Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:32 AM JST

PDB ID	:	7D0J / pdb_00007d0j
EMDB ID	:	EMD-30536
Title	:	Photosystem I-LHCI-LHCII of Chlamydomonas reinhardtii
Authors	:	Wang, W.D.; Shen, L.L.; Huang, Z.H.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on	:	2020-09-10
Resolution	:	3.42 Å(reported)

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

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

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

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

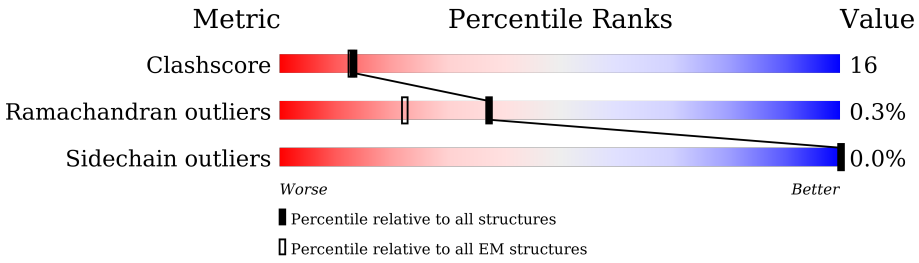
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

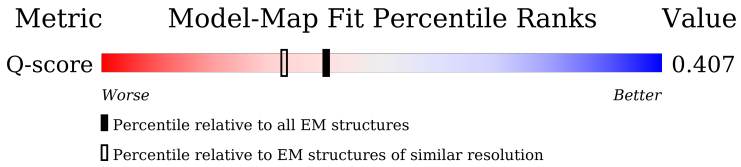
1 Overall quality at a glance

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

The reported resolution of this entry is 3.42 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	13959 (2.92 - 3.92)

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	20% 84% 16%
2	B	734	18% 82% 17%
3	C	80	21% 78% 20%
4	D	144	56% 78% 22%

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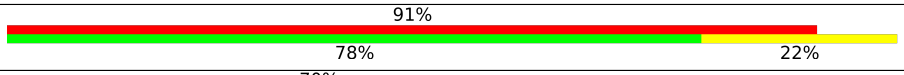
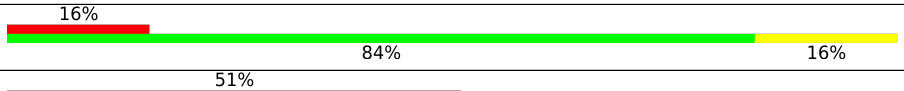
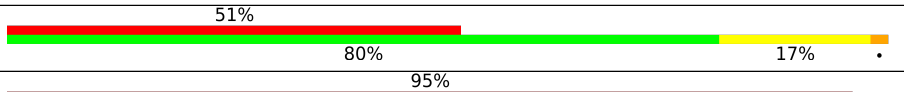
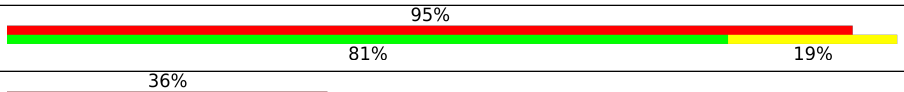
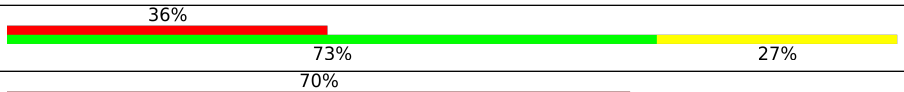
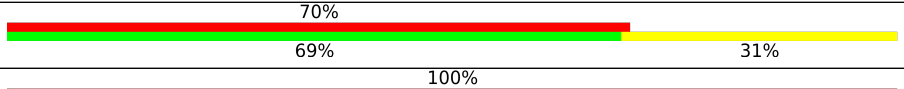
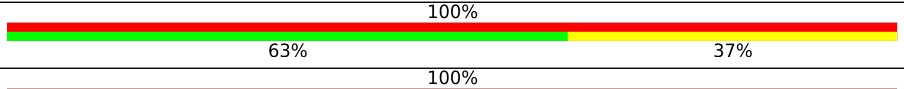
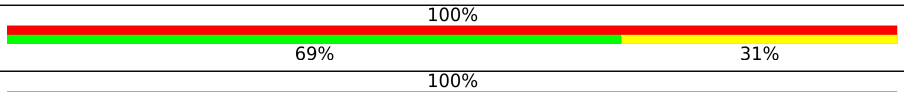
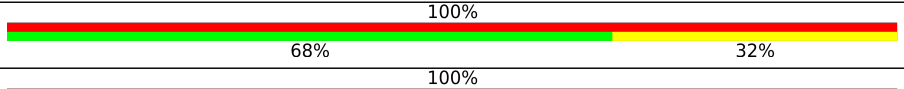
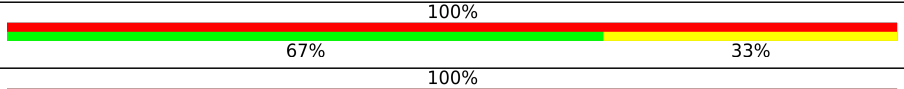
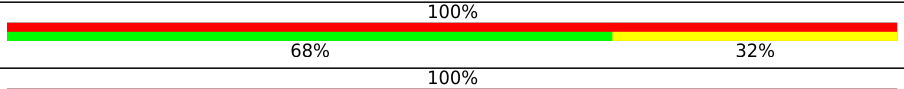
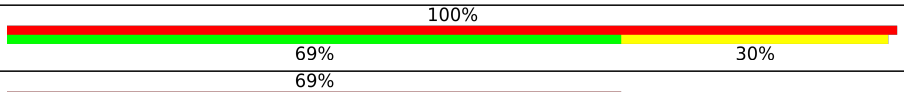
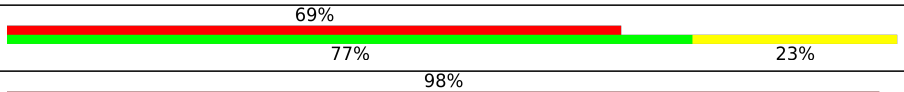
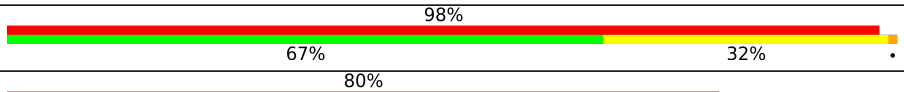
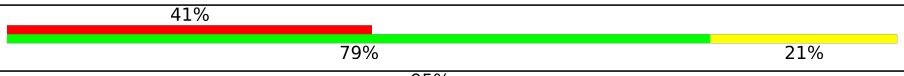
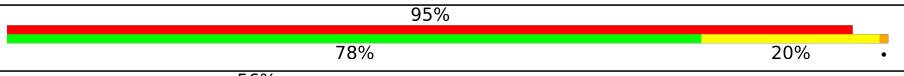
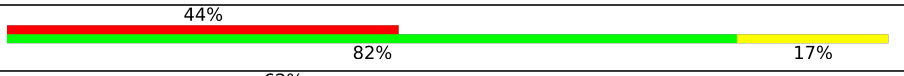
Mol	Chain	Length	Quality of chain
5	E	63	
6	F	165	
7	G	91	
8	H	100	
9	I	37	
10	J	41	
11	K	85	
12	L	159	
13	O	93	
14	P	219	
14	Q	219	
14	R	219	
14	T	219	
14	U	219	
15	S	234	
16	1	194	
16	a	194	
17	2	201	
18	3	203	
19	4	205	
20	5	225	
21	6	230	
22	7	213	
23	8	217	
24	9	182	

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
25	CLA	P	603	-	-	X	-
25	CLA	P	610	-	-	X	-
25	CLA	P	611	-	-	X	-
25	CLA	P	612	-	-	X	-
25	CLA	Q	603	-	-	X	-
25	CLA	R	603	-	-	X	-
25	CLA	R	610	-	-	X	-
25	CLA	R	612	-	-	X	-
33	CHL	P	609	-	-	X	-
33	CHL	Q	608	-	-	X	-
33	CHL	R	609	-	-	X	-
36	NEX	U	301	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 68860 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5811	3799	991	999	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5828	3827	978	1005	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1132	725	200	200	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			496	316	87	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	91	Total	C	N	O	0	0
			678	436	114	128		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	100	Total	C	N	O	S	0	0
			773	479	138	154	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1161	757	189	212	3		

- Molecule 13 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	93	Total	C	N	O	0	0
			720	477	118	125		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	Q	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	R	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	T	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	U	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	S	233	Total	C	N	O	P	S	0	0
			1717	1098	285	328	1	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
16	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	201	Total	C	N	O	S	0	0
			1545	1002	253	280	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	203	Total	C	N	O	S	0	0
			1560	1021	253	278	8		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	205	Total	C	N	O	S	0	0
			1590	1046	254	285	5		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	5	225	Total	C	N	O	S	0	0
			1757	1145	294	310	8		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	7	212	Total	C	N	O	S	0	0
			1644	1067	274	297	6		

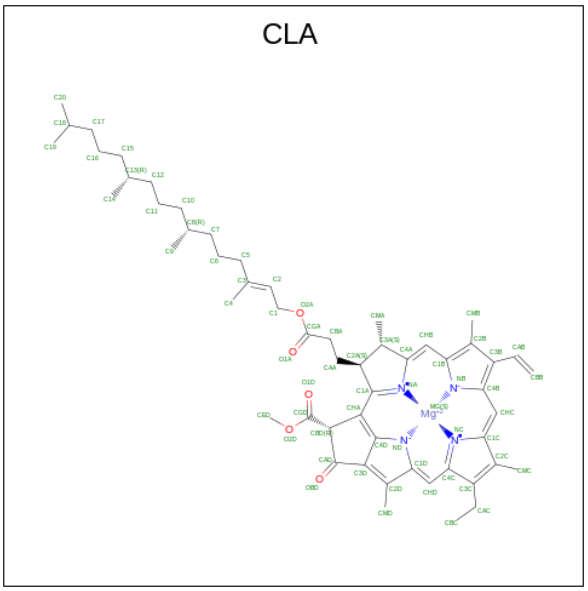
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	9	182	Total	C	N	O	S	0	0
			1392	903	231	251	7		

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	J	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	K	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
25	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
25	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	P	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	Q	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	T	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			54	47	1	4	2	
25	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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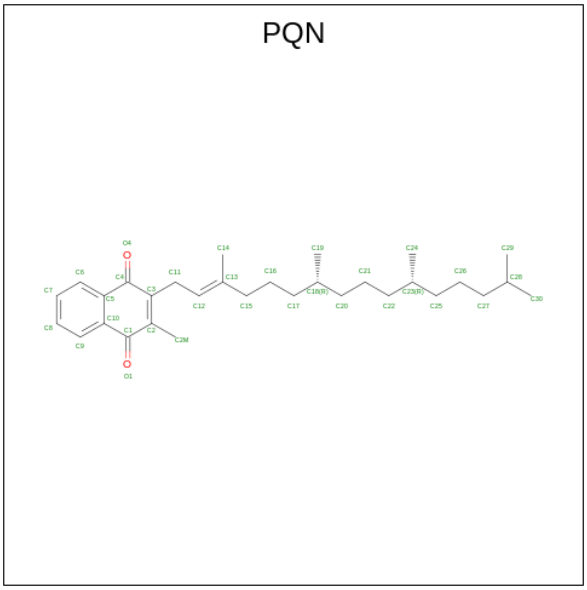
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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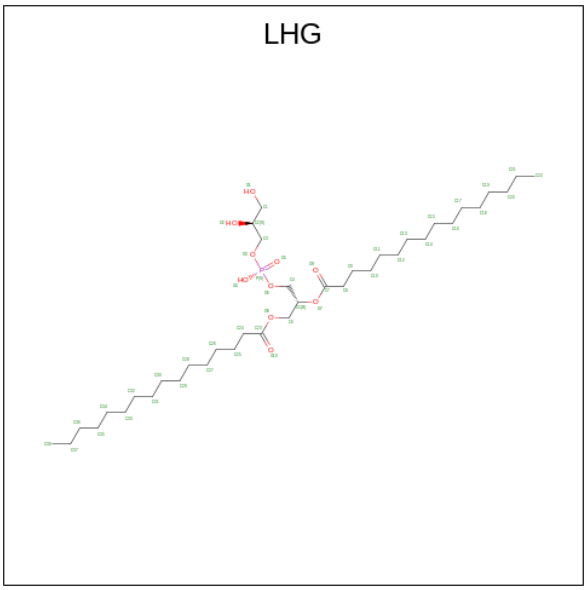
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			33	31	2	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			38	27	10	1	
27	A	1	Total	C	O	P	0
			48	37	10	1	
27	B	1	Total	C	O	P	0
			38	27	10	1	
27	P	1	Total	C	O	P	0
			49	38	10	1	
27	P	1	Total	C	O	P	0
			49	38	10	1	
27	Q	1	Total	C	O	P	0
			49	38	10	1	
27	R	1	Total	C	O	P	0
			49	38	10	1	
27	S	1	Total	C	O	P	0
			49	38	10	1	
27	T	1	Total	C	O	P	0
			49	38	10	1	

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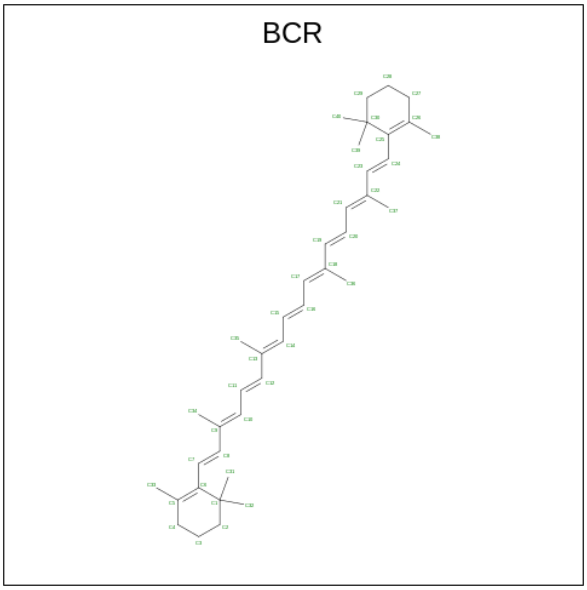
Mol	Chain	Residues	Atoms				AltConf
27	1	1	Total	C	O	P	0
			43	32	10	1	
27	2	1	Total	C	O	P	0
			49	38	10	1	
27	4	1	Total	C	O	P	0
			49	38	10	1	
27	4	1	Total	C	O	P	0
			32	21	10	1	
27	5	1	Total	C	O	P	0
			45	34	10	1	
27	5	1	Total	C	O	P	0
			37	26	10	1	
27	6	1	Total	C	O	P	0
			49	38	10	1	
27	7	1	Total	C	O	P	0
			37	26	10	1	
27	8	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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

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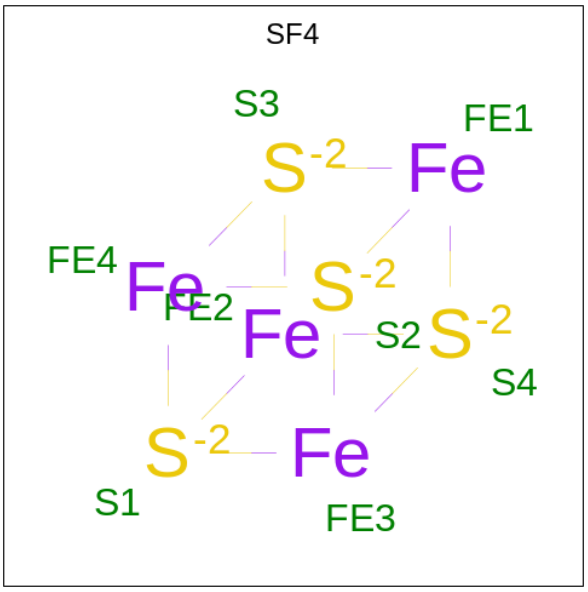
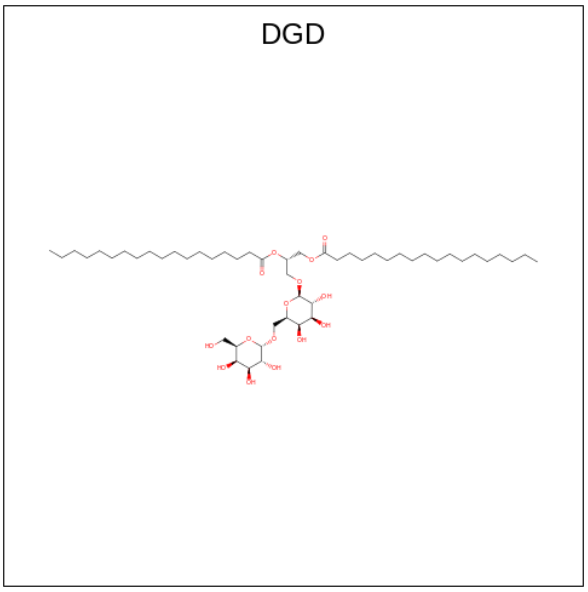
Mol	Chain	Residues	Atoms	AltConf
28	L	1	Total C 40 40	0
28	L	1	Total C 40 40	0
28	O	1	Total C 40 40	0
28	O	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	4	1	Total C 40 40	0
28	4	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	6	1	Total C 40 40	0
28	7	1	Total C 40 40	0
28	8	1	Total C 40 40	0
28	8	1	Total C 40 40	0

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



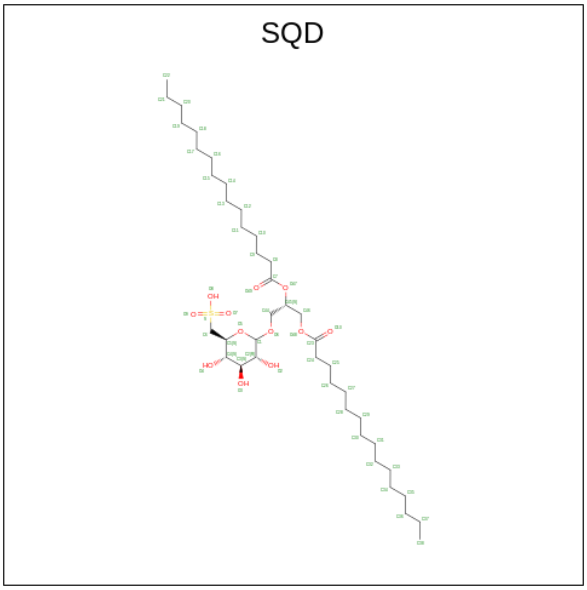
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



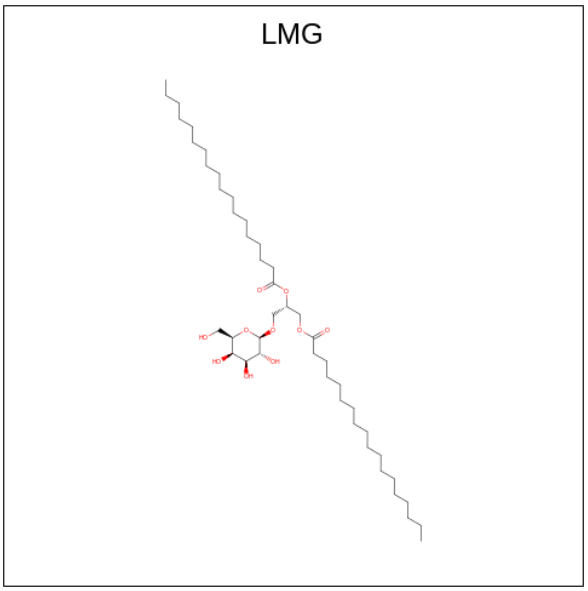
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total 66	C 51	O 15	0
30	B	1	Total 57	C 42	O 15	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



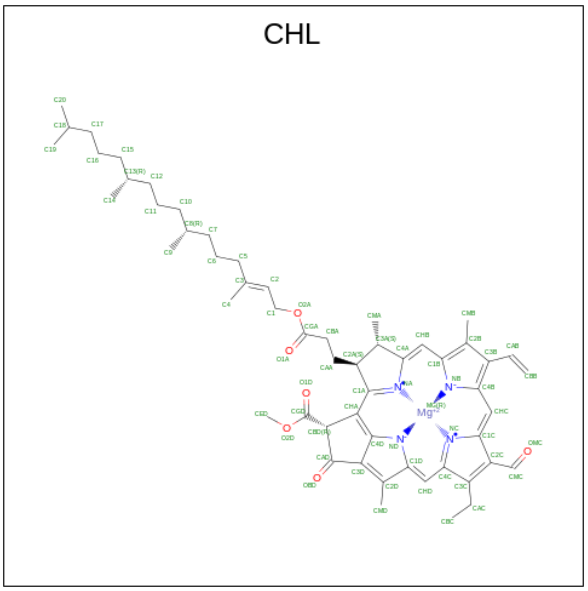
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total 51	C 38	O 12	S 1	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
32	H	1	Total C O 47 37 10	0
32	J	1	Total C O 40 30 10	0
32	J	1	Total C O 35 25 10	0
32	J	1	Total C O 55 45 10	0
32	1	1	Total C O 46 36 10	0
32	2	1	Total C O 41 31 10	0
32	4	1	Total C O 40 30 10	0
32	6	1	Total C O 40 30 10	0
32	7	1	Total C O 35 25 10	0
32	7	1	Total C O 36 26 10	0

- Molecule 33 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
33	P	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	P	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
33	P	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	P	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
33	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
33	P	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	P	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	Q	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	Q	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
33	Q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
33	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
33	R	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
33	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
33	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	R	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
33	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	S	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	T	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	T	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
33	T	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	T	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
33	T	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
33	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
33	U	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
33	U	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	U	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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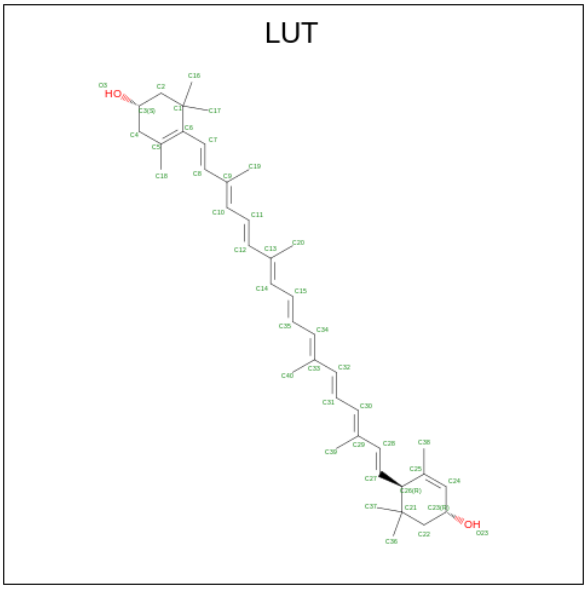
Mol	Chain	Residues	Atoms					AltConf
33	U	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
33	1	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
33	3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
33	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
33	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
33	6	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	6	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
33	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
33	8	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
33	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
33	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
33	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 34 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
34	P	1	Total C O 42 40 2	0
34	P	1	Total C O 42 40 2	0
34	Q	1	Total C O 42 40 2	0
34	Q	1	Total C O 42 40 2	0
34	R	1	Total C O 42 40 2	0
34	R	1	Total C O 42 40 2	0
34	S	1	Total C O 42 40 2	0
34	S	1	Total C O 42 40 2	0
34	T	1	Total C O 42 40 2	0
34	T	1	Total C O 42 40 2	0
34	U	1	Total C O 42 40 2	0
34	U	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	1	1	Total	C	O	0
			42	40	2	
34	1	1	Total	C	O	0
			42	40	2	
34	2	1	Total	C	O	0
			42	40	2	
34	2	1	Total	C	O	0
			42	40	2	
34	3	1	Total	C	O	0
			42	40	2	
34	3	1	Total	C	O	0
			42	40	2	
34	4	1	Total	C	O	0
			42	40	2	
34	4	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	

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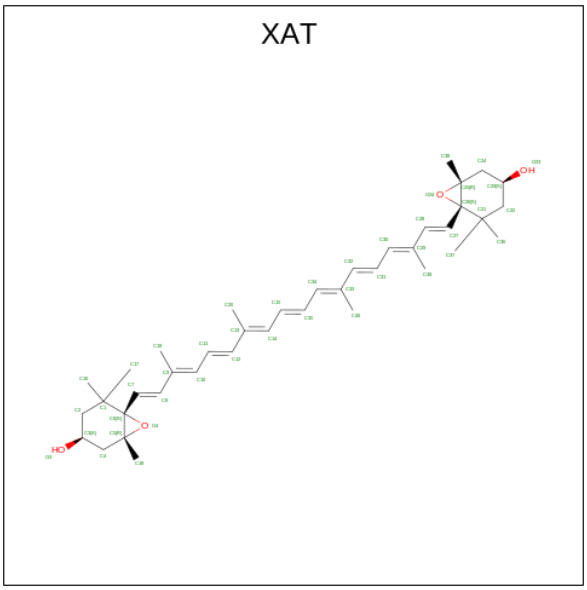
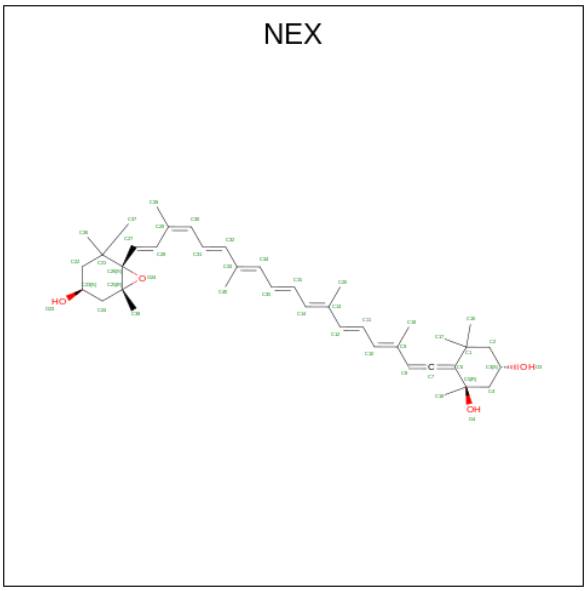
Mol	Chain	Residues	Atoms	AltConf
34	a	1	Total C O 42 40 2	0

- Molecule 35 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
35	P	1	Total C O 44 40 4	0
35	P	1	Total C O 44 40 4	0
35	P	1	Total C O 43 39 4	0
35	Q	1	Total C O 44 40 4	0
35	S	1	Total C O 44 40 4	0
35	T	1	Total C O 44 40 4	0

- Molecule 36 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2 ,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1, 3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



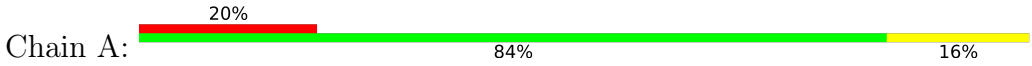
Mol	Chain	Residues	Atoms			AltConf
36	P	1	Total	C	O	0
			44	40	4	
36	P	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	T	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	

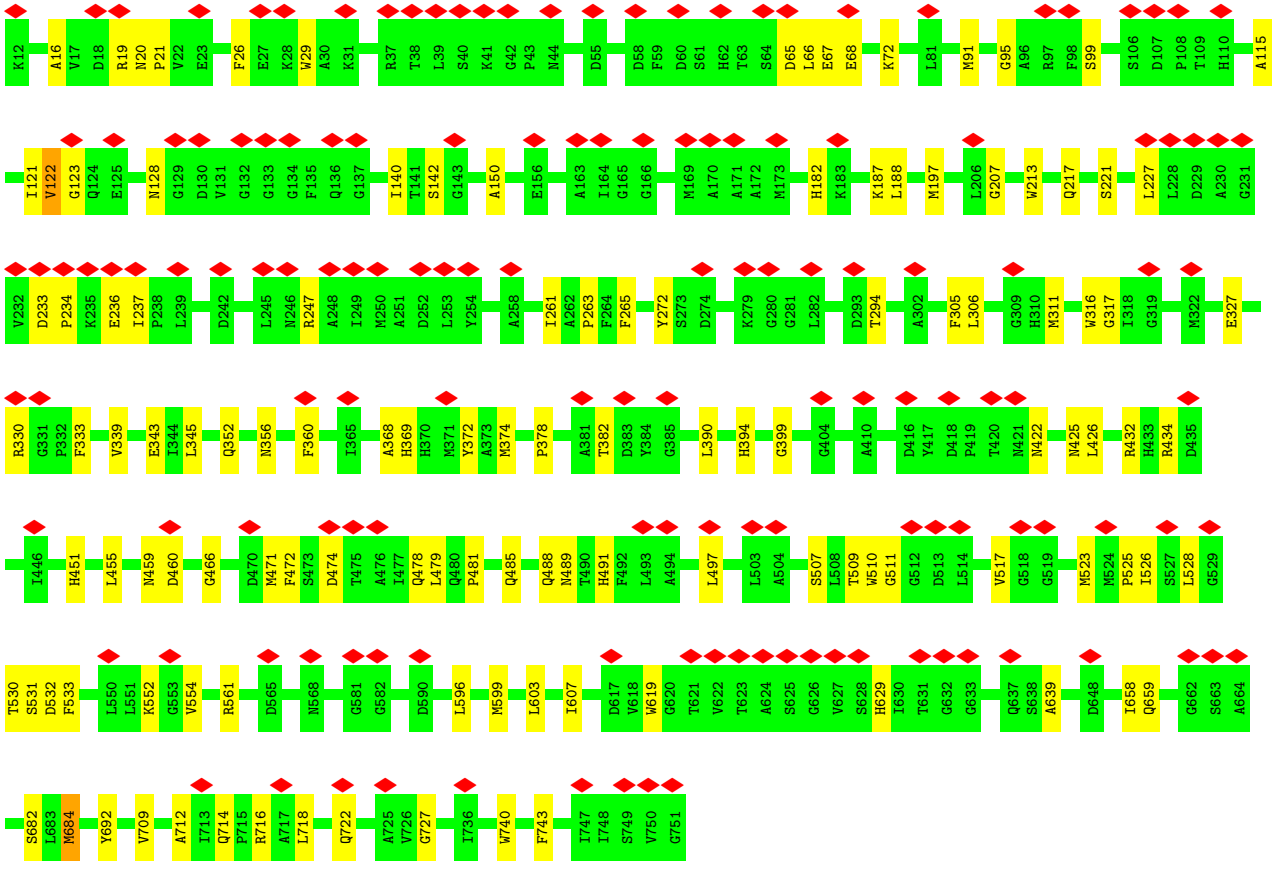
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

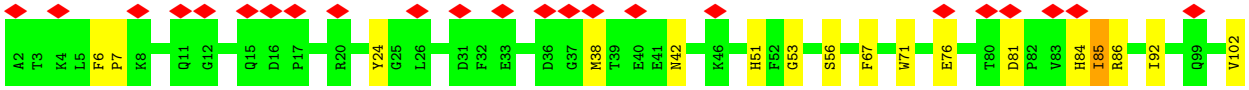
Chain A:

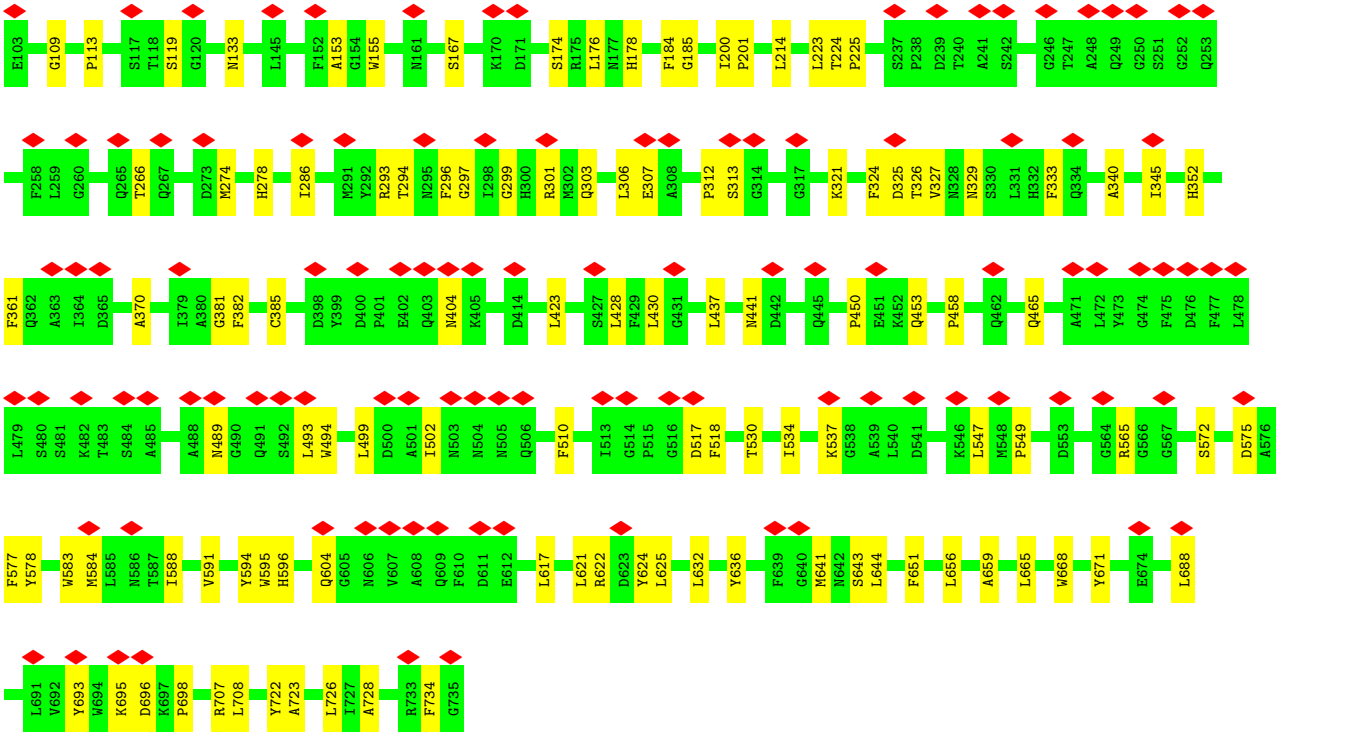




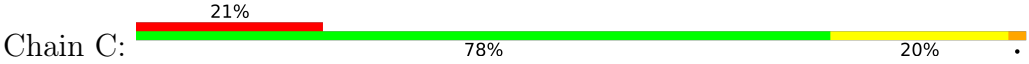
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

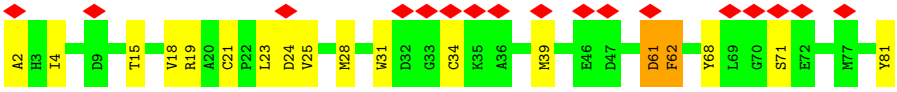
Chain B:



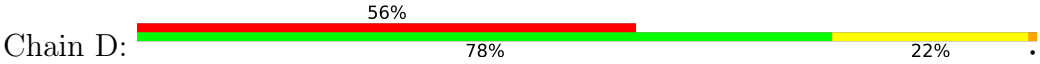


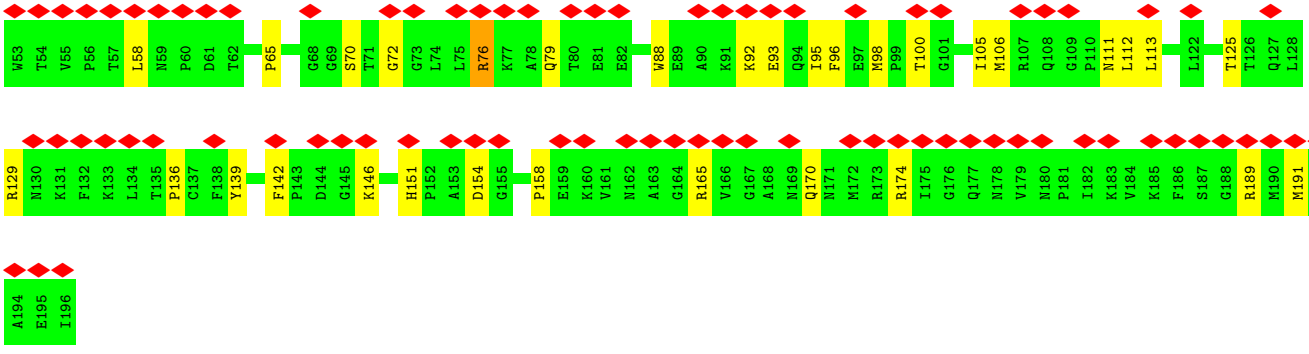
• Molecule 3: Photosystem I iron-sulfur center



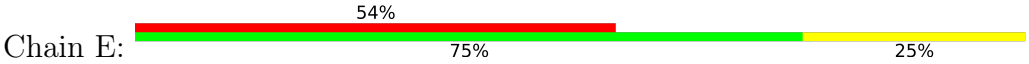


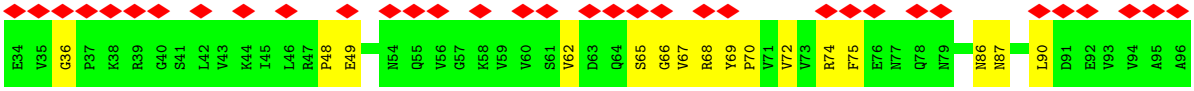
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic



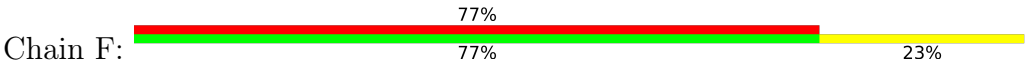


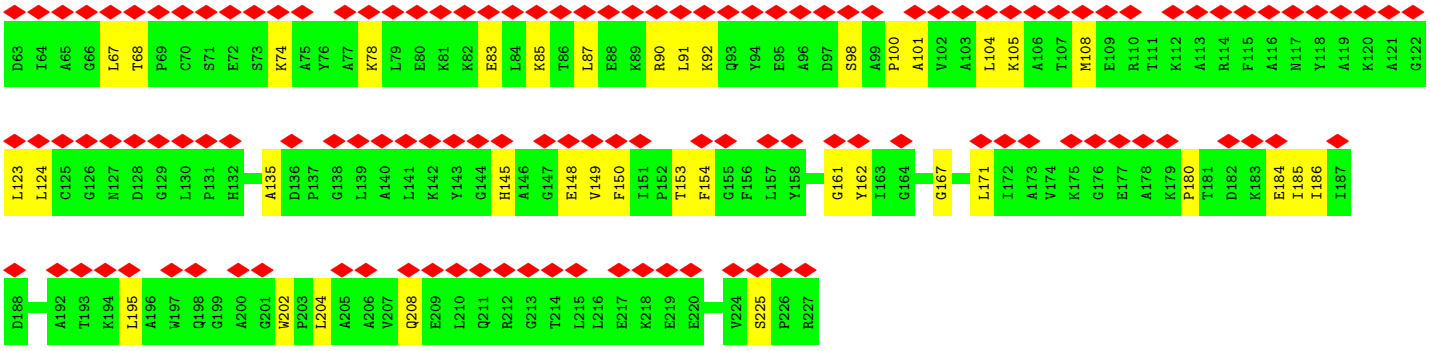
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



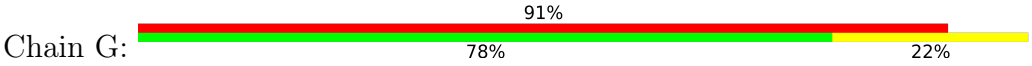


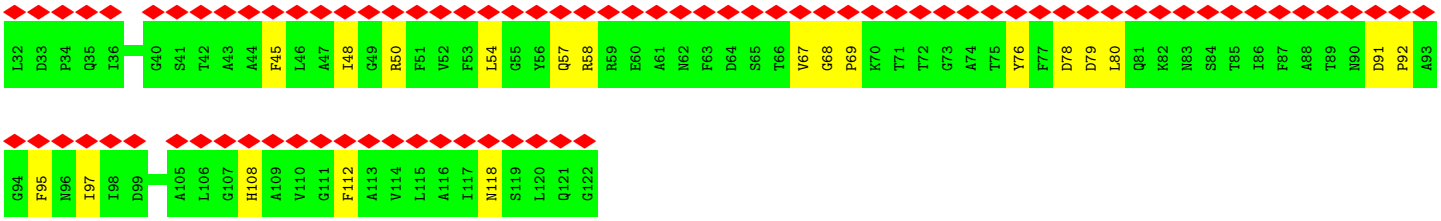
• Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic



