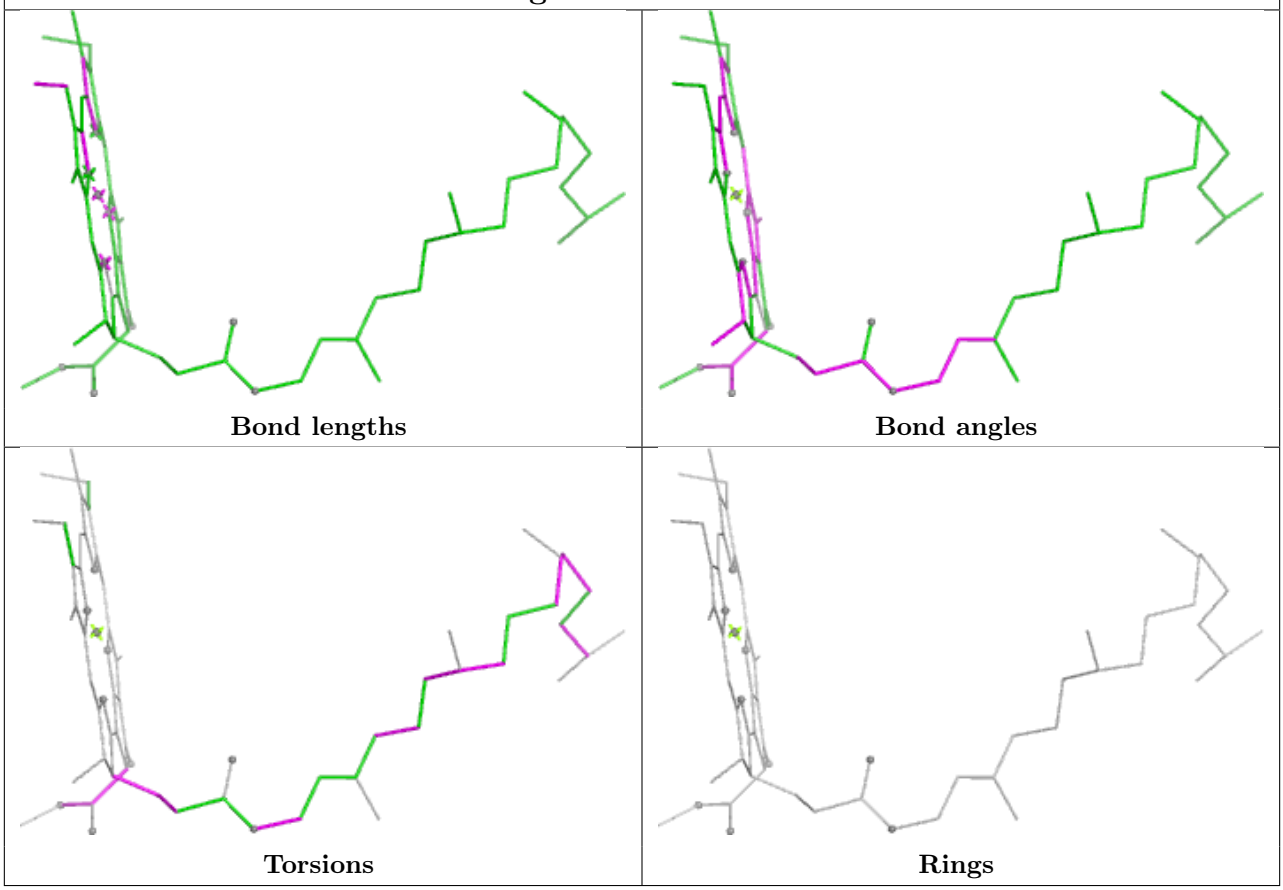


Torsions

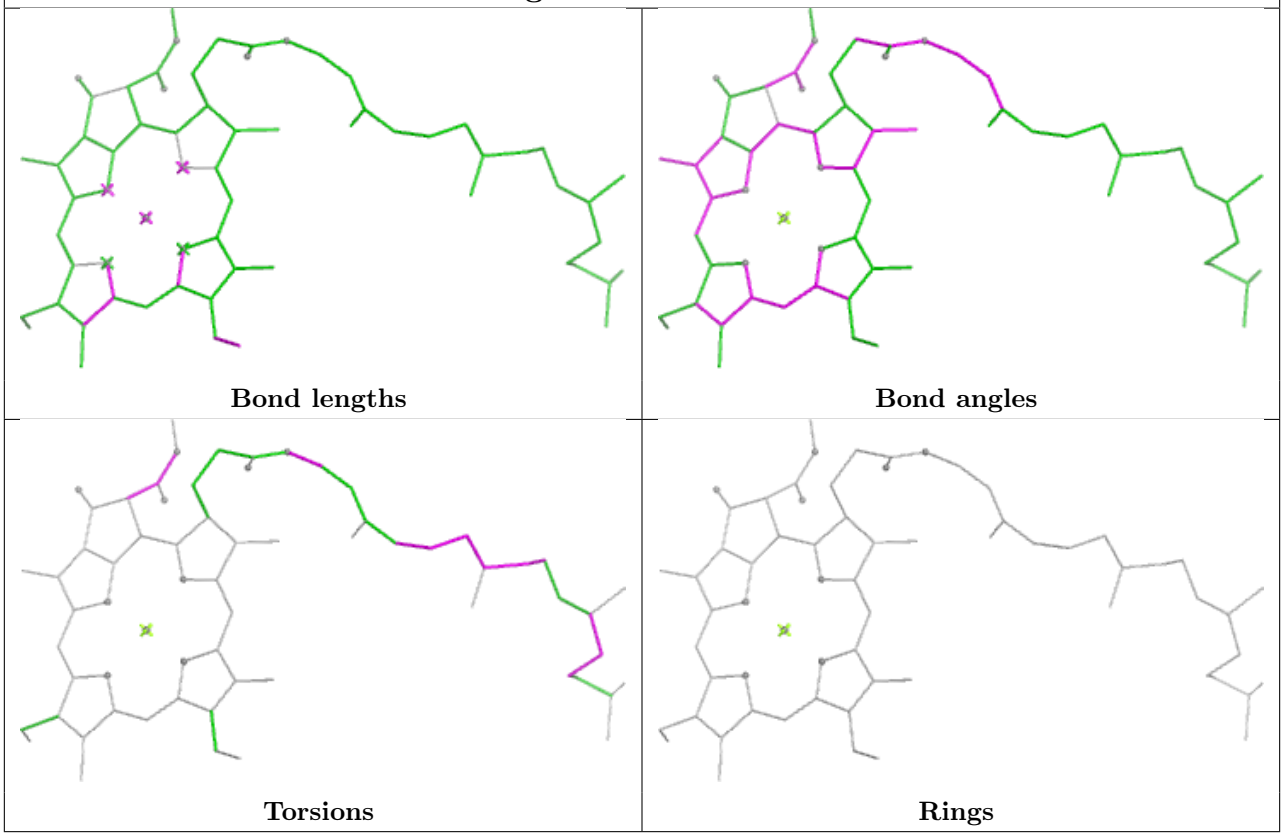


Rings

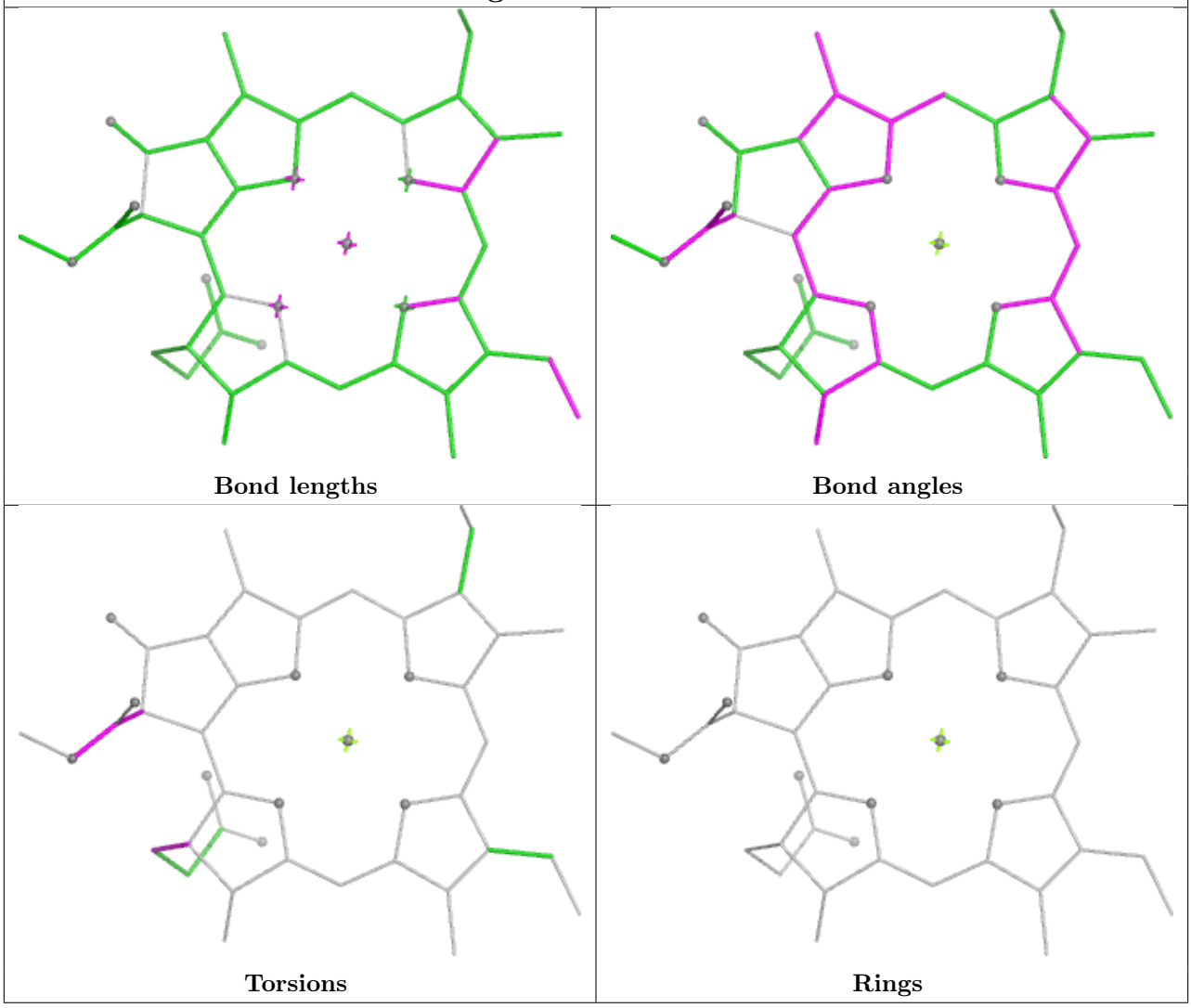
Ligand CLA 7 323



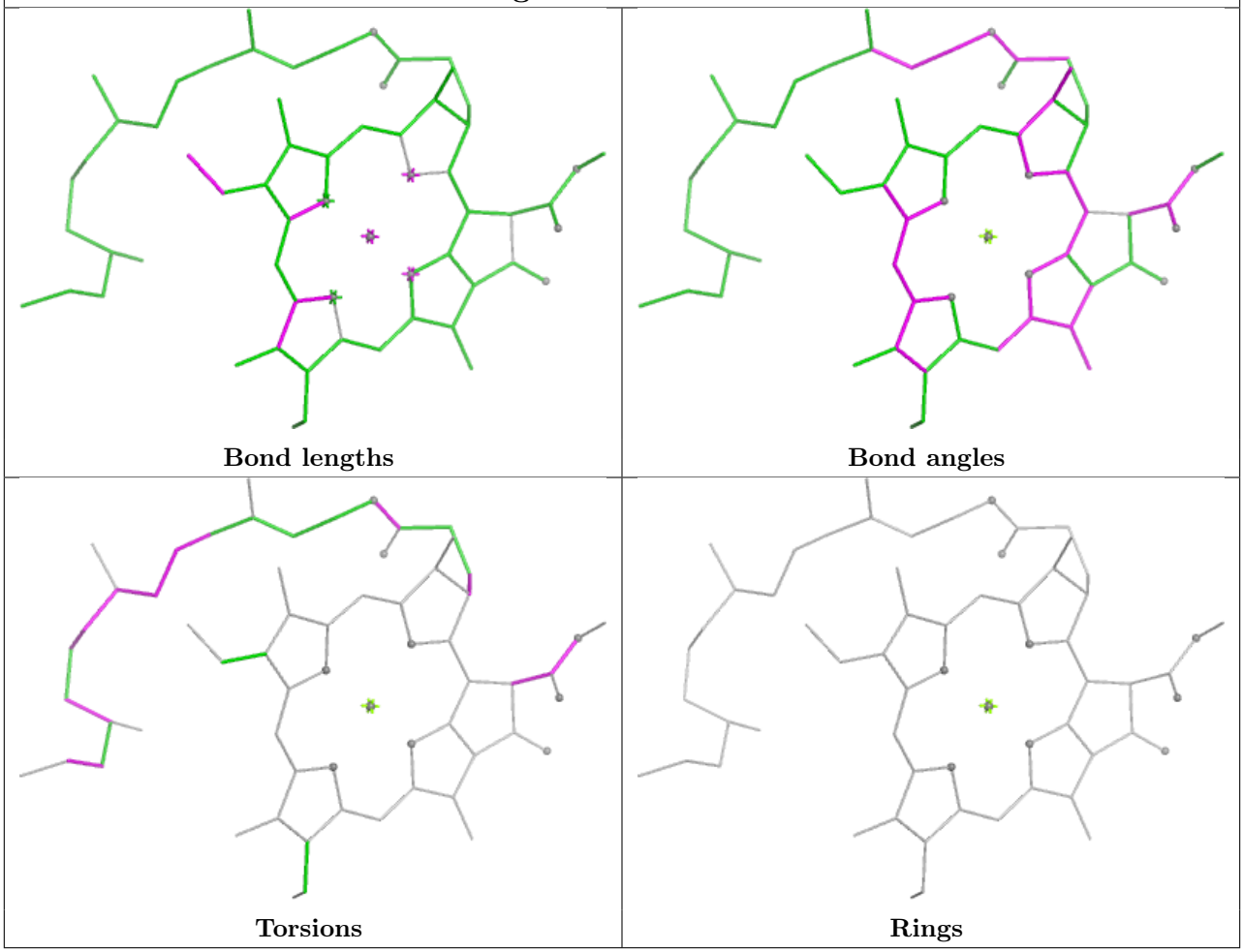
Ligand CLA B 801



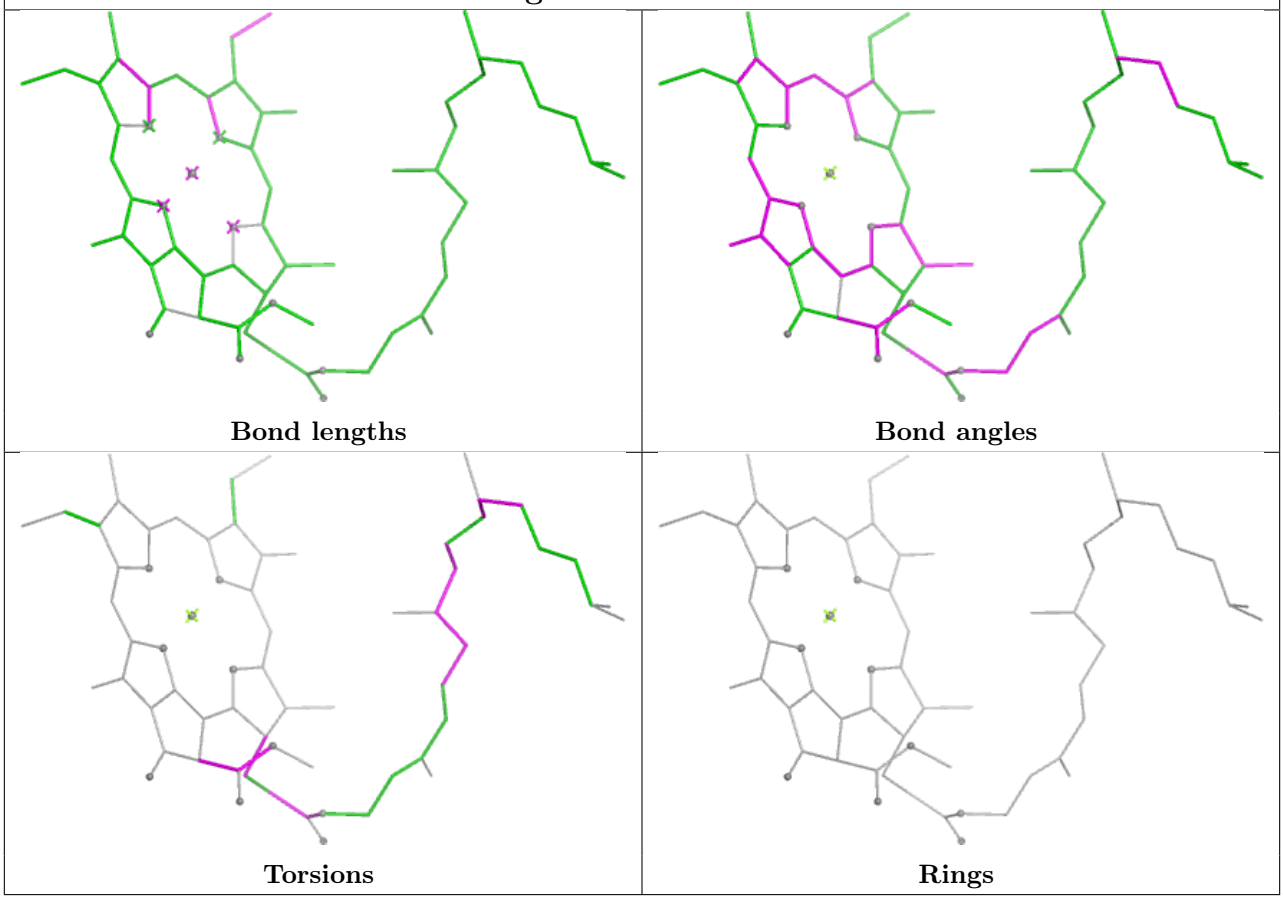
Ligand CLA B 836



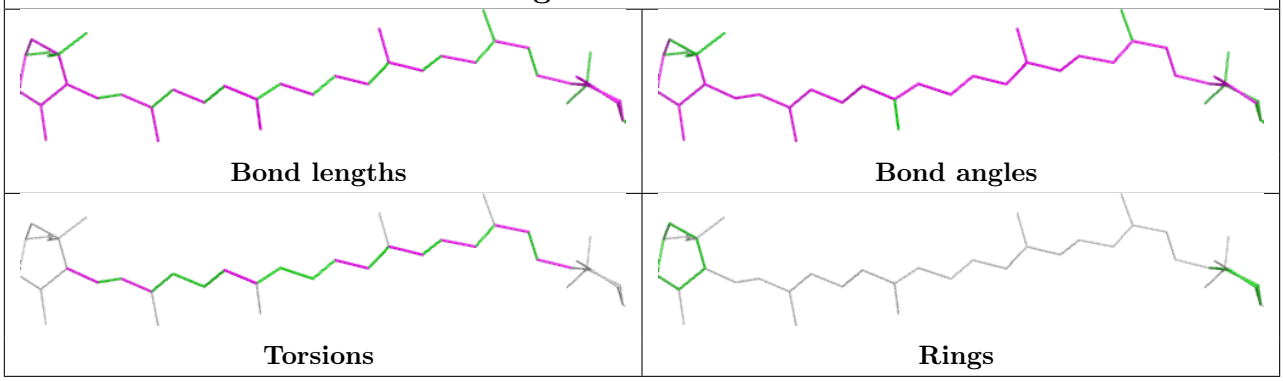