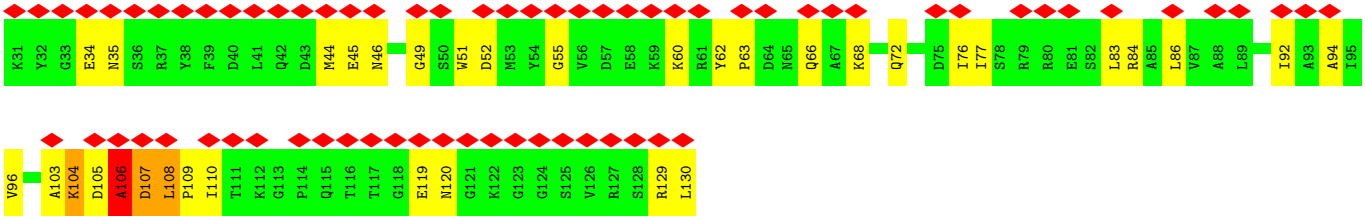


• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

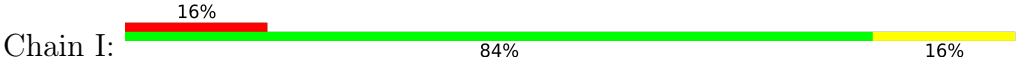


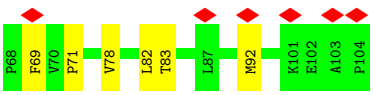


• Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



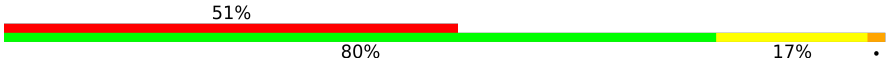
• Molecule 9: Photosystem I reaction center subunit VIII

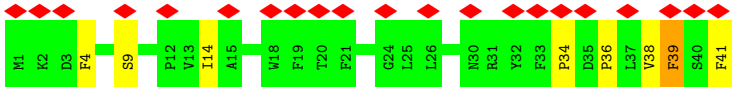




• Molecule 10: Photosystem I reaction center subunit IX

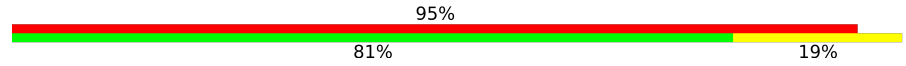
Chain J:

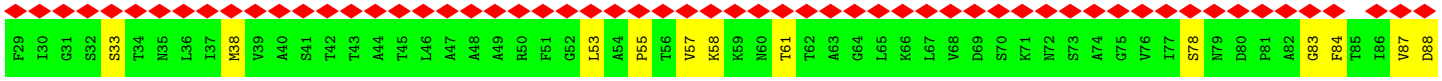


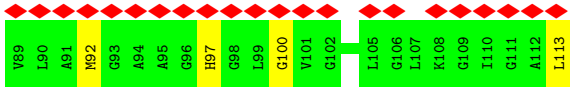


• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

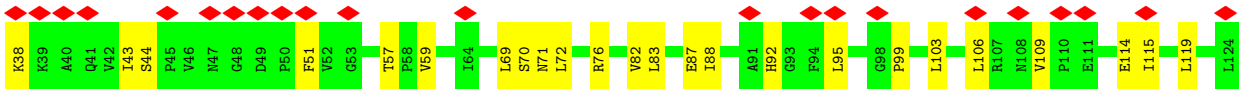


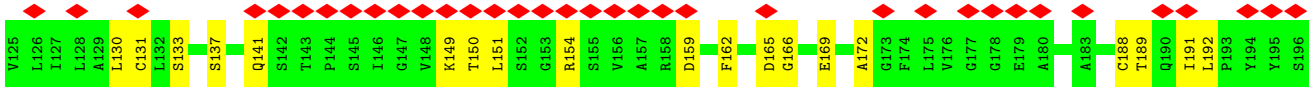




• Molecule 12: PSI subunit V

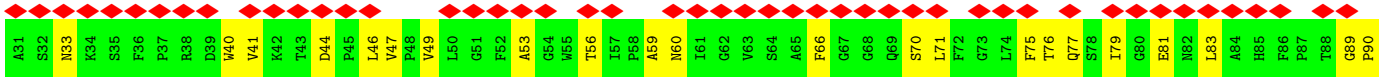
Chain L:

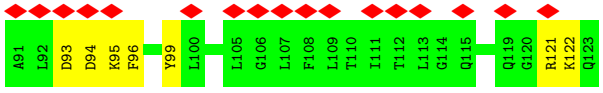




• Molecule 13: Photosystem I subunit O

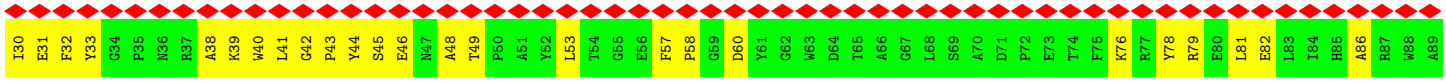
Chain O:

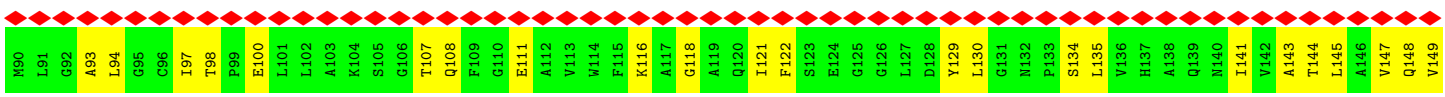




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain P:





I150 L151 M152 G153 L154 V155 E156 G157 Y158 R159 V160 N161 G162 G163 P164 A165 G166 E167 G168 L169 D170 P171 L172 Y173 P174 G175 E176 S177 F178 D179 P180 L181 G182 L183 A184 D185 D186 P187 D188 T189 F190 A191 E192 L193 K194 V195 K196 E197 I198 K199 N200 G201 R202 L203 A204 M205 F206 S207 M208 F209

G210 F211 F212 V213 Q214 A215 I216 V217 T218 G219 K220 G221 P222 I223 Q224 N225 L226 D227 D228 H229 L230 S231 N232 P233 T234 V235 N236 N237 A238 F239 A240 F241 A242 T243 K244 F245 T246 P247 S248

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

Chain Q:

I30 E31 F32 Y33 G34 P35 N36 R37 A38 K39 W40 L41 G42 P43 Y44 S45 E46 N47 A48 T49 P50 A51 Y52 L53 T54 G55 E56 F57 P58 G59 D60 Y61 G62 W63 D64 T65 A66 G67 L68 S69 A70 D71 P72 E73 T74 F75 K76 R77 Y78 R79 E80 L81 E82 L83 I84 H85 A86 R87 W88 A89

M90 L91 G92 A93 L94 G95 C96 I97 T98 P99 E100 L101 L102 A103 K104 S105 G106 T107 Q108 F109 G110 E111 A112 V113 W114 F115 K116 A117 G118 A119 Q120 I121 F122 S123 E124 G125 G126 L127 D128 Y129 L130 G131 N132 P133 S134 L135 V136 H137 A138 Q139 N140 I141 V142 A143 T144 L145 A146 V147 Q148 V149

I150 L151 M152 G153 L154 V155 E156 G157 Y158 R159 V160 N161 G162 G163 P164 A165 G166 E167 G168 L169 D170 P171 L172 Y173 P174 G175 E176 S177 F178 D179 P180 L181 G182 L183 A184 D185 D186 P187 D188 T189 F190 A191 E192 L193 K194 V195 K196 E197 I198 K199 N200 G201 R202 L203 A204 M205 F206 S207 M208 F209

G210 F211 F212 V213 Q214 A215 I216 V217 T218 G219 K220 G221 P222 I223 Q224 N225 L226 D227 D228 H229 L230 S231 N232 P233 T234 V235 N236 N237 A238 F239 A240 F241 A242 T243 K244 F245 T246 P247 S248

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

Chain R:

I30 E31 F32 Y33 G34 P35 N36 R37 A38 K39 W40 L41 G42 P43 Y44 S45 E46 N47 A48 T49 P50 A51 Y52 L53 T54 G55 E56 F57 P58 G59 D60 Y61 G62 W63 D64 T65 A66 G67 L68 S69 A70 D71 P72 E73 T74 F75 K76 R77 Y78 R79 E80 L81 E82 L83 I84 H85 A86 R87 W88 A89

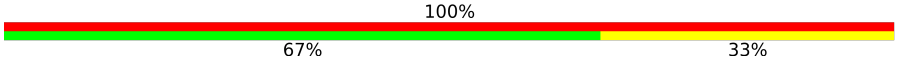
M90 L91 G92 A93 L94 G95 C96 I97 T98 P99 E100 L101 L102 A103 K104 S105 G106 T107 Q108 F109 G110 E111 A112 V113 W114 F115 K116 A117 G118 A119 Q120 I121 F122 S123 E124 G125 G126 L127 D128 Y129 L130 G131 N132 P133 S134 L135 V136 H137 A138 Q139 N140 I141 V142 A143 T144 L145 A146 V147 Q148 V149

I150 L151 M152 G153 L154 V155 E156 G157 Y158 R159 V160 N161 G162 G163 P164 A165 G166 E167 G168 L169 D170 P171 L172 Y173 P174 G175 E176 S177 F178 D179 P180 L181 G182 L183 A184 D185 D186 P187 D188 T189 F190 A191 E192 L193 K194 V195 K196 E197 I198 K199 N200 G201 R202 L203 A204 M205 F206 S207 M208 F209

G210 F211 F212 V213 Q214 A215 I216 V217 T218 G219 K220 G221 P222 I223 Q224 N225 L226 D227 D228 H229 L230 S231 N232 P233 T234 V235 N236 N237 A238 F239 A240 F241 A242 T243 K244 F245 T246 P247 S248

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

Chain T:



I30 E31 F32 Y33 G34 P35 N36 R37 A38 K39 W40 L41 G42 P43 Y44 S45 E46 N47 A48 T49 P50 A51 Y52 L53 T54 G55 E56 F57 P58 G59 D60 Y61 G62 W63 D64 T65 A66 G67 L68 S69 A70 D71 P72 E73 T74 F75 K76 R77 Y78 R79 E80 L81 E82 L83 I84 H85 A86 R87 W88 A89

M90 L91 G92 A93 L94 G95 C96 I97 T98 P99 E100 L101 L102 A103 K104 S105 G106 T107 Q108 F109 G110 E111 A112 V113 W114 F115 K116 A117 G118 A119 Q120 I121 F122 S123 E124 G125 G126 L127 D128 Y129 L130 G131 N132 P133 S134 L135 V136 H137 A138 Q139 N140 I141 V142 A143 T144 L145 A146 V147 Q148 V149

I150 L151 M152 G153 L154 V155 E156 G157 Y158 R159 V160 N161 G162 G163 P164 A165 G166 E167 G168 L169 D170 P171 L172 Y173 P174 G175 E176 S177 F178 D179 P180 L181 G182 L183 A184 D185 D186 P187 D188 T189 F190 A191 E192 L193 K194 V195 K196 E197 I198 K199 N200 G201 R202 L203 A204 M205 F206 S207 M208 F209

G210 F211 F212 V213 Q214 A215 I216 V217 T218 G219 K220 G221 P222 I223 Q224 N225 L226 D227 D228 H229 L230 S231 N232 P233 T234 V235 N236 N237 A238 F239 A240 F241 A242 T243 K244 F245 T246 P247 S248

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

Chain U:

I30 E31 F32 Y33 G34 P35 N36 R37 A38 K39 W40 L41 G42 P43 Y44 S45 E46 N47 A48 T49 P50 A51 Y52 L53 T54 G55 E56 F57 P58 G59 D60 Y61 G62 W63 D64 T65 A66 G67 L68 S69 A70 D71 P72 E73 T74 F75 K76 R77 Y78 R79 E80 L81 E82 L83 I84 H85 A86 R87 W88 A89

M90 L91 G92 A93 L94 G95 C96 I97 T98 P99 E100 L101 L102 A103 K104 S105 G106 T107 Q108 F109 G110 E111 A112 V113 W114 F115 K116 A117 G118 A119 Q120 I121 F122 S123 E124 G125 G126 L127 D128 Y129 L130 G131 N132 P133 S134 L135 V136 H137 A138 Q139 N140 I141 V142 A143 T144 L145 A146 V147 Q148 V149

I150 L151 M152 G153 L154 V155 E156 G157 Y158 R159 V160 N161 G162 G163 P164 A165 G166 E167 G168 L169 D170 P171 L172 Y173 P174 G175 E176 S177 F178 D179 P180 L181 G182 L183 A184 D185 D186 P187 D188 T189 F190 A191 E192 L193 K194 V195 K196 E197 I198 K199 N200 G201 R202 L203 A204 M205 F206 S207 M208 F209

G210 F211 F212 V213 Q214 A215 I216 V217 T218 G219 K220 G221 P222 I223 Q224 N225 L226 D227 D228 H229 L230 S231 N232 P233 T234 V235 N236 N237 A238 F239 A240 F241 A242 T243 K244 F245 T246 P247 S248

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

Chain S:

K21 K22 T23 A24 A25 K26 A27 A28 A29 P30 K31 S32 S33 G34 V35 E36 F37 Y38 G39 P40 N41 R42 A43 K44 W45 L46 G47 P48 Y49 S50 E51 N52 S53 T54 P55 A56 Y57 L58 T59 G60 E61 F62 P63 G64 D65 Y66 G67 W68 D69 T70 A71 G72 L73 S74 A75 D76 P77 E78 T79 F80

K81 R82 Y83 R84 E85 L86 E87 L88 I89 H90 A91 R92 W93 A94 M95 L96 G97 A98 L99 G100 C101 L102 T103 P104 E105 L106 L107 A108 K109 N110 G111 T112 K113 F114 G115 E116 A117 V118 W119 F120 K121 A122 G123 A124 Q125 I126 F127 S128 E129 G130 G131 L132 D133 Y134 L135 G136 N137 P138 S139 L140

V141 H142 A143 Q144 N145 I146 V147 A148 T149 L150 A151 V152 Q153 V154 I155 L156 M157 G158 L159 I160 E161 G162 Y163 R164 V165 N166 G167 G168 P169 A170 G171 E172 G173 L174 D175 P176 L177 Y178 P179 G180 E181 S182 F183 D184 P185 L186 G187 L188 A189 D190 D191 P192 D193 T194 F195 A196 E197 L198 K199 V200

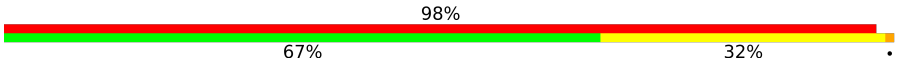
K201 E202 I203 K204 N205 G206 R207 L208 A209 M210 F211 S212 M213 F214 G215 F216 F217 V218 Q219 A220 I221 V222 T223 G224 K225 G226 P227 V228 Q229 N230 L231 D232 D233 H234 L235 A236 N237 P238 T239 V240 N241 N242 A243 F244 A245 F246 A247 T248 K249 F250 T251 P252 S253 ALA

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

Chain 1:

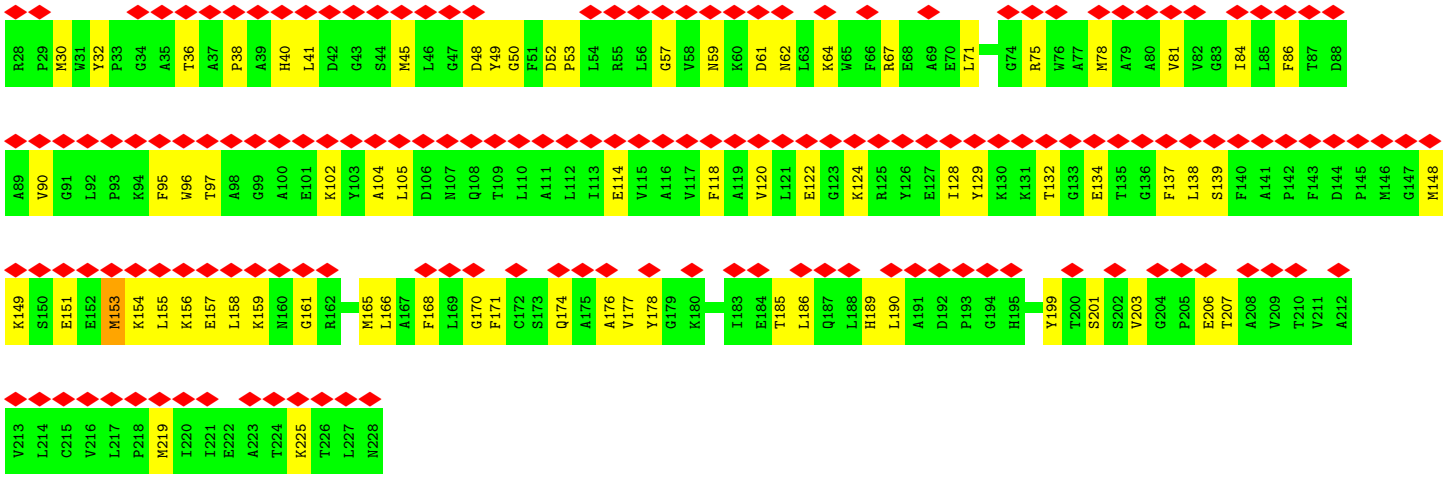
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain a:



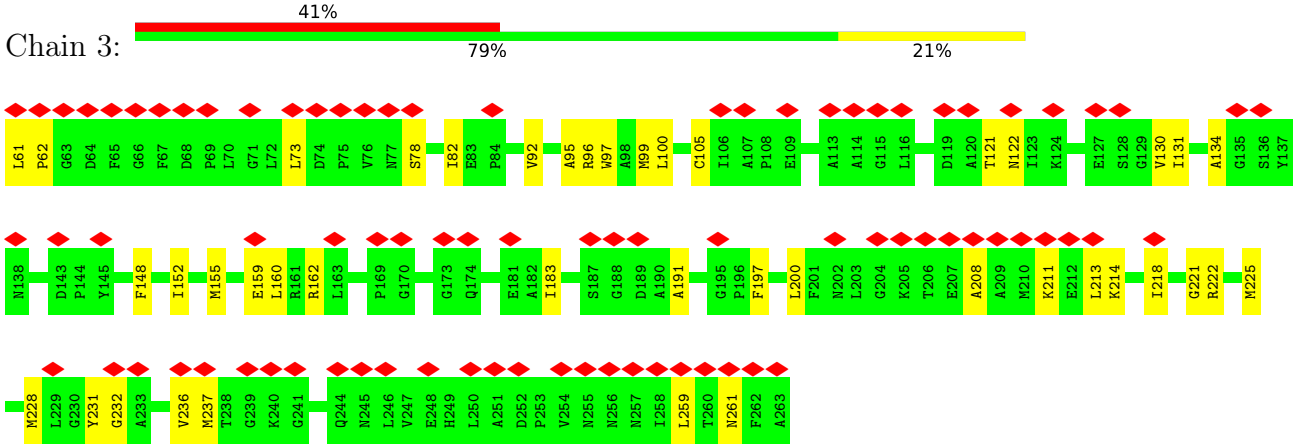
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



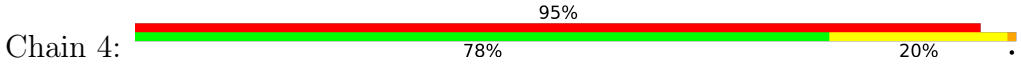
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



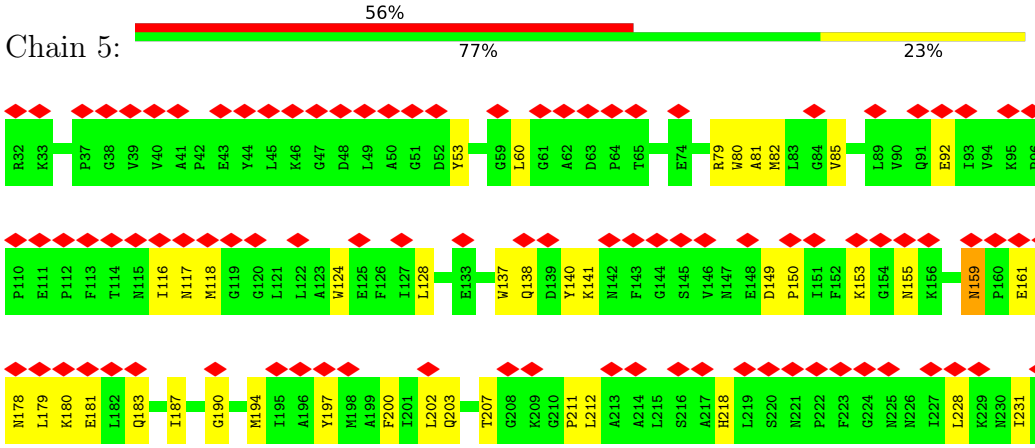
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

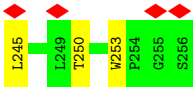
Chain 4:



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

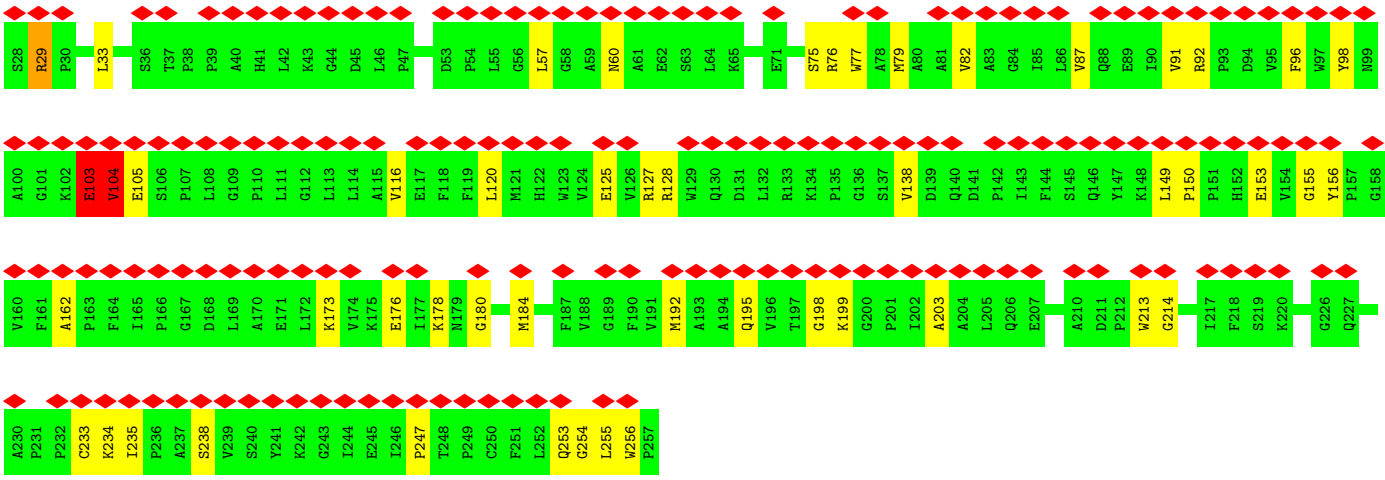
Chain 5:





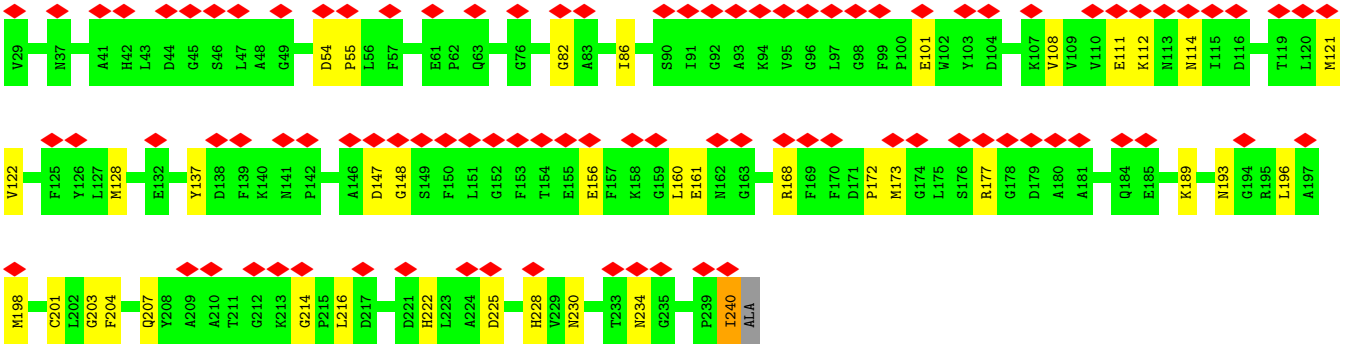
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



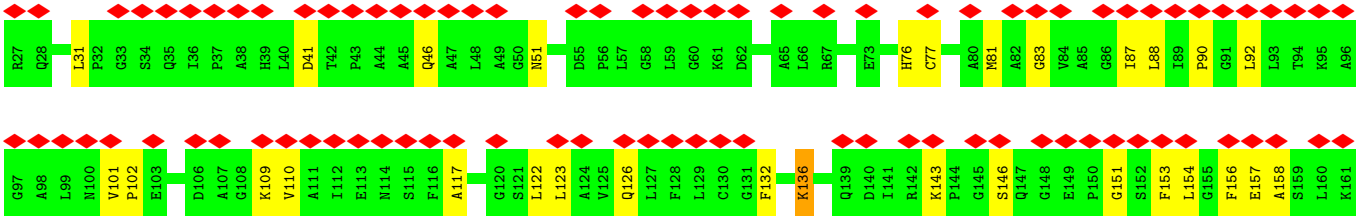
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

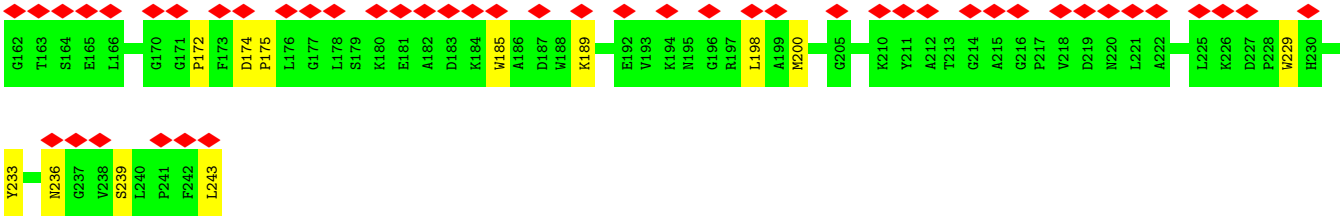
Chain 7:



• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

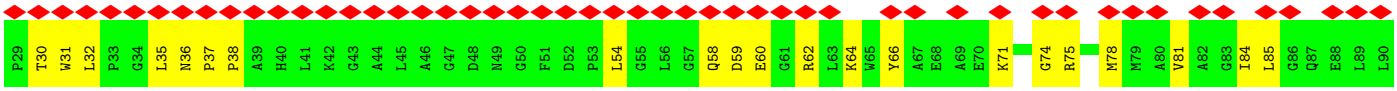
Chain 8:

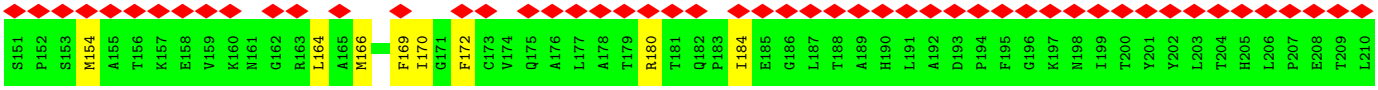




• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.004	Depositor
Minimum map value	-1.725	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	1	Depositor
Map size (Å)	470.52002, 470.52002, 470.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, BCR, SQD, CHL, NEX, LHG, XAT, DGD, PQN, CLA, LMG, TPO, LUT

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	0.54	1/6007 (0.0%)	0.54	1/8190 (0.0%)
2	B	0.50	0/6040	0.55	0/8247
3	C	0.48	0/610	0.55	0/826
4	D	0.43	0/1160	0.52	1/1567 (0.1%)
5	E	0.37	0/506	0.43	0/689
6	F	0.36	0/1291	0.49	0/1747
7	G	0.32	0/693	0.55	0/943
8	H	0.39	0/785	0.71	4/1055 (0.4%)
9	I	0.51	0/293	0.54	0/406
10	J	0.41	0/349	0.46	0/478
11	K	0.32	0/583	0.49	0/790
12	L	0.43	0/1190	0.58	0/1628
13	O	0.40	0/743	0.63	0/1013
14	P	0.27	0/1717	0.44	0/2339
14	Q	0.22	0/1717	0.42	0/2339
14	R	0.21	0/1717	0.43	0/2339
14	T	0.17	0/1717	0.40	0/2339
14	U	0.20	0/1717	0.43	0/2339
15	S	0.35	0/1748	0.69	3/2376 (0.1%)
16	1	0.35	0/1490	0.44	0/2028
16	a	0.54	4/1490 (0.3%)	0.53	1/2028 (0.0%)
17	2	0.42	0/1583	0.73	1/2148 (0.0%)
18	3	0.44	0/1606	0.54	0/2180
19	4	0.33	0/1645	0.52	1/2246 (0.0%)
20	5	0.43	0/1812	0.52	0/2469
21	6	0.38	0/1833	0.55	3/2505 (0.1%)
22	7	0.43	0/1696	0.51	0/2303
23	8	0.43	0/1700	0.51	1/2315 (0.0%)
24	9	0.34	0/1433	0.57	0/1949
All	All	0.41	5/46871 (0.0%)	0.53	16/63821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	2
10	J	0	1
15	S	0	1
17	2	0	2
19	4	0	2
21	6	0	1
22	7	0	1
24	9	0	1
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ASN	C-O	15.68	1.31	1.23
16	a	118	TRP	NE1-CE2	10.48	1.49	1.37
16	a	118	TRP	CE2-CZ2	-7.62	1.23	1.39
16	a	118	TRP	CB-CG	-6.70	1.29	1.50
16	a	118	TRP	CG-CD2	-6.24	1.32	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	153	MET	CG-SD-CE	-7.75	83.86	100.90
1	A	684	MET	CG-SD-CE	-7.27	84.90	100.90
23	8	136	LYS	CD-CE-NZ	-7.14	89.04	111.90
15	S	34	GLY	N-CA-C	-6.27	98.31	113.18
15	S	32	SER	CA-C-N	6.21	133.39	121.54
15	S	32	SER	C-N-CA	6.21	133.39	121.54
16	a	118	TRP	CD2-CE2-CZ2	6.09	128.49	122.40
21	6	104	VAL	N-CA-C	5.69	121.18	109.34
8	H	106	ALA	CA-C-N	5.39	131.83	121.54
8	H	106	ALA	C-N-CA	5.39	131.83	121.54
21	6	103	GLU	CA-C-N	5.31	131.53	121.97
21	6	103	GLU	C-N-CA	5.31	131.53	121.97
19	4	214	LYS	CB-CG-CD	-5.12	99.51	111.30
8	H	104	LYS	CA-C-N	5.07	131.22	121.54
8	H	104	LYS	C-N-CA	5.07	131.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	76	ARG	NE-CZ-NH1	-5.03	116.47	121.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	2	137	PHE	Peptide
17	2	32	TYR	Peptide
19	4	142	TYR	Peptide,Mainchain
21	6	29	ARG	Peptide
22	7	114	ASN	Peptide
24	9	142	PHE	Peptide
2	B	297	GLY	Peptide
2	B	668	TRP	Peptide
3	C	61	ASP	Peptide
3	C	62	PHE	Peptide
10	J	39	PHE	Peptide
15	S	33	SER	Mainchain

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	5811	0	5657	107	0
2	B	5828	0	5582	109	0
3	C	600	0	581	16	0
4	D	1132	0	1150	32	0
5	E	496	0	491	12	0
6	F	1265	0	1303	32	0
7	G	678	0	659	20	0
8	H	773	0	756	37	0
9	I	281	0	292	10	0
10	J	337	0	336	8	0
11	K	578	0	617	17	0
12	L	1161	0	1184	35	0
13	O	720	0	716	32	0
14	P	1669	0	1603	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	Q	1669	0	1602	88	0
14	R	1669	0	1603	94	0
14	T	1669	0	1603	61	0
14	U	1669	0	1602	76	0
15	S	1717	0	1625	82	0
16	1	1444	0	1392	39	0
16	a	1444	0	1393	76	0
17	2	1545	0	1552	89	0
18	3	1560	0	1527	34	0
19	4	1590	0	1536	46	0
20	5	1757	0	1736	62	0
21	6	1771	0	1772	52	0
22	7	1644	0	1579	29	0
23	8	1649	0	1626	39	0
24	9	1392	0	1369	49	0
25	1	722	0	734	33	0
25	2	681	0	606	35	0
25	3	761	0	704	20	0
25	4	515	0	432	18	0
25	5	799	0	710	27	0
25	6	752	0	670	27	0
25	7	616	0	534	12	0
25	8	680	0	592	13	0
25	9	461	0	380	7	0
25	A	2638	0	2751	108	0
25	B	2368	0	2443	72	0
25	F	45	0	33	2	0
25	G	96	0	72	2	0
25	H	175	0	126	6	0
25	J	100	0	86	6	0
25	K	232	0	173	6	0
25	L	278	0	274	9	0
25	O	117	0	67	1	0
25	P	399	0	384	108	0
25	Q	493	0	463	75	0
25	R	477	0	475	110	0
25	S	585	0	575	50	0
25	T	408	0	396	29	0
25	U	408	0	408	36	0
25	a	714	0	715	59	0
26	A	33	0	46	0	0
26	B	33	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	1	43	0	56	3	0
27	2	49	0	74	1	0
27	4	81	0	106	1	0
27	5	82	0	107	6	0
27	6	49	0	74	5	0
27	7	37	0	44	1	0
27	8	49	0	74	1	0
27	A	135	0	189	9	0
27	B	38	0	46	2	0
27	P	98	0	148	15	0
27	Q	49	0	74	4	0
27	R	49	0	74	7	0
27	S	49	0	74	3	0
27	T	49	0	74	5	0
27	a	43	0	56	6	0
28	3	120	0	168	10	0
28	4	80	0	111	10	0
28	5	80	0	112	8	0
28	6	40	0	56	2	0
28	7	40	0	56	2	0
28	8	80	0	112	3	0
28	A	240	0	336	23	0
28	B	280	0	390	20	0
28	F	80	0	112	3	0
28	G	40	0	53	1	0
28	I	40	0	53	5	0
28	J	80	0	112	7	0
28	K	40	0	56	0	0
28	L	160	0	222	4	0
28	O	80	0	112	3	0
29	A	8	0	0	0	0
29	C	16	0	0	1	0
30	B	123	0	168	6	0
31	B	51	0	69	5	0
32	1	46	0	65	1	0
32	2	41	0	52	5	0
32	4	40	0	50	1	0
32	6	40	0	50	1	0
32	7	71	0	82	2	0
32	H	47	0	64	3	0
32	J	130	0	176	4	0
33	1	101	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	3	53	0	41	1	0
33	4	240	0	169	9	0
33	5	145	0	103	4	0
33	6	200	0	148	9	0
33	7	54	0	43	2	0
33	8	53	0	41	4	0
33	9	93	0	64	1	0
33	P	416	0	326	70	0
33	Q	253	0	201	58	0
33	R	309	0	244	56	0
33	S	358	0	265	28	0
33	T	244	0	177	11	0
33	U	241	0	173	12	0
33	a	48	0	33	1	0
34	1	126	0	163	12	0
34	2	84	0	112	9	0
34	3	84	0	112	5	0
34	4	84	0	112	11	0
34	5	84	0	112	8	0
34	6	84	0	112	5	0
34	7	84	0	112	10	0
34	8	84	0	112	9	0
34	9	84	0	112	11	0
34	P	84	0	112	14	0
34	Q	84	0	112	12	0
34	R	84	0	112	14	0
34	S	84	0	112	11	0
34	T	84	0	112	8	0
34	U	84	0	112	12	0
34	a	126	0	163	17	0
35	P	131	0	165	23	0
35	Q	44	0	56	6	0
35	S	44	0	56	8	0
35	T	44	0	56	6	0
36	P	88	0	112	18	0
36	R	44	0	56	3	0
36	T	44	0	56	3	0
36	U	88	0	111	25	0
All	All	68860	0	68110	2228	0

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

All (2228) 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)
14:R:212:PHE:CB	33:R:609:CHL:H203	1.17	1.63
14:Q:212:PHE:CB	33:Q:608:CHL:H203	1.18	1.61
14:P:212:PHE:CB	33:P:609:CHL:H203	1.17	1.58
14:R:212:PHE:HB3	33:R:609:CHL:C20	1.15	1.57
25:R:610:CLA:H72	25:R:612:CLA:CMB	1.30	1.56
14:P:212:PHE:HB3	33:P:609:CHL:C20	1.16	1.54
14:Q:212:PHE:HB3	33:Q:608:CHL:C20	1.19	1.54
25:P:610:CLA:C7	25:P:612:CLA:HMB1	1.36	1.53
25:P:610:CLA:H72	25:P:612:CLA:CMB	1.34	1.53
25:R:610:CLA:C7	25:R:612:CLA:HMB1	1.34	1.48
25:R:610:CLA:C10	25:R:612:CLA:HMB2	1.42	1.47
25:P:610:CLA:C10	25:P:612:CLA:HMB2	1.44	1.46
25:R:610:CLA:C10	25:R:612:CLA:CMB	1.95	1.44
25:P:610:CLA:C10	25:P:612:CLA:CMB	1.96	1.43
25:R:610:CLA:C7	25:R:612:CLA:CMB	1.89	1.41
25:P:610:CLA:C7	25:P:612:CLA:CMB	1.92	1.38
25:P:611:CLA:CMA	36:P:621:NEX:H161	1.60	1.31
25:R:610:CLA:H102	25:R:612:CLA:CMB	1.59	1.30
14:P:212:PHE:CB	33:P:609:CHL:C20	1.86	1.23
14:R:212:PHE:CB	33:R:609:CHL:C20	1.86	1.21
25:R:611:CLA:H52	25:R:612:CLA:C2D	1.69	1.21
14:Q:212:PHE:CB	33:Q:608:CHL:C20	1.87	1.21
25:R:611:CLA:H52	25:R:612:CLA:C3D	1.70	1.20
25:R:612:CLA:H91	25:R:612:CLA:H121	1.22	1.19
25:Q:603:CLA:OBD	33:Q:608:CHL:CGA	1.90	1.18
25:P:603:CLA:OBD	33:P:609:CHL:CGA	1.92	1.17
25:R:603:CLA:OBD	33:R:609:CHL:CGA	1.93	1.16
14:R:193:LEU:CD2	25:R:612:CLA:HBA2	1.75	1.15
25:R:610:CLA:C8	25:R:612:CLA:CMB	2.25	1.15
25:R:603:CLA:C3B	33:R:609:CHL:H13	1.57	1.14
25:P:610:CLA:H102	25:P:612:CLA:CMB	1.64	1.13
25:P:603:CLA:C3B	33:P:609:CHL:H13	1.61	1.12
14:P:193:LEU:CD2	25:P:612:CLA:HBA2	1.79	1.12
14:P:81:LEU:HD12	33:P:609:CHL:O2D	1.48	1.11
25:P:610:CLA:C8	25:P:612:CLA:CMB	2.28	1.10
25:R:610:CLA:H101	25:R:612:CLA:HMB2	1.15	1.10
25:P:611:CLA:HMA2	36:P:621:NEX:H161	1.12	1.09
25:P:612:CLA:H91	25:P:612:CLA:H121	1.22	1.09
17:2:153:MET:HE1	17:2:156:LYS:HE2	1.28	1.09
14:P:43:PRO:HA	14:U:43:PRO:HD2	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:214:LYS:HD3	25:4:310:CLA:HAA2	1.30	1.08
25:R:610:CLA:C8	25:R:612:CLA:HMB2	1.82	1.07
25:P:610:CLA:H101	25:P:612:CLA:HMB2	1.10	1.06
25:P:610:CLA:C8	25:P:612:CLA:HMB2	1.86	1.06
25:Q:603:CLA:C3B	33:Q:608:CHL:H13	1.58	1.06
14:R:196:LYS:HD3	25:R:612:CLA:HBD	1.38	1.04
25:P:610:CLA:H102	25:P:612:CLA:HMB3	1.06	1.03
14:P:94:LEU:HD12	25:P:612:CLA:CBB	1.89	1.02
33:P:609:CHL:H152	33:P:609:CHL:H192	1.41	1.02
14:Q:212:PHE:HB2	33:Q:608:CHL:C20	1.86	1.02
1:A:67:GLU:HG2	1:A:188:LEU:HB2	1.36	1.02
25:R:610:CLA:H102	25:R:612:CLA:HMB3	1.03	1.01
14:P:212:PHE:HB2	33:P:609:CHL:C20	1.87	1.01
14:R:94:LEU:HD12	25:R:612:CLA:CBB	1.89	1.01
33:R:609:CHL:H152	33:R:609:CHL:H192	1.41	1.01
25:P:611:CLA:HMA2	36:P:621:NEX:C16	1.91	1.00
21:6:156:TYR:OH	21:6:176:GLU:OE2	1.79	1.00
14:P:94:LEU:HD12	25:P:612:CLA:HBB2	1.00	0.99
14:R:212:PHE:HB2	33:R:609:CHL:C20	1.88	0.99
14:R:94:LEU:HD12	25:R:612:CLA:HBB2	1.00	0.99
3:C:39:MET:HE2	4:D:170:GLN:HE21	1.23	0.99
33:Q:608:CHL:H152	33:Q:608:CHL:H192	1.41	0.97
23:8:136:LYS:NZ	23:8:153:PHE:HZ	1.62	0.97
33:U:308:CHL:CGA	25:U:310:CLA:HBC2	1.96	0.96
14:Q:152:MET:HE3	33:Q:606:CHL:HHB	1.47	0.96
25:R:610:CLA:C7	25:R:612:CLA:HMB2	1.76	0.96
14:R:212:PHE:CB	33:R:609:CHL:H201	1.94	0.95
14:P:212:PHE:CB	33:P:609:CHL:H201	1.95	0.95
33:T:606:CHL:CGA	25:T:608:CLA:HBC2	1.97	0.95
16:a:118:TRP:HH2	25:a:303:CLA:C4	1.80	0.95
1:A:507:SER:HB3	1:A:510:TRP:HE1	1.31	0.94
33:R:608:CHL:CGA	25:R:610:CLA:HBC2	1.97	0.94
33:P:608:CHL:CGA	25:P:610:CLA:HBC2	1.97	0.93
14:Q:212:PHE:CB	33:Q:608:CHL:H201	1.97	0.93
25:R:610:CLA:H51	25:R:612:CLA:HHB	1.51	0.93
25:P:610:CLA:C7	25:P:612:CLA:HMB2	1.80	0.93
25:P:610:CLA:H51	25:P:612:CLA:HHB	1.48	0.93
33:Q:607:CHL:CGA	25:Q:609:CLA:HBC2	1.98	0.92
25:R:603:CLA:CHC	33:R:609:CHL:H102	1.99	0.92
17:2:153:MET:HE1	17:2:156:LYS:CE	1.99	0.91
25:R:603:CLA:C3B	33:R:609:CHL:C13	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:43:PRO:HA	14:U:43:PRO:CD	2.01	0.89
25:R:612:CLA:H121	25:R:612:CLA:C9	2.00	0.89
14:P:94:LEU:CD1	25:P:612:CLA:HBB2	1.97	0.89
25:P:612:CLA:H121	25:P:612:CLA:C9	2.00	0.89
25:Q:603:CLA:C3B	33:Q:608:CHL:C13	2.51	0.89
28:A:854:BCR:H403	11:K:92:MET:HE1	1.54	0.89
14:P:196:LYS:HD3	25:P:612:CLA:HBD	1.53	0.89
2:B:596:HIS:HD1	2:B:624:TYR:HH	1.16	0.88
16:a:118:TRP:HH2	25:a:303:CLA:H42	1.37	0.88
25:R:611:CLA:C5	25:R:612:CLA:C2D	2.52	0.88
21:6:91:VAL:HG23	21:6:92:ARG:HG2	1.56	0.88
23:8:102:PRO:HG3	23:8:110:VAL:HG21	1.55	0.88
14:P:81:LEU:CD1	33:P:609:CHL:O2D	2.22	0.88
25:P:603:CLA:CHC	33:P:609:CHL:H102	2.04	0.88
25:Q:603:CLA:CHC	33:Q:608:CHL:H102	2.03	0.88
14:P:196:LYS:HG2	25:P:611:CLA:HED1	1.55	0.87
25:Q:618:CLA:HBD	36:U:301:NEX:H172	1.54	0.87
15:S:145:ASN:HD21	25:S:301:CLA:C4B	1.87	0.87
25:R:611:CLA:H71	25:R:612:CLA:C1D	2.05	0.86
2:B:67:PHE:CE1	9:I:69:PHE:HE2	1.92	0.86
35:P:623:XAT:H41	33:S:308:CHL:HAA2	1.57	0.86
1:A:369:HIS:HA	1:A:372:TYR:CE1	2.10	0.86
14:R:94:LEU:CD1	25:R:612:CLA:HBB2	1.97	0.86
15:S:178:TYR:OH	15:S:202:GLU:OE1	1.92	0.86
14:T:76:LYS:HA	14:T:79:ARG:HE	1.40	0.86
14:U:76:LYS:HA	14:U:79:ARG:HE	1.38	0.86
17:2:120:VAL:O	17:2:124:LYS:NZ	2.09	0.85
16:a:197:ALA:HA	16:a:223:ILE:HD11	1.56	0.85
14:P:76:LYS:HA	14:P:79:ARG:HE	1.41	0.85
14:Q:76:LYS:HA	14:Q:79:ARG:HE	1.40	0.85
14:R:76:LYS:HA	14:R:79:ARG:HE	1.39	0.85
2:B:693:TYR:OH	4:D:76:ARG:NH2	2.10	0.85
25:R:612:CLA:HHC	25:R:612:CLA:HBB1	1.59	0.85
23:8:136:LYS:HZ1	23:8:153:PHE:HZ	1.21	0.84
25:P:603:CLA:H51	25:Q:603:CLA:H51	1.58	0.84
14:R:196:LYS:HD2	25:R:612:CLA:HAA2	1.60	0.84
17:2:186:LEU:O	17:2:190:LEU:HB2	1.77	0.84
19:4:214:LYS:HD3	25:4:310:CLA:CAA	2.07	0.84
25:P:603:CLA:C3B	33:P:609:CHL:C13	2.53	0.84
33:P:608:CHL:CGA	25:P:610:CLA:CBC	2.57	0.83
14:R:193:LEU:HD23	25:R:612:CLA:HBA2	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:161:GLU:OE2	20:5:164:TYR:HD2	1.62	0.83
25:P:611:CLA:CBC	27:P:618:LHG:H332	2.09	0.83
25:R:610:CLA:C10	25:R:612:CLA:HMB3	1.83	0.83
25:P:612:CLA:HHC	25:P:612:CLA:HBB1	1.59	0.83
14:P:43:PRO:CA	14:U:43:PRO:HD2	2.09	0.83
12:L:165:ASP:OD1	12:L:166:GLY:N	2.11	0.82
16:a:117:THR:O	16:a:118:TRP:HD1	1.61	0.82
14:P:193:LEU:HD23	25:P:612:CLA:HBA2	1.60	0.82
2:B:76:GLU:OE1	2:B:133:ASN:ND2	2.12	0.82
11:K:58:LYS:HE3	11:K:83:GLY:HA3	1.61	0.82
14:P:196:LYS:HG2	25:P:611:CLA:CED	2.09	0.82
33:Q:607:CHL:CGA	25:Q:609:CLA:CBC	2.58	0.82
25:Q:604:CLA:HBC3	25:Q:609:CLA:H18	1.62	0.82
24:9:170:ILE:HD11	25:9:304:CLA:HBB2	1.62	0.81
14:P:180:PRO:HB2	17:2:139:SER:HB3	1.63	0.81
17:2:156:LYS:HD3	25:2:311:CLA:HBD	1.62	0.81
25:R:603:CLA:C1C	33:R:609:CHL:H102	2.11	0.81
16:a:118:TRP:CH2	25:a:303:CLA:H42	2.16	0.81
2:B:102:VAL:HG13	2:B:113:PRO:HG3	1.63	0.81
33:U:308:CHL:CGA	25:U:310:CLA:CBC	2.58	0.81
14:P:81:LEU:HA	33:P:609:CHL:CED	2.11	0.80
25:a:303:CLA:H12	34:a:316:LUT:H41	1.62	0.80
33:T:606:CHL:CGA	25:T:608:CLA:CBC	2.58	0.80
33:R:608:CHL:CGA	25:R:610:CLA:CBC	2.58	0.80
25:A:802:CLA:H152	25:A:839:CLA:HBB1	1.63	0.80
14:R:196:LYS:CD	25:R:612:CLA:HBD	2.11	0.80
1:A:236:GLU:N	1:A:236:GLU:OE1	2.13	0.80
14:Q:81:LEU:HA	33:Q:608:CHL:CED	2.11	0.80
14:R:81:LEU:HA	33:R:609:CHL:CED	2.11	0.80
20:5:194:MET:HE2	25:5:303:CLA:HMC3	1.62	0.80
7:G:50:ARG:HD2	7:G:95:PHE:CE2	2.17	0.80
16:a:96:GLU:OE2	16:a:203:ILE:HB	1.80	0.80
14:P:212:PHE:HB2	33:P:609:CHL:H201	1.61	0.80
16:a:206:LEU:HD12	34:a:314:LUT:H22	1.64	0.80
14:P:30:ILE:HA	36:P:621:NEX:H22	1.65	0.79
14:R:144:THR:HG22	33:R:605:CHL:HAC1	1.64	0.79
24:9:75:ARG:HA	24:9:78:MET:HE3	1.65	0.79
2:B:458:PRO:HG3	2:B:518:PHE:HB2	1.63	0.78
14:Q:212:PHE:HB2	33:Q:608:CHL:H201	1.60	0.78
25:R:603:CLA:C4B	33:R:609:CHL:H102	2.13	0.78
25:A:806:CLA:H61	28:A:846:BCR:HC8	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:62:PHE:CD1	15:S:63:PRO:HD2	2.18	0.78
16:1:206:LEU:HD12	34:1:615:LUT:H22	1.65	0.78
2:B:643:SER:OG	8:H:119:GLU:OE1	1.99	0.78
25:R:603:CLA:OBD	33:R:609:CHL:CBA	2.32	0.78
25:A:816:CLA:H51	28:3:319:BCR:H23C	1.66	0.78
25:P:610:CLA:C5	25:P:612:CLA:HHB	2.14	0.78
1:A:507:SER:HB3	1:A:510:TRP:NE1	1.99	0.78
16:a:118:TRP:CH2	25:a:303:CLA:C4	2.67	0.78
14:Q:144:THR:HG22	33:Q:605:CHL:HAC1	1.65	0.77
25:Q:603:CLA:C1C	33:Q:608:CHL:H102	2.12	0.77
25:P:603:CLA:C1C	33:P:609:CHL:H102	2.13	0.77
20:5:159:ASN:O	20:5:159:ASN:ND2	2.17	0.77
14:R:193:LEU:CD2	25:R:612:CLA:CBA	2.62	0.77
20:5:117:ASN:HD22	21:6:214:GLY:HA2	1.50	0.77
25:Q:603:CLA:OBD	33:Q:608:CHL:CBA	2.33	0.77
25:R:610:CLA:H71	25:R:612:CLA:CMB	2.14	0.76
25:B:834:CLA:H72	25:B:834:CLA:HBB1	1.66	0.76
25:P:603:CLA:OBD	33:P:609:CHL:CBA	2.33	0.76
8:H:34:GLU:CD	8:H:35:ASN:H	1.93	0.76
25:P:611:CLA:HMA3	36:P:621:NEX:H161	1.65	0.76
16:a:118:TRP:HH2	25:a:303:CLA:C3	1.99	0.76
25:L:206:CLA:HAA1	25:L:209:CLA:HAB	1.68	0.76
25:R:610:CLA:C5	25:R:612:CLA:HHB	2.15	0.76
15:S:225:LYS:HE2	15:S:229:GLN:HB3	1.67	0.76
20:5:202:LEU:HD13	25:5:313:CLA:HAC2	1.68	0.76
2:B:723:ALA:HB2	25:B:825:CLA:HBB1	1.67	0.76
25:P:610:CLA:H71	25:P:612:CLA:CMB	2.14	0.75
15:S:178:TYR:HE2	15:S:199:LYS:HG2	1.50	0.75
2:B:67:PHE:HE1	9:I:69:PHE:HE2	1.31	0.75
4:D:58:LEU:HB3	4:D:139:TYR:CE2	2.21	0.75
14:P:144:THR:HG22	33:P:605:CHL:HAC1	1.67	0.75
17:2:59:ASN:OD1	17:2:62:ASN:ND2	2.19	0.75
33:P:622:CHL:HBA2	33:S:310:CHL:HBA1	1.66	0.75
14:U:144:THR:HG22	33:U:305:CHL:HAC1	1.67	0.75
14:R:212:PHE:HB2	33:R:609:CHL:H201	1.60	0.75
25:3:302:CLA:HHC	25:3:302:CLA:HBB1	1.68	0.75
14:T:144:THR:HG22	33:T:604:CHL:HAC1	1.68	0.75
25:P:603:CLA:H72	25:Q:603:CLA:H8	1.66	0.75
3:C:39:MET:HE2	4:D:170:GLN:NE2	2.01	0.74
25:A:810:CLA:H101	28:J:106:BCR:H333	1.68	0.74
25:Q:603:CLA:C4B	33:Q:608:CHL:H102	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:P:609:CHL:CBB	33:R:601:CHL:H2	2.17	0.74
14:R:196:LYS:HD2	25:R:612:CLA:CAA	2.17	0.74
24:9:123:GLU:OE2	24:9:126:ARG:NH2	2.20	0.74
14:R:193:LEU:HD22	25:R:612:CLA:HBA2	1.69	0.74
35:S:318:XAT:H41	33:S:321:CHL:HAA2	1.70	0.73
14:U:86:ALA:HB1	14:U:201:GLY:HA3	1.70	0.73
22:7:101:GLU:OE1	22:7:214:GLY:HA3	1.87	0.73
18:3:121:THR:HG22	18:3:122:ASN:H	1.54	0.73
6:F:162:TYR:HE2	25:F:802:CLA:HBD	1.53	0.73
14:P:193:LEU:HD22	25:P:612:CLA:HBA2	1.70	0.73
25:P:603:CLA:C4B	33:P:609:CHL:H102	2.18	0.73
17:2:67:ARG:HH12	25:2:303:CLA:HED3	1.53	0.73
2:B:301:ARG:HH21	7:G:67:VAL:HG21	1.53	0.73
17:2:153:MET:CE	17:2:156:LYS:HE2	2.15	0.73
17:2:149:LYS:HE2	17:2:153:MET:HB2	1.71	0.73
22:7:160:LEU:HD23	22:7:161:GLU:HG3	1.71	0.73
15:S:247:ALA:HA	35:S:318:XAT:H22	1.69	0.72
20:5:202:LEU:HD22	25:5:313:CLA:HHD	1.71	0.72
14:P:247:PRO:HG3	33:P:619:CHL:HBA2	1.71	0.72
15:S:50:SER:HB2	15:S:54:THR:HG22	1.71	0.72
25:A:804:CLA:HBB1	28:J:101:BCR:H271	1.70	0.72
25:S:301:CLA:HHC	33:S:306:CHL:HBB2	1.70	0.72
1:A:128:ASN:O	6:F:90:ARG:NH1	2.23	0.72
14:Q:86:ALA:HB1	14:Q:201:GLY:HA3	1.70	0.72
23:8:154:LEU:HB2	25:a:302:CLA:H2	1.71	0.72
25:R:612:CLA:H91	25:R:612:CLA:C12	2.13	0.71
25:A:806:CLA:H11	25:A:807:CLA:HBB1	1.70	0.71
33:P:609:CHL:HHC	33:P:609:CHL:HBB1	1.73	0.71
19:4:159:TRP:HB2	33:4:322:CHL:H2	1.72	0.71
7:G:76:TYR:CD2	24:9:59:ASP:HB2	2.25	0.71
14:R:86:ALA:HB1	14:R:201:GLY:HA3	1.73	0.71
14:P:30:ILE:HG22	36:P:621:NEX:H22	1.72	0.70
15:S:153:GLN:HE22	33:S:308:CHL:HAC1	1.55	0.70
14:P:180:PRO:HB2	17:2:139:SER:CB	2.21	0.70
14:Q:140:ASN:ND2	14:U:230:LEU:O	2.24	0.70
33:4:322:CHL:HAB	16:a:59:PHE:CE2	2.26	0.70
25:6:623:CLA:H93	25:6:623:CLA:HBB1	1.71	0.70
13:O:60:ASN:HA	13:O:70:SER:HB3	1.72	0.70
33:Q:608:CHL:HHC	33:Q:608:CHL:HBB1	1.73	0.70
21:6:82:VAL:HG11	34:6:619:LUT:H12	1.72	0.70
14:P:86:ALA:HB1	14:P:201:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:81:LEU:HD12	33:Q:608:CHL:O2D	1.92	0.70
16:a:117:THR:C	16:a:118:TRP:HD1	2.00	0.70
7:G:97:ILE:HD11	24:9:32:LEU:HD21	1.73	0.70
14:P:107:THR:HG22	17:2:105:LEU:HD11	1.74	0.70
21:6:104:VAL:HG11	33:6:606:CHL:HAC1	1.74	0.70
25:P:612:CLA:H91	25:P:612:CLA:C12	2.13	0.70
14:P:193:LEU:CD2	25:P:612:CLA:CBA	2.65	0.70
15:S:81:LYS:O	15:S:84:ARG:HG2	1.91	0.70
2:B:572:SER:OG	2:B:575:ASP:OD2	2.08	0.69
14:R:212:PHE:CG	33:R:609:CHL:H203	2.21	0.69
2:B:67:PHE:CE1	9:I:69:PHE:CE2	2.79	0.69
14:T:86:ALA:HB1	14:T:201:GLY:HA3	1.75	0.69
21:6:156:TYR:HE1	21:6:173:LYS:HG2	1.56	0.69
1:A:121:ILE:O	1:A:123:GLY:N	2.25	0.69
25:P:610:CLA:H51	25:P:612:CLA:CHB	2.23	0.69
25:R:603:CLA:OBD	33:R:609:CHL:HBA2	1.91	0.69
16:a:138:MET:HG2	25:a:307:CLA:HMC2	1.74	0.69
25:B:810:CLA:H2	24:9:54:LEU:HD13	1.73	0.69
25:Q:603:CLA:OBD	33:Q:608:CHL:O1A	2.11	0.69
25:R:611:CLA:C9	25:R:612:CLA:HBC3	2.23	0.69
21:6:60:ASN:OD1	22:7:177:ARG:HG3	1.92	0.69
25:P:603:CLA:OBD	33:P:609:CHL:HBA2	1.93	0.69
14:Q:58:PRO:HB2	14:Q:198:ILE:HD12	1.74	0.69
16:1:142:GLU:OE1	16:1:145:ARG:NH2	2.25	0.69
15:S:57:TYR:HB3	15:S:80:PHE:CE2	2.28	0.68
25:S:301:CLA:CAB	33:S:306:CHL:HBB2	2.23	0.68
25:1:611:CLA:HBB1	34:1:615:LUT:H14	1.75	0.68
33:R:609:CHL:HBB1	33:R:609:CHL:HHC	1.73	0.68
15:S:68:TRP:CH2	33:S:302:CHL:HAA1	2.28	0.68
14:U:196:LYS:HG2	36:U:301:NEX:H173	1.74	0.68
16:a:118:TRP:O	16:a:120:GLY:N	2.25	0.68
1:A:712:ALA:HB3	6:F:184:GLU:OE1	1.93	0.68
14:U:118:GLY:HA2	33:U:306:CHL:HAC2	1.75	0.68
17:2:64:LYS:HD2	17:2:134:GLU:OE2	1.94	0.68
15:S:88:LEU:HD12	15:S:177:LEU:HD22	1.76	0.68
14:U:111:GLU:HG2	14:U:116:LYS:HB2	1.75	0.68
16:a:142:GLU:OE1	16:a:145:ARG:NH2	2.25	0.68
8:H:45:GLU:HG3	12:L:149:LYS:HG3	1.73	0.68
2:B:547:LEU:O	2:B:565:ARG:NH2	2.27	0.68
12:L:99:PRO:HB2	25:L:202:CLA:H2	1.75	0.68
14:P:118:GLY:HA2	33:P:606:CHL:HAC2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:610:CLA:H101	25:P:612:CLA:CMB	1.91	0.68
8:H:63:PRO:HG2	8:H:66:GLN:HE22	1.58	0.68
17:2:30:MET:HE1	17:2:50:GLY:HA3	1.74	0.68
17:2:178:TYR:HH	17:2:201:SER:HG	1.37	0.68
2:B:167:SER:OG	7:G:78:ASP:OD1	2.10	0.68
13:O:90:PRO:HB2	13:O:96:PHE:HZ	1.58	0.68
14:Q:118:GLY:HA2	33:Q:606:CHL:HAC2	1.75	0.68
25:R:610:CLA:C7	25:R:612:CLA:HHB	2.24	0.68
14:U:100:GLU:HB3	14:U:223:ILE:HD12	1.75	0.68
13:O:49:VAL:O	13:O:53:ALA:HB3	1.94	0.68
14:R:212:PHE:CB	33:R:609:CHL:C18	2.71	0.68
14:T:100:GLU:HB3	14:T:223:ILE:HD12	1.76	0.67
25:S:301:CLA:O1A	25:U:313:CLA:H3A	1.94	0.67
25:a:303:CLA:C1	34:a:316:LUT:H41	2.23	0.67
1:A:422:ASN:OD1	1:A:425:ASN:ND2	2.26	0.67
25:B:834:CLA:H151	28:F:803:BCR:H21C	1.75	0.67
16:a:73:ARG:HA	16:a:76:GLU:OE1	1.94	0.67
25:a:310:CLA:HBB1	34:a:314:LUT:H14	1.76	0.67
25:a:311:CLA:H101	27:a:317:LHG:H301	1.75	0.67
25:2:309:CLA:HAB	34:2:315:LUT:H32	1.76	0.67
25:B:802:CLA:CGA	25:B:802:CLA:H3A	2.24	0.67
25:5:324:CLA:H2	27:6:618:LHG:H152	1.76	0.67
17:2:156:LYS:HG3	25:2:310:CLA:OBD	1.94	0.67
11:K:58:LYS:CE	11:K:83:GLY:HA3	2.25	0.67
14:R:118:GLY:HA2	33:R:606:CHL:HAC2	1.76	0.67
14:T:118:GLY:HA2	33:T:605:CHL:HAC2	1.76	0.67
15:S:99:LEU:HD21	25:S:313:CLA:HAB	1.75	0.67
13:O:94:ASP:HB3	13:O:96:PHE:CE1	2.30	0.67
25:R:611:CLA:C5	25:R:612:CLA:CMD	2.73	0.67
31:B:850:SQD:H151	32:2:301:LMG:H311	1.76	0.66
8:H:62:TYR:HE2	12:L:83:LEU:HB3	1.59	0.66
14:R:212:PHE:HB3	33:R:609:CHL:C18	2.19	0.66
1:A:67:GLU:CG	1:A:188:LEU:HB2	2.19	0.66
14:P:100:GLU:HB3	14:P:223:ILE:HD12	1.76	0.66
14:P:81:LEU:CA	33:P:609:CHL:HED1	2.26	0.66
14:P:212:PHE:CB	33:P:609:CHL:C18	2.70	0.66
1:A:369:HIS:ND1	1:A:372:TYR:OH	2.23	0.66
8:H:62:TYR:OH	12:L:87:GLU:OE1	2.13	0.66
17:2:149:LYS:CE	17:2:153:MET:HB2	2.24	0.66
4:D:96:PHE:CD1	4:D:106:MET:HE2	2.31	0.66
25:P:603:CLA:OBD	33:P:609:CHL:O1A	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:610:CLA:H93	25:R:612:CLA:C15	2.26	0.66
25:R:611:CLA:H93	25:R:612:CLA:HBC3	1.78	0.66
15:S:225:LYS:CE	15:S:229:GLN:HB3	2.24	0.66
15:S:251:THR:HG21	33:S:321:CHL:HED1	1.78	0.66
25:P:611:CLA:H2A	36:P:621:NEX:H171	1.77	0.66
14:R:100:GLU:HB3	14:R:223:ILE:HD12	1.78	0.66
3:C:24:ASP:OD2	4:D:151:HIS:ND1	2.17	0.66
15:S:189:ALA:HA	15:S:195:PHE:CE2	2.31	0.66
2:B:86:ARG:HG2	8:H:129:ARG:HH21	1.61	0.66
14:Q:81:LEU:CA	33:Q:608:CHL:HED1	2.26	0.66
14:Q:111:GLU:HG2	14:Q:116:LYS:HB2	1.78	0.66
25:P:610:CLA:C7	25:P:612:CLA:HHB	2.26	0.65
14:R:164:PRO:HB3	36:R:617:NEX:H183	1.78	0.65
2:B:575:ASP:OD1	2:B:707:ARG:NH2	2.28	0.65
25:Q:603:CLA:OBD	33:Q:608:CHL:HBA2	1.94	0.65
14:R:81:LEU:CA	33:R:609:CHL:HED1	2.26	0.65
25:S:304:CLA:HED2	25:S:304:CLA:H2A	1.77	0.65
18:3:148:PHE:CZ	18:3:152:ILE:HD11	2.31	0.65
25:B:823:CLA:H92	25:B:833:CLA:H62	1.79	0.65
25:6:612:CLA:HBB1	34:6:619:LUT:C14	2.27	0.65
23:8:229:TRP:CZ3	25:8:314:CLA:H3A	2.32	0.65
1:A:489:ASN:HD22	13:O:93:ASP:HB2	1.62	0.65
25:B:803:CLA:HAA2	30:B:848:DGD:HD62	1.79	0.65
19:4:214:LYS:CD	25:4:310:CLA:HAA2	2.18	0.65
21:6:103:GLU:O	21:6:105:GLU:N	2.26	0.65
12:L:106:LEU:HD12	12:L:109:VAL:HG21	1.78	0.65
25:1:607:CLA:HBB1	25:1:607:CLA:H151	1.77	0.65
14:Q:100:GLU:HB3	14:Q:223:ILE:HD12	1.78	0.65
15:S:57:TYR:HB3	15:S:80:PHE:HE2	1.62	0.65
15:S:145:ASN:ND2	25:S:301:CLA:C4B	2.60	0.65
16:a:197:ALA:CA	16:a:223:ILE:HD11	2.27	0.65
25:a:306:CLA:HBB1	25:a:306:CLA:H151	1.77	0.65
14:T:164:PRO:HB3	36:T:616:NEX:H183	1.78	0.65
23:8:136:LYS:NZ	23:8:153:PHE:CZ	2.52	0.65
14:Q:212:PHE:HB3	33:Q:608:CHL:C18	2.21	0.65
14:R:81:LEU:HA	33:R:609:CHL:HED1	1.79	0.65
25:R:610:CLA:H101	25:R:612:CLA:CMB	1.96	0.64
25:R:610:CLA:H51	25:R:612:CLA:CHB	2.24	0.64
14:T:137:HIS:ND1	14:T:137:HIS:O	2.29	0.64
14:P:111:GLU:HG2	14:P:116:LYS:HB2	1.78	0.64
14:P:181:LEU:HD23	17:2:124:LYS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:611:CLA:H93	25:R:612:CLA:CHD	2.28	0.64
33:S:309:CHL:HHC	33:S:309:CHL:HBB1	1.79	0.64
16:a:109:TRP:CH2	16:a:116:ALA:HB2	2.32	0.64
1:A:434:ARG:NH2	4:D:100:THR:O	2.31	0.64
2:B:67:PHE:HE1	9:I:69:PHE:CE2	2.14	0.64
14:P:30:ILE:HA	36:P:621:NEX:C2	2.27	0.64
14:T:111:GLU:HG2	14:T:116:LYS:HB2	1.79	0.64
21:6:75:SER:O	21:6:79:MET:HG3	1.97	0.64
25:P:611:CLA:HBC1	27:P:618:LHG:H332	1.77	0.64
25:R:603:CLA:OBD	33:R:609:CHL:O1A	2.14	0.64
14:Q:212:PHE:CB	33:Q:608:CHL:C18	2.72	0.64
36:U:301:NEX:H161	25:U:311:CLA:CAD	2.28	0.64
23:8:136:LYS:HZ3	23:8:153:PHE:HZ	1.44	0.64
14:Q:76:LYS:HA	14:Q:79:ARG:NE	2.12	0.64
33:S:310:CHL:HAA2	14:U:65:THR:HG21	1.79	0.64
25:P:611:CLA:CMA	36:P:621:NEX:C16	2.55	0.64
25:4:308:CLA:H43	25:4:310:CLA:HBA1	1.78	0.64
14:Q:81:LEU:HA	33:Q:608:CHL:HED1	1.79	0.64
25:A:816:CLA:H71	28:3:319:BCR:H21C	1.79	0.64
2:B:214:LEU:O	24:9:180:ARG:NH1	2.31	0.64
8:H:63:PRO:HG2	8:H:66:GLN:NE2	2.14	0.64
15:S:62:PHE:CE1	15:S:84:ARG:NH2	2.66	0.64
14:U:164:PRO:HB3	36:U:316:NEX:H183	1.80	0.64
25:P:610:CLA:H93	25:P:612:CLA:C15	2.27	0.63
14:R:76:LYS:HA	14:R:79:ARG:NE	2.11	0.63
25:R:603:CLA:C2B	33:R:609:CHL:H13	2.25	0.63
19:4:105:ARG:NH1	33:4:306:CHL:OBD	2.27	0.63
17:2:118:PHE:O	17:2:122:GLU:HG2	1.97	0.63
25:P:610:CLA:H71	25:P:612:CLA:HMB2	1.75	0.63
14:R:211:PHE:CE2	34:R:615:LUT:H8	2.33	0.63
14:P:199:LYS:HE2	25:P:611:CLA:HMD2	1.79	0.63
25:P:603:CLA:C3D	33:P:609:CHL:H2	2.29	0.63
14:U:76:LYS:HA	14:U:79:ARG:NE	2.11	0.63
2:B:370:ALA:HB1	2:B:726:LEU:HD21	1.80	0.63
4:D:58:LEU:HB3	4:D:139:TYR:HE2	1.61	0.63
14:P:164:PRO:HB3	36:P:617:NEX:H183	1.80	0.63
14:Q:94:LEU:HA	14:Q:97:ILE:HG12	1.81	0.63
23:8:198:LEU:HD21	34:8:316:LUT:H191	1.81	0.63
16:a:109:TRP:CZ2	16:a:116:ALA:HB2	2.33	0.63
25:P:603:CLA:C2B	33:P:609:CHL:H13	2.27	0.63
16:1:160:PRO:HD2	34:1:615:LUT:H23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:4:308:CLA:H52	34:4:315:LUT:H28	1.79	0.63
1:A:740:TRP:HB2	25:A:828:CLA:HBB1	1.81	0.63
4:D:189:ARG:HH22	4:D:191:MET:CB	2.11	0.63
14:P:43:PRO:HA	14:U:43:PRO:CG	2.27	0.63
14:P:212:PHE:HB3	33:P:609:CHL:C18	2.19	0.63
25:Q:603:CLA:C3D	33:Q:608:CHL:H2	2.28	0.63
3:C:61:ASP:OD1	5:E:86:ASN:ND2	2.31	0.63
25:Q:603:CLA:C2B	33:Q:608:CHL:H13	2.25	0.63
14:Q:208:MET:CE	34:Q:615:LUT:H10	2.29	0.62
20:5:85:VAL:HG13	20:5:200:PHE:HE2	1.64	0.62
21:6:104:VAL:HG21	25:6:605:CLA:CAA	2.29	0.62
21:6:253:GLN:HG2	21:6:256:TRP:CZ2	2.34	0.62
16:a:118:TRP:CH2	25:a:303:CLA:C3	2.81	0.62
14:P:81:LEU:HA	33:P:609:CHL:HED1	1.79	0.62
25:A:840:CLA:HBB1	25:A:840:CLA:H71	1.80	0.62
2:B:385:CYS:HB3	2:B:577:PHE:HE1	1.63	0.62
12:L:70:SER:OG	15:S:21:LYS:HD2	1.98	0.62
25:1:612:CLA:H101	27:1:618:LHG:H301	1.79	0.62
17:2:138:LEU:HG	17:2:139:SER:H	1.63	0.62
25:A:804:CLA:HBB2	25:A:812:CLA:H102	1.80	0.62
25:S:304:CLA:HED3	34:U:315:LUT:H372	1.79	0.62
25:8:302:CLA:H61	25:8:314:CLA:H42	1.81	0.62
33:P:609:CHL:H192	33:P:609:CHL:C15	2.24	0.62
25:R:610:CLA:H71	25:R:612:CLA:HMB2	1.73	0.62
14:T:94:LEU:HA	14:T:97:ILE:HG12	1.82	0.62
4:D:142:PHE:HD2	4:D:146:LYS:HE2	1.63	0.62
14:P:208:MET:HE1	34:P:615:LUT:H10	1.80	0.62
14:U:156:GLU:OE1	14:U:159:ARG:NE	2.31	0.62
19:4:132:VAL:HG23	19:4:133:ALA:H	1.64	0.62
25:5:324:CLA:HBB1	27:6:618:LHG:H261	1.80	0.62
8:H:62:TYR:CE2	12:L:83:LEU:HB3	2.34	0.62
17:2:40:HIS:NE2	17:2:57:GLY:O	2.33	0.62
25:P:603:CLA:H102	25:Q:603:CLA:H102	1.81	0.62
25:Q:602:CLA:H92	25:Q:603:CLA:HMA3	1.82	0.62
17:2:78:MET:HE2	34:2:315:LUT:H34	1.82	0.62
2:B:530:THR:O	2:B:534:ILE:HD12	2.00	0.62
36:U:301:NEX:H171	25:U:311:CLA:CAD	2.30	0.62
19:4:142:TYR:O	19:4:143:PHE:HD1	1.83	0.62
6:F:91:LEU:HA	6:F:104:LEU:HD13	1.82	0.61
14:P:76:LYS:HA	14:P:79:ARG:NE	2.13	0.61
14:Q:164:PRO:HB3	36:U:301:NEX:H183	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:301:LHG:H122	25:7:312:CLA:HBA1	1.81	0.61
24:9:169:PHE:HA	24:9:172:PHE:HD2	1.65	0.61
7:G:50:ARG:HA	7:G:95:PHE:CZ	2.35	0.61
14:Q:212:PHE:CG	33:Q:608:CHL:H203	2.24	0.61
15:S:223:THR:HG21	25:S:314:CLA:HED1	1.82	0.61
19:4:214:LYS:HE2	25:4:310:CLA:HBD	1.81	0.61
20:5:140:TYR:HA	20:5:162:MET:CE	2.30	0.61
16:1:118:TRP:O	16:1:120:GLY:N	2.33	0.61
20:5:82:MET:HE2	20:5:190:GLY:CA	2.31	0.61
23:8:132:PHE:O	23:8:136:LYS:HG2	2.00	0.61
16:a:160:PRO:HD2	34:a:314:LUT:H23	1.82	0.61
25:A:810:CLA:HAB	25:J:103:CLA:HMD2	1.83	0.61
15:S:66:TYR:HB2	25:S:303:CLA:HMD3	1.83	0.61
24:9:59:ASP:HB3	24:9:62:ARG:HB2	1.81	0.61
25:9:302:CLA:HAB	25:9:303:CLA:HMD1	1.82	0.61
14:P:94:LEU:HA	14:P:97:ILE:HG12	1.82	0.61
14:P:212:PHE:CA	33:P:609:CHL:H203	2.23	0.61
8:H:77:ILE:HB	8:H:83:LEU:HB3	1.82	0.61
25:L:201:CLA:H52	25:L:205:CLA:H43	1.83	0.61
14:U:94:LEU:HA	14:U:97:ILE:HG12	1.81	0.61
1:A:491:HIS:ND1	1:A:510:TRP:CZ3	2.69	0.61
25:R:603:CLA:C3D	33:R:609:CHL:H2	2.30	0.61
25:R:611:CLA:C5	25:R:612:CLA:C3D	2.64	0.61
14:U:152:MET:HE3	14:U:156:GLU:HG2	1.81	0.61
21:6:79:MET:HE2	21:6:180:GLY:CA	2.31	0.61
8:H:83:LEU:HD11	12:L:133:SER:HB2	1.82	0.61
25:3:305:CLA:H11	22:7:240:ILE:HD13	1.82	0.61
12:L:131:CYS:HB3	28:L:207:BCR:H19C	1.82	0.60
15:S:178:TYR:CE2	15:S:199:LYS:HG2	2.33	0.60
20:5:150:PRO:HA	20:5:153:LYS:NZ	2.16	0.60
18:3:99:MET:HG2	34:3:315:LUT:C15	2.31	0.60
30:B:848:DGD:O5E	30:B:848:DGD:O4E	2.14	0.60
14:R:94:LEU:HA	14:R:97:ILE:HG12	1.83	0.60
19:4:163:ARG:HE	19:4:174:ALA:HB1	1.67	0.60
17:2:148:MET:HG2	17:2:149:LYS:H	1.66	0.60
18:3:105:CYS:SG	18:3:228:MET:HE1	2.42	0.60
1:A:682:SER:OG	1:A:727:GLY:O	2.18	0.60
20:5:161:GLU:OE1	20:5:161:GLU:N	2.34	0.60
1:A:68:GLU:OE1	1:A:72:LYS:HG3	2.02	0.60
7:G:45:PHE:HA	7:G:48:ILE:HG22	1.84	0.60
14:T:150:ILE:O	14:T:154:LEU:HD23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:624:LHG:O1	27:P:624:LHG:O3	2.19	0.60
14:T:76:LYS:HA	14:T:79:ARG:NE	2.12	0.60
19:4:160:VAL:HG21	28:4:317:BCR:H362	1.84	0.60
25:6:603:CLA:H2A	25:6:603:CLA:HED3	1.81	0.60
2:B:493:LEU:HG	2:B:494:TRP:CE3	2.37	0.60
14:P:156:GLU:OE1	14:P:159:ARG:NE	2.35	0.60
17:2:190:LEU:HD21	25:2:312:CLA:HMA2	1.83	0.60
24:9:84:ILE:HG13	34:9:313:LUT:H182	1.84	0.60
16:a:55:GLY:H	16:a:175:LEU:HD23	1.67	0.60
1:A:317:GLY:H	11:K:57:VAL:HG13	1.67	0.59
25:A:851:CLA:HHB	25:B:801:CLA:H202	1.83	0.59
25:P:602:CLA:H92	25:P:603:CLA:HMA3	1.84	0.59
14:T:156:GLU:OE1	14:T:159:ARG:NE	2.35	0.59
1:A:305:PHE:HE1	25:A:822:CLA:HAB	1.67	0.59
13:O:77:GLN:O	13:O:81:GLU:HB2	2.02	0.59
32:2:301:LMG:H341	25:2:304:CLA:H52	1.83	0.59
25:P:611:CLA:HBC3	27:P:618:LHG:H332	1.83	0.59
33:Q:608:CHL:H192	33:Q:608:CHL:C15	2.24	0.59
25:U:302:CLA:H92	25:U:303:CLA:HMA3	1.84	0.59
25:Q:609:CLA:HBB1	25:Q:611:CLA:H3A	1.84	0.59
17:2:86:PHE:CZ	17:2:90:VAL:HG21	2.36	0.59
32:4:320:LMG:O5	32:4:320:LMG:O4	2.20	0.59
33:1:601:CHL:HMD3	23:8:153:PHE:HE1	1.67	0.59
19:4:142:TYR:O	19:4:143:PHE:CD1	2.54	0.59
21:6:91:VAL:HG21	25:6:605:CLA:HMD1	1.84	0.59
1:A:607:ILE:HD12	1:A:743:PHE:HE2	1.68	0.59
25:A:826:CLA:H111	25:A:837:CLA:H71	1.83	0.59
2:B:313:SER:OG	27:B:847:LHG:O5	2.21	0.59
2:B:693:TYR:CZ	4:D:76:ARG:NH1	2.71	0.59
7:G:118:ASN:O	7:G:118:ASN:ND2	2.36	0.59
18:3:159:GLU:OE1	18:3:162:ARG:NH2	2.25	0.59
20:5:116:ILE:HD11	21:6:213:TRP:CZ3	2.38	0.59
35:P:620:XAT:H403	27:R:618:LHG:H132	1.82	0.59
14:T:242:ALA:HA	35:T:615:XAT:H22	1.84	0.59
33:4:314:CHL:HBB2	28:4:317:BCR:H10C	1.84	0.59
2:B:266:THR:HG22	2:B:361:PHE:H	1.67	0.59
25:T:602:CLA:HAB	34:T:614:LUT:H32	1.85	0.59
25:1:605:CLA:HHC	25:1:605:CLA:HBB1	1.84	0.59
23:8:109:LYS:HG2	33:8:307:CHL:OBD	2.02	0.59
12:L:114:GLU:HG2	12:L:189:THR:HG21	1.85	0.59
25:R:612:CLA:C9	25:R:612:CLA:C12	2.78	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:4:310:CLA:HBB1	34:4:315:LUT:C14	2.32	0.59
1:A:345:LEU:O	1:A:352:GLN:NE2	2.36	0.59
3:C:15:THR:HG22	3:C:28:MET:HE2	1.84	0.59
24:9:64:LYS:HD2	24:9:135:THR:HG21	1.85	0.59
25:S:303:CLA:H52	34:S:317:LUT:H30	1.84	0.58
17:2:81:VAL:HG11	34:2:315:LUT:H12	1.85	0.58
19:4:137:ALA:O	19:4:142:TYR:OH	2.19	0.58
2:B:688:LEU:HD12	25:L:205:CLA:H42	1.84	0.58
25:B:823:CLA:HMA1	28:B:844:BCR:H14C	1.85	0.58
25:Q:618:CLA:CBD	36:U:301:NEX:H172	2.28	0.58
14:R:81:LEU:HD12	33:R:609:CHL:O2D	2.04	0.58
2:B:301:ARG:NH2	7:G:67:VAL:HG11	2.18	0.58
20:5:194:MET:HE1	25:5:303:CLA:CHC	2.33	0.58
1:A:247:ARG:NH1	27:A:852:LHG:O5	2.37	0.58
33:4:322:CHL:HMA3	16:a:40:LEU:HD13	1.85	0.58
17:2:38:PRO:HG2	17:2:41:LEU:HB2	1.85	0.58
24:9:94:PRO:HG3	24:9:102:LYS:HD2	1.85	0.58
1:A:261:ILE:HD13	28:A:854:BCR:HC21	1.85	0.58
14:P:43:PRO:HA	14:U:43:PRO:HG2	1.85	0.58
35:P:620:XAT:H22	14:R:242:ALA:HA	1.86	0.58
27:S:319:LHG:O3	27:S:319:LHG:O1	2.17	0.58
25:B:810:CLA:HBB2	25:B:818:CLA:H102	1.85	0.58
14:P:208:MET:HE1	34:P:615:LUT:H8	1.84	0.58
14:Q:242:ALA:HA	35:Q:616:XAT:H22	1.86	0.58
25:S:301:CLA:CBB	33:S:306:CHL:HBB2	2.34	0.58
23:8:172:PRO:HA	16:a:62:LEU:HD22	1.85	0.58
24:9:169:PHE:CD2	34:9:313:LUT:H12	2.39	0.58
1:A:121:ILE:HG12	1:A:122:VAL:H	1.68	0.58
6:F:90:ARG:HH21	6:F:104:LEU:HD21	1.69	0.58
14:P:30:ILE:HG13	14:P:31:GLU:CD	2.29	0.58
14:P:196:LYS:HD2	25:P:612:CLA:CAA	2.34	0.58
25:P:602:CLA:H52	34:P:615:LUT:H28	1.86	0.58