Ligand CLA 8 308



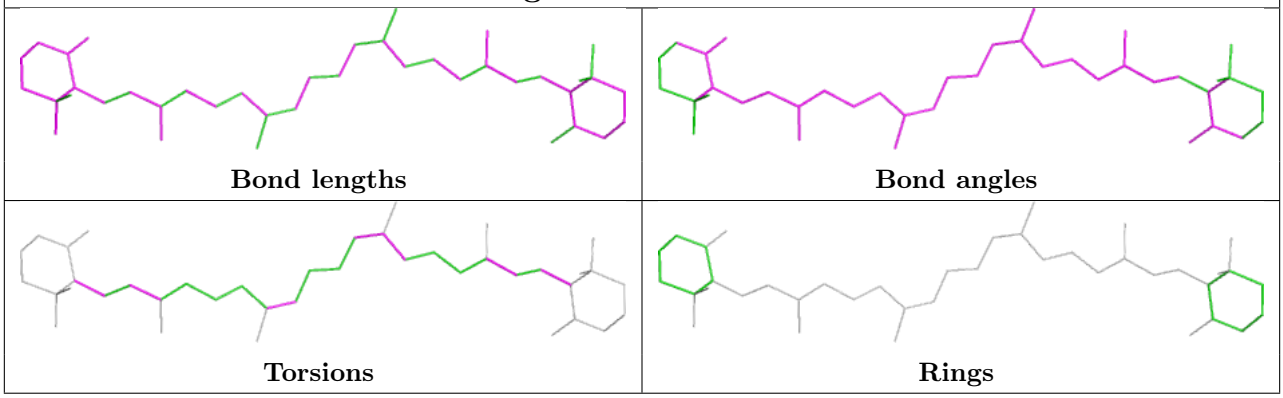
Ligand CLA B 826



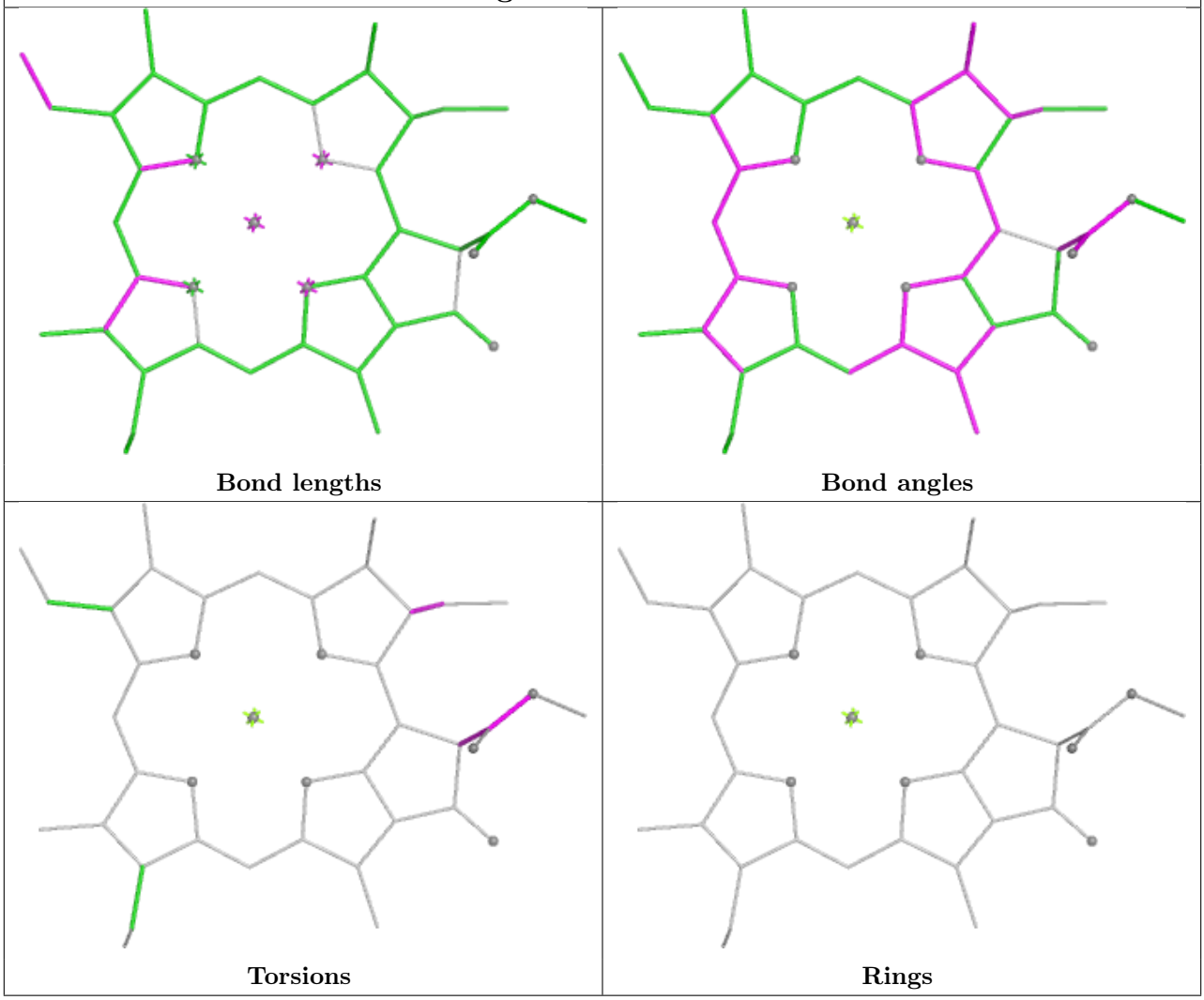
Ligand C7Z J 105



Ligand BCR B 844



Ligand CLA 7 316



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	144:PRO	C	158:ARG	N	6.44

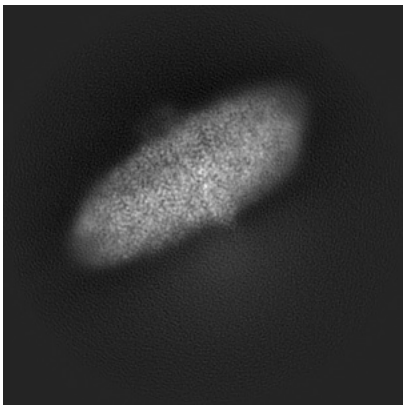
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-16732. These allow visual inspection of the internal detail of the map and identification of artifacts.

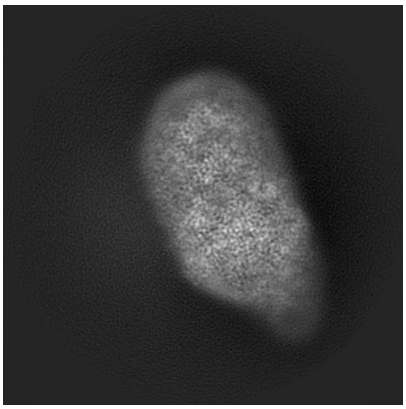
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

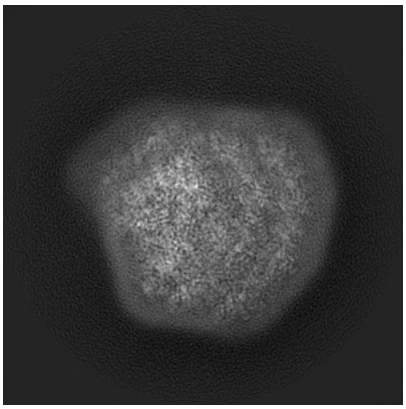
6.1.1 Primary map



X

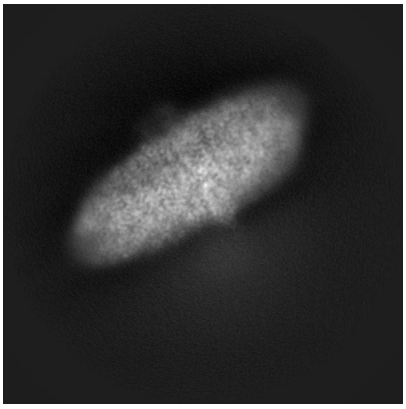


Y

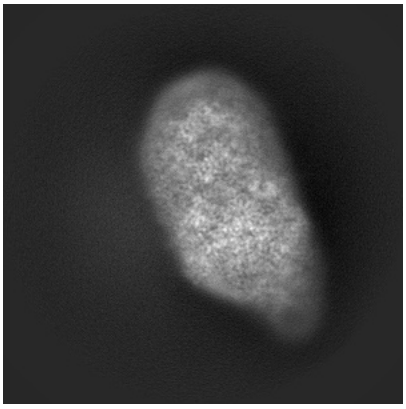


Z

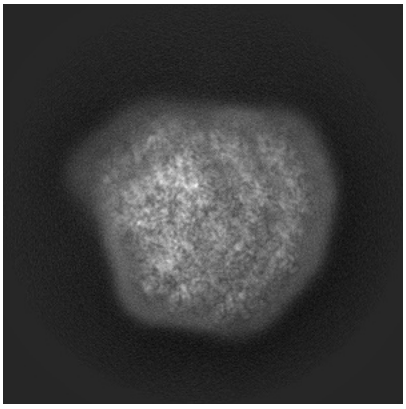
6.1.2 Raw map



X



Y

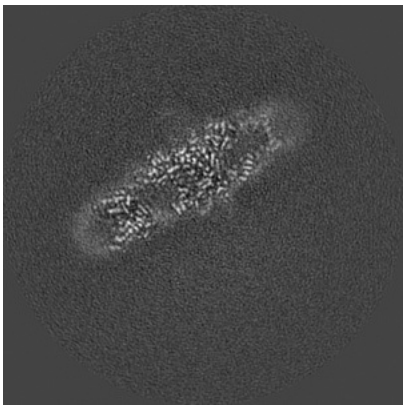


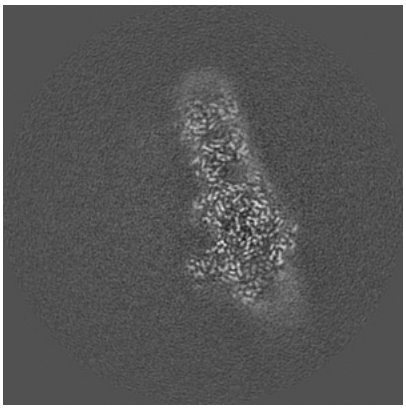
Z

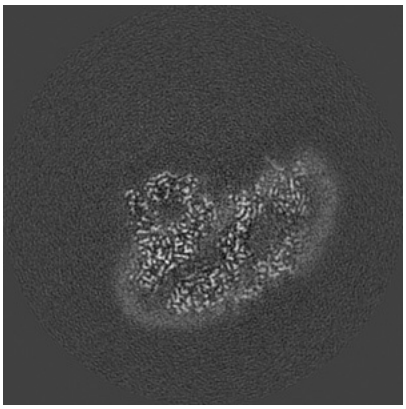
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