15:S:235:LEU:HD22	25:S:315:CLA:HBB1	1.84	0.58
20:5:53:TYR:OH	27:5:321:LHG:O5	2.15	0.58
20:5:161:GLU:OE2	20:5:164:TYR:CD2	2.50	0.58
23:8:156:PHE:CE2	25:a:302:CLA:H72	2.38	0.58
14:U:152:MET:HE3	14:U:156:GLU:CG	2.33	0.57
25:3:314:CLA:H43	20:5:231:ILE:HD13	1.85	0.57
21:6:155:GLY:C	21:6:156:TYR:HD2	2.11	0.57
6:F:104:LEU:O	6:F:108:MET:HG2	2.04	0.57
7:G:79:ASP:OD1	24:9:58:GLN:OE1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:40:LEU:HD13	33:1:601:CHL:HMA3	1.85	0.57
17:2:81:VAL:HA	17:2:84:ILE:HG22	1.86	0.57
16:a:109:TRP:CD1	16:a:109:TRP:H	2.21	0.57
1:A:714:GLN:OE1	1:A:716:ARG:NH2	2.36	0.57
25:A:816:CLA:H91	27:A:852:LHG:H191	1.86	0.57
2:B:352:HIS:ND1	25:B:815:CLA:OBD	2.38	0.57
9:I:78:VAL:O	9:I:82:LEU:HG	2.05	0.57
14:P:242:ALA:HA	35:P:616:XAT:H22	1.87	0.57
25:R:602:CLA:H92	25:R:603:CLA:HMA3	1.87	0.57
25:T:608:CLA:HBB1	25:T:610:CLA:H3A	1.87	0.57
6:F:123:LEU:HD21	10:J:38:VAL:HG11	1.85	0.57
6:F:135:ALA:HA	6:F:149:VAL:HG21	1.84	0.57
25:T:602:CLA:CAB	34:T:614:LUT:H32	2.34	0.57
25:U:310:CLA:HBB1	25:U:311:CLA:H3A	1.85	0.57
17:2:64:LYS:O	17:2:129:TYR:OH	2.22	0.57
14:P:212:PHE:CG	33:P:609:CHL:H203	2.23	0.57
16:a:67:GLU:OE1	16:a:67:GLU:N	2.37	0.57
17:2:86:PHE:CE2	17:2:90:VAL:HG21	2.40	0.57
17:2:168:PHE:CZ	34:2:316:LUT:H10	2.40	0.57
2:B:293:ARG:HA	2:B:299:GLY:HA3	1.87	0.57
25:B:821:CLA:HAB	25:B:828:CLA:HMD1	1.87	0.57
2:B:325:ASP:O	2:B:329:ASN:ND2	2.36	0.57
6:F:85:LYS:HE2	6:F:85:LYS:HA	1.86	0.57
25:P:611:CLA:HMA2	36:P:621:NEX:C1	2.34	0.57
25:A:802:CLA:H3A	25:A:802:CLA:CGA	2.34	0.57
3:C:4:ILE:HB	3:C:68:TYR:HB2	1.86	0.57
35:P:623:XAT:H22	14:U:242:ALA:HA	1.87	0.57
19:4:111:VAL:HG11	34:4:315:LUT:H12	1.87	0.57
18:3:95:ALA:HB1	18:3:221:GLY:HA3	1.87	0.56
1:A:497:LEU:HD21	13:O:66:PHE:CE1	2.40	0.56
28:A:845:BCR:H362	28:A:846:BCR:H21C	1.87	0.56
2:B:81:ASP:OD2	2:B:84:HIS:ND1	2.37	0.56
14:P:145:LEU:HD21	35:P:620:XAT:C13	2.35	0.56
25:P:612:CLA:C9	25:P:612:CLA:C12	2.78	0.56
33:Q:606:CHL:HMB3	33:Q:608:CHL:HAC1	1.88	0.56
14:R:111:GLU:HG2	14:R:116:LYS:HB2	1.87	0.56
25:R:603:CLA:CHC	33:R:609:CHL:H122	2.35	0.56
15:S:81:LYS:HA	15:S:84:ARG:HD3	1.87	0.56
25:U:302:CLA:CAB	34:U:315:LUT:H32	2.36	0.56
20:5:242:VAL:HG12	20:5:243:GLN:H	1.71	0.56
24:9:106:ILE:HB	24:9:111:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:9:123:GLU:HG2	25:9:308:CLA:C1B	2.35	0.56
16:a:218:PHE:HA	16:a:221:ASN:CG	2.30	0.56
1:A:479:LEU:HB2	1:A:530:THR:HG23	1.88	0.56
1:A:531:SER:HB3	1:A:639:ALA:HB3	1.88	0.56
25:R:610:CLA:H51	25:R:612:CLA:C3A	2.35	0.56
17:2:155:LEU:HA	17:2:158:LEU:HG	1.87	0.56
17:2:171:PHE:HE1	34:2:315:LUT:H41	1.70	0.56
25:U:302:CLA:HAB	34:U:315:LUT:H32	1.86	0.56
20:5:85:VAL:HG11	34:5:318:LUT:H12	1.86	0.56
1:A:29:TRP:HE1	25:A:812:CLA:HBA1	1.71	0.56
8:H:76:ILE:HD11	25:H:202:CLA:HMA1	1.88	0.56
33:P:601:CHL:HBB2	35:P:623:XAT:H23	1.88	0.56
25:P:602:CLA:HAB	34:P:615:LUT:H32	1.86	0.56
25:Q:618:CLA:HBD	36:U:301:NEX:C17	2.30	0.56
14:U:42:GLY:O	14:U:45:SER:HB3	2.06	0.56
17:2:71:LEU:O	17:2:75:ARG:HB2	2.06	0.56
17:2:153:MET:HE1	17:2:156:LYS:CD	2.36	0.56
7:G:50:ARG:HA	7:G:95:PHE:HZ	1.70	0.56
11:K:33:SER:OG	11:K:113:LEU:HD11	2.06	0.56
25:Q:602:CLA:HAB	34:Q:615:LUT:H32	1.88	0.56
18:3:208:ALA:HA	18:3:211:LYS:HZ1	1.71	0.56
21:6:104:VAL:HG21	25:6:605:CLA:HAA1	1.87	0.56
21:6:173:LYS:O	21:6:176:GLU:HG2	2.05	0.56
24:9:74:GLY:N	24:9:166:MET:HE2	2.20	0.56
32:H:204:LMG:H352	12:L:130:LEU:HD11	1.87	0.56
14:R:237:ASN:ND2	25:R:614:CLA:O1D	2.39	0.56
25:S:320:CLA:HMA2	25:S:320:CLA:H2	1.87	0.56
25:1:611:CLA:HBB1	34:1:615:LUT:C14	2.36	0.56
20:5:118:MET:HE3	28:5:323:BCR:H353	1.88	0.56
4:D:125:THR:HG22	4:D:129:ARG:HD3	1.88	0.56
14:Q:208:MET:HE3	34:Q:615:LUT:H10	1.88	0.56
14:R:196:LYS:CD	25:R:612:CLA:HAA2	2.35	0.56
19:4:194:PRO:HB2	19:4:198:PHE:CD2	2.40	0.56
28:4:317:BCR:HC22	27:a:317:LHG:HC81	1.88	0.56
25:P:610:CLA:H51	25:P:612:CLA:C3A	2.35	0.55
35:T:615:XAT:H41	33:U:307:CHL:HAA2	1.88	0.55
27:T:617:LHG:O3	27:T:617:LHG:O1	2.22	0.55
21:6:104:VAL:HG22	21:6:104:VAL:O	2.05	0.55
14:P:196:LYS:CD	25:P:612:CLA:HAA2	2.36	0.55
25:P:602:CLA:CAB	34:P:615:LUT:H32	2.36	0.55
25:Q:602:CLA:CAB	34:Q:615:LUT:H32	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:192:MET:HE3	25:6:620:CLA:HAA2	1.87	0.55
23:8:77:CYS:O	23:8:81:MET:HG3	2.06	0.55
19:4:82:ASP:OD1	34:4:316:LUT:O23	2.24	0.55
22:7:122:VAL:HG11	25:8:314:CLA:HED1	1.86	0.55
23:8:117:ALA:HB3	23:8:122:LEU:HD11	1.87	0.55
2:B:708:LEU:HD11	30:B:846:DGD:HB51	1.89	0.55
25:B:824:CLA:HBB1	25:B:831:CLA:HMA2	1.88	0.55
11:K:78:SER:OG	25:K:204:CLA:O1D	2.24	0.55
25:1:613:CLA:HBC1	34:1:615:LUT:H162	1.88	0.55
8:H:103:ALA:HA	8:H:110:ILE:HG21	1.88	0.55
1:A:658:ILE:HG13	1:A:659:GLN:HG3	1.89	0.55
2:B:274:MET:O	2:B:278:HIS:ND1	2.40	0.55
14:R:213:VAL:HG11	25:R:613:CLA:HAC2	1.89	0.55
33:U:309:CHL:HBB1	33:U:309:CHL:HHC	1.87	0.55
25:3:302:CLA:H111	25:3:307:CLA:H43	1.88	0.55
24:9:31:TRP:CD1	24:9:31:TRP:H	2.25	0.55
28:A:854:BCR:C40	11:K:92:MET:HE1	2.32	0.55
14:P:122:PHE:CE1	14:R:239:PHE:HB3	2.42	0.55
14:P:196:LYS:HD2	25:P:612:CLA:HAA2	1.87	0.55
33:Q:607:CHL:CGA	25:Q:609:CLA:HBC1	2.37	0.55
25:T:602:CLA:H52	34:T:614:LUT:H28	1.89	0.55
17:2:84:ILE:HD11	17:2:95:PHE:CD1	2.42	0.55
17:2:148:MET:SD	25:2:309:CLA:H11	2.46	0.55
18:3:222:ARG:HA	18:3:225:MET:HE3	1.89	0.55
19:4:226:PHE:HA	19:4:229:PHE:HD2	1.72	0.55
10:J:39:PHE:HA	32:J:107:LMG:H112	1.88	0.55
21:6:184:MET:HE1	25:6:603:CLA:HHC	1.88	0.55
25:J:103:CLA:HED2	25:J:103:CLA:H2A	1.88	0.55
27:Q:617:LHG:O3	27:Q:617:LHG:O1	2.18	0.55
14:R:211:PHE:HE2	34:R:615:LUT:H8	1.72	0.55
25:2:310:CLA:HAC2	25:2:312:CLA:H202	1.88	0.55
20:5:194:MET:HE1	25:5:303:CLA:HHC	1.87	0.55
24:9:60:GLU:OE1	24:9:60:GLU:HA	2.07	0.55
25:a:304:CLA:HHC	25:a:304:CLA:HBB1	1.88	0.55
14:P:229:HIS:ND1	25:P:613:CLA:HAA2	2.21	0.54
14:U:40:TRP:NE1	14:U:46:GLU:OE2	2.38	0.54
18:3:208:ALA:HA	18:3:211:LYS:NZ	2.22	0.54
20:5:138:GLN:OE1	20:5:138:GLN:HA	2.06	0.54
21:6:87:VAL:O	21:6:91:VAL:HG22	2.07	0.54
21:6:195:GLN:HA	21:6:235:ILE:CD1	2.38	0.54
16:a:144:GLN:HG3	25:a:306:CLA:HMC2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:LEU:HG	2:B:494:TRP:HE3	1.71	0.54
25:R:611:CLA:H51	25:R:612:CLA:CMD	2.37	0.54
15:S:97:GLY:HA2	34:S:317:LUT:H181	1.89	0.54
17:2:120:VAL:C	17:2:124:LYS:HZ3	2.07	0.54
2:B:517:ASP:OD1	2:B:594:TYR:OH	2.20	0.54
5:E:67:VAL:HG13	5:E:70:PRO:HG3	1.89	0.54
25:R:603:CLA:HBC2	33:R:609:CHL:HMD2	1.88	0.54
1:A:740:TRP:NE1	25:A:828:CLA:O1A	2.38	0.54
14:P:199:LYS:HB3	25:P:611:CLA:HMD2	1.88	0.54
15:S:83:TYR:HB3	25:S:303:CLA:HHB	1.88	0.54
14:T:237:ASN:ND2	25:T:612:CLA:O1D	2.41	0.54
16:a:84:TRP:CZ2	25:a:306:CLA:HED2	2.42	0.54
14:Q:156:GLU:OE1	14:Q:159:ARG:NE	2.37	0.54
25:a:312:CLA:HBC1	34:a:314:LUT:H162	1.90	0.54
3:C:18:VAL:HG11	4:D:158:PRO:O	2.08	0.54
12:L:82:VAL:HG22	12:L:169:GLU:HB3	1.89	0.54
15:S:218:VAL:HG21	25:S:314:CLA:HAC2	1.90	0.54
14:T:94:LEU:HD13	25:T:608:CLA:H142	1.90	0.54
8:H:105:ASP:O	8:H:107:ASP:N	2.41	0.54
14:P:44:TYR:HE2	25:Q:618:CLA:HAB	1.72	0.54
33:P:608:CHL:CGA	25:P:610:CLA:HBC1	2.36	0.54
25:R:602:CLA:HAB	34:R:616:LUT:H32	1.89	0.54
25:R:611:CLA:C3	25:R:612:CLA:HMD1	2.38	0.54
16:1:67:GLU:OE1	16:1:67:GLU:N	2.40	0.54
24:9:97:TRP:CD1	24:9:98:GLU:HG3	2.43	0.54
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.90	0.54
25:R:602:CLA:CAB	34:R:616:LUT:H32	2.38	0.54
22:7:108:VAL:O	22:7:112:LYS:HB2	2.08	0.54
1:A:507:SER:O	1:A:510:TRP:HD1	1.91	0.54
25:P:603:CLA:HBC2	33:P:609:CHL:HMD2	1.89	0.54
27:5:301:LHG:H131	25:5:315:CLA:HBC1	1.90	0.54
28:8:318:BCR:H353	25:a:302:CLA:H112	1.89	0.54
1:A:95:GLY:O	1:A:99:SER:OG	2.23	0.53
2:B:510:PHE:HE1	25:B:833:CLA:HED1	1.73	0.53
2:B:604:GLN:HG2	2:B:734:PHE:HZ	1.73	0.53
14:P:151:LEU:HD21	33:P:606:CHL:H43	1.91	0.53
25:5:306:CLA:HBB1	33:5:307:CHL:OMC	2.07	0.53
24:9:74:GLY:CA	24:9:166:MET:HE2	2.38	0.53
1:A:265:PHE:HA	25:K:203:CLA:HBC3	1.90	0.53
4:D:189:ARG:HH22	4:D:191:MET:HB2	1.72	0.53
13:O:75:PHE:HB3	13:O:99:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:247:PRO:HG3	33:P:619:CHL:CBA	2.37	0.53
33:P:622:CHL:HMB2	15:S:158:GLY:HA3	1.90	0.53
33:R:606:CHL:HMB3	33:R:609:CHL:HAC1	1.89	0.53
14:T:76:LYS:HA	14:T:79:ARG:HH21	1.73	0.53
19:4:157:PHE:HZ	28:4:317:BCR:H373	1.73	0.53
25:R:611:CLA:H71	25:R:612:CLA:ND	2.23	0.53
25:1:607:CLA:H192	25:1:607:CLA:HBC3	1.91	0.53
19:4:133:ALA:HB3	19:4:136:ASP:HB2	1.90	0.53
6:F:67:LEU:HD11	6:F:124:LEU:HB3	1.89	0.53
33:T:606:CHL:CGA	25:T:608:CLA:HBC1	2.38	0.53
20:5:92:GLU:HG2	20:5:212:LEU:HB2	1.88	0.53
20:5:140:TYR:HA	20:5:162:MET:HE2	1.90	0.53
24:9:31:TRP:CZ3	24:9:32:LEU:HG	2.43	0.53
1:A:330:ARG:H	25:A:842:CLA:HBC3	1.74	0.53
33:P:606:CHL:HMB3	33:P:609:CHL:HAC1	1.89	0.53
17:2:170:GLY:O	17:2:174:GLN:HG2	2.09	0.53
2:B:119:SER:OG	25:B:807:CLA:OBD	2.26	0.53
14:P:147:VAL:O	14:P:151:LEU:HD13	2.09	0.53
14:R:76:LYS:CA	14:R:79:ARG:HH21	2.22	0.53
14:R:212:PHE:CA	33:R:609:CHL:H203	2.23	0.53
17:2:53:PRO:HD2	34:2:316:LUT:H23	1.90	0.53
20:5:137:TRP:CZ2	20:5:141:LYS:HD2	2.43	0.53
16:a:102:ASN:OD1	16:a:105:ASP:N	2.41	0.53
25:a:310:CLA:HBB1	34:a:314:LUT:C14	2.39	0.53
33:R:609:CHL:H192	33:R:609:CHL:C15	2.24	0.53
33:S:310:CHL:H11	34:U:315:LUT:H363	1.90	0.53
14:T:121:ILE:HG23	14:T:122:PHE:CD1	2.44	0.53
16:a:138:MET:HG2	25:a:307:CLA:CMC	2.38	0.53
14:P:76:LYS:CA	14:P:79:ARG:HH21	2.22	0.53
21:6:104:VAL:HG21	25:6:605:CLA:HAA2	1.91	0.53
21:6:233:CYS:HB3	21:6:256:TRP:HH2	1.73	0.53
25:B:812:CLA:HMA2	28:B:842:BCR:H282	1.90	0.53
14:R:191:ALA:O	14:R:195:VAL:HG23	2.09	0.53
14:T:76:LYS:CA	14:T:79:ARG:HH21	2.22	0.53
14:U:191:ALA:O	14:U:195:VAL:HG23	2.09	0.53
25:A:806:CLA:H51	25:A:814:CLA:H12	1.91	0.53
25:A:827:CLA:HHC	25:A:827:CLA:HBB1	1.91	0.53
4:D:95:ILE:HG12	4:D:105:ILE:HG12	1.91	0.53
14:R:76:LYS:HA	14:R:79:ARG:HH21	1.74	0.53
15:S:144:GLN:HB2	25:S:301:CLA:HAB	1.91	0.53
22:7:234:ASN:ND2	25:7:311:CLA:OBD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:9:164:LEU:HD22	34:9:312:LUT:H202	1.90	0.53
24:9:169:PHE:CZ	34:9:313:LUT:H10	2.44	0.53
25:B:805:CLA:HHB	25:B:827:CLA:HAB	1.90	0.52
14:P:237:ASN:ND2	25:S:301:CLA:O1D	2.42	0.52
25:R:613:CLA:H161	27:R:618:LHG:H351	1.90	0.52
14:U:132:ASN:HB3	14:U:135:LEU:HD13	1.90	0.52
33:6:608:CHL:HBB2	33:6:617:CHL:C1C	2.39	0.52
25:A:851:CLA:H11	2:B:617:LEU:HD12	1.92	0.52
7:G:54:LEU:HD12	7:G:95:PHE:CZ	2.43	0.52
14:T:191:ALA:O	14:T:195:VAL:HG23	2.09	0.52
20:5:194:MET:CE	25:5:303:CLA:HMC3	2.36	0.52
8:H:84:ARG:NH2	12:L:137:SER:OG	2.34	0.52
14:P:213:VAL:HG11	25:P:613:CLA:HAC2	1.91	0.52
14:Q:76:LYS:CA	14:Q:79:ARG:HH21	2.22	0.52
25:R:602:CLA:H52	34:R:616:LUT:H28	1.90	0.52
33:U:308:CHL:CGA	25:U:310:CLA:HBC1	2.40	0.52
16:a:218:PHE:HA	16:a:221:ASN:ND2	2.24	0.52
2:B:345:ILE:HD12	25:B:816:CLA:H71	1.90	0.52
2:B:489:ASN:HB3	25:B:832:CLA:HED2	1.91	0.52
14:Q:132:ASN:HB3	14:Q:135:LEU:HD13	1.92	0.52
14:U:196:LYS:NZ	25:U:311:CLA:O1A	2.34	0.52
17:2:154:LYS:HA	17:2:157:GLU:CD	2.35	0.52
24:9:170:ILE:CD1	25:9:304:CLA:HBB2	2.37	0.52
1:A:316:TRP:CD1	11:K:87:VAL:HG21	2.44	0.52
25:B:809:CLA:H121	8:H:94:ALA:HB1	1.90	0.52
15:S:141:VAL:HG13	33:S:306:CHL:ND	2.25	0.52
16:a:182:ARG:HA	16:a:185:MET:HE3	1.90	0.52
25:a:304:CLA:HBB2	33:a:305:CHL:CBB	2.40	0.52
14:P:196:LYS:CG	25:P:611:CLA:HED1	2.35	0.52
14:Q:237:ASN:ND2	25:Q:613:CLA:O1D	2.42	0.52
14:R:132:ASN:HB3	14:R:135:LEU:HD13	1.91	0.52
15:S:243:ALA:HA	25:S:314:CLA:OBD	2.10	0.52
14:U:213:VAL:HG11	25:U:312:CLA:HAC2	1.91	0.52
17:2:199:TYR:HB3	24:9:109:GLN:HG3	1.90	0.52
18:3:130:VAL:HG21	34:3:316:LUT:H22	1.90	0.52
21:6:180:GLY:O	21:6:184:MET:HG3	2.10	0.52
22:7:137:TYR:CZ	23:8:31:LEU:HD21	2.45	0.52
4:D:79:GLN:NE2	8:H:49:GLY:O	2.42	0.52
15:S:247:ALA:O	33:S:321:CHL:HBD	2.08	0.52
14:U:76:LYS:CA	14:U:79:ARG:HH21	2.23	0.52
23:8:76:HIS:HB3	23:8:200:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:67:LEU:CD1	6:F:124:LEU:HB3	2.40	0.52
21:6:178:LYS:NZ	25:6:611:CLA:O1D	2.34	0.52
1:A:234:PRO:HA	1:A:237:ILE:HD12	1.92	0.52
25:A:815:CLA:H62	27:A:852:LHG:H371	1.91	0.52
7:G:50:ARG:HD2	7:G:95:PHE:CZ	2.45	0.52
14:Q:76:LYS:HA	14:Q:79:ARG:HH21	1.74	0.52
14:R:152:MET:HA	14:R:155:VAL:HG22	1.92	0.52
14:U:94:LEU:HD13	25:U:310:CLA:H142	1.91	0.52
25:a:306:CLA:H192	25:a:306:CLA:HBC3	1.92	0.52
6:F:150:PHE:O	6:F:153:THR:HG22	2.10	0.52
12:L:38:LYS:HD2	13:O:121:ARG:O	2.08	0.52
25:P:603:CLA:H61	25:P:603:CLA:CMA	2.40	0.52
14:R:76:LYS:CA	14:R:79:ARG:HE	2.18	0.52
25:U:302:CLA:H52	34:U:315:LUT:H28	1.90	0.52
18:3:92:VAL:HG21	18:3:191:ALA:HB1	1.92	0.52
24:9:62:ARG:NH2	24:9:66:TYR:OH	2.42	0.52
2:B:294:THR:O	2:B:296:PHE:N	2.42	0.51
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.91	0.51
8:H:76:ILE:HD11	25:H:202:CLA:CMA	2.40	0.51
14:P:230:LEU:HD22	33:S:306:CHL:HMB3	1.91	0.51
14:R:170:ASP:HB2	14:R:174:PRO:HA	1.91	0.51
15:S:225:LYS:HZ2	15:S:233:ASP:CG	2.18	0.51
17:2:171:PHE:CE1	34:2:315:LUT:H41	2.45	0.51
22:7:101:GLU:CD	22:7:214:GLY:HA3	2.35	0.51
25:8:306:CLA:HBC2	33:8:307:CHL:HHD	1.91	0.51
13:O:76:THR:HA	13:O:79:ILE:HG22	1.92	0.51
14:P:76:LYS:HA	14:P:79:ARG:HH21	1.74	0.51
14:Q:81:LEU:CD1	33:Q:608:CHL:O2D	2.57	0.51
25:Q:603:CLA:CHC	33:Q:608:CHL:H122	2.39	0.51
25:Q:603:CLA:HBC2	33:Q:608:CHL:HMD2	1.91	0.51
14:R:76:LYS:CB	14:R:79:ARG:HH21	2.24	0.51
14:R:156:GLU:OE1	14:R:159:ARG:NE	2.39	0.51
14:U:76:LYS:HA	14:U:79:ARG:HH21	1.75	0.51
21:6:153:GLU:H	21:6:153:GLU:CD	2.19	0.51
1:A:460:ASP:OD1	2:B:636:TYR:OH	2.19	0.51
11:K:38:MET:HE1	11:K:97:HIS:HA	1.91	0.51
12:L:71:ASN:HA	12:L:76:ARG:HH11	1.76	0.51
15:S:144:GLN:OE1	25:S:301:CLA:HBB2	2.10	0.51
14:T:213:VAL:HG11	25:T:611:CLA:HAC2	1.92	0.51
16:1:109:TRP:CE2	16:1:116:ALA:HB2	2.46	0.51
17:2:49:TYR:HD2	25:2:302:CLA:HMC2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2:203:VAL:O	17:2:203:VAL:HG13	2.11	0.51
19:4:250:ASP:OD2	19:4:253:SER:OG	2.18	0.51
23:8:233:TYR:O	23:8:239:SER:OG	2.28	0.51
25:B:806:CLA:H12	9:I:83:THR:HG21	1.92	0.51
14:P:30:ILE:HD13	15:S:169:PRO:CA	2.40	0.51
14:P:43:PRO:O	14:P:44:TYR:HD1	1.93	0.51
33:1:601:CHL:HMD3	23:8:153:PHE:CE1	2.43	0.51
17:2:128:ILE:O	17:2:132:THR:HG22	2.11	0.51
22:7:54:ASP:OD1	34:7:315:LUT:O23	2.27	0.51
25:A:820:CLA:H8	25:A:820:CLA:HAB	1.91	0.51
2:B:441:ASN:OD1	2:B:453:GLN:HB2	2.10	0.51
3:C:34:CYS:HA	5:E:67:VAL:HG23	1.92	0.51
7:G:68:GLY:H	7:G:69:PRO:HD2	1.75	0.51
25:P:603:CLA:CHC	33:P:609:CHL:H122	2.41	0.51
14:U:237:ASN:ND2	25:U:313:CLA:O1D	2.44	0.51
17:2:156:LYS:HD3	25:2:311:CLA:HAA2	1.91	0.51
17:2:156:LYS:CD	25:2:311:CLA:HBD	2.36	0.51
21:6:149:LEU:HD23	21:6:150:PRO:O	2.11	0.51
2:B:437:LEU:HD12	25:J:103:CLA:HAB	1.92	0.51
13:O:44:ASP:HB3	13:O:47:VAL:HG23	1.92	0.51
14:P:94:LEU:HD13	25:P:610:CLA:H142	1.93	0.51
14:P:208:MET:CE	34:P:615:LUT:H10	2.40	0.51
14:Q:212:PHE:CA	33:Q:608:CHL:H203	2.23	0.51
17:2:190:LEU:HD12	25:2:313:CLA:C1C	2.41	0.51
22:7:55:PRO:HD2	34:7:315:LUT:H23	1.93	0.51
28:A:849:BCR:H362	25:A:851:CLA:C4	2.41	0.51
8:H:108:LEU:H	8:H:109:PRO:HD3	1.74	0.51
25:Q:602:CLA:H52	34:Q:615:LUT:H28	1.93	0.51
25:R:610:CLA:H72	25:R:612:CLA:C2B	2.28	0.51
25:R:611:CLA:C5	25:R:612:CLA:HMD1	2.40	0.51
14:Q:190:PHE:CE2	14:Q:194:LYS:HE3	2.45	0.51
36:U:301:NEX:H171	25:U:311:CLA:CBD	2.41	0.51
16:1:102:ASN:OD1	16:1:105:ASP:N	2.38	0.51
20:5:202:LEU:HD23	20:5:202:LEU:C	2.35	0.51
25:P:610:CLA:HBB1	25:P:612:CLA:CHB	2.41	0.51
15:S:166:ASN:ND2	14:U:44:TYR:HB3	2.26	0.51
14:T:132:ASN:HB3	14:T:135:LEU:HD13	1.93	0.51
14:U:170:ASP:HB2	14:U:174:PRO:HA	1.93	0.51
22:7:173:MET:HG3	34:7:314:LUT:H222	1.93	0.51
25:7:304:CLA:HBB1	33:7:305:CHL:OMC	2.11	0.51
23:8:143:LYS:HB2	23:8:146:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:822:CLA:HMB2	25:A:825:CLA:HMA3	1.92	0.50
25:B:829:CLA:HBC3	28:F:803:BCR:H362	1.92	0.50
14:P:82:GLU:OE2	14:P:202:ARG:NH2	2.44	0.50
15:S:214:PHE:HE2	34:S:317:LUT:C40	2.24	0.50
20:5:118:MET:HE3	28:5:323:BCR:C35	2.41	0.50
16:a:98:LEU:HD22	16:a:119:PHE:HE1	1.76	0.50
35:Q:616:XAT:H403	27:Q:617:LHG:H132	1.93	0.50
14:U:82:GLU:OE2	14:U:202:ARG:NH2	2.44	0.50
16:a:118:TRP:CD1	16:a:118:TRP:N	2.78	0.50
1:A:488:GLN:NE2	1:A:526:ILE:O	2.39	0.50
4:D:65:PRO:HG2	4:D:113:LEU:HD11	1.92	0.50
25:A:818:CLA:C4D	25:A:818:CLA:H12	2.41	0.50
25:A:840:CLA:H151	28:L:204:BCR:H15C	1.93	0.50
8:H:86:LEU:HD13	32:2:301:LMG:H141	1.94	0.50
11:K:55:PRO:HB3	11:K:61:THR:HG23	1.92	0.50
12:L:150:THR:HG22	12:L:154:ARG:H	1.77	0.50
14:Q:82:GLU:OE2	14:Q:202:ARG:NH2	2.44	0.50
14:Q:191:ALA:O	14:Q:195:VAL:HG23	2.11	0.50
14:R:193:LEU:HD21	25:R:612:CLA:HBA2	1.83	0.50
25:1:605:CLA:HBB2	33:1:606:CHL:CBB	2.41	0.50
17:2:96:TRP:CD1	17:2:97:THR:HG23	2.46	0.50
19:4:61:TRP:CZ3	19:4:62:MET:HE3	2.46	0.50
33:8:307:CHL:HHC	33:8:307:CHL:HBB1	1.94	0.50
24:9:35:LEU:HD12	24:9:36:ASN:N	2.27	0.50
24:9:129:GLY:HA3	24:9:138:PHE:CZ	2.46	0.50
1:A:489:ASN:ND2	13:O:93:ASP:HB2	2.25	0.50
1:A:709:VAL:O	1:A:709:VAL:HG12	2.11	0.50
14:P:44:TYR:CZ	35:P:623:XAT:H221	2.47	0.50
14:R:121:ILE:HG23	14:R:122:PHE:CD1	2.47	0.50
14:T:76:LYS:CA	14:T:79:ARG:HE	2.20	0.50
16:1:89:VAL:O	16:1:93:LEU:HD23	2.12	0.50
18:3:160:LEU:HD23	25:3:320:CLA:H2A	1.94	0.50
21:6:79:MET:HE2	21:6:180:GLY:HA3	1.93	0.50
22:7:121:MET:HE2	23:8:243:LEU:HD11	1.94	0.50
16:a:116:ALA:HB3	16:a:123:VAL:HB	1.92	0.50
1:A:65:ASP:OD1	1:A:66:LEU:N	2.45	0.50
13:O:95:LYS:O	13:O:95:LYS:HG2	2.12	0.50
14:P:191:ALA:O	14:P:195:VAL:HG23	2.11	0.50
14:Q:76:LYS:CA	14:Q:79:ARG:HE	2.19	0.50
14:R:93:ALA:HB1	34:R:615:LUT:H12	1.92	0.50
15:S:166:ASN:HD21	14:U:44:TYR:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:231:TYR:HE1	34:3:315:LUT:H41	1.77	0.50
19:4:150:PHE:CZ	16:a:227:PHE:HZ	2.29	0.50
25:a:303:CLA:HBA2	25:a:303:CLA:C4A	2.41	0.50
25:A:822:CLA:H72	28:A:848:BCR:H12C	1.94	0.50
8:H:92:ILE:O	8:H:96:VAL:HG12	2.12	0.50
14:R:82:GLU:OE2	14:R:202:ARG:NH2	2.45	0.50
17:2:203:VAL:HG22	17:2:206:GLU:OE2	2.11	0.50
18:3:197:PHE:O	18:3:200:LEU:HD22	2.12	0.50
20:5:181:GLU:H	20:5:181:GLU:CD	2.19	0.50
20:5:250:THR:HG21	27:5:301:LHG:H262	1.93	0.50
5:E:48:PRO:HB2	6:F:225:SER:OG	2.11	0.50
14:Q:198:ILE:O	14:Q:202:ARG:HG3	2.12	0.50
14:U:76:LYS:CB	14:U:79:ARG:HH21	2.24	0.50
20:5:128:LEU:HD12	28:5:320:BCR:C15	2.41	0.50
21:6:199:LYS:HE2	21:6:203:ALA:HB1	1.94	0.50
23:8:158:ALA:HB1	16:a:67:GLU:OE1	2.11	0.50
6:F:180:PRO:O	6:F:184:GLU:HG3	2.12	0.50
25:R:603:CLA:C4B	33:R:609:CHL:C10	2.87	0.50
22:7:196:LEU:HD21	34:7:314:LUT:H191	1.94	0.50
23:8:109:LYS:HG3	33:8:307:CHL:CGD	2.42	0.50
23:8:175:PRO:HD2	34:8:316:LUT:H23	1.93	0.50
2:B:306:LEU:HD12	2:B:324:PHE:HB2	1.94	0.49
2:B:549:PRO:HD2	3:C:62:PHE:CE1	2.47	0.49
35:P:616:XAT:H403	27:P:618:LHG:H132	1.94	0.49
14:Q:94:LEU:HD13	25:Q:609:CLA:H142	1.93	0.49
25:S:314:CLA:HBB2	27:S:319:LHG:H301	1.93	0.49
14:T:82:GLU:OE2	14:T:202:ARG:NH2	2.45	0.49
17:2:84:ILE:HD11	17:2:95:PHE:CG	2.47	0.49
24:9:30:THR:HG21	24:9:35:LEU:HD23	1.93	0.49
16:a:117:THR:O	16:a:118:TRP:CD1	2.52	0.49
14:P:40:TRP:NE1	14:P:46:GLU:OE2	2.42	0.49
14:P:134:SER:C	14:P:135:LEU:HD12	2.37	0.49
14:Q:76:LYS:CB	14:Q:79:ARG:HH21	2.24	0.49
14:P:76:LYS:CB	14:P:79:ARG:HH21	2.26	0.49
22:7:111:GLU:OE1	22:7:112:LYS:HG3	2.12	0.49
25:A:831:CLA:O1D	12:L:43:ILE:HD13	2.12	0.49
7:G:108:HIS:O	7:G:112:PHE:HD2	1.94	0.49
25:H:202:CLA:HBB1	32:2:301:LMG:H171	1.95	0.49
14:P:30:ILE:HB	36:P:621:NEX:H42	1.93	0.49
14:R:207:SER:O	14:R:211:PHE:HD2	1.96	0.49
25:R:610:CLA:H72	25:R:612:CLA:HHB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:206:LEU:O	16:1:210:LEU:HD13	2.13	0.49
19:4:194:PRO:HB2	19:4:198:PHE:HD2	1.77	0.49
19:4:244:LEU:HD22	34:4:315:LUT:H163	1.94	0.49
24:9:31:TRP:CE3	24:9:32:LEU:HG	2.48	0.49
14:P:76:LYS:CA	14:P:79:ARG:HE	2.20	0.49
14:P:180:PRO:HB2	17:2:139:SER:OG	2.13	0.49
25:R:611:CLA:H93	25:R:612:CLA:C4C	2.42	0.49
14:U:93:ALA:HB1	34:U:314:LUT:H12	1.94	0.49
16:a:73:ARG:NH1	25:a:302:CLA:O1A	2.46	0.49
2:B:184:PHE:HE1	25:B:811:CLA:H52	1.76	0.49
6:F:101:ALA:C	6:F:105:LYS:HZ2	2.21	0.49
8:H:52:ASP:OD1	8:H:55:GLY:HA3	2.13	0.49
8:H:105:ASP:C	8:H:107:ASP:N	2.71	0.49
14:P:129:TYR:HD2	14:P:135:LEU:HD23	1.77	0.49
14:Q:213:VAL:HG11	25:Q:612:CLA:HAC2	1.94	0.49
15:S:213:MET:HG3	15:S:217:PHE:CE2	2.47	0.49
14:U:121:ILE:HG23	14:U:122:PHE:CD1	2.47	0.49
33:6:608:CHL:HBB2	33:6:617:CHL:CHC	2.42	0.49
25:A:811:CLA:H12	25:A:813:CLA:H43	1.95	0.49
12:L:88:ILE:HG23	12:L:92:HIS:CE1	2.48	0.49
14:P:42:GLY:O	14:U:43:PRO:HG2	2.13	0.49
27:P:618:LHG:O3	27:P:618:LHG:O1	2.22	0.49
14:Q:40:TRP:NE1	14:Q:46:GLU:OE2	2.41	0.49
16:a:118:TRP:CH2	25:a:303:CLA:C2	2.96	0.49
16:a:118:TRP:CZ2	25:a:303:CLA:C1	2.96	0.49
16:a:188:PHE:CD2	34:a:315:LUT:H12	2.47	0.49
1:A:509:THR:HG22	1:A:523:MET:CE	2.43	0.49
6:F:150:PHE:CE1	6:F:154:PHE:HE2	2.31	0.49
15:S:144:GLN:HB2	25:S:301:CLA:CAB	2.43	0.49
16:1:59:PHE:HB3	25:1:602:CLA:CAD	2.43	0.49
20:5:80:TRP:CE2	33:5:308:CHL:HED2	2.48	0.49
20:5:202:LEU:HD22	25:5:313:CLA:CHD	2.42	0.49
24:9:85:LEU:HD11	24:9:172:PHE:CZ	2.48	0.49
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.95	0.49
2:B:155:TRP:HE1	31:B:850:SQD:H383	1.77	0.49
14:Q:121:ILE:HG23	14:Q:122:PHE:CD1	2.48	0.49
33:R:608:CHL:CGA	25:R:610:CLA:HBC1	2.39	0.49
14:T:76:LYS:CB	14:T:79:ARG:HH21	2.25	0.49
14:T:170:ASP:HB2	14:T:174:PRO:HA	1.94	0.49
19:4:203:TRP:CZ3	25:4:308:CLA:H42	2.48	0.49
32:6:602:LMG:O5	32:6:602:LMG:O4	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:807:CLA:H143	25:B:807:CLA:H161	1.65	0.49
16:a:91:GLY:O	16:a:95:VAL:HG23	2.12	0.49
2:B:382:PHE:N	2:B:584:MET:HE2	2.26	0.48
25:B:822:CLA:O1A	25:B:822:CLA:H2A	2.11	0.48
14:P:44:TYR:CE2	25:Q:618:CLA:HAB	2.47	0.48
14:R:211:PHE:CZ	34:R:615:LUT:H8	2.48	0.48
15:S:84:ARG:HH21	15:S:177:LEU:CD1	2.25	0.48
33:T:607:CHL:HHC	33:T:607:CHL:HBB1	1.95	0.48
25:3:305:CLA:H12	22:7:240:ILE:HG21	1.94	0.48
24:9:154:MET:HE2	25:9:309:CLA:H12	1.94	0.48
1:A:425:ASN:OD1	1:A:426:LEU:N	2.46	0.48
8:H:68:LYS:O	8:H:72:GLN:HG2	2.13	0.48
25:P:613:CLA:H2	25:P:613:CLA:H61	1.60	0.48
14:R:208:MET:HE2	14:R:208:MET:HA	1.94	0.48
14:T:40:TRP:NE1	14:T:46:GLU:OE2	2.45	0.48
2:B:109:GLY:H	8:H:120:ASN:HD22	1.62	0.48
25:Q:618:CLA:HBD	36:U:301:NEX:H21	1.95	0.48
14:R:32:PHE:HE2	25:R:611:CLA:HED3	1.78	0.48
25:R:603:CLA:C4B	33:R:609:CHL:C12	2.91	0.48
17:2:81:VAL:O	17:2:84:ILE:HG22	2.13	0.48
1:A:382:THR:HG21	1:A:517:VAL:HB	1.95	0.48
25:A:821:CLA:HAA2	11:K:87:VAL:HG13	1.95	0.48
8:H:77:ILE:HG13	12:L:172:ALA:HB1	1.95	0.48
14:Q:152:MET:HA	14:Q:155:VAL:HG22	1.95	0.48
14:T:42:GLY:O	14:T:45:SER:HB3	2.14	0.48
16:1:109:TRP:CZ2	16:1:116:ALA:HB2	2.49	0.48
17:2:149:LYS:CE	17:2:153:MET:CB	2.91	0.48
25:B:836:CLA:H93	28:I:201:BCR:H382	1.96	0.48
21:6:198:GLY:HA3	21:6:234:LYS:HG2	1.95	0.48
25:6:603:CLA:H203	27:6:618:LHG:H332	1.96	0.48
22:7:198:MET:HE1	25:7:301:CLA:CBB	2.44	0.48
25:a:303:CLA:H41	25:a:303:CLA:H62	1.37	0.48
1:A:68:GLU:CD	1:A:72:LYS:HZ2	2.19	0.48
25:B:836:CLA:HAB	26:B:839:PQN:H151	1.95	0.48
3:C:31:TRP:HZ2	5:E:68:ARG:HH22	1.59	0.48
13:O:90:PRO:CB	13:O:96:PHE:HZ	2.24	0.48
16:1:126:ASP:OD1	16:1:127:LEU:N	2.47	0.48
16:a:59:PHE:HB3	25:a:301:CLA:CAD	2.44	0.48
16:a:118:TRP:CZ2	25:a:303:CLA:O2A	2.66	0.48
1:A:345:LEU:HB3	25:A:825:CLA:HBC3	1.95	0.48
1:A:369:HIS:HA	1:A:372:TYR:HE1	1.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:811:CLA:H92	25:B:822:CLA:H42	1.96	0.48
25:B:825:CLA:H3A	25:B:825:CLA:HBA2	1.45	0.48
14:P:190:PHE:CE2	14:P:194:LYS:HE3	2.48	0.48
14:Q:162:GLY:HA3	14:Q:168:GLY:H	1.79	0.48
25:R:602:CLA:H13	25:R:602:CLA:H172	1.69	0.48
15:S:145:ASN:ND2	25:S:301:CLA:C3B	2.75	0.48
20:5:197:TYR:CZ	34:5:322:LUT:H10	2.49	0.48
21:6:125:GLU:OE1	21:6:128:ARG:NH2	2.30	0.48
25:a:303:CLA:O2A	34:a:316:LUT:H41	2.14	0.48
25:a:306:CLA:HBB1	25:a:306:CLA:H121	1.95	0.48
25:B:825:CLA:H2	25:B:825:CLA:H62	1.61	0.48
4:D:112:LEU:C	4:D:113:LEU:HD12	2.39	0.48
6:F:204:LEU:O	6:F:208:GLN:HG2	2.14	0.48
12:L:191:ILE:O	12:L:191:ILE:HG23	2.13	0.48
33:P:619:CHL:HMC	14:Q:148:GLN:HE22	1.79	0.48
15:S:214:PHE:HE2	34:S:317:LUT:H401	1.79	0.48
25:1:610:CLA:HBB2	28:8:318:BCR:H312	1.95	0.48
16:a:139:ALA:HA	25:a:307:CLA:HAB	1.94	0.48
4:D:125:THR:HG23	4:D:136:PRO:HG2	1.95	0.48
13:O:49:VAL:O	13:O:53:ALA:CB	2.62	0.48
14:P:93:ALA:HB1	34:P:614:LUT:H12	1.96	0.48
35:P:623:XAT:H403	27:P:624:LHG:H132	1.94	0.48
16:1:98:LEU:HD22	16:1:119:PHE:HE1	1.79	0.48
20:5:81:ALA:O	20:5:85:VAL:HG23	2.13	0.48
1:A:121:ILE:HG12	1:A:122:VAL:HG13	1.96	0.48
25:A:801:CLA:HBD	25:A:801:CLA:HED3	1.71	0.48
25:A:819:CLA:CGA	25:A:819:CLA:H3A	2.41	0.48
14:P:247:PRO:HG2	33:P:619:CHL:HED1	1.95	0.48
14:Q:170:ASP:HB2	14:Q:174:PRO:HA	1.96	0.48
27:R:618:LHG:O3	27:R:618:LHG:O1	2.24	0.48
15:S:185:PRO:HD2	34:S:316:LUT:H23	1.96	0.48
15:S:204:LYS:HB3	25:S:312:CLA:HMD1	1.96	0.48
14:U:190:PHE:CE2	14:U:194:LYS:HE3	2.49	0.48
17:2:36:THR:HG21	17:2:225:LYS:HE2	1.94	0.48
17:2:45:MET:HB2	17:2:48:ASP:HB2	1.96	0.48
25:2:303:CLA:CBB	34:2:316:LUT:H32	2.43	0.48
25:2:309:CLA:H62	25:2:309:CLA:H41	1.74	0.48
20:5:82:MET:HE2	20:5:190:GLY:HA3	1.95	0.48
20:5:179:LEU:O	20:5:183:GLN:HG3	2.14	0.48
25:5:313:CLA:H2A	25:5:313:CLA:O1D	2.13	0.48
25:A:801:CLA:H102	25:A:801:CLA:H62	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:252:PRO:O	15:S:253:SER:HB2	2.14	0.47
14:T:190:PHE:CE2	14:T:194:LYS:HE3	2.49	0.47
14:U:30:ILE:HG22	14:U:30:ILE:O	2.14	0.47
34:1:617:LUT:H31	34:1:617:LUT:H391	1.75	0.47
25:6:610:CLA:H91	25:6:610:CLA:H112	1.68	0.47
16:a:89:VAL:O	16:a:93:LEU:HD23	2.13	0.47
25:A:833:CLA:O1D	25:A:833:CLA:H2A	2.14	0.47
14:P:170:ASP:HB2	14:P:174:PRO:HA	1.96	0.47
14:Q:164:PRO:HB3	36:U:301:NEX:C18	2.43	0.47
14:R:32:PHE:CE2	25:R:611:CLA:HED3	2.49	0.47
14:R:212:PHE:C	33:R:609:CHL:C20	2.87	0.47
25:R:613:CLA:H101	27:R:618:LHG:H131	1.95	0.47
19:4:183:ASN:HB3	33:4:314:CHL:C2D	2.44	0.47
25:A:811:CLA:H13	28:A:846:BCR:H372	1.96	0.47
25:A:834:CLA:H2A	25:A:834:CLA:O2D	2.15	0.47
2:B:578:TYR:CE1	2:B:707:ARG:HB3	2.50	0.47
14:P:212:PHE:C	33:P:609:CHL:C20	2.87	0.47
35:P:620:XAT:H34	25:R:613:CLA:H122	1.97	0.47
25:Q:603:CLA:C2	25:Q:603:CLA:HMA1	2.45	0.47
25:S:315:CLA:H2A	25:S:315:CLA:O1D	2.14	0.47
14:T:97:ILE:HD13	25:T:610:CLA:HBB2	1.96	0.47
17:2:178:TYR:OH	17:2:201:SER:OG	2.14	0.47
18:3:61:LEU:O	18:3:61:LEU:HD23	2.14	0.47
25:4:309:CLA:NC	27:4:318:LHG:HC42	2.29	0.47
27:5:301:LHG:H241	25:5:315:CLA:C3C	2.44	0.47
21:6:75:SER:HB2	21:6:180:GLY:HA3	1.95	0.47
6:F:162:TYR:CE2	25:F:802:CLA:HBD	2.41	0.47