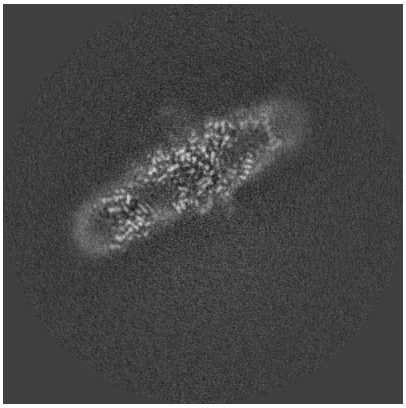
6.2.1 Primary map

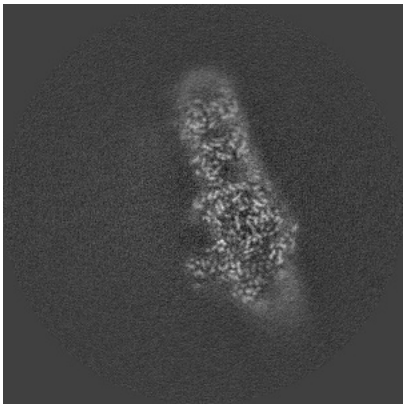

X Index: 250

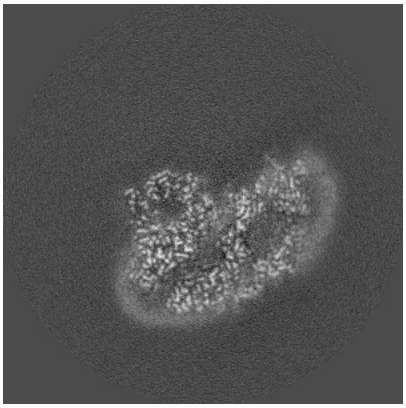

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

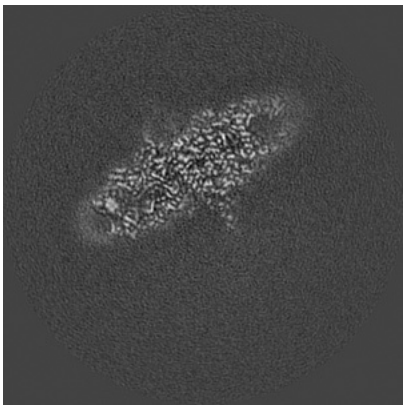

Y Index: 250

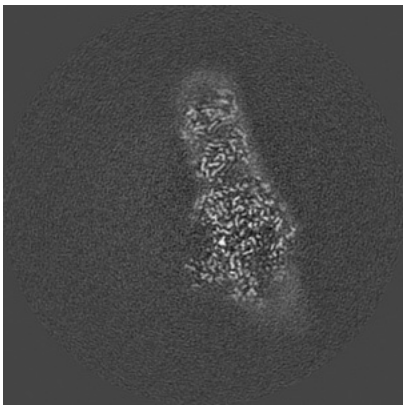

Z Index: 250

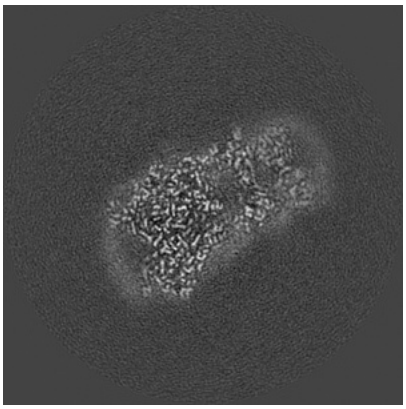
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

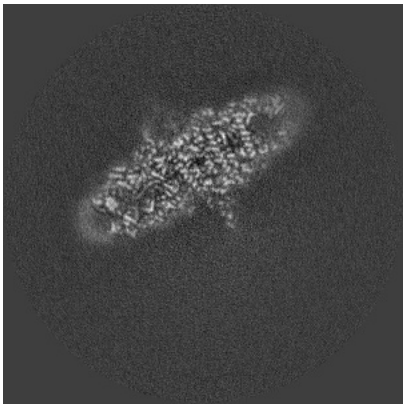
6.3.1 Primary map

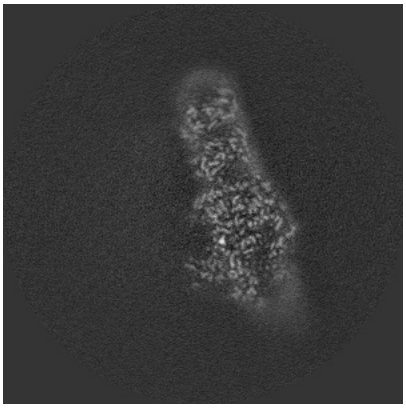

X Index: 218

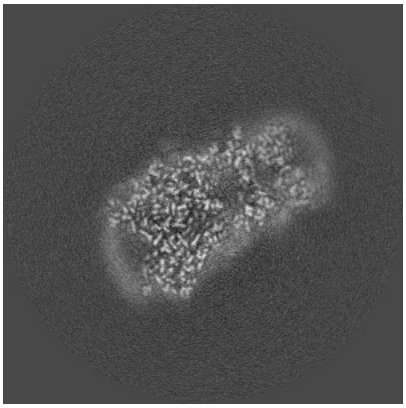

Y Index: 252


Z Index: 289

6.3.2 Raw map


X Index: 218

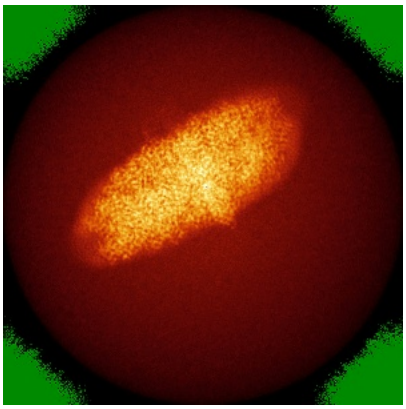

Y Index: 252

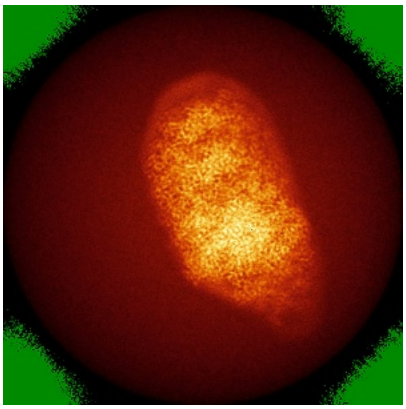

Z Index: 289

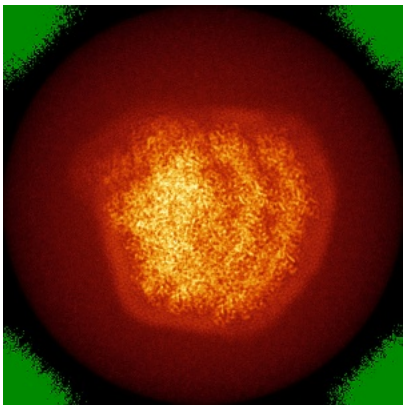
The images above show the largest variance slices of the map in three orthogonal directions.

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

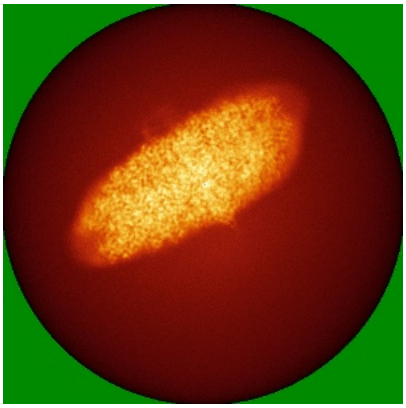
6.4.1 Primary map

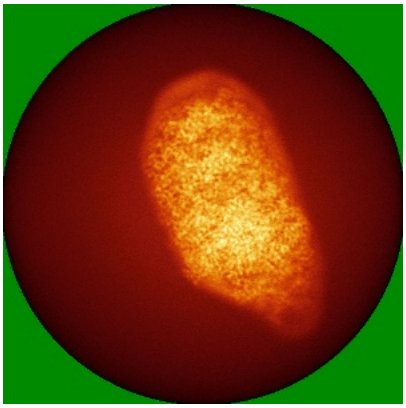

X

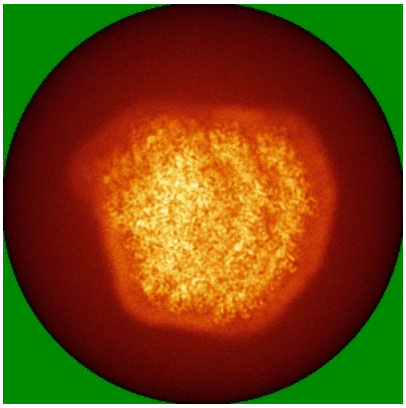

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

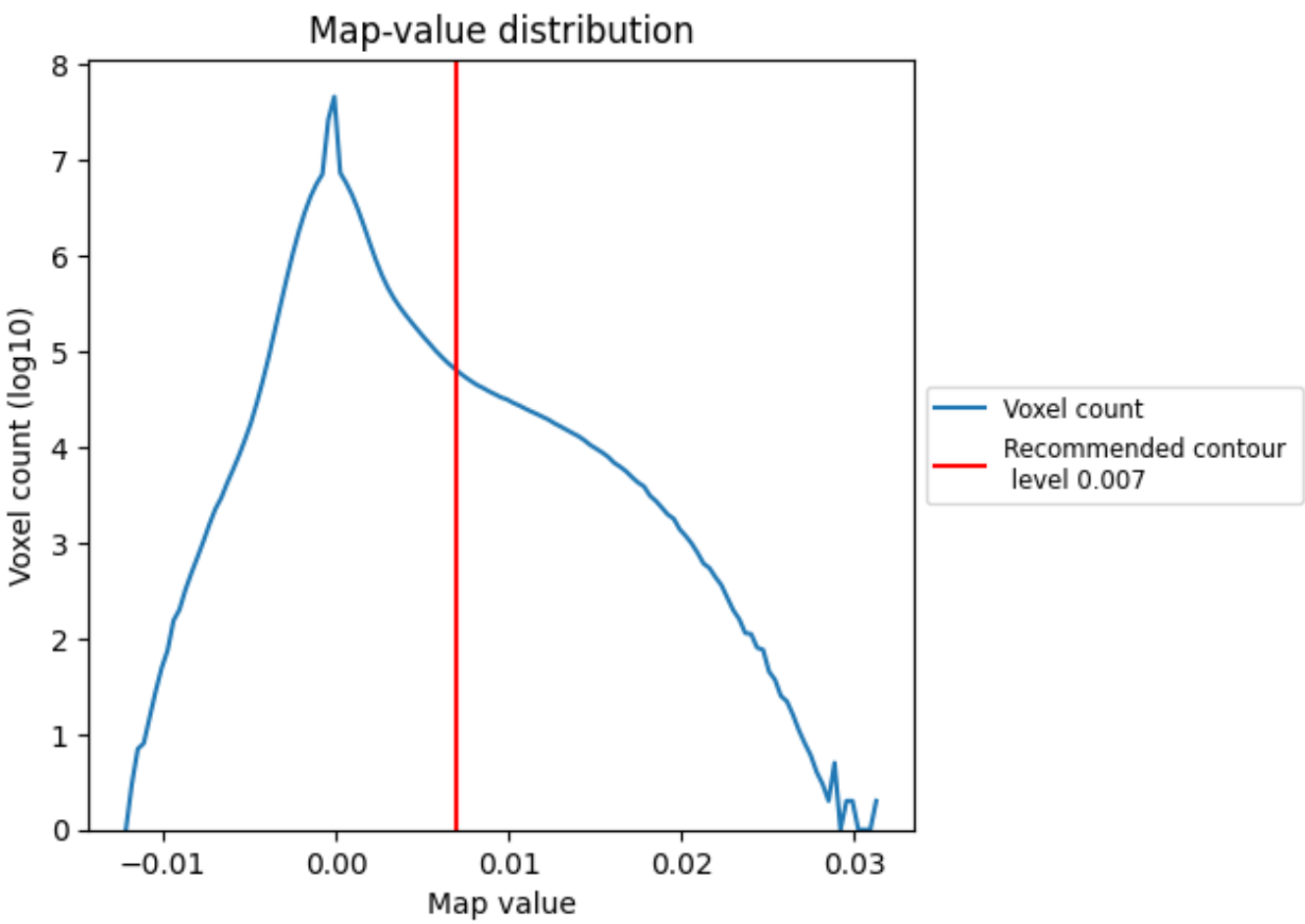
6.6 Mask visualisation (i)

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

7 Map analysis (i)

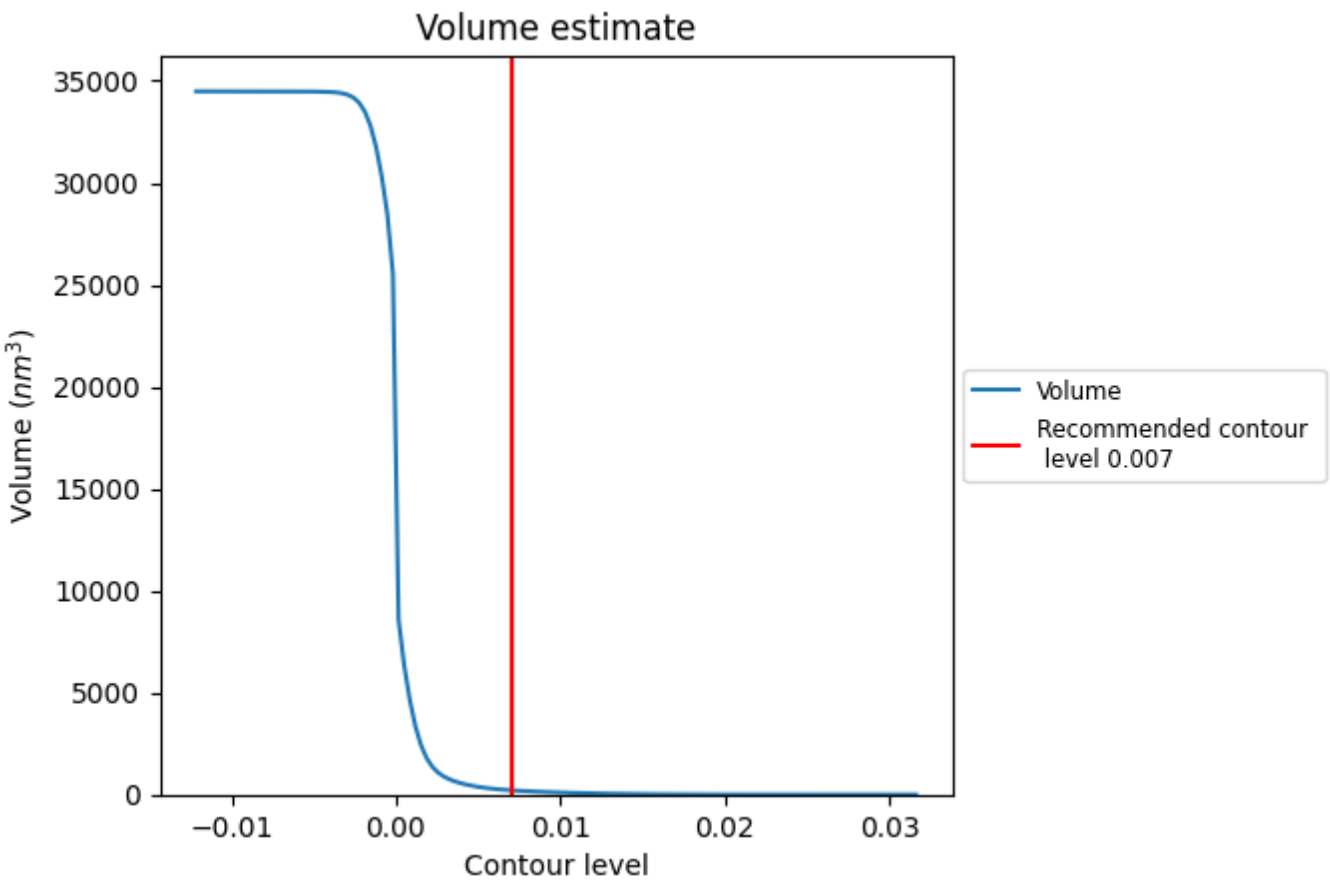
This section contains the results of statistical analysis of the map.

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.