13:O:40:TRP:CE3	13:O:41:VAL:HG23	2.49	0.47
14:P:44:TYR:CE2	35:P:623:XAT:H221	2.50	0.47
14:Q:42:GLY:O	14:Q:45:SER:HB3	2.15	0.47
25:R:603:CLA:NB	33:R:609:CHL:H102	2.29	0.47
15:S:147:VAL:HG13	25:U:313:CLA:O1A	2.14	0.47
16:1:179:LYS:NZ	25:1:610:CLA:O1D	2.44	0.47
17:2:64:LYS:HA	17:2:134:GLU:OE2	2.14	0.47
17:2:186:LEU:HD12	17:2:190:LEU:HG	1.96	0.47
25:2:302:CLA:HED3	24:9:121:PHE:HA	1.95	0.47
25:2:304:CLA:H161	25:2:304:CLA:H141	1.65	0.47
18:3:231:TYR:CE1	34:3:315:LUT:H41	2.50	0.47
21:6:91:VAL:HG21	25:6:605:CLA:CMD	2.43	0.47
22:7:172:PRO:HD2	34:7:314:LUT:H23	1.96	0.47
34:7:314:LUT:H35	34:7:314:LUT:H401	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:173:GLY:HA2	33:S:309:CHL:HBC1	1.94	0.47
14:T:81:LEU:HD12	33:T:607:CHL:OBD	2.14	0.47
18:3:96:ARG:HA	18:3:99:MET:HE3	1.97	0.47
28:3:318:BCR:H361	28:3:318:BCR:H20C	1.34	0.47
19:4:86:LEU:HD13	25:4:301:CLA:H42	1.96	0.47
1:A:658:ILE:HD12	2:B:622:ARG:HG3	1.97	0.47
28:A:849:BCR:H361	28:A:849:BCR:H20C	1.60	0.47
32:J:104:LMG:O5	32:J:104:LMG:O4	2.29	0.47
14:P:233:PRO:CB	25:S:301:CLA:HMB2	2.44	0.47
14:Q:212:PHE:C	33:Q:608:CHL:C20	2.87	0.47
15:S:249:LYS:O	35:S:318:XAT:O3	2.32	0.47
15:S:251:THR:CG2	33:S:321:CHL:HED1	2.43	0.47
14:U:97:ILE:HD13	25:U:311:CLA:HBB2	1.97	0.47
33:U:307:CHL:H2	33:U:307:CHL:H62	1.50	0.47
27:1:618:LHG:H302	27:1:618:LHG:H151	1.97	0.47
25:2:307:CLA:HBA1	25:2:307:CLA:H3A	1.34	0.47
20:5:150:PRO:HA	20:5:153:LYS:HZ1	1.79	0.47
21:6:116:VAL:O	21:6:120:LEU:HD23	2.15	0.47
1:A:554:VAL:HG21	28:A:848:BCR:HC31	1.96	0.47
1:A:599:MET:SD	1:A:603:LEU:HD12	2.54	0.47
1:A:684:MET:HB2	1:A:684:MET:HE3	1.34	0.47
1:A:718:LEU:HD13	1:A:722:GLN:OE1	2.14	0.47
25:A:832:CLA:HBB2	12:L:103:LEU:HD12	1.97	0.47
2:B:698:PRO:O	3:C:81:TYR:OH	2.31	0.47
28:J:106:BCR:H15C	28:J:106:BCR:H351	1.73	0.47
14:Q:134:SER:C	14:Q:135:LEU:HD12	2.40	0.47
14:Q:142:VAL:HG23	25:U:313:CLA:CAB	2.44	0.47
14:R:148:GLN:HE22	33:R:607:CHL:HMC	1.79	0.47
25:R:603:CLA:H202	25:R:603:CLA:H161	1.72	0.47
15:S:53:SER:O	15:S:54:THR:OG1	2.23	0.47
15:S:66:TYR:CD1	25:S:303:CLA:HMD2	2.50	0.47
25:S:320:CLA:HMA2	25:S:320:CLA:H61	1.96	0.47
25:T:611:CLA:H101	27:T:617:LHG:H131	1.96	0.47
17:2:186:LEU:HD12	17:2:190:LEU:CB	2.45	0.47
19:4:171:PRO:HB3	19:4:191:PRO:HG3	1.96	0.47
19:4:258:GLN:OE1	28:4:321:BCR:H332	2.15	0.47
20:5:79:ARG:NH1	33:5:308:CHL:OBD	2.39	0.47
24:9:104:TYR:O	24:9:107:PRO:HB3	2.15	0.47
1:A:16:ALA:HB1	1:A:187:LYS:HD3	1.96	0.47
11:K:53:LEU:HD12	25:K:205:CLA:C4D	2.44	0.47
14:P:148:GLN:HE22	33:P:607:CHL:HMC	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:93:ALA:HB1	34:T:613:LUT:H12	1.95	0.47
14:U:211:PHE:CE2	34:U:314:LUT:H8	2.50	0.47
20:5:79:ARG:HH22	20:5:164:TYR:HD1	1.59	0.47
21:6:195:GLN:HA	21:6:235:ILE:HD13	1.96	0.47
1:A:474:ASP:O	1:A:478:GLN:NE2	2.48	0.47
25:A:853:CLA:OBD	6:F:171:LEU:HD21	2.14	0.47
30:B:848:DGD:HG32	30:B:848:DGD:HD2	1.58	0.47
3:C:21:CYS:SG	3:C:25:VAL:HG22	2.54	0.47
25:H:203:CLA:HBA2	25:H:203:CLA:H3A	1.55	0.47
25:L:201:CLA:H143	25:L:201:CLA:H111	1.78	0.47
14:Q:220:LYS:NZ	14:Q:225:ASN:OD1	2.45	0.47
14:R:190:PHE:CE2	14:R:194:LYS:HE3	2.50	0.47
16:1:84:TRP:CE2	25:1:607:CLA:HED2	2.50	0.47
19:4:58:LEU:N	19:4:59:PRO:HD2	2.29	0.47
25:6:615:CLA:HBA2	25:6:615:CLA:H3A	1.73	0.47
25:6:615:CLA:HBC3	25:6:620:CLA:HMC2	1.96	0.47
16:a:189:LEU:O	16:a:192:VAL:HG12	2.15	0.47
2:B:565:ARG:NH2	3:C:62:PHE:HE1	2.12	0.47
14:P:44:TYR:CE1	27:P:624:LHG:HC2	2.50	0.47
14:P:199:LYS:NZ	25:P:611:CLA:O1D	2.48	0.47
14:Q:211:PHE:CE2	34:Q:614:LUT:H8	2.49	0.47
25:S:301:CLA:HHC	33:S:306:CHL:CBB	2.42	0.47
35:T:615:XAT:H35	35:T:615:XAT:H401	1.76	0.47
20:5:82:MET:HE2	20:5:190:GLY:HA2	1.97	0.47
16:a:55:GLY:H	16:a:175:LEU:CD2	2.27	0.47
1:A:368:ALA:HB2	1:A:394:HIS:HB2	1.96	0.46
1:A:596:LEU:HD21	25:A:830:CLA:HBC1	1.97	0.46
25:A:815:CLA:H101	25:A:817:CLA:H101	1.95	0.46
25:A:825:CLA:H161	25:A:825:CLA:H141	1.70	0.46
2:B:24:TYR:CE1	30:B:846:DGD:HG11	2.49	0.46
3:C:2:ALA:N	3:C:71:SER:O	2.48	0.46
5:E:67:VAL:HG22	5:E:69:TYR:H	1.79	0.46
34:P:614:LUT:H35	34:P:614:LUT:H401	1.76	0.46
25:R:603:CLA:C4B	33:R:609:CHL:C11	2.93	0.46
25:U:312:CLA:H2	25:U:312:CLA:H61	1.56	0.46
21:6:127:ARG:HD2	33:6:608:CHL:OMC	2.15	0.46
25:6:613:CLA:H3A	25:6:613:CLA:HBA2	1.64	0.46
25:B:830:CLA:H171	25:B:834:CLA:H171	1.97	0.46
10:J:36:PRO:HG2	25:J:103:CLA:HAA2	1.97	0.46
14:P:162:GLY:HA3	14:P:168:GLY:H	1.80	0.46
25:P:603:CLA:H143	25:P:603:CLA:H111	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:212:PHE:CA	33:Q:608:CHL:C20	2.86	0.46
14:R:42:GLY:O	14:R:45:SER:HB3	2.15	0.46
15:S:83:TYR:CB	25:S:303:CLA:HMA1	2.45	0.46
25:S:312:CLA:H61	25:S:312:CLA:H92	1.70	0.46
35:S:318:XAT:H15	35:S:318:XAT:H201	1.78	0.46
33:S:321:CHL:HMC	14:T:148:GLN:HE22	1.81	0.46
16:1:139:ALA:HA	25:1:608:CLA:HAB	1.96	0.46
17:2:186:LEU:HD12	17:2:190:LEU:HB2	1.98	0.46
20:5:242:VAL:HG12	20:5:243:GLN:N	2.30	0.46
1:A:343:GLU:OE1	1:A:343:GLU:N	2.48	0.46
25:A:808:CLA:H72	25:A:810:CLA:H92	1.97	0.46
25:A:814:CLA:H172	25:A:814:CLA:H13	1.71	0.46
25:A:827:CLA:H2	25:A:827:CLA:H61	1.69	0.46
25:B:830:CLA:H112	25:B:830:CLA:H152	1.43	0.46
6:F:74:LYS:NZ	6:F:78:LYS:HD3	2.30	0.46
25:L:205:CLA:H91	25:L:205:CLA:H111	1.60	0.46
33:P:622:CHL:CMB	15:S:158:GLY:HA3	2.45	0.46
14:R:46:GLU:O	14:R:48:ALA:N	2.41	0.46
14:U:162:GLY:HA3	14:U:168:GLY:H	1.81	0.46
25:3:308:CLA:H141	25:3:308:CLA:H162	1.63	0.46
28:3:318:BCR:H11C	28:3:318:BCR:H341	1.57	0.46
28:4:321:BCR:H24C	28:4:321:BCR:H371	1.57	0.46
22:7:189:LYS:O	22:7:193:ASN:ND2	2.48	0.46
32:7:319:LMG:O5	32:7:319:LMG:O4	2.28	0.46
25:A:815:CLA:H102	27:A:852:LHG:H362	1.97	0.46
36:R:617:NEX:H401	36:R:617:NEX:H35	1.63	0.46
25:U:303:CLA:C2	25:U:303:CLA:HMA1	2.46	0.46
20:5:97:ASP:OD1	20:5:98:VAL:N	2.48	0.46
28:5:320:BCR:H313	25:6:611:CLA:HAB	1.97	0.46
22:7:201:CYS:HA	22:7:204:PHE:HD2	1.81	0.46
1:A:217:GLN:NE2	25:A:820:CLA:O1D	2.48	0.46
1:A:511:GLY:HA2	1:A:525:PRO:HB3	1.97	0.46
25:A:830:CLA:H41	25:A:830:CLA:H61	1.34	0.46
27:A:844:LHG:H241	27:A:844:LHG:H111	1.97	0.46
28:A:845:BCR:H383	28:A:854:BCR:HC8	1.96	0.46
15:S:212:SER:HA	34:S:316:LUT:H182	1.97	0.46
19:4:199:ASP:OD1	34:4:315:LUT:O23	2.31	0.46
25:6:623:CLA:H11	25:6:623:CLA:H52	1.77	0.46
1:A:374:MET:HG2	1:A:507:SER:HB2	1.98	0.46
25:A:816:CLA:H61	18:3:236:VAL:HG21	1.97	0.46
2:B:423:LEU:HG	25:B:835:CLA:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:189:ARG:NH2	4:D:191:MET:HB2	2.30	0.46
14:P:181:LEU:CD2	17:2:124:LYS:HD2	2.45	0.46
17:2:149:LYS:HG3	17:2:149:LYS:O	2.15	0.46
18:3:131:ILE:HG22	18:3:134:ALA:H	1.80	0.46
20:5:60:LEU:HD13	25:5:303:CLA:H42	1.96	0.46
24:9:164:LEU:HD21	34:9:312:LUT:H191	1.98	0.46
25:A:808:CLA:H161	25:A:810:CLA:H111	1.96	0.46
25:A:814:CLA:H111	25:A:814:CLA:H93	1.64	0.46
25:A:838:CLA:HBC3	25:A:853:CLA:C1C	2.46	0.46
2:B:595:TRP:HD1	25:B:833:CLA:HAC1	1.80	0.46
25:B:823:CLA:H52	25:B:838:CLA:H201	1.98	0.46
28:B:841:BCR:H15C	28:B:841:BCR:H351	1.77	0.46
14:P:121:ILE:HD13	14:P:141:ILE:HB	1.96	0.46
25:P:610:CLA:H91	25:P:610:CLA:H111	1.71	0.46
25:1:602:CLA:H92	25:1:602:CLA:H61	1.69	0.46
17:2:124:LYS:O	17:2:128:ILE:HG22	2.16	0.46
19:4:214:LYS:HD3	25:4:310:CLA:CBA	2.46	0.46
23:8:154:LEU:HB2	25:a:302:CLA:C2	2.45	0.46
16:a:191:PHE:HE1	34:a:314:LUT:H41	1.80	0.46
25:A:822:CLA:H141	25:A:822:CLA:H161	1.71	0.46
25:B:809:CLA:H142	25:B:809:CLA:H111	1.83	0.46
6:F:167:GLY:O	6:F:171:LEU:HD23	2.16	0.46
25:K:202:CLA:HED2	25:K:202:CLA:H2A	1.98	0.46
25:P:603:CLA:H62	25:Q:603:CLA:H41	1.98	0.46
15:S:45:TRP:O	33:S:302:CHL:HBB1	2.16	0.46
34:U:314:LUT:H15	34:U:314:LUT:H201	1.79	0.46
16:1:122:GLU:CD	16:1:122:GLU:H	2.24	0.46
25:4:308:CLA:H62	25:4:308:CLA:H41	1.72	0.46
16:a:98:LEU:HD22	16:a:119:PHE:CE1	2.51	0.46
25:a:311:CLA:H142	25:a:311:CLA:H112	1.74	0.46
25:B:815:CLA:HBA2	25:B:815:CLA:H3A	1.33	0.46
25:B:828:CLA:H3A	25:B:828:CLA:HBA2	1.44	0.46
31:B:850:SQD:H81	31:B:850:SQD:H111	1.73	0.46
27:P:624:LHG:H131	25:U:312:CLA:H101	1.97	0.46
14:R:39:LYS:HD2	14:R:45:SER:HB2	1.98	0.46
14:R:57:PHE:HB2	14:R:60:ASP:OD2	2.16	0.46
14:R:193:LEU:HD21	25:R:612:CLA:CBA	2.43	0.46
25:R:603:CLA:HBC2	33:R:609:CHL:CMD	2.45	0.46
16:1:48:TRP:CD1	16:1:49:LEU:HD22	2.51	0.46
21:6:127:ARG:HH11	21:6:138:VAL:HB	1.81	0.46
33:7:305:CHL:HBA2	32:7:319:LMG:HC72	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:7:308:CLA:H13	34:7:314:LUT:H403	1.96	0.46
23:8:41:ASP:OD1	23:8:46:GLN:NE2	2.49	0.46
24:9:35:LEU:HD12	24:9:36:ASN:H	1.80	0.46
12:L:115:ILE:O	12:L:119:LEU:HD23	2.16	0.46
14:P:30:ILE:HD13	15:S:169:PRO:N	2.30	0.46
33:P:601:CHL:HHC	33:P:601:CHL:HBB1	1.98	0.46
25:1:610:CLA:C4D	25:1:611:CLA:HMD3	2.46	0.46
1:A:207:GLY:HA3	1:A:306:LEU:HD12	1.98	0.45
2:B:153:ALA:HB2	25:9:301:CLA:HBC2	1.97	0.45
2:B:176:LEU:HA	2:B:176:LEU:HD23	1.83	0.45
2:B:370:ALA:CB	2:B:726:LEU:HD21	2.47	0.45
36:P:617:NEX:H35	36:P:617:NEX:H401	1.64	0.45
14:Q:97:ILE:CD1	25:Q:611:CLA:HBB2	2.46	0.45
14:R:129:TYR:CD2	14:R:130:LEU:HG	2.51	0.45
14:R:198:ILE:O	14:R:202:ARG:HG3	2.15	0.45
14:U:198:ILE:O	14:U:202:ARG:HG3	2.16	0.45
25:A:803:CLA:H2	2:B:656:LEU:HD22	1.99	0.45
2:B:200:ILE:HB	2:B:201:PRO:HD3	1.97	0.45
2:B:340:ALA:HB2	28:B:844:BCR:H372	1.97	0.45
25:B:837:CLA:H193	9:I:92:MET:HE2	1.98	0.45
25:B:838:CLA:H91	25:B:838:CLA:H112	1.76	0.45
4:D:92:LYS:HE2	4:D:92:LYS:HB3	1.82	0.45
6:F:161:GLY:HA3	6:F:202:TRP:CH2	2.51	0.45
25:L:201:CLA:H41	25:L:201:CLA:H61	1.44	0.45
13:O:46:LEU:HA	13:O:49:VAL:HG12	1.97	0.45
13:O:79:ILE:HD11	28:O:204:BCR:H343	1.98	0.45
14:P:40:TRP:HH2	14:P:49:THR:HG22	1.80	0.45
14:P:122:PHE:CE1	14:R:239:PHE:CB	2.98	0.45
35:P:616:XAT:H15	35:P:616:XAT:H201	1.74	0.45
14:Q:97:ILE:HD13	25:Q:611:CLA:HBB2	1.98	0.45
33:S:302:CHL:HHC	35:S:318:XAT:H383	1.97	0.45
27:T:617:LHG:H171	27:T:617:LHG:H142	1.78	0.45
14:U:114:TRP:CZ2	14:U:115:PHE:HE1	2.35	0.45
23:8:83:GLY:O	23:8:87:ILE:HG12	2.16	0.45
16:a:122:GLU:H	16:a:122:GLU:CD	2.24	0.45
1:A:459:ASN:HB3	1:A:471:MET:HE3	1.98	0.45
1:A:489:ASN:HD22	13:O:93:ASP:CB	2.29	0.45
25:A:807:CLA:H192	25:A:807:CLA:H161	1.67	0.45
8:H:84:ARG:HD3	32:H:204:LMG:H302	1.98	0.45
14:P:44:TYR:HE1	33:P:622:CHL:HAC1	1.80	0.45
25:P:603:CLA:C5	25:Q:603:CLA:H51	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:618:LHG:H142	27:P:618:LHG:H171	1.78	0.45
25:Q:603:CLA:NB	33:Q:608:CHL:H102	2.31	0.45
25:Q:603:CLA:HMD3	33:Q:608:CHL:HBA1	1.97	0.45
14:R:151:LEU:HD22	36:R:617:NEX:C15	2.46	0.45
14:R:196:LYS:HD2	25:R:612:CLA:HAA1	1.96	0.45
25:R:603:CLA:HMD3	33:R:609:CHL:HBA1	1.98	0.45
15:S:93:TRP:CD1	33:S:310:CHL:HMD3	2.51	0.45
14:T:36:ASN:HA	14:T:39:LYS:NZ	2.32	0.45
14:T:97:ILE:CD1	25:T:610:CLA:HBB2	2.47	0.45
25:1:610:CLA:CBB	25:a:307:CLA:H42	2.46	0.45
24:9:129:GLY:HA3	24:9:138:PHE:HZ	1.82	0.45
16:a:99:GLY:O	16:a:100:TYR:CD1	2.69	0.45
16:a:117:THR:C	16:a:118:TRP:CD1	2.88	0.45
5:E:65:SER:OG	5:E:66:GLY:N	2.50	0.45
6:F:87:LEU:HG	6:F:108:MET:SD	2.56	0.45
12:L:151:LEU:HG	15:S:22:LYS:HE3	1.97	0.45
13:O:79:ILE:O	13:O:83:LEU:HB2	2.16	0.45
14:P:130:LEU:HD13	17:2:105:LEU:HD22	1.99	0.45
14:P:233:PRO:HB2	25:S:301:CLA:HMB2	1.99	0.45
36:U:301:NEX:H35	36:U:301:NEX:H401	1.64	0.45
16:1:188:PHE:CD2	34:1:616:LUT:H12	2.51	0.45
19:4:145:PRO:O	19:4:149:LEU:HD23	2.17	0.45
20:5:250:THR:OG1	27:5:301:LHG:H251	2.16	0.45
2:B:578:TYR:OH	2:B:665:LEU:HD21	2.16	0.45
25:T:611:CLA:H61	25:T:611:CLA:H2	1.59	0.45
14:U:93:ALA:HA	14:U:208:MET:CE	2.45	0.45
25:U:303:CLA:H61	25:U:303:CLA:CMA	2.47	0.45
25:U:304:CLA:HAB	36:U:316:NEX:H362	1.98	0.45
20:5:218:HIS:CG	25:5:313:CLA:HAA2	2.52	0.45
21:6:76:ARG:NH1	33:6:608:CHL:OBD	2.46	0.45
16:a:59:PHE:HB3	25:a:301:CLA:C3D	2.46	0.45
2:B:693:TYR:CE2	4:D:76:ARG:NH1	2.85	0.45
4:D:98:MET:HE2	12:L:51:PHE:HE1	1.81	0.45
6:F:98:SER:HB2	6:F:100:PRO:HD2	1.99	0.45
25:P:603:CLA:HBC2	33:P:609:CHL:CMD	2.46	0.45
35:P:616:XAT:H35	35:P:616:XAT:H401	1.78	0.45
25:Q:603:CLA:C4B	33:Q:608:CHL:C12	2.95	0.45
25:Q:603:CLA:HBC2	33:Q:608:CHL:CMD	2.47	0.45
15:S:225:LYS:CD	15:S:229:GLN:HB3	2.47	0.45
14:T:32:PHE:HE2	25:T:609:CLA:HED3	1.81	0.45
25:U:312:CLA:H111	25:U:312:CLA:H152	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:155:MET:HE2	18:3:155:MET:HA	1.98	0.45
25:6:620:CLA:H3A	25:6:620:CLA:HBA1	1.64	0.45
27:a:317:LHG:H302	27:a:317:LHG:H151	1.97	0.45
1:A:509:THR:HG22	1:A:523:MET:HE2	1.98	0.45
1:A:684:MET:HE2	25:A:802:CLA:NC	2.32	0.45
25:A:804:CLA:H2A	25:A:804:CLA:O1D	2.16	0.45
4:D:88:TRP:NE1	4:D:111:ASN:HD22	2.14	0.45
28:I:201:BCR:H11C	28:I:201:BCR:H341	1.83	0.45
14:P:53:LEU:O	14:P:53:LEU:HD12	2.16	0.45
25:Q:603:CLA:C4B	33:Q:608:CHL:C10	2.91	0.45
25:S:320:CLA:H61	25:S:320:CLA:CMA	2.46	0.45
14:T:198:ILE:O	14:T:202:ARG:HG3	2.17	0.45
36:T:616:NEX:H191	36:T:616:NEX:H11	1.71	0.45
14:U:33:TYR:CZ	14:U:191:ALA:HB1	2.51	0.45
14:U:42:GLY:O	14:U:45:SER:N	2.50	0.45
14:U:76:LYS:CA	14:U:79:ARG:HE	2.18	0.45
16:1:191:PHE:HE1	34:1:615:LUT:H41	1.81	0.45
27:6:618:LHG:H182	27:6:618:LHG:H211	1.77	0.45
24:9:71:LYS:O	24:9:75:ARG:HG3	2.16	0.45
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.79	0.45
2:B:493:LEU:HD21	2:B:494:TRP:CZ3	2.52	0.45
28:B:840:BCR:H11C	28:B:840:BCR:H341	1.71	0.45
35:P:620:XAT:H203	25:R:613:CLA:C3	2.47	0.45
14:Q:93:ALA:HB1	34:Q:614:LUT:H12	1.99	0.45
25:Q:618:CLA:HED3	14:U:32:PHE:CE2	2.52	0.45
14:R:211:PHE:HE2	34:R:615:LUT:C8	2.30	0.45
33:S:302:CHL:H51	33:T:607:CHL:HBB1	1.98	0.45
14:T:162:GLY:HA3	14:T:168:GLY:H	1.82	0.45
25:2:306:CLA:HHC	25:2:306:CLA:HBB1	1.99	0.45
19:4:159:TRP:CZ2	28:4:317:BCR:H331	2.52	0.45
19:4:182:ASN:OD1	19:4:183:ASN:N	2.50	0.45
19:4:214:LYS:CE	25:4:310:CLA:HBD	2.46	0.45
25:6:601:CLA:H142	25:6:601:CLA:H111	1.66	0.45
1:A:261:ILE:O	1:A:261:ILE:HG22	2.17	0.45
25:A:813:CLA:H92	25:A:813:CLA:HBB1	1.98	0.45
25:A:818:CLA:H91	25:A:818:CLA:H111	1.80	0.45
25:B:826:CLA:H92	25:B:826:CLA:H61	1.78	0.45
25:B:834:CLA:H141	25:B:834:CLA:H161	1.73	0.45
14:Q:152:MET:HE2	36:U:301:NEX:H32	1.99	0.45
33:Q:601:CHL:HHC	33:Q:601:CHL:HBB1	1.98	0.45
25:Q:603:CLA:H141	25:Q:603:CLA:H162	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:303:CLA:H92	25:S:304:CLA:HMA1	1.99	0.45
35:T:615:XAT:H403	27:T:617:LHG:H132	1.97	0.45
14:U:97:ILE:HG13	14:U:98:THR:N	2.32	0.45
17:2:59:ASN:HB3	17:2:61:ASP:H	1.80	0.45
21:6:254:GLY:C	21:6:255:LEU:HD12	2.42	0.45
22:7:203:GLY:O	22:7:207:GLN:HB2	2.17	0.45
24:9:37:PRO:HA	24:9:38:PRO:HD3	1.83	0.45
16:a:72:LYS:O	16:a:75:THR:OG1	2.30	0.45
25:a:309:CLA:C4D	25:a:310:CLA:HMD3	2.47	0.45
11:K:92:MET:N	11:K:92:MET:SD	2.90	0.45
25:Q:612:CLA:H122	35:Q:616:XAT:H34	1.99	0.45
14:U:40:TRP:HH2	14:U:49:THR:HG22	1.82	0.45
19:4:109:LEU:CD2	25:4:308:CLA:HMC3	2.47	0.45
25:8:310:CLA:CBB	34:8:316:LUT:H32	2.46	0.45
16:a:86:MET:CE	16:a:180:ASN:HB3	2.47	0.45
34:a:316:LUT:H201	34:a:316:LUT:H15	1.61	0.45
1:A:19:ARG:NE	18:3:78:SER:O	2.49	0.44
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.97	0.44
25:A:836:CLA:C4A	25:A:836:CLA:HBA2	2.46	0.44
25:B:808:CLA:H12	28:I:201:BCR:H10C	1.99	0.44
25:B:837:CLA:C19	9:I:92:MET:HE2	2.47	0.44
11:K:38:MET:SD	11:K:100:GLY:HA3	2.56	0.44
28:L:208:BCR:H15C	28:L:208:BCR:H351	1.74	0.44
25:P:613:CLA:H122	35:P:616:XAT:H34	1.99	0.44
14:Q:53:LEU:HD12	14:Q:53:LEU:O	2.18	0.44
33:R:601:CHL:HHC	33:R:601:CHL:HBB1	1.98	0.44
25:1:608:CLA:HBA2	25:1:608:CLA:H3A	1.54	0.44
20:5:149:ASP:HB2	20:5:155:ASN:HB2	1.98	0.44
21:6:155:GLY:O	21:6:156:TYR:HD2	1.99	0.44
25:8:309:CLA:HBA1	25:8:309:CLA:H3A	1.78	0.44
25:a:301:CLA:H61	25:a:301:CLA:H41	1.59	0.44
25:a:303:CLA:H2A	25:a:303:CLA:O1D	2.17	0.44
1:A:311:MET:HE1	25:A:822:CLA:C2D	2.47	0.44
1:A:466:GLY:HA2	2:B:641:MET:SD	2.57	0.44
28:A:845:BCR:H402	28:3:319:BCR:H382	1.99	0.44
2:B:381:GLY:C	2:B:584:MET:HE2	2.42	0.44
2:B:695:LYS:HE3	12:L:141:GLN:HE21	1.83	0.44
28:J:106:BCR:HC8	28:J:106:BCR:H331	1.99	0.44
14:P:199:LYS:HB3	25:P:611:CLA:CMD	2.47	0.44
36:P:617:NEX:H11	36:P:617:NEX:H191	1.72	0.44
14:R:196:LYS:HD3	25:R:612:CLA:CBD	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:84:ARG:HH21	15:S:177:LEU:HD13	1.81	0.44
25:S:320:CLA:H202	25:S:320:CLA:H161	1.77	0.44
14:T:32:PHE:CE2	25:T:609:CLA:HED3	2.53	0.44
14:T:97:ILE:HG13	14:T:98:THR:N	2.32	0.44
14:T:220:LYS:NZ	14:T:225:ASN:OD1	2.48	0.44
14:U:39:LYS:HD2	14:U:45:SER:HB2	1.98	0.44
21:6:253:GLN:HA	21:6:256:TRP:NE1	2.32	0.44
22:7:156:GLU:OE2	22:7:168:ARG:HD3	2.17	0.44
16:a:64:LEU:HD13	25:a:301:CLA:H42	1.99	0.44
16:a:148:ALA:O	16:a:151:VAL:HG23	2.18	0.44
16:a:152:VAL:HG23	16:a:153:TYR:CD2	2.53	0.44
27:A:843:LHG:H241	27:A:843:LHG:H271	1.63	0.44
2:B:71:TRP:CE2	9:I:71:PRO:HG2	2.53	0.44
8:H:104:LYS:HE2	25:H:203:CLA:C1B	2.46	0.44
25:J:103:CLA:HBA2	25:J:103:CLA:H3A	1.59	0.44
35:P:620:XAT:H15	35:P:620:XAT:H201	1.77	0.44
36:P:621:NEX:H11	36:P:621:NEX:H191	1.81	0.44
14:R:53:LEU:HD12	14:R:53:LEU:O	2.17	0.44
25:R:603:CLA:H61	25:R:603:CLA:CMA	2.47	0.44
14:T:134:SER:C	14:T:135:LEU:HD12	2.43	0.44
34:1:615:LUT:H401	34:1:615:LUT:H35	1.74	0.44
25:3:320:CLA:H41	25:3:320:CLA:H62	1.74	0.44
28:8:318:BCR:H15C	28:8:318:BCR:H351	1.67	0.44
25:a:303:CLA:HMA2	25:a:304:CLA:C3C	2.47	0.44
34:a:314:LUT:H15	34:a:314:LUT:H201	1.89	0.44
25:A:802:CLA:C1D	2:B:583:TRP:HE1	2.31	0.44
25:B:823:CLA:CAD	25:B:833:CLA:HBB1	2.47	0.44
28:O:205:BCR:H24C	28:O:205:BCR:H371	1.79	0.44
27:P:624:LHG:H332	25:Q:618:CLA:HAC1	2.00	0.44
25:R:610:CLA:H51	25:R:612:CLA:H3A	1.99	0.44
18:3:78:SER:OG	18:3:82:ILE:O	2.34	0.44
25:5:303:CLA:HAB	34:5:322:LUT:H32	2.00	0.44
28:5:320:BCR:H20C	28:5:320:BCR:H361	1.74	0.44
28:5:323:BCR:H11C	28:5:323:BCR:H341	1.46	0.44
21:6:77:TRP:CZ2	25:6:609:CLA:HBC3	2.52	0.44
33:6:606:CHL:HBC2	33:6:607:CHL:HBC3	1.99	0.44
23:8:46:GLN:HA	23:8:51:ASN:HD22	1.82	0.44
23:8:174:ASP:OD1	34:8:316:LUT:O23	2.32	0.44
25:9:303:CLA:H61	25:9:303:CLA:H92	1.55	0.44
1:A:91:MET:HE1	25:A:809:CLA:H2A	2.00	0.44
2:B:696:ASP:OD1	2:B:696:ASP:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:844:BCR:H11C	28:B:844:BCR:H341	1.85	0.44
14:P:129:TYR:CD2	14:P:130:LEU:HG	2.52	0.44
25:Q:603:CLA:H61	25:Q:603:CLA:CMA	2.48	0.44
25:Q:618:CLA:HED3	14:U:32:PHE:HE2	1.83	0.44
14:R:81:LEU:CD1	33:R:609:CHL:O2D	2.65	0.44
25:R:610:CLA:HBB1	25:R:612:CLA:CHB	2.48	0.44
34:R:615:LUT:H31	34:R:615:LUT:H391	1.88	0.44
14:T:46:GLU:O	14:T:48:ALA:N	2.39	0.44
14:U:53:LEU:O	14:U:53:LEU:HD12	2.17	0.44
25:1:607:CLA:HBB1	25:1:607:CLA:H121	1.99	0.44
28:4:317:BCR:H313	27:a:317:LHG:C11	2.47	0.44
20:5:85:VAL:HG13	20:5:200:PHE:CE2	2.49	0.44
22:7:225:ASP:OD2	22:7:228:HIS:HB2	2.17	0.44
34:8:317:LUT:H15	34:8:317:LUT:H201	1.80	0.44
24:9:132:GLN:HG3	24:9:133:THR:HG23	1.99	0.44
25:a:307:CLA:H143	25:a:307:CLA:H161	1.84	0.44
25:A:836:CLA:H41	25:A:836:CLA:H62	1.46	0.44
25:Q:618:CLA:HBD	36:U:301:NEX:H163	2.00	0.44
14:R:33:TYR:CZ	14:R:191:ALA:HB1	2.52	0.44
14:R:212:PHE:CD2	33:R:609:CHL:H18	2.52	0.44
15:S:157:MET:HE2	15:S:157:MET:HA	1.98	0.44
15:S:247:ALA:HA	35:S:318:XAT:H42	1.99	0.44
33:T:605:CHL:HMB1	33:T:607:CHL:HAC1	1.99	0.44
14:U:134:SER:C	14:U:135:LEU:HD12	2.43	0.44
25:U:303:CLA:H91	25:U:303:CLA:H112	1.67	0.44
33:U:305:CHL:H3A	33:U:305:CHL:HBA2	1.36	0.44
16:1:170:SER:O	16:1:174:LYS:HG3	2.18	0.44
25:1:604:CLA:HMA2	25:1:605:CLA:C3C	2.48	0.44
25:1:609:CLA:H2A	25:1:609:CLA:O1D	2.18	0.44
18:3:97:TRP:CE2	33:3:306:CHL:HED2	2.53	0.44
20:5:245:LEU:C	20:5:245:LEU:HD12	2.42	0.44
2:B:38:MET:HE3	2:B:42:ASN:HB3	1.98	0.44
8:H:106:ALA:HB3	8:H:110:ILE:HG22	2.00	0.44
10:J:39:PHE:O	10:J:41:PHE:N	2.51	0.44
12:L:188:CYS:O	12:L:192:LEU:HB2	2.18	0.44
14:P:152:MET:HG2	33:P:609:CHL:OMC	2.18	0.44
35:Q:616:XAT:H173	35:Q:616:XAT:H3	1.77	0.44
14:R:78:TYR:HB3	25:R:602:CLA:HMA1	2.00	0.44
25:R:610:CLA:H91	25:R:610:CLA:H111	1.74	0.44
15:S:74:SER:O	15:S:79:THR:OG1	2.35	0.44
36:U:301:NEX:H162	36:U:301:NEX:H193	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:U:306:CHL:HMB1	33:U:309:CHL:HAC1	2.00	0.44
34:U:315:LUT:H31	34:U:315:LUT:H391	1.83	0.44
24:9:184:ILE:HD12	24:9:184:ILE:H	1.82	0.44
16:a:185:MET:HG2	34:a:315:LUT:C35	2.47	0.44
25:A:802:CLA:H122	28:A:849:BCR:H23C	2.00	0.44
36:P:621:NEX:H3	36:P:621:NEX:H173	1.49	0.44
14:T:88:TRP:CE2	33:T:606:CHL:HED2	2.53	0.44
14:U:152:MET:HA	14:U:155:VAL:HG22	1.98	0.44
25:2:312:CLA:H111	25:2:312:CLA:HAB	2.00	0.44
25:6:601:CLA:H112	25:6:601:CLA:H72	1.72	0.44
23:8:90:PRO:HB3	23:8:101:VAL:HG21	2.00	0.44
23:8:185:TRP:HH2	25:8:310:CLA:HED3	1.82	0.44
25:8:310:CLA:H91	25:8:310:CLA:H111	1.66	0.44
28:A:848:BCR:H11C	28:A:848:BCR:H341	1.69	0.44
10:J:34:PRO:O	32:J:107:LMG:O2	2.35	0.44
25:P:611:CLA:HMB3	15:S:156:LEU:HD23	1.99	0.44
34:P:615:LUT:H35	34:P:615:LUT:H401	1.87	0.44
14:Q:97:ILE:HG13	14:Q:98:THR:N	2.33	0.44
25:Q:603:CLA:H91	25:Q:603:CLA:H112	1.69	0.44
33:Q:606:CHL:CMB	33:Q:608:CHL:HAC1	2.48	0.44
25:Q:612:CLA:H101	27:Q:617:LHG:H131	2.00	0.44
25:T:603:CLA:HAB	36:T:616:NEX:H362	2.00	0.44
17:2:156:LYS:CE	25:2:311:CLA:HBD	2.48	0.44
19:4:142:TYR:C	19:4:143:PHE:CD1	2.96	0.44
19:4:221:LEU:HD21	34:4:315:LUT:H191	2.00	0.44
21:6:96:PHE:CE2	21:6:98:TYR:HB3	2.53	0.44
25:7:308:CLA:CBB	34:7:314:LUT:H32	2.48	0.44
23:8:198:LEU:CD2	34:8:316:LUT:H11	2.48	0.44
25:A:807:CLA:HBA2	25:A:807:CLA:O1D	2.18	0.43
25:A:812:CLA:H143	25:A:812:CLA:H161	1.58	0.43
25:A:828:CLA:H202	28:J:106:BCR:H17C	2.00	0.43
2:B:224:THR:HB	2:B:225:PRO:HD3	1.99	0.43
25:B:817:CLA:H203	25:B:822:CLA:H171	2.00	0.43
5:E:90:LEU:HD23	5:E:90:LEU:HA	1.86	0.43
28:I:201:BCR:H15C	28:I:201:BCR:H351	1.91	0.43
14:P:39:LYS:HD2	14:P:45:SER:HB2	1.99	0.43
25:S:303:CLA:H193	25:S:303:CLA:H161	1.87	0.43
14:T:78:TYR:HB3	25:T:602:CLA:HMA1	1.99	0.43
14:T:211:PHE:CE2	34:T:613:LUT:H8	2.53	0.43
16:1:160:PRO:HG3	25:1:607:CLA:H41	2.00	0.43
17:2:219:MET:HA	17:2:219:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:183:ILE:HD11	18:3:197:PHE:CB	2.48	0.43
25:3:302:CLA:H141	25:3:302:CLA:H162	1.87	0.43
19:4:76:PRO:O	19:4:216:ILE:HD13	2.17	0.43
34:5:318:LUT:H35	34:5:318:LUT:H401	1.79	0.43
1:A:432:ARG:HG2	4:D:70:SER:HA	1.99	0.43
25:B:837:CLA:H3A	25:B:837:CLA:HBA2	1.69	0.43
12:L:69:LEU:HD11	25:L:201:CLA:H2	2.00	0.43
14:P:46:GLU:O	14:P:48:ALA:N	2.42	0.43
25:P:610:CLA:H51	25:P:612:CLA:H3A	2.00	0.43
14:Q:40:TRP:HH2	14:Q:49:THR:HG22	1.82	0.43
14:Q:142:VAL:HG23	25:U:313:CLA:HAB	2.00	0.43
25:Q:603:CLA:HMD3	33:Q:608:CHL:CBA	2.48	0.43
25:Q:611:CLA:HMB3	25:Q:611:CLA:H121	1.99	0.43
14:R:212:PHE:HD2	33:R:609:CHL:H18	1.83	0.43
34:5:322:LUT:H35	34:5:322:LUT:H401	1.80	0.43
34:9:313:LUT:H35	34:9:313:LUT:H401	1.83	0.43
16:a:185:MET:HG2	34:a:315:LUT:C15	2.48	0.43
25:a:309:CLA:HBC3	27:a:317:LHG:HC62	2.01	0.43
25:A:828:CLA:H3A	25:A:828:CLA:HBA2	1.58	0.43
2:B:51:HIS:HE1	25:B:804:CLA:H171	1.83	0.43
28:B:851:BCR:H15C	28:B:851:BCR:H351	1.87	0.43
25:J:103:CLA:H102	25:J:103:CLA:H61	1.84	0.43
13:O:75:PHE:CD1	13:O:99:TYR:HB3	2.53	0.43
14:Q:58:PRO:HG3	14:Q:194:LYS:HB3	2.00	0.43
15:S:235:LEU:CD2	25:S:315:CLA:HBB1	2.49	0.43
25:1:602:CLA:H61	25:1:602:CLA:H41	1.57	0.43
25:1:604:CLA:H62	25:1:604:CLA:H41	1.82	0.43
25:2:313:CLA:HBD	25:2:313:CLA:HBA1	1.99	0.43
25:a:308:CLA:H92	25:a:308:CLA:H61	1.82	0.43
25:A:816:CLA:H122	18:3:232:GLY:HA3	2.00	0.43
2:B:6:PHE:HA	2:B:7:PRO:HA	1.76	0.43
28:B:843:BCR:H24C	28:B:843:BCR:H371	1.83	0.43
25:G:202:CLA:HBA1	25:G:202:CLA:H3A	1.72	0.43
27:P:624:LHG:H142	27:P:624:LHG:H171	1.76	0.43
14:Q:212:PHE:HB2	33:Q:608:CHL:C18	2.46	0.43
14:T:53:LEU:HD12	14:T:53:LEU:O	2.18	0.43
25:T:609:CLA:H51	25:T:610:CLA:O2D	2.19	0.43
14:U:97:ILE:CD1	25:U:311:CLA:HBB2	2.48	0.43
25:1:602:CLA:HED2	25:1:602:CLA:H2A	2.00	0.43
17:2:102:LYS:HG3	17:2:104:ALA:HB3	2.01	0.43
17:2:206:GLU:OE2	25:2:314:CLA:C4C	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:3:305:CLA:H122	28:3:319:BCR:H312	2.01	0.43
25:4:302:CLA:HBB1	34:4:316:LUT:C35	2.48	0.43
16:a:179:LYS:NZ	25:a:309:CLA:O1D	2.48	0.43
1:A:692:TYR:CE1	2:B:537:LYS:HD2	2.53	0.43
25:A:811:CLA:CBB	25:A:814:CLA:H142	2.48	0.43
3:C:23:LEU:HD12	29:C:101:SF4:S3	2.59	0.43
4:D:92:LYS:HG2	4:D:93:GLU:N	2.32	0.43
4:D:142:PHE:CD2	4:D:146:LYS:HE2	2.49	0.43
8:H:46:ASN:HD22	8:H:51:TRP:HE1	1.67	0.43
8:H:60:LYS:HE2	15:S:187:GLY:HA2	2.00	0.43
14:P:212:PHE:CD2	33:P:609:CHL:H18	2.53	0.43
25:P:603:CLA:C4B	33:P:609:CHL:C10	2.92	0.43
33:P:609:CHL:H152	33:P:609:CHL:C19	2.27	0.43
14:Q:46:GLU:O	14:Q:48:ALA:N	2.40	0.43
25:Q:604:CLA:HAB	36:U:301:NEX:H362	2.01	0.43
14:R:32:PHE:HE1	14:R:38:ALA:HB3	1.83	0.43
14:R:134:SER:C	14:R:135:LEU:HD12	2.43	0.43
25:R:603:CLA:H143	25:R:603:CLA:H111	1.73	0.43
14:U:148:GLN:HE22	33:U:307:CHL:HMC	1.82	0.43
20:5:155:ASN:HB3	33:5:317:CHL:C2D	2.48	0.43
20:5:194:MET:CE	25:5:303:CLA:HHC	2.48	0.43
21:6:120:LEU:HD12	28:6:621:BCR:C15	2.48	0.43
1:A:227:LEU:HD22	1:A:237:ILE:HG23	2.01	0.43
25:A:815:CLA:H102	27:A:852:LHG:C36	2.45	0.43
28:A:846:BCR:H371	28:A:846:BCR:H24C	1.84	0.43
2:B:659:ALA:HB3	25:B:802:CLA:HBB2	2.00	0.43
7:G:92:PRO:HG2	25:G:202:CLA:HBC2	2.00	0.43
13:O:79:ILE:HD13	25:S:315:CLA:HBB2	2.00	0.43
25:Q:609:CLA:H51	25:Q:611:CLA:HMA3	1.99	0.43
34:R:616:LUT:H35	34:R:616:LUT:H401	1.82	0.43
15:S:46:LEU:HD12	33:S:302:CHL:CBB	2.49	0.43
25:S:312:CLA:H91	25:S:312:CLA:H111	1.83	0.43
14:T:37:ARG:O	14:T:39:LYS:HD2	2.18	0.43
25:U:303:CLA:H202	25:U:303:CLA:H161	1.78	0.43
25:U:310:CLA:H51	25:U:311:CLA:HMA3	2.01	0.43
34:6:619:LUT:H401	34:6:619:LUT:H35	1.71	0.43
27:7:317:LHG:H291	27:7:317:LHG:H102	2.00	0.43
28:A:845:BCR:H371	28:A:845:BCR:H24C	1.79	0.43
25:B:810:CLA:H3A	25:B:810:CLA:HBA2	1.82	0.43
7:G:57:GLN:OE1	7:G:58:ARG:NH1	2.52	0.43
32:H:204:LMG:H122	32:2:301:LMG:H312	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:79:ILE:HD12	25:O:202:CLA:HMD1	2.00	0.43
14:P:42:GLY:O	14:P:45:SER:HB3	2.18	0.43
25:P:613:CLA:H101	27:P:618:LHG:H131	2.00	0.43
14:Q:222:PRO:O	14:Q:225:ASN:HB2	2.19	0.43
25:Q:603:CLA:NB	33:Q:608:CHL:C10	2.82	0.43
14:R:162:GLY:HA3	14:R:168:GLY:H	1.83	0.43
25:R:613:CLA:H111	25:R:613:CLA:H152	1.53	0.43
18:3:73:LEU:HG	25:3:301:CLA:HAA2	2.01	0.43
25:3:308:CLA:H142	25:3:308:CLA:H111	1.83	0.43
21:6:153:GLU:N	21:6:153:GLU:OE2	2.51	0.43
25:8:302:CLA:HBA1	25:8:302:CLA:H3A	1.65	0.43
25:a:308:CLA:O1D	25:a:308:CLA:H2A	2.18	0.43
1:A:356:ASN:O	1:A:360:PHE:HB2	2.19	0.43
2:B:53:GLY:O	2:B:56:SER:OG	2.27	0.43
2:B:722:TYR:HB2	25:B:801:CLA:HED3	2.00	0.43
25:B:838:CLA:H192	25:B:838:CLA:H161	1.75	0.43
28:B:840:BCR:H15C	28:B:840:BCR:H351	1.84	0.43
11:K:92:MET:HA	11:K:92:MET:HE3	2.01	0.43
14:P:30:ILE:HG21	15:S:169:PRO:CG	2.49	0.43
14:P:211:PHE:CE2	34:P:614:LUT:H8	2.54	0.43
25:P:610:CLA:CBB	25:P:612:CLA:CHB	2.97	0.43
25:R:603:CLA:NB	33:R:609:CHL:C10	2.80	0.43
14:T:152:MET:HA	14:T:155:VAL:HG22	2.01	0.43
16:1:59:PHE:HB3	25:1:602:CLA:C3D	2.48	0.43
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.82	0.43
25:A:823:CLA:H2A	11:K:61:THR:OG1	2.17	0.43
25:A:839:CLA:H91	25:A:839:CLA:H112	1.78	0.43
25:B:813:CLA:H11	25:B:813:CLA:H51	1.83	0.43
13:O:71:LEU:O	13:O:75:PHE:HE1	2.01	0.43
25:P:603:CLA:NB	33:P:609:CHL:H102	2.34	0.43
15:S:84:ARG:HE	15:S:177:LEU:HD11	1.84	0.43
15:S:244:PHE:CE2	14:T:145:LEU:HD22	2.54	0.43
14:T:76:LYS:HA	14:T:79:ARG:NH2	2.34	0.43
25:T:611:CLA:H122	35:T:615:XAT:H34	2.00	0.43
25:U:310:CLA:H91	25:U:310:CLA:H111	1.76	0.43
16:1:206:LEU:HD23	16:1:210:LEU:HD13	2.00	0.43
34:1:617:LUT:H201	34:1:617:LUT:H15	1.63	0.43
19:4:132:VAL:HG23	19:4:133:ALA:N	2.30	0.43
19:4:214:LYS:HG3	25:4:309:CLA:OBD	2.18	0.43
20:5:177:GLY:C	20:5:179:LEU:H	2.26	0.43
24:9:64:LYS:HD2	24:9:135:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:84:TRP:CE2	25:a:306:CLA:HED2	2.54	0.43
1:A:451:HIS:O	1:A:455:LEU:HG	2.19	0.43
25:A:825:CLA:H2	25:A:825:CLA:H62	1.70	0.43
2:B:499:LEU:HA	2:B:499:LEU:HD23	1.89	0.43
25:B:820:CLA:H92	25:B:820:CLA:H62	1.84	0.43
5:E:36:GLY:HA3	5:E:62:VAL:HG11	2.00	0.43
25:K:201:CLA:HBA2	25:K:201:CLA:H3A	1.66	0.43
14:Q:39:LYS:HD2	14:Q:45:SER:HB2	2.00	0.43
34:Q:614:LUT:H35	34:Q:614:LUT:H401	1.79	0.43
34:Q:615:LUT:H35	34:Q:615:LUT:H401	1.79	0.43
25:T:608:CLA:H51	25:T:610:CLA:HMA3	2.01	0.43
14:U:46:GLU:O	14:U:48:ALA:N	2.39	0.43
34:1:617:LUT:H35	34:1:617:LUT:H401	1.75	0.43
18:3:213:LEU:HD13	25:3:308:CLA:O1A	2.18	0.43
20:5:124:TRP:O	20:5:128:LEU:HD23	2.19	0.43
21:6:57:LEU:HD13	25:6:603:CLA:H42	2.01	0.43
23:8:151:GLY:N	23:8:157:GLU:OE1	2.52	0.43
24:9:30:THR:CG2	24:9:35:LEU:HD23	2.48	0.43
1:A:142:SER:OG	25:A:809:CLA:O1D	2.36	0.42
1:A:233:ASP:N	1:A:233:ASP:OD1	2.50	0.42
1:A:374:MET:HE3	1:A:374:MET:HB2	1.82	0.42
25:A:817:CLA:H93	25:A:817:CLA:H111	1.70	0.42
25:A:822:CLA:H202	28:A:847:BCR:H272	2.01	0.42
28:A:847:BCR:H24C	28:A:847:BCR:H371	1.78	0.42
28:B:842:BCR:H15C	28:B:842:BCR:H351	1.85	0.42
31:B:850:SQD:H341	31:B:850:SQD:H372	1.91	0.42
14:P:32:PHE:HE1	14:P:38:ALA:HB3	1.82	0.42
14:P:152:MET:HE2	14:P:152:MET:HA	2.01	0.42
14:P:159:ARG:HH21	33:P:609:CHL:HMA2	1.84	0.42
25:P:603:CLA:H202	25:P:603:CLA:H161	1.78	0.42
33:P:622:CHL:H41	33:P:622:CHL:H61	1.72	0.42
33:Q:605:CHL:HBB1	14:U:230:LEU:HD12	2.00	0.42
34:Q:615:LUT:H31	34:Q:615:LUT:H391	1.84	0.42
15:S:50:SER:HB2	15:S:54:THR:CG2	2.44	0.42
14:T:176:GLU:O	14:T:178:PHE:N	2.46	0.42
25:T:608:CLA:H91	25:T:608:CLA:H111	1.78	0.42
25:T:609:CLA:H3A	25:T:609:CLA:HBA1	1.29	0.42
27:2:317:LHG:H331	27:2:317:LHG:H361	1.74	0.42
1:A:528:LEU:HA	1:A:532:ASP:OD2	2.19	0.42
25:A:816:CLA:H101	28:3:319:BCR:H19C	2.01	0.42
28:A:845:BCR:H11C	28:A:845:BCR:H341	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:LYS:O	6:F:85:LYS:HD3	2.19	0.42
25:K:203:CLA:HBC2	25:K:203:CLA:HMC1	2.01	0.42
14:P:33:TYR:CZ	14:P:191:ALA:HB1	2.54	0.42
25:P:610:CLA:H72	25:P:612:CLA:HHB	1.97	0.42
25:3:302:CLA:H152	25:3:302:CLA:H112	1.71	0.42
28:4:317:BCR:H351	28:4:317:BCR:H15C	1.75	0.42
20:5:203:GLN:O	20:5:207:THR:HG22	2.19	0.42
25:5:316:CLA:HBA2	27:6:618:LHG:H372	2.01	0.42
28:5:323:BCR:H15C	28:5:323:BCR:H351	1.87	0.42
25:6:610:CLA:H62	25:6:610:CLA:H41	1.62	0.42
28:6:621:BCR:H11C	28:6:621:BCR:H341	1.67	0.42
25:7:310:CLA:HBC1	25:7:311:CLA:H201	2.01	0.42
25:7:311:CLA:H93	25:7:311:CLA:H61	1.76	0.42
34:9:313:LUT:H31	34:9:313:LUT:H391	1.87	0.42
16:a:99:GLY:O	16:a:100:TYR:HD1	2.01	0.42
16:a:100:TYR:HE2	16:a:119:PHE:HA	1.84	0.42
1:A:327:GLU:HG2	1:A:339:VAL:HG22	2.00	0.42
28:B:845:BCR:H15C	28:B:845:BCR:H351	1.89	0.42
7:G:91:ASP:OD2	7:G:95:PHE:HD2	2.03	0.42
12:L:44:SER:HB2	13:O:33:ASN:HB3	2.01	0.42
12:L:95:LEU:HD22	25:L:206:CLA:HBC2	2.00	0.42
35:P:616:XAT:H31	35:P:616:XAT:H391	1.76	0.42
36:P:621:NEX:H15	36:P:621:NEX:H201	1.70	0.42
14:Q:33:TYR:CZ	14:Q:191:ALA:HB1	2.54	0.42
25:Q:603:CLA:NC	33:Q:608:CHL:H102	2.34	0.42
14:R:212:PHE:C	33:R:609:CHL:H201	2.44	0.42
25:T:609:CLA:HAC1	27:T:617:LHG:H332	2.01	0.42
34:T:613:LUT:H35	34:T:613:LUT:H401	1.79	0.42
16:1:98:LEU:HD22	16:1:119:PHE:CE1	2.54	0.42
17:2:153:MET:HE1	17:2:156:LYS:HD2	2.00	0.42
25:2:303:CLA:H93	25:2:304:CLA:H93	2.00	0.42
18:3:183:ILE:HG21	18:3:183:ILE:HD13	1.73	0.42
16:a:106:ALA:O	16:a:109:TRP:CD1	2.72	0.42
1:A:21:PRO:HD2	1:A:182:HIS:O	2.20	0.42
1:A:197:MET:HE2	25:A:814:CLA:CHD	2.49	0.42
25:A:830:CLA:H193	25:A:830:CLA:H161	1.84	0.42
11:K:84:PHE:CZ	11:K:88:ASP:OD1	2.73	0.42
14:P:40:TRP:CD1	14:P:41:LEU:HG	2.54	0.42
14:P:196:LYS:HG2	25:P:611:CLA:HED3	1.98	0.42
14:Q:212:PHE:C	33:Q:608:CHL:H201	2.44	0.42
14:R:76:LYS:HA	14:R:79:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:603:CLA:HMD3	33:R:609:CHL:CBA	2.49	0.42
15:S:213:MET:HG2	34:S:317:LUT:H12	2.01	0.42
35:S:318:XAT:H191	35:S:318:XAT:H11	1.67	0.42
14:T:40:TRP:HH2	14:T:49:THR:HG22	1.83	0.42
35:T:615:XAT:H15	35:T:615:XAT:H201	1.76	0.42
14:U:43:PRO:O	14:U:44:TYR:HD1	2.02	0.42
25:3:314:CLA:HBC1	20:5:228:LEU:HD23	2.01	0.42
34:3:315:LUT:H35	34:3:315:LUT:H401	1.88	0.42
21:6:127:ARG:NH1	21:6:138:VAL:HB	2.35	0.42
24:9:81:VAL:HG11	34:9:312:LUT:H10	2.02	0.42
16:a:65:GLY:O	16:a:71:LEU:HD12	2.20	0.42
25:a:312:CLA:H2	25:a:312:CLA:H61	1.79	0.42
1:A:510:TRP:HZ2	25:A:827:CLA:HMC3	1.85	0.42
25:A:816:CLA:HBB1	28:A:854:BCR:C33	2.49	0.42
2:B:327:VAL:HG22	2:B:333:PHE:CE2	2.55	0.42
3:C:15:THR:OG1	3:C:19:ARG:NH1	2.52	0.42
8:H:44:MET:HE2	8:H:44:MET:HB2	1.89	0.42
10:J:9:SER:HA	10:J:14:ILE:HD11	2.01	0.42
14:P:97:ILE:HG13	14:P:98:THR:N	2.33	0.42
14:P:152:MET:HA	14:P:155:VAL:HG22	2.01	0.42
14:Q:32:PHE:CE2	25:Q:610:CLA:HED3	2.54	0.42
25:Q:611:CLA:H61	25:Q:611:CLA:H102	1.82	0.42
25:Q:612:CLA:H61	25:Q:612:CLA:H2	1.58	0.42
14:R:96:CYS:HB3	14:R:211:PHE:CE1	2.53	0.42
34:R:616:LUT:H31	34:R:616:LUT:H391	1.84	0.42
36:U:316:NEX:H401	36:U:316:NEX:H35	1.64	0.42
25:1:613:CLA:H112	25:1:613:CLA:H142	1.76	0.42
17:2:157:GLU:HB3	25:2:309:CLA:HMB2	2.01	0.42
17:2:206:GLU:OE2	25:2:314:CLA:CHD	2.67	0.42
28:4:317:BCR:H313	27:a:317:LHG:H111	2.01	0.42
20:5:200:PHE:HE1	34:5:318:LUT:H41	1.83	0.42
25:8:313:CLA:C4A	25:8:313:CLA:HBA2	2.49	0.42
34:a:314:LUT:H11	34:a:314:LUT:H191	1.88	0.42
25:A:840:CLA:H101	25:A:840:CLA:H13	1.88	0.42
28:A:849:BCR:H362	25:A:851:CLA:H42	2.01	0.42
2:B:588:ILE:HA	2:B:591:VAL:HG22	2.01	0.42
25:B:818:CLA:HBB1	28:B:840:BCR:H17C	2.00	0.42
25:H:201:CLA:HBA1	25:H:201:CLA:H3A	1.45	0.42
28:J:101:BCR:H11C	28:J:101:BCR:H341	1.93	0.42
14:P:76:LYS:HA	14:P:79:ARG:NH2	2.35	0.42
14:P:212:PHE:HD2	33:P:609:CHL:H18	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:32:PHE:HE2	25:Q:610:CLA:HED3	1.83	0.42
25:R:603:CLA:C4B	33:R:609:CHL:H122	2.50	0.42
25:R:603:CLA:C2	25:R:603:CLA:HMA1	2.49	0.42
25:R:611:CLA:HAC1	27:R:618:LHG:H332	2.02	0.42
25:S:303:CLA:CMC	34:S:317:LUT:H402	2.50	0.42
35:S:318:XAT:H35	35:S:318:XAT:H401	1.90	0.42
14:U:102:LEU:HD23	14:U:102:LEU:HA	1.90	0.42
16:1:64:LEU:HD13	25:1:602:CLA:H42	2.00	0.42
25:2:305:CLA:H41	25:2:305:CLA:H61	1.54	0.42
25:A:823:CLA:HBA2	25:A:823:CLA:H3A	1.13	0.42
34:R:615:LUT:H35	34:R:615:LUT:H401	1.77	0.42
14:T:129:TYR:CD2	14:T:130:LEU:HG	2.53	0.42
16:1:140:ALA:O	16:1:144:GLN:HG2	2.20	0.42
25:1:604:CLA:HMA2	25:1:605:CLA:CAC	2.50	0.42
25:1:610:CLA:HBC3	27:1:618:LHG:HC62	2.02	0.42
25:3:320:CLA:H62	25:3:320:CLA:H92	1.65	0.42
25:5:302:CLA:H161	25:5:302:CLA:H141	1.71	0.42
23:8:185:TRP:NE1	23:8:189:LYS:HE3	2.35	0.42
25:a:307:CLA:H3A	25:a:307:CLA:HBA2	1.55	0.42
25:A:803:CLA:H152	25:B:802:CLA:H192	2.01	0.42
25:A:814:CLA:H41	25:A:814:CLA:H61	1.55	0.42
6:F:145:HIS:O	6:F:148:GLU:HG2	2.19	0.42
25:P:611:CLA:HBC3	27:P:618:LHG:C33	2.47	0.42
14:Q:159:ARG:HH21	33:Q:608:CHL:HMA2	1.84	0.42
25:Q:611:CLA:H2	25:Q:611:CLA:H62	1.78	0.42
25:S:320:CLA:H112	25:S:320:CLA:H91	1.66	0.42
14:T:81:LEU:HG	14:T:85:HIS:CD2	2.54	0.42
14:U:192:GLU:O	14:U:196:LYS:HG3	2.19	0.42
17:2:151:GLU:C	17:2:153:MET:H	2.28	0.42
25:2:303:CLA:H112	25:2:303:CLA:H142	1.82	0.42
28:3:319:BCR:H20C	28:3:319:BCR:H361	1.62	0.42
22:7:128:MET:HB2	22:7:128:MET:HE2	1.83	0.42
34:7:314:LUT:H15	34:7:314:LUT:H201	1.85	0.42
25:8:302:CLA:H43	27:8:319:LHG:H142	2.01	0.42
25:a:303:CLA:HMA2	25:a:304:CLA:CAC	2.49	0.42
25:A:802:CLA:HBA2	2:B:428:LEU:HD23	2.02	0.42
25:A:828:CLA:H52	25:A:828:CLA:H8	1.64	0.42
25:A:830:CLA:H2A	25:A:830:CLA:O2D	2.20	0.42
25:A:837:CLA:O2D	25:A:837:CLA:H2A	2.20	0.42
25:B:831:CLA:HBB1	28:B:844:BCR:H332	2.01	0.42
8:H:60:LYS:HG3	15:S:187:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:57:THR:HG22	12:L:59:VAL:H	1.85	0.42
13:O:122:LYS:HE2	13:O:122:LYS:HB2	1.90	0.42
14:P:212:PHE:C	33:P:609:CHL:H201	2.44	0.42
25:Q:618:CLA:CHA	36:U:301:NEX:H163	2.49	0.42
25:S:303:CLA:H142	25:S:303:CLA:H112	1.84	0.42
19:4:111:VAL:CG1	34:4:315:LUT:H12	2.49	0.42
25:8:303:CLA:H102	25:8:303:CLA:H62	1.85	0.42
16:a:48:TRP:CD1	16:a:49:LEU:HD22	2.55	0.42
25:a:306:CLA:H141	25:a:306:CLA:H161	1.88	0.42
1:A:115:ALA:HB3	1:A:140:ILE:HG21	2.02	0.42
25:A:801:CLA:H2A	25:A:801:CLA:O1D	2.20	0.42
25:A:842:CLA:O1A	25:A:842:CLA:H3A	2.20	0.42
2:B:517:ASP:CG	2:B:594:TYR:HH	2.23	0.42
2:B:632:LEU:HD21	2:B:651:PHE:CG	2.55	0.42
2:B:644:LEU:HD12	2:B:728:ALA:HB1	2.00	0.42
25:P:603:CLA:C4B	33:P:609:CHL:C12	2.97	0.42
14:Q:121:ILE:HD13	14:Q:141:ILE:HB	2.01	0.42
14:Q:129:TYR:CD2	14:Q:130:LEU:HG	2.55	0.42
25:Q:618:CLA:HBD	36:U:301:NEX:C1	2.50	0.42
14:R:193:LEU:HD21	25:R:612:CLA:CGA	2.50	0.42
25:R:603:CLA:NC	33:R:609:CHL:H102	2.33	0.42
14:U:129:TYR:CD2	14:U:130:LEU:HG	2.55	0.42
25:U:311:CLA:H121	25:U:311:CLA:HMB3	2.02	0.42
17:2:185:THR:HB	25:2:312:CLA:HED2	2.02	0.42
20:5:187:ILE:HD12	20:5:187:ILE:HA	1.92	0.42
20:5:197:TYR:CD2	34:5:322:LUT:H12	2.55	0.42
28:7:316:BCR:H15C	28:7:316:BCR:H351	1.75	0.42
33:9:306:CHL:HHC	33:9:306:CHL:HBB1	2.01	0.42
25:A:825:CLA:H111	25:A:825:CLA:H142	1.75	0.41
2:B:185:GLY:HA3	2:B:286:ILE:HG13	2.02	0.41
14:P:43:PRO:CB	33:P:622:CHL:OMC	2.68	0.41
14:P:229:HIS:CE1	25:P:613:CLA:HBA1	2.55	0.41
33:P:606:CHL:CMB	33:P:609:CHL:HAC1	2.50	0.41
35:P:620:XAT:H12	27:R:618:LHG:H211	2.01	0.41
34:Q:614:LUT:H15	34:Q:614:LUT:H201	1.85	0.41
14:T:57:PHE:HB2	14:T:60:ASP:OD2	2.20	0.41
25:T:602:CLA:H93	25:T:602:CLA:H111	1.94	0.41
14:U:78:TYR:HB3	25:U:302:CLA:HMA1	2.02	0.41
16:1:93:LEU:HD21	16:1:191:PHE:HZ	1.84	0.41
16:1:118:TRP:CG	16:1:119:PHE:H	2.38	0.41
18:3:214:LYS:O	18:3:218:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:82:MET:SD	25:5:310:CLA:HAB	2.60	0.41
21:6:33:LEU:O	21:6:33:LEU:HD23	2.20	0.41
21:6:238:SER:HA	21:6:247:PRO:HA	2.02	0.41
33:6:608:CHL:HBA2	33:6:608:CHL:H3A	1.90	0.41
34:a:315:LUT:H31	34:a:315:LUT:H391	1.91	0.41
1:A:26:PHE:CD2	10:J:4:PHE:HB2	2.55	0.41
2:B:71:TRP:CZ2	9:I:71:PRO:HG2	2.55	0.41
2:B:86:ARG:NE	8:H:130:LEU:O	2.52	0.41
25:B:830:CLA:H18	25:B:834:CLA:H152	2.02	0.41
12:L:159:ASP:HB3	12:L:162:PHE:HD2	1.85	0.41
14:P:42:GLY:HA3	14:P:43:PRO:HD3	1.83	0.41
14:P:233:PRO:HB3	25:S:301:CLA:C2B	2.50	0.41
25:P:602:CLA:H172	25:P:602:CLA:H13	1.71	0.41
25:Q:603:CLA:C4B	33:Q:608:CHL:C11	2.97	0.41
25:S:304:CLA:H2	25:S:304:CLA:HMA2	2.02	0.41
27:S:319:LHG:H142	27:S:319:LHG:H171	1.74	0.41
14:T:33:TYR:CZ	14:T:191:ALA:HB1	2.56	0.41
14:U:93:ALA:HA	14:U:208:MET:HE1	2.02	0.41
17:2:156:LYS:CD	25:2:311:CLA:HAA2	2.50	0.41
25:2:304:CLA:H41	25:2:304:CLA:H61	1.63	0.41
25:2:304:CLA:H92	25:2:304:CLA:H62	1.81	0.41
25:3:314:CLA:H2	25:5:315:CLA:O2D	2.20	0.41
20:5:200:PHE:CD1	20:5:211:PRO:HB3	2.54	0.41
34:8:316:LUT:H35	34:8:316:LUT:H401	1.77	0.41
16:a:197:ALA:HA	16:a:223:ILE:CD1	2.39	0.41
1:A:459:ASN:OD1	1:A:472:PHE:N	2.44	0.41
1:A:481:PRO:HG3	1:A:533:PHE:HB2	2.02	0.41
25:A:811:CLA:H141	25:A:811:CLA:H162	1.85	0.41
25:A:818:CLA:C4A	25:A:818:CLA:HBA2	2.49	0.41
27:A:852:LHG:H121	27:A:852:LHG:H152	1.88	0.41
28:A:854:BCR:H11C	28:A:854:BCR:H341	1.92	0.41
25:B:826:CLA:H3A	25:B:826:CLA:HBA2	1.64	0.41
26:B:839:PQN:H162	28:B:845:BCR:H382	2.02	0.41
4:D:174:ARG:NH2	5:E:49:GLU:OE2	2.46	0.41
5:E:74:ARG:HG2	5:E:75:PHE:N	2.35	0.41
6:F:161:GLY:HA3	6:F:202:TRP:CZ2	2.56	0.41
7:G:79:ASP:O	7:G:79:ASP:CG	2.63	0.41
13:O:83:LEU:CD1	28:O:204:BCR:H323	2.50	0.41
33:Q:608:CHL:C15	33:Q:608:CHL:C19	2.94	0.41
14:T:58:PRO:HG3	14:T:194:LYS:HB3	2.02	0.41
25:U:303:CLA:H143	25:U:303:CLA:H111	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:176:LYS:HD3	25:1:611:CLA:HBA1	2.01	0.41
17:2:124:LYS:HD3	17:2:124:LYS:N	2.35	0.41
17:2:155:LEU:O	17:2:159:LYS:HB2	2.21	0.41
25:5:304:CLA:H3A	25:5:304:CLA:HBA1	1.85	0.41
25:5:306:CLA:HBA2	28:5:320:BCR:H19C	2.03	0.41
34:5:322:LUT:H15	34:5:322:LUT:H201	1.89	0.41
22:7:82:GLY:O	22:7:86:ILE:HG12	2.19	0.41
25:a:301:CLA:H2A	25:a:301:CLA:HED2	2.01	0.41
25:A:839:CLA:H61	25:A:839:CLA:H102	1.67	0.41
2:B:312:PRO:O	2:B:313:SER:OG	2.35	0.41
34:P:614:LUT:H11	34:P:614:LUT:H191	1.90	0.41
14:Q:179:ASP:OD1	34:Q:614:LUT:H24	2.20	0.41
14:Q:212:PHE:CD2	33:Q:608:CHL:H18	2.54	0.41
17:2:166:LEU:HD11	25:2:303:CLA:HBC1	2.01	0.41
18:3:100:LEU:HG	25:3:303:CLA:HAB	2.02	0.41
28:3:319:BCR:H24C	28:3:319:BCR:H371	1.73	0.41
19:4:103:ASN:C	19:4:223:MET:HE2	2.45	0.41
33:4:322:CHL:H3A	33:4:322:CHL:HBA2	1.70	0.41
21:6:103:GLU:HB3	21:6:104:VAL:H	1.71	0.41
33:6:606:CHL:HBB1	33:6:606:CHL:HHC	2.02	0.41
23:8:136:LYS:HB3	23:8:136:LYS:HE3	1.52	0.41
34:8:316:LUT:H27	34:8:316:LUT:H361	1.91	0.41
1:A:333:PHE:HD2	27:A:844:LHG:HC5	1.85	0.41
25:A:808:CLA:H2A	25:A:810:CLA:HED1	2.02	0.41
25:A:826:CLA:OBD	25:A:835:CLA:HBB1	2.19	0.41
2:B:85:ILE:HG23	8:H:130:LEU:HD22	2.02	0.41
2:B:510:PHE:CE1	25:B:833:CLA:HED1	2.54	0.41
4:D:154:ASP:OD2	4:D:165:ARG:NE	2.32	0.41
5:E:72:VAL:HG22	5:E:87:ASN:OD1	2.20	0.41
14:P:169:LEU:HD12	14:P:170:ASP:CG	2.46	0.41
25:P:611:CLA:HMA2	36:P:621:NEX:C7	2.51	0.41
14:Q:212:PHE:HD2	33:Q:608:CHL:H18	1.84	0.41
25:Q:602:CLA:H193	25:Q:602:CLA:H161	1.85	0.41
25:R:603:CLA:H91	25:R:603:CLA:H112	1.71	0.41
25:S:304:CLA:C9	25:U:302:CLA:H102	2.51	0.41
14:U:76:LYS:HA	14:U:79:ARG:NH2	2.35	0.41
22:7:216:LEU:O	22:7:216:LEU:HD23	2.20	0.41
25:a:306:CLA:H2	25:a:306:CLA:H62	1.85	0.41
1:A:213:TRP:HE1	1:A:217:GLN:NE2	2.18	0.41
25:A:809:CLA:H2	25:A:828:CLA:H92	2.01	0.41
25:A:832:CLA:H202	28:L:207:BCR:H10C	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:837:CLA:H41	25:B:837:CLA:H61	1.66	0.41
28:G:203:BCR:H11C	28:G:203:BCR:H341	1.88	0.41
8:H:104:LYS:N	8:H:104:LYS:HD2	2.36	0.41
32:J:102:LMG:H152	32:J:102:LMG:H182	1.78	0.41
14:Q:142:VAL:HG23	25:U:313:CLA:CBB	2.51	0.41
25:Q:610:CLA:HAC1	27:Q:617:LHG:H332	2.03	0.41
15:S:95:MET:HE2	15:S:206:GLY:CA	2.51	0.41
14:U:169:LEU:HD12	14:U:170:ASP:CG	2.46	0.41
16:1:86:MET:HE2	16:1:180:ASN:HB3	2.01	0.41
25:1:607:CLA:H141	25:1:607:CLA:H161	1.85	0.41
25:1:613:CLA:H2	25:1:613:CLA:H61	1.83	0.41
17:2:124:LYS:HB2	17:2:124:LYS:HE2	1.55	0.41
17:2:154:LYS:HA	17:2:157:GLU:OE1	2.21	0.41
17:2:161:GLY:O	17:2:165:MET:HG3	2.20	0.41
28:3:317:BCR:H24C	28:3:317:BCR:H21C	1.80	0.41
19:4:58:LEU:N	19:4:59:PRO:CD	2.84	0.41
25:5:302:CLA:H91	25:5:302:CLA:H111	1.75	0.41
34:8:316:LUT:H31	34:8:316:LUT:H391	1.95	0.41
1:A:263:PRO:HB2	1:A:272:TYR:CZ	2.55	0.41
1:A:485:GLN:NE2	1:A:528:LEU:O	2.49	0.41
1:A:561:ARG:NH1	4:D:72:GLY:HA2	2.35	0.41
2:B:303:GLN:O	2:B:307:GLU:HG2	2.21	0.41
2:B:307:GLU:OE1	2:B:321:LYS:HD2	2.20	0.41
30:B:846:DGD:HA21	30:B:846:DGD:HA51	1.89	0.41
25:P:611:CLA:CBC	27:P:618:LHG:C33	2.92	0.41
33:P:622:CHL:HBB1	33:P:622:CHL:HHC	2.01	0.41
15:S:26:LYS:C	15:S:28:ALA:H	2.28	0.41
15:S:244:PHE:HE2	14:T:145:LEU:HD22	1.86	0.41
34:S:317:LUT:H15	34:S:317:LUT:H201	1.86	0.41
14:T:80:GLU:O	14:T:84:ILE:HG12	2.20	0.41
14:U:176:GLU:O	14:U:178:PHE:N	2.48	0.41
16:1:170:SER:OG	16:1:174:LYS:NZ	2.54	0.41
32:1:619:LMG:H252	32:1:619:LMG:H221	1.87	0.41
17:2:206:GLU:HG3	17:2:207:THR:N	2.36	0.41
25:5:324:CLA:HBA2	25:5:324:CLA:H3A	1.52	0.41
1:A:26:PHE:HD2	10:J:4:PHE:HB2	1.86	0.41
25:B:823:CLA:H142	25:B:823:CLA:H112	1.89	0.41
6:F:92:LYS:HE3	6:F:92:LYS:HB2	1.62	0.41
35:P:623:XAT:H201	35:P:623:XAT:H15	1.76	0.41
14:Q:94:LEU:HD22	25:Q:604:CLA:CMC	2.50	0.41
14:Q:169:LEU:HD12	14:Q:170:ASP:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:179:ASP:OD1	34:R:615:LUT:H24	2.21	0.41
25:R:610:CLA:CBB	25:R:612:CLA:CHB	2.99	0.41
15:S:188:LEU:O	15:S:195:PHE:HZ	2.04	0.41
15:S:208:LEU:HD21	25:S:312:CLA:HAC2	2.02	0.41
25:T:610:CLA:H121	25:T:610:CLA:HMB3	2.03	0.41
34:T:613:LUT:H27	34:T:613:LUT:H361	1.84	0.41
14:U:81:LEU:HD12	33:U:309:CHL:OBD	2.20	0.41
16:1:72:LYS:O	16:1:75:THR:OG1	2.37	0.41
25:2:314:CLA:C4A	25:2:314:CLA:HBA2	2.51	0.41
21:6:162:ALA:HB2	25:6:610:CLA:HBD	2.03	0.41
25:6:611:CLA:H41	25:6:611:CLA:H61	1.53	0.41
34:6:622:LUT:H15	34:6:622:LUT:H201	1.85	0.41
23:8:88:LEU:O	23:8:92:LEU:N	2.45	0.41
25:a:302:CLA:H61	25:a:302:CLA:H41	1.92	0.41
1:A:217:GLN:HA	1:A:221:SER:HB2	2.02	0.41
1:A:294:THR:HG23	25:A:820:CLA:HMA3	2.03	0.41
1:A:491:HIS:HB2	1:A:510:TRP:CE3	2.55	0.41
25:A:802:CLA:H41	25:A:802:CLA:H62	1.60	0.41
2:B:86:ARG:HG2	8:H:129:ARG:NH2	2.32	0.41
2:B:174:SER:O	2:B:178:HIS:ND1	2.44	0.41
2:B:223:LEU:N	2:B:223:LEU:HD12	2.34	0.41
2:B:450:PRO:HD2	6:F:83:GLU:OE2	2.20	0.41
2:B:465:GLN:NE2	25:B:833:CLA:OBD	2.50	0.41
25:B:805:CLA:H161	25:B:805:CLA:H192	1.84	0.41
25:B:805:CLA:H71	25:B:805:CLA:H111	1.85	0.41
25:B:810:CLA:H142	34:9:313:LUT:H363	2.03	0.41
25:B:834:CLA:H3A	25:B:834:CLA:HBA2	1.82	0.41
25:B:836:CLA:H13	28:I:201:BCR:H21C	2.03	0.41
28:B:842:BCR:H24C	28:B:842:BCR:H371	1.59	0.41
31:B:850:SQD:H241	31:B:850:SQD:H271	1.76	0.41
4:D:189:ARG:HH22	4:D:191:MET:HG3	1.85	0.41
28:F:803:BCR:H341	28:F:803:BCR:H11C	1.64	0.41
7:G:76:TYR:CZ	7:G:80:LEU:HD11	2.55	0.41
12:L:165:ASP:OD1	12:L:165:ASP:C	2.62	0.41
13:O:89:GLY:HA2	13:O:90:PRO:HD3	1.93	0.41
14:P:57:PHE:HB2	14:P:60:ASP:OD2	2.20	0.41
14:P:78:TYR:HB3	25:P:602:CLA:HMA1	2.01	0.41
14:P:108:GLN:N	14:P:108:GLN:OE1	2.54	0.41
14:P:212:PHE:CA	33:P:609:CHL:C20	2.85	0.41
14:R:33:TYR:CE2	14:R:191:ALA:HB1	2.55	0.41
33:R:606:CHL:CMB	33:R:609:CHL:HAC1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:618:LHG:H142	27:R:618:LHG:H171	1.76	0.41
15:S:83:TYR:HB3	25:S:303:CLA:HMA1	2.03	0.41
14:T:179:ASP:OD1	34:T:613:LUT:H24	2.20	0.41
14:U:58:PRO:HG3	14:U:194:LYS:HB3	2.03	0.41
36:U:301:NEX:H11	36:U:301:NEX:H191	1.67	0.41
36:U:316:NEX:H15	36:U:316:NEX:H201	1.86	0.41
16:1:87:LEU:HD23	16:1:87:LEU:HA	1.91	0.41
16:1:134:GLU:O	16:1:138:MET:HG2	2.21	0.41
17:2:52:ASP:OD1	34:2:316:LUT:O23	2.33	0.41
17:2:64:LYS:HE3	17:2:64:LYS:HB3	1.95	0.41
25:2:312:CLA:H93	25:2:312:CLA:H62	1.82	0.41
18:3:148:PHE:O	18:3:152:ILE:HG12	2.21	0.41
19:4:226:PHE:CE2	19:4:230:ILE:HD11	2.55	0.41
34:4:315:LUT:H31	34:4:315:LUT:H391	1.91	0.41
20:5:234:CYS:SG	20:5:253:TRP:NE1	2.94	0.41
22:7:147:ASP:OD1	22:7:148:GLY:N	2.54	0.41
34:9:312:LUT:H35	34:9:312:LUT:H401	1.75	0.41
16:a:123:VAL:HG11	25:a:304:CLA:HMD1	2.03	0.41
25:a:301:CLA:H61	25:a:301:CLA:H92	1.65	0.41
2:B:326:THR:HG21	2:B:404:ASN:HD21	1.86	0.41
2:B:621:LEU:HD12	2:B:625:LEU:HD12	2.02	0.41
25:B:812:CLA:H2	28:B:842:BCR:H362	2.02	0.41
28:B:851:BCR:H11C	28:B:851:BCR:H341	1.97	0.41
6:F:67:LEU:HD12	6:F:68:THR:N	2.36	0.41
6:F:185:ILE:HG23	6:F:186:ILE:HG13	2.03	0.41
14:P:208:MET:SD	34:P:615:LUT:H10	2.61	0.41
14:R:108:GLN:OE1	14:R:108:GLN:N	2.54	0.41
25:S:320:CLA:H2	25:S:320:CLA:H61	1.87	0.41
25:T:610:CLA:H62	25:T:610:CLA:H2	1.76	0.41
16:1:65:GLY:O	16:1:71:LEU:HD12	2.20	0.41
17:2:189:HIS:CD2	17:2:190:LEU:HD22	2.56	0.41
25:3:307:CLA:HBA2	25:3:307:CLA:H3A	1.44	0.41
19:4:108:MET:CE	25:4:308:CLA:HAB	2.51	0.41
25:6:605:CLA:H171	33:6:608:CHL:HBA1	2.03	0.41
34:6:619:LUT:H15	34:6:619:LUT:H201	1.80	0.41
34:a:315:LUT:H35	34:a:315:LUT:H401	1.86	0.41
25:B:807:CLA:C4A	25:B:807:CLA:HBA2	2.51	0.40
28:B:845:BCR:H20C	28:B:845:BCR:H361	1.84	0.40
6:F:195:LEU:HD23	6:F:195:LEU:HA	1.91	0.40
14:P:145:LEU:O	14:P:149:VAL:HG23	2.21	0.40
14:P:230:LEU:HD13	33:S:306:CHL:CMB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:603:CLA:C4B	33:P:609:CHL:C11	2.99	0.40
35:P:620:XAT:H35	35:P:620:XAT:H401	1.79	0.40
35:P:623:XAT:H401	35:P:623:XAT:H35	1.79	0.40
14:Q:76:LYS:HA	14:Q:79:ARG:NH2	2.35	0.40
14:Q:78:TYR:HB3	25:Q:602:CLA:HMA1	2.01	0.40
14:Q:230:LEU:HD21	25:Q:613:CLA:HMC3	2.02	0.40
14:R:143:ALA:HB3	33:R:605:CHL:HMC	2.02	0.40
34:R:615:LUT:H15	34:R:615:LUT:H201	1.80	0.40
25:S:314:CLA:C1D	25:S:314:CLA:H42	2.51	0.40
25:4:307:CLA:HHC	25:4:307:CLA:HBB1	2.02	0.40
22:7:222:HIS:CG	25:7:311:CLA:HAA2	2.57	0.40
28:7:316:BCR:H11C	28:7:316:BCR:H341	1.87	0.40
23:8:236:ASN:ND2	25:8:313:CLA:OBD	2.54	0.40
24:9:121:PHE:O	24:9:122:LEU:C	2.64	0.40
24:9:135:THR:O	24:9:135:THR:HG22	2.21	0.40
24:9:169:PHE:CE2	34:9:313:LUT:H12	2.55	0.40
16:a:93:LEU:C	16:a:97:LEU:HD13	2.46	0.40
16:a:93:LEU:O	16:a:97:LEU:HD13	2.20	0.40
1:A:509:THR:CG2	1:A:523:MET:HE2	2.51	0.40
2:B:430:LEU:HD23	2:B:430:LEU:HA	1.93	0.40
4:D:189:ARG:HH22	4:D:191:MET:CG	2.34	0.40
12:L:69:LEU:HD23	12:L:69:LEU:HA	1.91	0.40
12:L:72:LEU:HD23	12:L:72:LEU:HA	1.80	0.40
33:P:609:CHL:C15	33:P:609:CHL:C19	2.94	0.40
25:P:612:CLA:HMB3	34:P:614:LUT:C32	2.51	0.40
14:Q:80:GLU:O	14:Q:84:ILE:HG12	2.21	0.40
25:Q:603:CLA:H202	25:Q:603:CLA:H161	1.77	0.40
25:Q:612:CLA:C3	35:Q:616:XAT:H203	2.51	0.40
14:R:222:PRO:O	14:R:225:ASN:HB2	2.21	0.40
34:S:316:LUT:H11	34:S:316:LUT:H191	1.93	0.40
14:U:179:ASP:OD1	34:U:314:LUT:H24	2.21	0.40
36:U:301:NEX:H15	36:U:301:NEX:H201	1.89	0.40
18:3:237:MET:HE2	18:3:261:ASN:O	2.22	0.40
33:4:306:CHL:OMC	33:4:314:CHL:HMC	2.21	0.40
20:5:200:PHE:CE1	20:5:211:PRO:HB3	2.56	0.40
22:7:230:ASN:HB2	25:7:312:CLA:HED1	2.02	0.40
25:7:313:CLA:HBA2	25:7:313:CLA:H3A	1.64	0.40
23:8:123:LEU:HA	23:8:126:GLN:HG2	2.03	0.40
1:A:510:TRP:CD1	1:A:510:TRP:H	2.39	0.40
25:A:808:CLA:CBB	28:J:106:BCR:HC32	2.51	0.40
28:A:854:BCR:H323	28:A:854:BCR:HC31	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:PRO:HG2	27:B:847:LHG:HC31	2.03	0.40
28:B:844:BCR:H15C	28:B:844:BCR:H351	1.73	0.40
13:O:56:THR:HA	13:O:59:ALA:HB3	2.03	0.40
13:O:94:ASP:OD2	13:O:96:PHE:HE1	2.05	0.40
25:P:613:CLA:C3	35:P:616:XAT:H203	2.51	0.40
34:P:615:LUT:H31	34:P:615:LUT:H391	1.83	0.40
14:R:40:TRP:CD1	14:R:41:LEU:HG	2.56	0.40
15:S:99:LEU:HD23	15:S:102:LEU:HD12	2.03	0.40
34:S:317:LUT:H31	34:S:317:LUT:H391	1.72	0.40
14:U:76:LYS:HB2	14:U:79:ARG:HH21	1.86	0.40
14:U:196:LYS:CG	36:U:301:NEX:H173	2.47	0.40
34:U:315:LUT:H35	34:U:315:LUT:H401	1.84	0.40
16:1:214:TRP:HB3	23:8:117:ALA:HB2	2.04	0.40
17:2:102:LYS:HA	17:2:102:LYS:HD3	1.83	0.40
18:3:61:LEU:N	18:3:62:PRO:HD3	2.36	0.40
18:3:259:LEU:H	18:3:259:LEU:HD23	1.87	0.40
25:3:303:CLA:H141	25:3:303:CLA:H162	1.77	0.40
34:4:315:LUT:H35	34:4:315:LUT:H401	1.75	0.40
25:5:303:CLA:CGA	25:5:303:CLA:H3A	2.52	0.40
25:5:324:CLA:O1D	25:5:324:CLA:H2A	2.21	0.40
25:7:309:CLA:H2A	25:7:309:CLA:O2D	2.20	0.40
1:A:619:TRP:O	1:A:629:HIS:ND1	2.43	0.40
25:A:819:CLA:H3A	25:A:819:CLA:HBA2	1.59	0.40
2:B:604:GLN:CG	2:B:734:PHE:HZ	2.35	0.40
25:B:823:CLA:H141	25:B:823:CLA:H162	1.82	0.40
13:O:79:ILE:HD13	13:O:79:ILE:HG21	1.91	0.40
14:P:143:ALA:HB3	33:P:605:CHL:HMC	2.04	0.40
33:P:622:CHL:HMB2	33:S:310:CHL:HAB	2.03	0.40
14:Q:152:MET:HE1	36:U:301:NEX:H30	2.02	0.40
25:Q:611:CLA:H122	25:Q:611:CLA:H8	1.86	0.40
35:Q:616:XAT:H11	35:Q:616:XAT:H191	1.94	0.40
14:R:163:GLY:HA3	14:R:164:PRO:HD2	1.96	0.40
25:T:602:CLA:H193	25:T:602:CLA:H161	1.90	0.40
25:T:609:CLA:H61	25:T:609:CLA:H41	1.82	0.40
34:1:615:LUT:H11	34:1:615:LUT:H191	1.95	0.40
20:5:178:ASN:C	20:5:180:LYS:H	2.29	0.40
16:a:126:ASP:OD1	16:a:127:LEU:N	2.51	0.40
1:A:497:LEU:HD21	13:O:66:PHE:HE1	1.85	0.40
1:A:552:LYS:HD3	2:B:671:TYR:HE1	1.86	0.40
25:B:832:CLA:HBA2	25:B:832:CLA:H3A	1.61	0.40
28:B:843:BCR:H11C	28:B:843:BCR:H341	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:58:PRO:HG3	14:P:194:LYS:HB3	2.04	0.40
25:P:603:CLA:HMA1	25:P:603:CLA:C2	2.50	0.40
25:S:304:CLA:HMD3	33:S:310:CHL:HBA2	2.04	0.40
33:S:307:CHL:HMB1	33:S:310:CHL:HAC1	2.04	0.40
14:T:93:ALA:HA	14:T:208:MET:SD	2.61	0.40
33:T:601:CHL:HHC	33:T:601:CHL:HBB1	2.02	0.40
34:U:315:LUT:H15	34:U:315:LUT:H201	1.86	0.40
16:1:80:ILE:HD13	16:1:80:ILE:HA	1.87	0.40
25:1:613:CLA:H112	25:1:613:CLA:H91	1.86	0.40
17:2:114:GLU:CD	25:2:306:CLA:C1B	2.87	0.40
33:4:322:CHL:HAB	16:a:59:PHE:CD2	2.56	0.40
34:7:314:LUT:H27	34:7:314:LUT:H361	1.91	0.40
24:9:105:ASP:OD1	24:9:105:ASP:N	2.54	0.40
16:a:118:TRP:CE2	25:a:303:CLA:O2A	2.75	0.40
25:a:312:CLA:H142	25:a:312:CLA:H112	1.76	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%)	698 (95%)	39 (5%)	1 (0%)	48 78
2	B	732/734 (100%)	675 (92%)	56 (8%)	1 (0%)	48 78
3	C	78/80 (98%)	73 (94%)	5 (6%)	0	100 100
4	D	142/144 (99%)	127 (89%)	15 (11%)	0	100 100
5	E	61/63 (97%)	56 (92%)	5 (8%)	0	100 100
6	F	163/165 (99%)	152 (93%)	11 (7%)	0	100 100
7	G	89/91 (98%)	83 (93%)	6 (7%)	0	100 100
8	H	98/100 (98%)	77 (79%)	18 (18%)	3 (3%)	3 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
11	K	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
12	L	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
13	O	91/93 (98%)	76 (84%)	15 (16%)	0	100	100
14	P	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	Q	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	R	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	T	217/219 (99%)	190 (88%)	27 (12%)	0	100	100
14	U	217/219 (99%)	190 (88%)	27 (12%)	0	100	100
15	S	230/234 (98%)	192 (84%)	36 (16%)	2 (1%)	14	41
16	1	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
16	a	192/194 (99%)	175 (91%)	16 (8%)	1 (0%)	24	54
17	2	199/201 (99%)	169 (85%)	28 (14%)	2 (1%)	12	39
18	3	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
19	4	203/205 (99%)	186 (92%)	16 (8%)	1 (0%)	24	54
20	5	223/225 (99%)	200 (90%)	23 (10%)	0	100	100
21	6	228/230 (99%)	209 (92%)	16 (7%)	3 (1%)	9	33
22	7	210/213 (99%)	195 (93%)	15 (7%)	0	100	100
23	8	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
24	9	180/182 (99%)	154 (86%)	25 (14%)	1 (1%)	21	49
All	All	5864/5925 (99%)	5297 (90%)	552 (9%)	15 (0%)	37	65