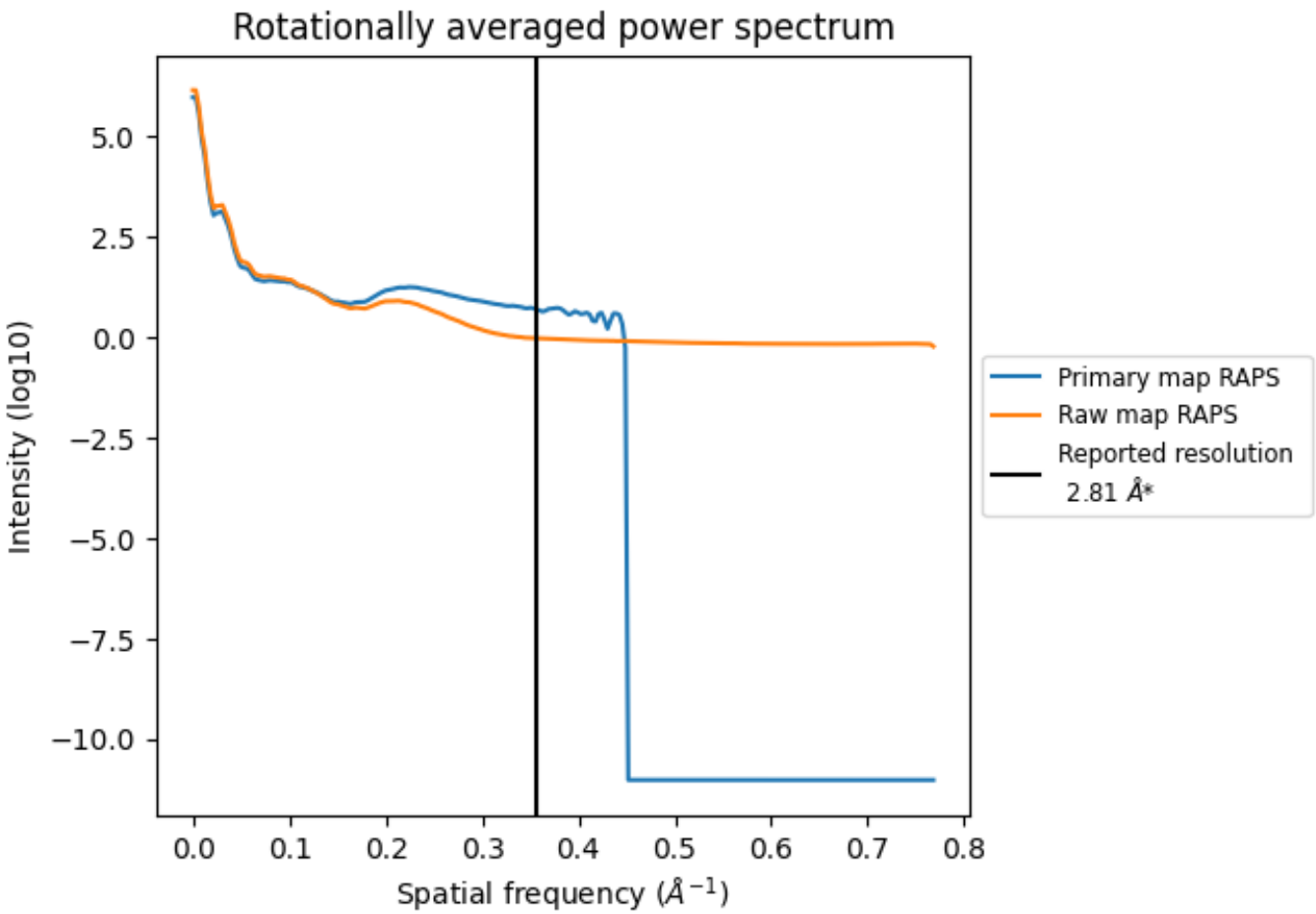
7.2 Volume estimate (i)



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 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)

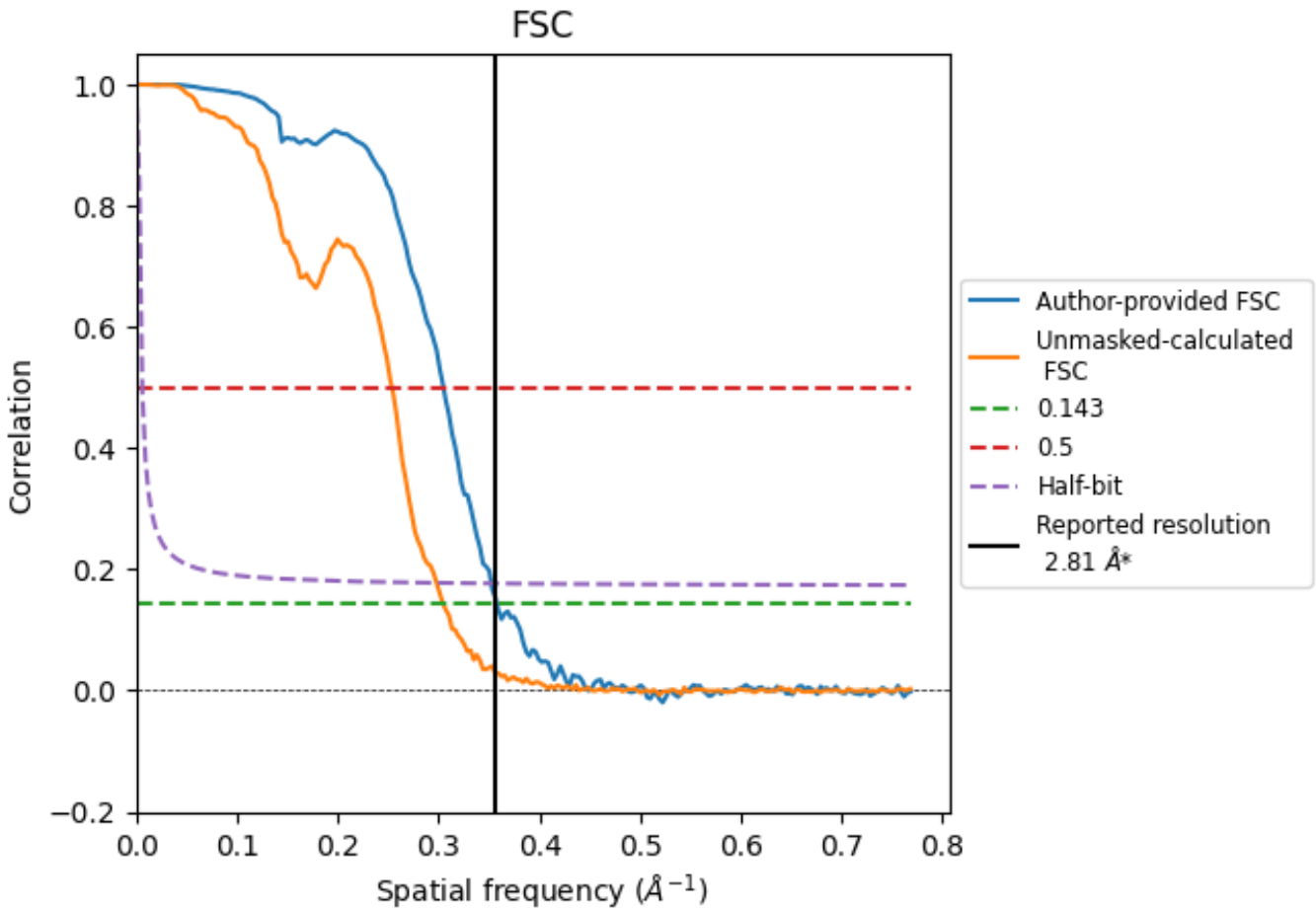


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

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 0.356 Å^{-1}

8.2 Resolution estimates (i)

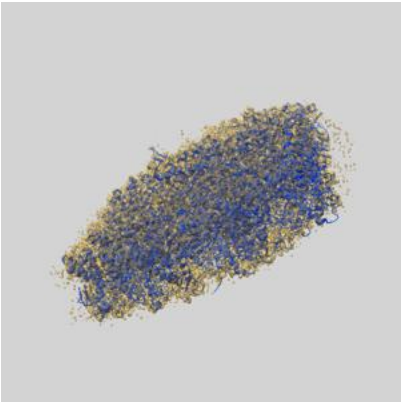
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.79	3.28	2.84
Unmasked-calculated*	3.28	3.94	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.81 by more than 10 %

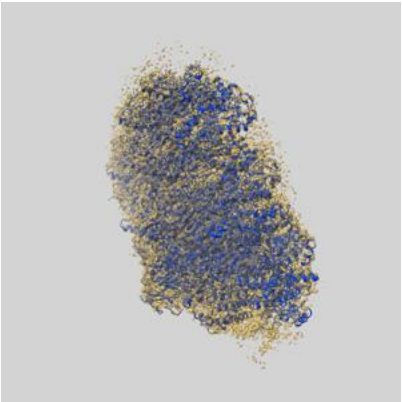
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16732 and PDB model 8CMO. Per-residue inclusion information can be found in section 3 on page 36.