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
21	6	104	VAL
8	H	106	ALA
19	4	143	PHE
15	S	54	THR
21	6	103	GLU
21	6	29	ARG
16	a	119	PHE
17	2	176	ALA

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Mol	Chain	Res	Type
17	2	177	VAL
8	H	107	ASP
8	H	108	LEU
2	B	85	ILE
15	S	47	GLY
24	9	107	PRO

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	600/600 (100%)	600 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	68/68 (100%)	68 (100%)	0	100	100
8	H	80/81 (99%)	80 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/59 (100%)	59 (100%)	0	100	100
12	L	121/121 (100%)	121 (100%)	0	100	100
13	O	75/75 (100%)	75 (100%)	0	100	100
14	P	168/170 (99%)	168 (100%)	0	100	100
14	Q	168/170 (99%)	168 (100%)	0	100	100
14	R	168/170 (99%)	168 (100%)	0	100	100
14	T	168/170 (99%)	168 (100%)	0	100	100
14	U	168/170 (99%)	168 (100%)	0	100	100
15	S	164/177 (93%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1	137/137 (100%)	137 (100%)	0	100 100
16	a	137/137 (100%)	137 (100%)	0	100 100
17	2	159/159 (100%)	159 (100%)	0	100 100
18	3	155/155 (100%)	155 (100%)	0	100 100
19	4	161/162 (99%)	161 (100%)	0	100 100
20	5	182/182 (100%)	181 (100%)	1 (0%)	81 80
21	6	184/184 (100%)	184 (100%)	0	100 100
22	7	164/164 (100%)	163 (99%)	1 (1%)	78 80
23	8	163/163 (100%)	163 (100%)	0	100 100
24	9	139/140 (99%)	139 (100%)	0	100 100
All	All	4623/4649 (99%)	4621 (100%)	2 (0%)	100 100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	5	159	ASN
22	7	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	110	HIS
1	A	217	GLN
1	A	225	ASN
1	A	241	HIS
1	A	489	ASN
2	B	133	ASN
2	B	219	HIS
2	B	453	GLN
2	B	506	GLN
4	D	120	GLN
4	D	148	GLN
4	D	180	ASN
6	F	132	HIS
7	G	81	GLN
8	H	66	GLN

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Mol	Chain	Res	Type
12	L	47	ASN
14	P	237	ASN
14	Q	85	HIS
14	Q	148	GLN
14	Q	237	ASN
14	R	120	GLN
14	R	237	ASN
15	S	110	ASN
15	S	153	GLN
15	S	230	ASN
15	S	234	HIS
14	T	237	ASN
14	U	148	GLN
14	U	237	ASN
16	1	56	ASN
17	2	62	ASN
18	3	202	ASN
18	3	220	ASN
18	3	257	ASN
19	4	218	ASN
20	5	117	ASN
20	5	142	ASN
20	5	189	ASN
20	5	205	GLN
22	7	113	ASN
22	7	193	ASN
23	8	126	GLN
23	8	147	GLN
23	8	195	ASN
23	8	209	GLN
24	9	40	HIS
24	9	128	GLN
24	9	140	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	TPO	S	23	15	8,10,11	0.88	0	10,14,16	1.70	1 (10%)

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
15	TPO	S	23	15	-	3/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	S	23	TPO	P-OG1-CB	-4.90	108.41	123.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	S	23	TPO	N-CA-CB-OG1
15	S	23	TPO	C-CA-CB-CG2
15	S	23	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