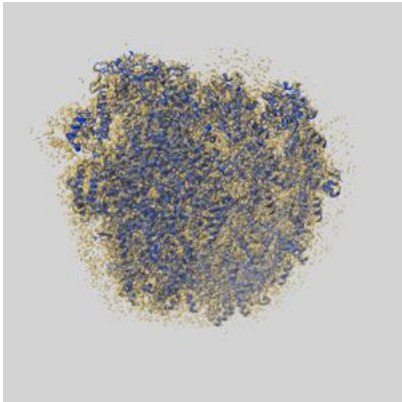
9.1 Map-model overlay (i)



X



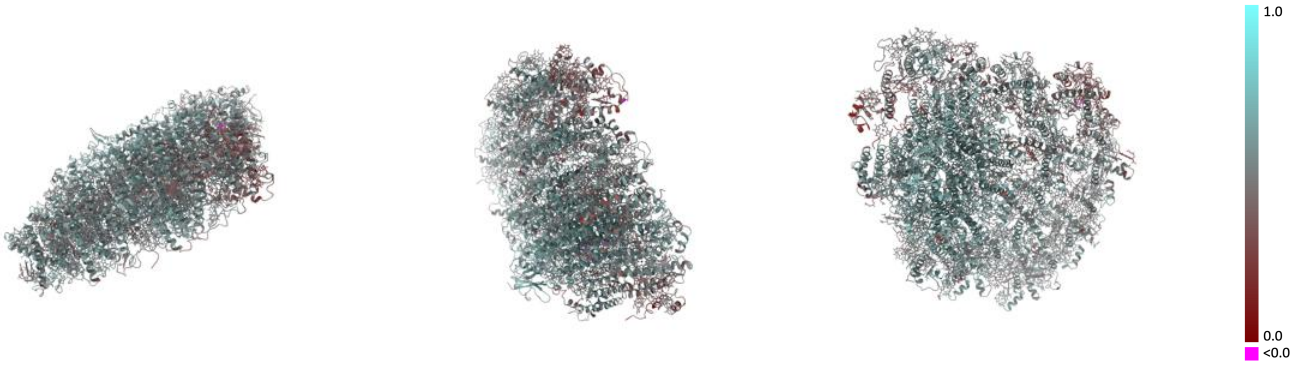
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

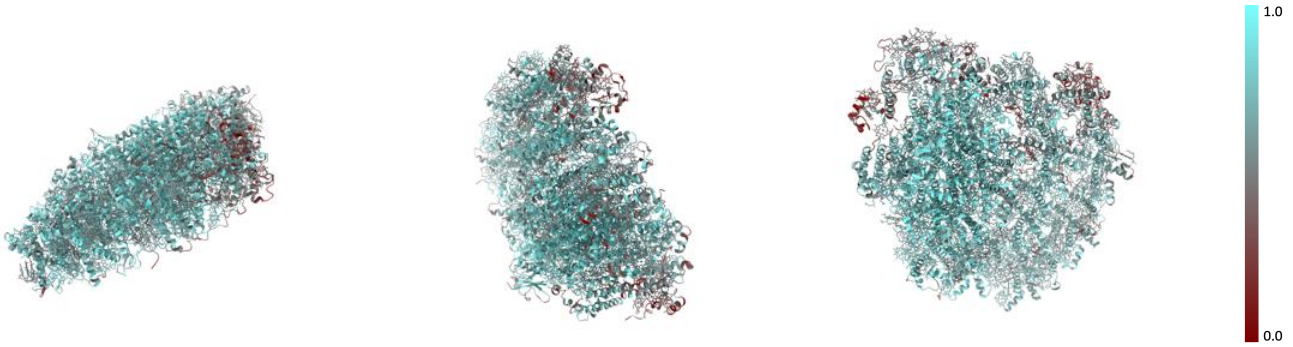
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

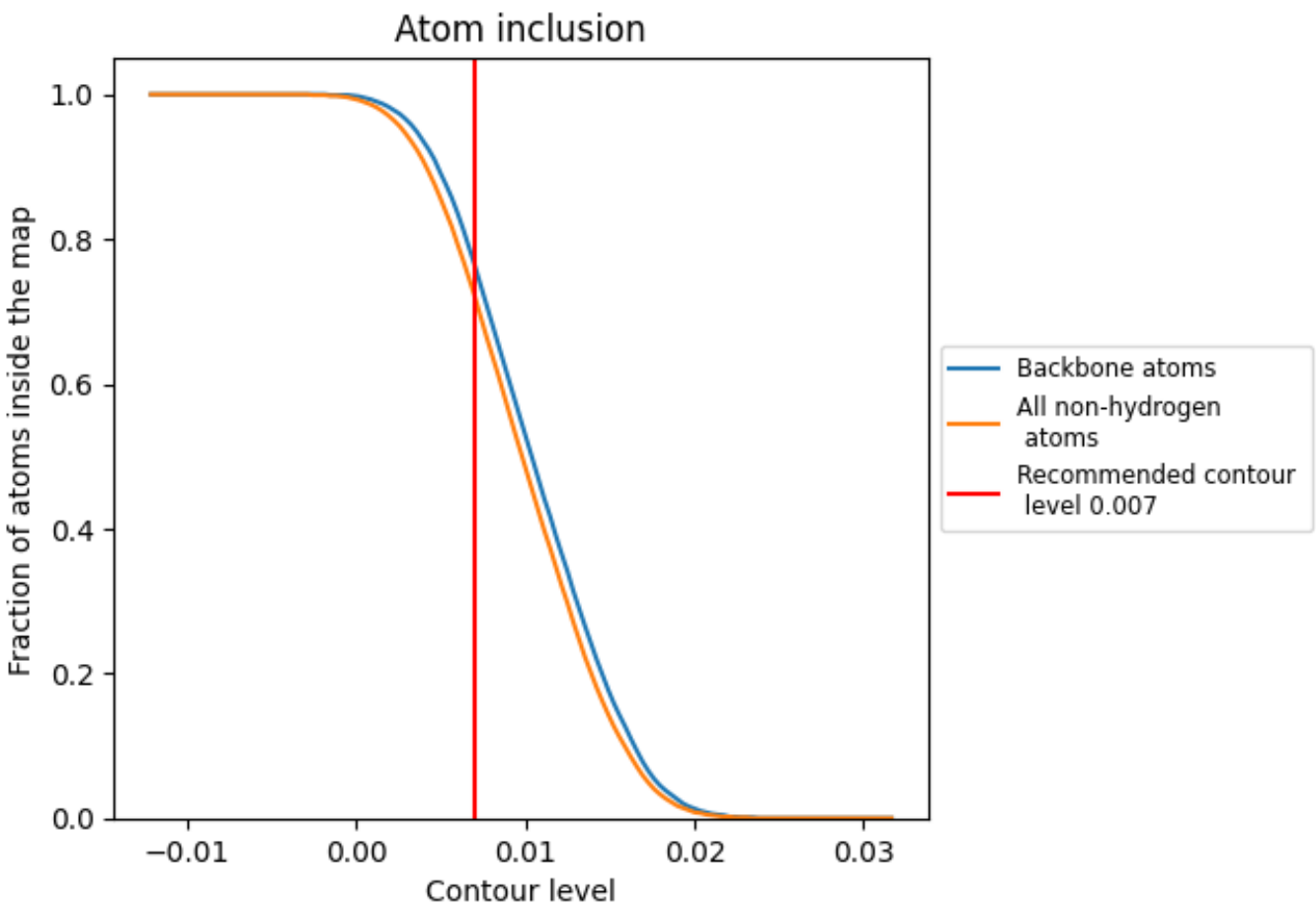
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.5370
1	0.6350	0.4980
2	0.3310	0.3380
3	0.7710	0.5610
4	0.6470	0.5050
5	0.6780	0.5150
6	0.6810	0.5140
7	0.7840	0.5510
8	0.7410	0.5310
9	0.5380	0.4770
A	0.8270	0.5920
B	0.8210	0.5830
C	0.7720	0.6020
D	0.6520	0.5660
E	0.6830	0.5660
F	0.6980	0.5310
G	0.4660	0.4150
I	0.6720	0.5270
J	0.7000	0.5310
K	0.7110	0.5230
L	0.6550	0.5030
Z	0.4730	0.4100