453 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	4	301	-	64,68,73	1.30	12 (18%)	77,107,113	1.35	6 (7%)
33	CHL	R	608	-	48,52,74	2.18	17 (35%)	53,87,114	3.18	24 (45%)
33	CHL	Q	607	-	48,52,74	2.18	18 (37%)	53,87,114	3.19	24 (45%)
25	CLA	8	310	-	64,68,73	1.31	10 (15%)	77,107,113	1.32	7 (9%)
25	CLA	A	811	1	69,73,73	1.26	10 (14%)	83,113,113	1.41	7 (8%)
25	CLA	R	602	-	69,73,73	1.27	8 (11%)	83,113,113	1.29	9 (10%)
27	LHG	B	847	32	37,37,48	1.03	2 (5%)	40,43,54	1.20	5 (12%)
25	CLA	1	609	16	64,68,73	1.26	13 (20%)	77,107,113	1.63	11 (14%)
25	CLA	Q	613	-	52,56,73	1.48	8 (15%)	62,92,113	1.46	8 (12%)
33	CHL	P	605	14	52,56,74	2.22	20 (38%)	58,92,114	3.24	27 (46%)
25	CLA	T	610	-	64,68,73	1.32	8 (12%)	77,107,113	1.37	6 (7%)
25	CLA	S	301	15	51,55,73	1.48	8 (15%)	61,91,113	1.64	10 (16%)
25	CLA	2	309	-	64,68,73	1.31	11 (17%)	77,107,113	1.35	7 (9%)
25	CLA	1	614	-	50,54,73	1.45	10 (20%)	60,90,113	1.50	6 (10%)
25	CLA	7	307	-	54,58,73	1.40	10 (18%)	65,95,113	1.43	4 (6%)
25	CLA	5	302	20	69,73,73	1.27	11 (15%)	83,113,113	1.37	8 (9%)
33	CHL	5	317	-	47,51,74	2.11	18 (38%)	52,86,114	3.32	24 (46%)
33	CHL	8	307	23	57,61,74	2.07	19 (33%)	64,98,114	3.32	30 (46%)
35	XAT	S	318	-	39,47,47	0.98	1 (2%)	54,74,74	2.87	22 (40%)
27	LHG	5	321	-	36,36,48	1.03	2 (5%)	39,42,54	1.29	5 (12%)
25	CLA	1	611	-	56,60,73	1.41	11 (19%)	67,97,113	1.39	7 (10%)
28	BCR	A	845	-	41,41,41	0.83	1 (2%)	56,56,56	2.08	21 (37%)
36	NEX	R	617	-	38,46,46	0.98	1 (2%)	50,70,70	2.79	19 (38%)
27	LHG	A	843	-	48,48,48	0.90	2 (4%)	51,54,54	1.13	3 (5%)
25	CLA	S	312	15	64,68,73	1.30	8 (12%)	77,107,113	1.32	7 (9%)
25	CLA	a	304	-	56,60,73	1.42	9 (16%)	67,97,113	1.30	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	BCR	3	317	-	41,41,41	0.94	2 (4%)	56,56,56	2.33	17 (30%)
25	CLA	7	308	-	64,68,73	1.35	12 (18%)	77,107,113	1.37	8 (10%)
33	CHL	S	302	-	57,61,74	2.03	19 (33%)	64,98,114	3.09	29 (45%)
28	BCR	G	203	28	41,41,41	0.84	1 (2%)	56,56,56	2.09	16 (28%)
33	CHL	U	309	-	52,56,74	2.31	18 (34%)	58,92,114	3.06	24 (41%)
25	CLA	5	306	-	59,63,73	1.35	11 (18%)	71,101,113	1.36	6 (8%)
25	CLA	B	812	2	64,68,73	1.31	10 (15%)	77,107,113	1.36	6 (7%)
28	BCR	B	843	-	41,41,41	0.86	2 (4%)	56,56,56	1.86	18 (32%)
33	CHL	R	605	14	50,54,74	2.26	19 (38%)	56,90,114	3.23	27 (48%)
25	CLA	A	823	-	53,57,73	1.42	11 (20%)	62,93,113	1.53	8 (12%)
32	LMG	J	104	-	35,35,55	1.06	2 (5%)	43,43,63	1.25	5 (11%)
25	CLA	B	827	2	69,73,73	1.27	10 (14%)	83,113,113	1.34	9 (10%)
25	CLA	A	805	1	59,63,73	1.38	11 (18%)	71,101,113	1.44	5 (7%)
25	CLA	B	806	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
25	CLA	B	831	2	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
25	CLA	Q	618	14	43,48,73	1.63	10 (23%)	52,82,113	1.75	10 (19%)
25	CLA	B	820	2	63,67,73	1.31	10 (15%)	75,105,113	1.44	7 (9%)
32	LMG	4	320	-	40,40,55	1.06	3 (7%)	48,48,63	1.30	6 (12%)
25	CLA	G	201	-	54,58,73	1.41	10 (18%)	65,95,113	1.44	8 (12%)
25	CLA	A	822	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	8 (9%)
25	CLA	B	817	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	8 (9%)
25	CLA	6	620	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	7 (11%)
25	CLA	B	808	2	69,73,73	1.28	11 (15%)	83,113,113	1.35	9 (10%)
34	LUT	1	615	-	42,43,43	0.96	2 (4%)	51,60,60	1.87	16 (31%)
34	LUT	S	317	-	42,43,43	0.77	0	51,60,60	1.65	9 (17%)
27	LHG	A	844	25	37,37,48	1.05	3 (8%)	40,43,54	1.20	3 (7%)
25	CLA	A	814	1	69,73,73	1.32	11 (15%)	83,113,113	1.43	9 (10%)
34	LUT	R	615	-	42,43,43	0.76	0	51,60,60	1.93	14 (27%)
33	CHL	1	606	-	52,56,74	2.20	20 (38%)	58,92,114	2.95	23 (39%)
25	CLA	S	304	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
34	LUT	2	316	-	42,43,43	0.86	1 (2%)	51,60,60	1.66	13 (25%)
28	BCR	A	854	-	41,41,41	0.88	1 (2%)	56,56,56	1.96	16 (28%)
34	LUT	9	312	-	42,43,43	0.84	2 (4%)	51,60,60	1.60	13 (25%)
28	BCR	K	206	-	41,41,41	0.81	0	56,56,56	2.35	20 (35%)
25	CLA	7	311	-	69,73,73	1.26	11 (15%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	SF4	C	102	3	0,12,12	-	-	-		
28	BCR	7	316	-	41,41,41	0.89	1 (2%)	56,56,56	2.00	16 (28%)
28	BCR	L	203	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	15 (26%)
25	CLA	6	605	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	6 (7%)
28	BCR	5	320	-	41,41,41	0.82	1 (2%)	56,56,56	1.92	16 (28%)
25	CLA	1	610	27	69,73,73	1.26	10 (14%)	83,113,113	1.24	7 (8%)
25	CLA	A	821	1	49,53,73	1.49	10 (20%)	59,89,113	1.66	10 (16%)
25	CLA	B	833	-	64,68,73	1.32	11 (17%)	77,107,113	1.35	8 (10%)
33	CHL	6	617	21	47,51,74	2.15	18 (38%)	52,86,114	3.30	24 (46%)
34	LUT	2	315	-	42,43,43	0.83	1 (2%)	51,60,60	1.84	13 (25%)
33	CHL	5	307	-	55,59,74	2.09	20 (36%)	62,96,114	3.10	28 (45%)
27	LHG	4	319	-	31,31,48	1.13	2 (6%)	34,37,54	1.23	4 (11%)
25	CLA	a	310	-	56,60,73	1.40	10 (17%)	67,97,113	1.39	4 (5%)
25	CLA	4	309	27	59,63,73	1.36	9 (15%)	71,101,113	1.32	8 (11%)
25	CLA	B	832	-	49,53,73	1.49	11 (22%)	59,89,113	1.49	6 (10%)
25	CLA	U	304	-	54,58,73	1.41	8 (14%)	65,95,113	1.47	8 (12%)
25	CLA	9	302	-	50,54,73	1.43	8 (16%)	60,90,113	1.41	5 (8%)
25	CLA	a	303	16,34	61,65,73	1.66	16 (26%)	73,103,113	3.46	21 (28%)
25	CLA	6	612	-	56,60,73	1.44	10 (17%)	67,97,113	1.37	5 (7%)
34	LUT	U	315	-	42,43,43	0.78	0	51,60,60	1.81	17 (33%)
25	CLA	6	615	21	50,54,73	1.47	11 (22%)	60,90,113	1.56	8 (13%)
25	CLA	5	304	20	50,54,73	1.47	10 (20%)	60,90,113	1.50	7 (11%)
33	CHL	6	606	-	57,61,74	1.99	17 (29%)	64,98,114	3.00	28 (43%)
25	CLA	S	320	-	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
25	CLA	J	105	-	46,50,73	1.49	10 (21%)	55,85,113	1.51	7 (12%)
25	CLA	6	601	19	65,69,73	1.28	10 (15%)	78,108,113	1.36	6 (7%)
25	CLA	B	826	-	69,73,73	1.29	10 (14%)	83,113,113	1.40	9 (10%)
25	CLA	B	804	2	69,73,73	1.30	11 (15%)	83,113,113	1.40	8 (9%)
25	CLA	a	312	16	69,73,73	1.26	10 (14%)	83,113,113	1.31	8 (9%)
35	XAT	P	623	-	38,46,47	0.97	1 (2%)	52,72,74	3.12	22 (42%)
28	BCR	J	106	-	41,41,41	0.86	2 (4%)	56,56,56	2.25	18 (32%)
25	CLA	1	604	34	61,65,73	1.34	12 (19%)	73,103,113	1.34	8 (10%)
34	LUT	T	614	-	42,43,43	0.76	0	51,60,60	1.73	14 (27%)
25	CLA	3	312	18	49,53,73	1.48	9 (18%)	59,89,113	1.48	8 (13%)
34	LUT	6	622	-	42,43,43	0.88	1 (2%)	51,60,60	1.50	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	836	1	69,73,73	1.28	11 (15%)	83,113,113	1.40	7 (8%)
25	CLA	B	828	-	54,58,73	1.41	11 (20%)	65,95,113	1.46	6 (9%)
25	CLA	L	202	1,28	69,73,73	1.26	11 (15%)	83,113,113	1.32	6 (7%)
33	CHL	1	601	16	57,61,74	1.99	19 (33%)	64,98,114	3.05	28 (43%)
25	CLA	P	611	-	45,49,73	1.80	11 (24%)	54,84,113	2.15	20 (37%)
25	CLA	Q	603	33	69,73,73	1.25	7 (10%)	83,113,113	1.38	6 (7%)
36	NEX	U	301	14	38,46,46	1.08	2 (5%)	50,70,70	2.95	18 (36%)
25	CLA	3	320	22	69,73,73	1.25	12 (17%)	83,113,113	1.36	7 (8%)
25	CLA	4	307	-	54,58,73	1.42	10 (18%)	65,95,113	1.33	6 (9%)
25	CLA	7	313	22	50,54,73	1.45	10 (20%)	60,90,113	1.44	6 (10%)
25	CLA	B	819	2	50,54,73	1.45	11 (22%)	60,90,113	1.53	9 (15%)
25	CLA	T	611	-	64,68,73	1.30	8 (12%)	77,107,113	1.32	6 (7%)
25	CLA	3	301	-	64,68,73	1.32	10 (15%)	77,107,113	1.40	8 (10%)
25	CLA	1	612	16	69,73,73	1.29	10 (14%)	83,113,113	1.97	14 (16%)
33	CHL	R	601	-	55,59,74	2.26	18 (32%)	62,96,114	2.94	27 (43%)
31	SQD	B	850	-	50,51,54	1.21	4 (8%)	59,62,65	1.21	7 (11%)
25	CLA	A	809	1	69,73,73	1.26	12 (17%)	83,113,113	1.36	8 (9%)
25	CLA	H	205	12	46,50,73	1.51	11 (23%)	55,85,113	1.81	10 (18%)
25	CLA	U	310	-	68,72,73	1.27	7 (10%)	81,111,113	1.29	8 (9%)
25	CLA	6	604	-	50,54,73	1.48	11 (22%)	60,90,113	1.46	6 (10%)
25	CLA	4	308	19	64,68,73	1.28	10 (15%)	77,107,113	1.35	6 (7%)
25	CLA	2	313	-	59,63,73	1.37	10 (16%)	71,101,113	1.47	11 (15%)
25	CLA	A	807	-	69,73,73	1.30	11 (15%)	83,113,113	1.42	8 (9%)
25	CLA	8	305	-	50,54,73	1.46	11 (22%)	60,90,113	1.44	6 (10%)
25	CLA	5	310	-	64,68,73	1.29	12 (18%)	77,107,113	1.33	8 (10%)
25	CLA	B	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
25	CLA	U	311	-	58,62,73	1.38	9 (15%)	64,97,113	1.28	6 (9%)
32	LMG	7	318	-	35,35,55	1.10	2 (5%)	43,43,63	1.11	2 (4%)
25	CLA	4	302	25	50,54,73	1.47	10 (20%)	60,90,113	1.44	5 (8%)
33	CHL	4	304	-	46,50,74	2.24	16 (34%)	51,85,114	3.20	24 (47%)
34	LUT	P	615	-	42,43,43	0.81	0	51,60,60	1.78	18 (35%)
34	LUT	5	318	-	42,43,43	0.92	2 (4%)	51,60,60	1.68	13 (25%)
33	CHL	S	321	-	55,59,74	2.12	19 (34%)	62,96,114	3.06	28 (45%)
34	LUT	5	322	-	42,43,43	1.01	2 (4%)	51,60,60	1.64	13 (25%)
33	CHL	U	307	-	57,61,74	2.09	17 (29%)	64,98,114	3.01	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CHL	U	305	14	50,54,74	2.24	18 (36%)	56,90,114	3.16	28 (50%)
25	CLA	K	204	-	49,53,73	1.48	10 (20%)	59,89,113	1.54	7 (11%)
33	CHL	P	606	-	54,58,74	2.13	18 (33%)	59,94,114	3.09	25 (42%)
25	CLA	A	820	1	69,73,73	1.28	12 (17%)	83,113,113	1.35	8 (9%)
30	DGD	B	848	-	58,58,67	0.96	4 (6%)	72,72,81	1.37	11 (15%)
25	CLA	P	604	-	54,58,73	1.42	10 (18%)	65,95,113	1.49	7 (10%)
28	BCR	L	204	25	41,41,41	1.01	2 (4%)	56,56,56	2.21	23 (41%)
35	XAT	T	615	-	39,47,47	0.92	0	54,74,74	3.00	21 (38%)
25	CLA	8	304	23	49,53,73	1.49	10 (20%)	59,89,113	1.51	6 (10%)
25	CLA	B	810	-	69,73,73	1.27	9 (13%)	83,113,113	1.37	7 (8%)
25	CLA	4	311	19	60,64,73	1.33	9 (15%)	72,102,113	1.44	6 (8%)
34	LUT	1	617	25	42,43,43	0.79	0	51,60,60	2.17	18 (35%)
34	LUT	R	616	-	42,43,43	0.78	0	51,60,60	1.83	18 (35%)
25	CLA	B	813	2	61,65,73	1.31	11 (18%)	73,103,113	1.37	6 (8%)
34	LUT	8	317	-	42,43,43	0.92	2 (4%)	51,60,60	1.56	12 (23%)
33	CHL	T	605	-	54,58,74	2.13	19 (35%)	59,94,114	3.08	24 (40%)
25	CLA	L	201	-	69,73,73	1.26	11 (15%)	83,113,113	1.34	6 (7%)
28	BCR	8	301	-	41,41,41	0.78	0	56,56,56	1.88	15 (26%)
25	CLA	1	608	-	69,73,73	1.24	11 (15%)	83,113,113	1.22	6 (7%)
33	CHL	6	607	-	57,61,74	2.02	19 (33%)	64,98,114	3.05	27 (42%)
25	CLA	3	309	-	45,49,73	1.49	11 (24%)	54,84,113	1.53	8 (14%)
25	CLA	a	307	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	6 (7%)
32	LMG	2	301	-	41,41,55	1.03	2 (4%)	49,49,63	1.19	4 (8%)
25	CLA	A	830	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	10 (12%)
25	CLA	A	818	1	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
25	CLA	R	612	-	64,68,73	1.26	7 (10%)	77,107,113	1.57	10 (12%)
25	CLA	S	314	-	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
33	CHL	S	309	-	56,60,74	2.07	18 (32%)	63,97,114	3.06	27 (42%)
28	BCR	I	201	25	41,41,41	0.93	2 (4%)	56,56,56	2.42	22 (39%)
25	CLA	5	313	-	60,64,73	1.37	11 (18%)	72,102,113	1.68	12 (16%)
25	CLA	B	836	-	69,73,73	1.26	11 (15%)	83,113,113	1.33	7 (8%)
33	CHL	4	305	-	55,59,74	2.23	20 (36%)	62,96,114	2.97	26 (41%)
35	XAT	P	616	-	39,47,47	0.93	0	54,74,74	3.03	20 (37%)
33	CHL	R	606	-	54,58,74	2.13	19 (35%)	59,94,114	3.04	26 (44%)
25	CLA	a	313	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LHG	P	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	8	311	27	50,54,73	1.46	11 (22%)	60,90,113	1.40	6 (10%)
25	CLA	4	303	-	54,58,73	1.38	11 (20%)	65,95,113	1.46	7 (10%)
32	LMG	1	619	27	46,46,55	0.98	2 (4%)	54,54,63	1.17	3 (5%)
34	LUT	S	316	-	42,43,43	0.79	0	51,60,60	1.82	16 (31%)
34	LUT	a	315	25	42,43,43	0.87	0	51,60,60	1.83	15 (29%)
25	CLA	3	308	-	69,73,73	1.27	11 (15%)	83,113,113	1.32	6 (7%)
25	CLA	A	835	-	55,59,73	1.44	10 (18%)	66,96,113	1.51	9 (13%)
25	CLA	2	308	-	47,51,73	1.49	10 (21%)	56,86,113	1.47	7 (12%)
33	CHL	3	306	-	57,61,74	1.96	18 (31%)	64,98,114	3.05	27 (42%)
25	CLA	8	303	-	66,70,73	1.32	12 (18%)	79,109,113	1.38	6 (7%)
25	CLA	2	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.43	9 (10%)
25	CLA	7	301	-	69,73,73	1.29	11 (15%)	83,113,113	1.29	8 (9%)
25	CLA	B	825	2	69,73,73	1.29	10 (14%)	83,113,113	1.40	9 (10%)
25	CLA	T	608	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	7 (8%)
25	CLA	a	308	16	64,68,73	1.25	10 (15%)	77,107,113	1.68	12 (15%)
25	CLA	B	837	2	69,73,73	1.27	10 (14%)	83,113,113	1.48	6 (7%)
25	CLA	1	605	-	56,60,73	1.42	9 (16%)	67,97,113	1.40	8 (11%)
25	CLA	G	202	-	50,54,73	1.47	9 (18%)	60,90,113	1.55	9 (15%)
25	CLA	5	324	-	69,73,73	1.26	11 (15%)	83,113,113	1.31	5 (6%)
36	NEX	T	616	-	38,46,46	0.98	1 (2%)	50,70,70	2.76	16 (32%)
25	CLA	2	307	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	7 (10%)
25	CLA	A	829	-	69,73,73	1.29	11 (15%)	83,113,113	1.41	8 (9%)
25	CLA	S	311	-	64,68,73	1.30	9 (14%)	77,107,113	1.29	7 (9%)
28	BCR	L	208	-	41,41,41	0.87	2 (4%)	56,56,56	1.98	18 (32%)
25	CLA	P	613	-	62,66,73	1.33	8 (12%)	74,104,113	1.34	6 (8%)
25	CLA	1	613	16	69,73,73	1.27	10 (14%)	83,113,113	1.33	8 (9%)
33	CHL	S	306	-	52,56,74	2.19	17 (32%)	58,92,114	3.18	29 (50%)
34	LUT	7	315	-	42,43,43	0.93	2 (4%)	51,60,60	1.56	12 (23%)
33	CHL	4	306	-	55,59,74	2.03	18 (32%)	62,96,114	3.02	26 (41%)
33	CHL	T	601	-	54,58,74	2.29	18 (33%)	59,94,114	2.98	26 (44%)
25	CLA	O	201	-	45,49,73	1.49	10 (22%)	54,84,113	1.58	7 (12%)
25	CLA	2	304	-	69,73,73	1.27	10 (14%)	83,113,113	1.36	7 (8%)
25	CLA	R	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.57	10 (15%)
25	CLA	B	801	-	69,73,73	1.27	10 (14%)	83,113,113	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMG	J	107	-	55,55,55	0.90	2 (3%)	63,63,63	1.23	8 (12%)
28	BCR	B	842	-	41,41,41	1.02	2 (4%)	56,56,56	2.27	20 (35%)
25	CLA	U	312	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
25	CLA	B	824	2	69,73,73	1.28	11 (15%)	83,113,113	1.38	10 (12%)
27	LHG	Q	617	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
34	LUT	1	616	25	42,43,43	0.95	2 (4%)	51,60,60	1.84	18 (35%)
33	CHL	P	607	-	56,60,74	2.10	18 (32%)	63,97,114	3.05	29 (46%)
34	LUT	Q	614	-	42,43,43	0.73	0	51,60,60	1.84	12 (23%)
25	CLA	5	312	-	56,60,73	1.42	10 (17%)	67,97,113	1.42	7 (10%)
25	CLA	R	611	-	64,68,73	1.34	7 (10%)	77,107,113	1.57	9 (11%)
33	CHL	T	604	14	52,56,74	2.19	18 (34%)	58,92,114	3.17	28 (48%)
34	LUT	Q	615	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	16 (31%)
25	CLA	6	609	-	54,58,73	1.39	11 (20%)	65,95,113	1.46	7 (10%)
28	BCR	4	321	-	41,41,41	0.94	2 (4%)	56,56,56	2.73	24 (42%)
25	CLA	A	834	1	49,53,73	1.49	10 (20%)	59,89,113	1.54	3 (5%)
28	BCR	F	803	-	41,41,41	0.91	2 (4%)	56,56,56	2.20	20 (35%)
33	CHL	P	601	-	55,59,74	2.26	18 (32%)	62,96,114	2.95	28 (45%)
33	CHL	9	306	-	46,50,74	2.22	19 (41%)	51,85,114	3.34	25 (49%)
25	CLA	a	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	8 (9%)
25	CLA	8	313	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	7 (8%)
25	CLA	8	302	23	69,73,73	1.25	10 (14%)	83,113,113	1.27	9 (10%)
25	CLA	6	614	-	49,53,73	1.46	10 (20%)	59,89,113	1.48	7 (11%)
25	CLA	A	832	1	69,73,73	1.27	11 (15%)	83,113,113	1.36	5 (6%)
25	CLA	L	206	-	46,50,73	1.51	11 (23%)	55,85,113	1.54	6 (10%)
25	CLA	L	209	-	45,49,73	1.50	10 (22%)	54,84,113	1.67	8 (14%)
33	CHL	Q	608	25	70,74,74	1.35	8 (11%)	80,114,114	1.80	12 (15%)
28	BCR	3	319	-	41,41,41	0.80	1 (2%)	56,56,56	2.42	16 (28%)
34	LUT	a	314	-	42,43,43	0.88	2 (4%)	51,60,60	1.87	16 (31%)
25	CLA	P	602	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
25	CLA	6	611	27	59,63,73	1.36	9 (15%)	71,101,113	1.32	5 (7%)
27	LHG	S	319	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
25	CLA	K	203	-	50,54,73	1.46	12 (24%)	60,90,113	1.47	6 (10%)
25	CLA	6	616	21,27	50,54,73	1.45	9 (18%)	60,90,113	1.48	7 (11%)
33	CHL	R	607	-	56,60,74	2.10	18 (32%)	63,97,114	3.05	29 (46%)
35	XAT	Q	616	-	39,47,47	0.96	1 (2%)	54,74,74	3.04	24 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	T	602	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	9 (10%)
25	CLA	7	303	-	60,64,73	1.37	11 (18%)	72,102,113	1.42	6 (8%)
25	CLA	A	826	-	69,73,73	1.29	11 (15%)	83,113,113	1.28	7 (8%)
25	CLA	H	202	-	45,49,73	1.52	9 (20%)	54,84,113	1.66	7 (12%)
25	CLA	B	811	-	69,73,73	1.31	10 (14%)	83,113,113	1.44	9 (10%)
33	CHL	P	622	-	57,61,74	2.18	18 (31%)	64,98,114	3.08	33 (51%)
25	CLA	9	311	24	49,53,73	1.50	10 (20%)	59,89,113	1.41	8 (13%)
25	CLA	R	603	33	69,73,73	1.28	6 (8%)	83,113,113	1.29	6 (7%)
34	LUT	P	614	-	42,43,43	0.74	0	51,60,60	1.92	15 (29%)
25	CLA	9	304	-	50,54,73	1.47	9 (18%)	60,90,113	1.48	5 (8%)
25	CLA	A	810	1	69,73,73	1.25	11 (15%)	83,113,113	1.36	8 (9%)
25	CLA	4	310	19	56,60,73	1.46	12 (21%)	67,97,113	1.64	10 (14%)
25	CLA	5	315	20	50,54,73	1.45	9 (18%)	60,90,113	1.45	5 (8%)
25	CLA	B	823	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	7 (8%)
25	CLA	B	830	2	69,73,73	1.29	12 (17%)	83,113,113	1.36	9 (10%)
25	CLA	B	803	2	49,53,73	1.47	10 (20%)	59,89,113	1.62	8 (13%)
25	CLA	4	313	19	45,49,73	1.51	9 (20%)	54,84,113	1.58	8 (14%)
25	CLA	K	202	-	49,53,73	1.47	12 (24%)	59,89,113	1.48	5 (8%)
25	CLA	A	813	1	58,62,73	1.40	11 (18%)	69,99,113	1.48	7 (10%)
25	CLA	6	610	-	64,68,73	1.34	9 (14%)	77,107,113	1.36	7 (9%)
33	CHL	T	607	-	56,60,74	2.19	18 (32%)	63,97,114	2.96	29 (46%)
25	CLA	2	314	-	50,54,73	1.46	10 (20%)	60,90,113	1.39	5 (8%)
33	CHL	7	305	-	58,62,74	2.00	21 (36%)	65,99,114	3.01	24 (36%)
25	CLA	A	802	25	69,73,73	1.29	12 (17%)	83,113,113	1.41	12 (14%)
25	CLA	P	603	33	69,73,73	1.25	8 (11%)	83,113,113	1.36	7 (8%)
25	CLA	2	303	17	69,73,73	1.27	11 (15%)	83,113,113	1.31	7 (8%)
33	CHL	S	307	-	54,58,74	2.21	17 (31%)	59,94,114	3.05	24 (40%)
25	CLA	A	839	1,25	69,73,73	1.26	10 (14%)	83,113,113	1.43	7 (8%)
28	BCR	F	801	-	41,41,41	0.90	2 (4%)	56,56,56	2.10	17 (30%)
25	CLA	A	817	-	61,65,73	1.36	9 (14%)	73,103,113	1.35	5 (6%)
25	CLA	6	613	-	60,64,73	1.34	10 (16%)	72,102,113	1.49	7 (9%)
33	CHL	S	308	-	56,60,74	2.08	18 (32%)	63,97,114	3.03	28 (44%)
33	CHL	Q	605	14	46,50,74	2.32	18 (39%)	51,85,114	3.37	25 (49%)
25	CLA	A	819	1	69,73,73	1.28	10 (14%)	83,113,113	1.42	9 (10%)
25	CLA	A	840	-	69,73,73	1.29	10 (14%)	83,113,113	1.42	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	814	2	59,63,73	1.37	11 (18%)	71,101,113	1.43	8 (11%)
25	CLA	A	831	1	54,58,73	1.42	11 (20%)	65,95,113	1.50	8 (12%)
25	CLA	a	302	16	61,65,73	1.35	10 (16%)	73,103,113	1.36	5 (6%)
25	CLA	H	201	-	50,54,73	1.45	10 (20%)	60,90,113	1.45	5 (8%)
25	CLA	A	851	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	6 (7%)
25	CLA	F	802	-	49,53,73	1.50	11 (22%)	59,89,113	1.45	7 (11%)
27	LHG	a	317	25	42,42,48	0.95	2 (4%)	45,48,54	1.21	4 (8%)
36	NEX	P	617	-	38,46,46	1.01	1 (2%)	50,70,70	2.80	18 (36%)
25	CLA	5	314	-	49,53,73	1.49	10 (20%)	59,89,113	1.44	8 (13%)
36	NEX	U	316	-	38,46,46	0.99	1 (2%)	50,70,70	2.72	18 (36%)
25	CLA	A	827	-	69,73,73	1.30	11 (15%)	83,113,113	1.38	9 (10%)
25	CLA	Q	602	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	8 (9%)
28	BCR	A	846	-	41,41,41	1.00	2 (4%)	56,56,56	2.10	20 (35%)
25	CLA	T	612	-	52,56,73	1.44	7 (13%)	62,92,113	1.48	6 (9%)
25	CLA	T	609	-	64,68,73	1.32	8 (12%)	77,107,113	1.43	10 (12%)
25	CLA	5	311	-	59,63,73	1.35	10 (16%)	71,101,113	1.34	7 (9%)
33	CHL	T	606	-	48,52,74	2.19	17 (35%)	53,87,114	3.22	25 (47%)
25	CLA	B	816	2	64,68,73	1.31	10 (15%)	77,107,113	1.43	8 (10%)
25	CLA	3	310	-	50,54,73	1.47	10 (20%)	60,90,113	1.48	7 (11%)
25	CLA	Q	612	-	64,68,73	1.31	7 (10%)	77,107,113	1.36	9 (11%)
27	LHG	A	852	25	46,46,48	0.95	2 (4%)	48,51,54	1.20	5 (10%)
25	CLA	2	306	17	45,49,73	1.53	10 (22%)	54,84,113	1.64	9 (16%)
28	BCR	A	848	-	41,41,41	0.91	1 (2%)	56,56,56	1.97	16 (28%)
33	CHL	9	307	-	55,59,74	2.10	19 (34%)	62,96,114	3.00	26 (41%)
25	CLA	K	205	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	5 (8%)
28	BCR	5	323	-	41,41,41	0.96	2 (4%)	56,56,56	3.15	22 (39%)
33	CHL	S	310	15	56,60,74	2.13	17 (30%)	63,97,114	2.96	26 (41%)
25	CLA	Q	611	-	64,68,73	1.37	9 (14%)	77,107,113	1.31	9 (11%)
33	CHL	Q	606	-	54,58,74	2.16	17 (31%)	59,94,114	3.13	23 (38%)
25	CLA	9	301	-	58,62,73	1.43	11 (18%)	73,100,113	1.43	9 (12%)
25	CLA	a	309	27	69,73,73	1.26	10 (14%)	83,113,113	1.26	7 (8%)
34	LUT	T	613	-	42,43,43	0.72	0	51,60,60	1.91	13 (25%)
35	XAT	P	620	-	39,47,47	0.89	0	54,74,74	2.97	23 (42%)
25	CLA	P	610	-	64,68,73	1.31	9 (14%)	77,107,113	1.29	7 (9%)
25	CLA	U	303	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CHL	5	308	-	55,59,74	1.99	20 (36%)	62,96,114	3.15	30 (48%)
25	CLA	A	801	-	69,73,73	1.28	10 (14%)	83,113,113	1.29	8 (9%)
25	CLA	5	303	-	69,73,73	1.28	12 (17%)	83,113,113	1.42	7 (8%)
28	BCR	O	205	-	41,41,41	0.82	1 (2%)	56,56,56	2.18	16 (28%)
34	LUT	a	316	25	42,43,43	0.74	0	51,60,60	2.13	15 (29%)
25	CLA	B	818	2	60,64,73	1.34	10 (16%)	72,102,113	1.48	7 (9%)
25	CLA	3	302	-	69,73,73	1.30	10 (14%)	83,113,113	1.34	8 (9%)
28	BCR	B	841	-	41,41,41	0.95	2 (4%)	56,56,56	2.24	18 (32%)
25	CLA	A	833	1	54,58,73	1.41	11 (20%)	65,95,113	1.52	6 (9%)
25	CLA	9	308	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	9 (13%)
34	LUT	U	314	-	42,43,43	0.73	0	51,60,60	1.91	14 (27%)
27	LHG	T	617	-	48,48,48	0.94	2 (4%)	51,54,54	0.93	2 (3%)
28	BCR	B	844	-	41,41,41	0.96	2 (4%)	56,56,56	2.11	16 (28%)
25	CLA	7	302	-	50,54,73	1.48	10 (20%)	60,90,113	1.50	7 (11%)
33	CHL	R	609	25	70,74,74	1.35	8 (11%)	80,114,114	1.80	12 (15%)
32	LMG	7	319	-	36,36,55	1.12	3 (8%)	44,44,63	1.25	5 (11%)
25	CLA	U	302	-	69,73,73	1.27	9 (13%)	83,113,113	1.29	10 (12%)
25	CLA	3	313	-	50,54,73	1.45	11 (22%)	60,90,113	1.46	6 (10%)
25	CLA	R	610	-	68,72,73	1.29	8 (11%)	81,111,113	1.32	9 (11%)
25	CLA	B	809	2,28	69,73,73	1.27	11 (15%)	83,113,113	1.34	7 (8%)
25	CLA	5	319	-	50,54,73	1.46	10 (20%)	60,90,113	1.50	7 (11%)
28	BCR	B	845	-	41,41,41	1.03	3 (7%)	56,56,56	2.16	18 (32%)
27	LHG	1	618	25	42,42,48	0.96	2 (4%)	45,48,54	1.22	4 (8%)
28	BCR	B	840	28	41,41,41	0.93	1 (2%)	56,56,56	2.11	15 (26%)
25	CLA	4	312	19	49,53,73	1.47	9 (18%)	59,89,113	1.40	6 (10%)
28	BCR	A	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.00	18 (32%)
25	CLA	A	838	1	69,73,73	1.27	10 (14%)	83,113,113	1.41	8 (9%)
25	CLA	B	807	-	69,73,73	1.24	10 (14%)	83,113,113	1.52	9 (10%)
25	CLA	T	603	-	54,58,73	1.42	7 (12%)	65,95,113	1.47	6 (9%)
25	CLA	Q	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.52	7 (10%)
34	LUT	4	315	-	42,43,43	0.89	1 (2%)	51,60,60	1.94	17 (33%)
25	CLA	1	603	16	69,73,73	1.26	11 (15%)	83,113,113	1.28	7 (8%)
25	CLA	R	613	-	69,73,73	1.25	7 (10%)	83,113,113	1.34	8 (9%)
25	CLA	2	305	-	56,60,73	1.39	9 (16%)	67,97,113	1.43	6 (8%)
33	CHL	4	322	16,19	57,61,74	2.02	19 (33%)	64,98,114	3.18	29 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	8	312	25	56,60,73	1.39	10 (17%)	67,97,113	1.40	4 (5%)
25	CLA	A	812	-	69,73,73	1.27	10 (14%)	83,113,113	1.36	9 (10%)
25	CLA	A	825	-	69,73,73	1.30	10 (14%)	83,113,113	1.40	11 (13%)
25	CLA	S	305	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	6 (9%)
34	LUT	3	316	-	42,43,43	0.97	2 (4%)	51,60,60	1.65	15 (29%)
25	CLA	J	103	-	62,66,73	1.31	10 (16%)	74,104,113	1.41	7 (9%)
25	CLA	a	306	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	9 (10%)
25	CLA	B	802	-	69,73,73	1.28	11 (15%)	83,113,113	1.44	8 (9%)
25	CLA	a	311	16	69,73,73	1.25	9 (13%)	83,113,113	1.51	8 (9%)
25	CLA	Q	609	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	8 (9%)
28	BCR	3	318	-	41,41,41	0.84	1 (2%)	56,56,56	2.79	24 (42%)
25	CLA	A	804	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
33	CHL	Q	601	-	55,59,74	2.26	18 (32%)	62,96,114	2.95	27 (43%)
36	NEX	P	621	-	38,46,46	0.86	0	50,70,70	3.27	27 (54%)
25	CLA	B	835	2	51,55,73	1.46	11 (21%)	61,91,113	1.39	6 (9%)
25	CLA	7	304	-	46,50,73	1.53	11 (23%)	55,85,113	1.41	6 (10%)
25	CLA	P	612	-	64,68,73	1.27	7 (10%)	77,107,113	1.59	10 (12%)
25	CLA	7	310	-	56,60,73	1.40	10 (17%)	67,97,113	1.45	6 (8%)
33	CHL	a	305	-	52,56,74	2.21	18 (34%)	58,92,114	2.95	23 (39%)
25	CLA	6	603	-	69,73,73	1.29	11 (15%)	83,113,113	1.34	7 (8%)
25	CLA	B	849	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
27	LHG	6	618	25	48,48,48	0.87	2 (4%)	51,54,54	1.22	4 (7%)
30	DGD	B	846	-	67,67,67	0.80	3 (4%)	81,81,81	1.18	5 (6%)
25	CLA	B	815	-	63,67,73	1.35	10 (15%)	75,105,113	1.54	11 (14%)
34	LUT	4	316	-	42,43,43	0.88	2 (4%)	51,60,60	1.53	11 (21%)
25	CLA	1	607	-	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
25	CLA	A	803	-	69,73,73	1.30	9 (13%)	83,113,113	1.25	5 (6%)
25	CLA	8	309	-	50,54,73	1.44	10 (20%)	60,90,113	1.47	4 (6%)
25	CLA	8	306	-	46,50,73	1.51	10 (21%)	55,85,113	1.46	7 (12%)
25	CLA	L	205	12	69,73,73	1.25	10 (14%)	83,113,113	1.39	9 (10%)
25	CLA	9	309	-	64,68,73	1.31	9 (14%)	77,107,113	1.40	8 (10%)
33	CHL	U	306	-	54,58,74	2.14	18 (33%)	59,94,114	3.08	25 (42%)
28	BCR	4	317	19	41,41,41	0.88	0	56,56,56	2.30	19 (33%)
25	CLA	S	315	15	52,56,73	1.42	10 (19%)	62,92,113	1.39	7 (11%)
25	CLA	9	305	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	BCR	8	318	-	41,41,41	0.82	1 (2%)	56,56,56	2.16	20 (35%)
25	CLA	H	203	-	50,54,73	1.44	10 (20%)	60,90,113	1.49	7 (11%)
25	CLA	A	828	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	7 (8%)
33	CHL	6	608	-	55,59,74	2.03	18 (32%)	62,96,114	3.25	32 (51%)
25	CLA	A	816	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
28	BCR	6	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.23	18 (32%)
25	CLA	7	312	22	47,51,73	1.50	11 (23%)	56,86,113	1.51	7 (12%)
25	CLA	S	303	15	69,73,73	1.28	10 (14%)	83,113,113	1.40	10 (12%)
32	LMG	6	602	-	40,40,55	1.03	2 (5%)	48,48,63	1.41	6 (12%)
29	SF4	C	101	3	0,12,12	-	-	-		
25	CLA	2	311	-	56,60,73	1.41	10 (17%)	67,97,113	1.41	7 (10%)
25	CLA	5	316	-	47,51,73	1.51	11 (23%)	56,86,113	1.57	6 (10%)
25	CLA	2	310	-	45,49,73	1.54	10 (22%)	54,84,113	1.48	6 (11%)
25	CLA	3	304	-	46,50,73	1.53	10 (21%)	55,85,113	1.46	5 (9%)
25	CLA	1	602	-	69,73,73	1.28	10 (14%)	83,113,113	1.25	6 (7%)
25	CLA	A	837	1	69,73,73	1.25	10 (14%)	83,113,113	1.36	8 (9%)
27	LHG	P	624	-	48,48,48	0.94	2 (4%)	51,54,54	0.96	2 (3%)
28	BCR	J	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.08	19 (33%)
25	CLA	B	834	2	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
25	CLA	S	313	-	64,68,73	1.31	8 (12%)	77,107,113	1.31	7 (9%)
25	CLA	9	310	24	54,58,73	1.40	10 (18%)	65,95,113	1.49	6 (9%)
25	CLA	7	309	27	45,49,73	1.51	12 (26%)	54,84,113	1.52	8 (14%)
27	LHG	4	318	25	48,48,48	0.92	2 (4%)	51,54,54	1.09	3 (5%)
25	CLA	A	853	-	69,73,73	1.26	11 (15%)	83,113,113	1.34	7 (8%)
25	CLA	3	307	-	54,58,73	1.43	11 (20%)	65,95,113	1.41	7 (10%)
25	CLA	6	623	-	64,68,73	1.28	9 (14%)	77,107,113	1.48	8 (10%)
25	CLA	3	303	-	69,73,73	1.27	11 (15%)	83,113,113	1.38	8 (9%)
25	CLA	3	305	18	64,68,73	1.30	10 (15%)	77,107,113	1.38	8 (10%)
25	CLA	A	806	-	69,73,73	1.30	11 (15%)	83,113,113	1.44	9 (10%)
25	CLA	8	314	-	59,63,73	1.35	11 (18%)	71,101,113	1.40	9 (12%)
26	PQN	B	839	-	34,34,34	1.35	2 (5%)	42,45,45	1.33	4 (9%)
28	BCR	O	204	-	41,41,41	0.86	2 (4%)	56,56,56	2.34	21 (37%)
25	CLA	A	842	27	56,60,73	1.39	10 (17%)	67,97,113	1.70	13 (19%)
25	CLA	7	306	-	54,58,73	1.42	10 (18%)	65,95,113	1.47	8 (12%)
25	CLA	5	309	-	54,58,73	1.42	11 (20%)	65,95,113	1.41	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	A	808	1	69,73,73	1.27	10 (14%)	83,113,113	1.33	8 (9%)
28	BCR	L	207	-	41,41,41	0.93	2 (4%)	56,56,56	2.00	13 (23%)
25	CLA	8	315	23	50,54,73	1.46	10 (20%)	60,90,113	1.44	4 (6%)
26	PQN	A	841	-	34,34,34	1.37	2 (5%)	42,45,45	1.33	6 (14%)
34	LUT	8	316	-	42,43,43	0.90	1 (2%)	51,60,60	1.78	14 (27%)
25	CLA	B	805	-	69,73,73	1.29	12 (17%)	83,113,113	1.38	5 (6%)
25	CLA	O	203	-	41,46,73	1.65	10 (24%)	52,81,113	1.63	7 (13%)
33	CHL	P	619	-	56,60,74	2.10	18 (32%)	63,97,114	3.06	29 (46%)
33	CHL	P	609	25	70,74,74	1.35	8 (11%)	80,114,114	1.80	13 (16%)
34	LUT	3	315	-	42,43,43	0.92	2 (4%)	51,60,60	1.65	13 (25%)
25	CLA	8	308	-	54,58,73	1.40	11 (20%)	65,95,113	1.56	7 (10%)
29	SF4	A	850	2,1	0,12,12	-	-	-		
25	CLA	A	815	1,27	64,68,73	1.33	11 (17%)	77,107,113	1.36	6 (7%)
28	BCR	A	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.08	17 (30%)
25	CLA	B	829	-	53,57,73	1.41	11 (20%)	62,93,113	1.48	7 (11%)
34	LUT	9	313	-	42,43,43	0.90	1 (2%)	51,60,60	1.61	14 (27%)
27	LHG	R	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	K	201	1	55,59,73	1.40	11 (20%)	66,96,113	1.52	9 (13%)
33	CHL	P	608	-	48,52,74	2.18	18 (37%)	53,87,114	3.19	24 (45%)
27	LHG	5	301	-	44,44,48	0.96	2 (4%)	47,50,54	1.05	3 (6%)
25	CLA	O	202	-	40,46,73	1.63	11 (27%)	48,80,113	1.60	8 (16%)
28	BCR	B	851	-	41,41,41	0.83	2 (4%)	56,56,56	2.12	19 (33%)
33	CHL	4	314	19	47,51,74	2.16	18 (38%)	52,86,114	3.25	23 (44%)
33	CHL	U	308	-	48,52,74	2.18	17 (35%)	53,87,114	3.18	23 (43%)
25	CLA	2	302	17	50,54,73	1.50	11 (22%)	60,90,113	1.54	7 (11%)
27	LHG	7	317	25	36,36,48	1.00	2 (5%)	39,42,54	1.31	4 (10%)
25	CLA	3	314	-	60,64,73	1.36	10 (16%)	72,102,113	1.42	6 (8%)
25	CLA	R	614	-	52,56,73	1.44	7 (13%)	62,92,113	1.52	7 (11%)
25	CLA	A	824	-	59,63,73	1.36	11 (18%)	71,101,113	1.43	7 (9%)
27	LHG	2	317	-	48,48,48	0.90	2 (4%)	51,54,54	0.99	2 (3%)
34	LUT	6	619	-	42,43,43	0.89	1 (2%)	51,60,60	1.82	14 (27%)
25	CLA	9	303	-	64,68,73	1.31	11 (17%)	77,107,113	1.34	6 (7%)
25	CLA	B	838	-	69,73,73	1.27	12 (17%)	83,113,113	1.34	5 (6%)
32	LMG	J	102	-	40,40,55	0.99	2 (5%)	48,48,63	1.11	5 (10%)
34	LUT	7	314	-	42,43,43	0.96	2 (4%)	51,60,60	1.74	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LHG	8	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	3	311	-	59,63,73	1.34	10 (16%)	71,101,113	1.46	7 (9%)
25	CLA	B	821	2	64,68,73	1.31	11 (17%)	77,107,113	1.35	6 (7%)
25	CLA	5	305	-	54,58,73	1.43	11 (20%)	65,95,113	1.49	8 (12%)
25	CLA	Q	610	-	43,48,73	1.56	8 (18%)	52,82,113	1.69	9 (17%)
25	CLA	U	313	-	49,53,73	1.44	7 (14%)	59,89,113	1.60	8 (13%)
32	LMG	H	204	-	47,47,55	0.95	2 (4%)	55,55,63	1.16	5 (9%)

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
25	CLA	4	301	-	-	13/33/109/115	-
33	CHL	R	608	-	-	7/15/91/117	-
33	CHL	Q	607	-	-	7/15/91/117	-
25	CLA	8	310	-	-	10/33/109/115	-
25	CLA	A	811	1	-	6/39/115/115	-
25	CLA	R	602	-	-	8/39/115/115	-
27	LHG	B	847	32	-	17/42/42/53	-
25	CLA	1	609	16	-	7/33/109/115	-
25	CLA	Q	613	-	-	11/19/95/115	-
33	CHL	P	605	14	-	6/20/96/117	-
25	CLA	T	610	-	-	12/33/109/115	-
25	CLA	S	301	15	-	9/18/94/115	-
25	CLA	2	309	-	-	13/33/109/115	-
25	CLA	1	614	-	-	6/17/93/115	-
25	CLA	7	307	-	-	4/21/97/115	-
25	CLA	5	302	20	-	12/39/115/115	-
33	CHL	5	317	-	-	4/14/90/117	-
33	CHL	8	307	23	-	11/26/102/117	-
35	XAT	S	318	-	-	4/31/93/93	0/4/4/4
27	LHG	5	321	-	-	13/41/41/53	-
25	CLA	1	611	-	-	10/24/100/115	-
28	BCR	A	845	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	R	617	-	-	6/27/83/83	0/3/3/3
27	LHG	A	843	-	-	18/53/53/53	-
25	CLA	S	312	15	-	11/33/109/115	-
25	CLA	a	304	-	-	2/24/100/115	-
28	BCR	3	317	-	-	6/29/63/63	0/2/2/2
25	CLA	7	308	-	-	12/33/109/115	-
33	CHL	S	302	-	-	15/26/102/117	-
28	BCR	G	203	28	-	1/29/63/63	0/2/2/2
33	CHL	U	309	-	-	3/20/96/117	-
25	CLA	5	306	-	-	4/27/103/115	-
25	CLA	B	812	2	-	12/33/109/115	-
28	BCR	B	843	-	-	5/29/63/63	0/2/2/2
33	CHL	R	605	14	-	5/17/93/117	-
25	CLA	A	823	-	-	12/20/96/115	-
32	LMG	J	104	-	-	13/30/50/70	0/1/1/1
25	CLA	B	827	2	-	9/39/115/115	-
25	CLA	A	805	1	-	10/27/103/115	-
25	CLA	B	806	2	-	12/39/115/115	-
25	CLA	B	831	2	-	12/39/115/115	-
25	CLA	Q	618	14	-	2/10/82/115	-
25	CLA	B	820	2	-	4/32/108/115	-
32	LMG	4	320	-	-	6/35/55/70	0/1/1/1
25	CLA	G	201	-	-	5/21/97/115	-
25	CLA	A	822	-	-	14/39/115/115	-
25	CLA	B	817	-	-	7/39/115/115	-
25	CLA	6	620	-	-	8/15/91/115	-
25	CLA	B	808	2	-	10/39/115/115	-
34	LUT	1	615	-	-	2/29/67/67	0/2/2/2
34	LUT	S	317	-	-	6/29/67/67	0/2/2/2
27	LHG	A	844	25	-	14/42/42/53	-
25	CLA	A	814	1	-	19/39/115/115	-
34	LUT	R	615	-	-	2/29/67/67	0/2/2/2
33	CHL	1	606	-	-	8/20/96/117	-
25	CLA	S	304	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LUT	2	316	-	-	0/29/67/67	0/2/2/2
28	BCR	A	854	-	-	2/29/63/63	0/2/2/2
34	LUT	9	312	-	-	2/29/67/67	0/2/2/2
28	BCR	K	206	-	-	10/29/63/63	0/2/2/2
25	CLA	7	311	-	-	15/39/115/115	-
29	SF4	C	102	3	-	-	0/6/5/5
28	BCR	7	316	-	-	2/29/63/63	0/2/2/2
28	BCR	L	203	-	-	4/29/63/63	0/2/2/2
25	CLA	6	605	-	-	13/39/115/115	-
28	BCR	5	320	-	-	9/29/63/63	0/2/2/2
25	CLA	1	610	27	-	10/39/115/115	-
25	CLA	A	821	1	-	3/15/91/115	-
25	CLA	B	833	-	-	5/33/109/115	-
33	CHL	6	617	21	-	6/14/90/117	-
34	LUT	2	315	-	-	6/29/67/67	0/2/2/2
33	CHL	5	307	-	-	11/23/99/117	-
27	LHG	4	319	-	-	7/36/36/53	-
25	CLA	a	310	-	-	10/24/100/115	-
25	CLA	4	309	27	-	10/27/103/115	-
25	CLA	B	832	-	-	7/15/91/115	-
25	CLA	U	304	-	-	8/21/97/115	-
25	CLA	9	302	-	-	11/17/93/115	-
25	CLA	a	303	16,34	-	12/30/106/115	-
25	CLA	6	612	-	-	5/24/100/115	-
34	LUT	U	315	-	-	2/29/67/67	0/2/2/2
25	CLA	6	615	21	-	6/17/93/115	-
25	CLA	5	304	20	-	5/17/93/115	-
33	CHL	6	606	-	-	7/26/102/117	-
25	CLA	S	320	-	-	13/39/115/115	-
25	CLA	J	105	-	-	8/12/88/115	-
25	CLA	6	601	19	-	15/35/111/115	-
25	CLA	B	826	-	-	18/39/115/115	-
25	CLA	B	804	2	-	15/39/115/115	-
25	CLA	a	312	16	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	XAT	P	623	-	-	3/29/91/93	0/4/4/4
28	BCR	J	106	-	-	6/29/63/63	0/2/2/2
25	CLA	1	604	34	-	10/30/106/115	-
34	LUT	T	614	-	-	2/29/67/67	0/2/2/2
25	CLA	3	312	18	-	6/15/91/115	-
34	LUT	6	622	-	-	1/29/67/67	0/2/2/2
25	CLA	A	836	1	-	16/39/115/115	-
25	CLA	B	828	-	-	5/21/97/115	-
25	CLA	L	202	1,28	-	14/39/115/115	-
33	CHL	1	601	16	-	5/26/102/117	-
25	CLA	P	611	-	-	6/10/86/115	-
25	CLA	Q	603	33	-	13/39/115/115	-
36	NEX	U	301	14	-	6/27/83/83	0/3/3/3
25	CLA	3	320	22	-	18/39/115/115	-
25	CLA	4	307	-	-	7/21/97/115	-
25	CLA	7	313	22	-	10/17/93/115	-
25	CLA	B	819	2	-	8/17/93/115	-
25	CLA	T	611	-	-	13/33/109/115	-
25	CLA	3	301	-	-	3/33/109/115	-
25	CLA	1	612	16	-	16/39/115/115	-
33	CHL	R	601	-	-	8/23/99/117	-
31	SQD	B	850	-	-	16/46/66/69	0/1/1/1
25	CLA	A	809	1	-	15/39/115/115	-
25	CLA	H	205	12	-	2/12/88/115	-
25	CLA	U	310	-	-	10/38/114/115	-
25	CLA	6	604	-	-	5/17/93/115	-
25	CLA	4	308	19	-	14/33/109/115	-
25	CLA	2	313	-	-	5/27/103/115	-
25	CLA	A	807	-	-	23/39/115/115	-
25	CLA	8	305	-	-	6/17/93/115	-
25	CLA	5	310	-	-	7/33/109/115	-
25	CLA	B	822	-	-	16/39/115/115	-
25	CLA	U	311	-	-	9/27/96/115	-
32	LMG	7	318	-	-	11/30/50/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	302	25	-	5/17/93/115	-
33	CHL	4	304	-	-	3/12/88/117	-
34	LUT	P	615	-	-	2/29/67/67	0/2/2/2
34	LUT	5	318	-	-	0/29/67/67	0/2/2/2
33	CHL	S	321	-	-	9/23/99/117	-
34	LUT	5	322	-	-	0/29/67/67	0/2/2/2
33	CHL	U	307	-	-	11/26/102/117	-
33	CHL	U	305	14	-	8/17/93/117	-
25	CLA	K	204	-	-	9/15/91/115	-
33	CHL	P	606	-	-	7/22/98/117	-
25	CLA	A	820	1	-	12/39/115/115	-
30	DGD	B	848	-	-	16/46/86/95	0/2/2/2
25	CLA	P	604	-	-	8/21/97/115	-
28	BCR	L	204	25	-	7/29/63/63	0/2/2/2
35	XAT	T	615	-	-	4/31/93/93	0/4/4/4
25	CLA	8	304	23	-	10/15/91/115	-
25	CLA	B	810	-	-	13/39/115/115	-
25	CLA	4	311	19	-	16/29/105/115	-
34	LUT	1	617	25	-	6/29/67/67	0/2/2/2
34	LUT	R	616	-	-	2/29/67/67	0/2/2/2
25	CLA	B	813	2	-	8/30/106/115	-
34	LUT	8	317	-	-	1/29/67/67	0/2/2/2
33	CHL	T	605	-	-	7/22/98/117	-
25	CLA	L	201	-	-	12/39/115/115	-
28	BCR	8	301	-	-	3/29/63/63	0/2/2/2
25	CLA	1	608	-	-	13/39/115/115	-
33	CHL	6	607	-	-	10/26/102/117	-
25	CLA	3	309	-	-	6/10/86/115	-
25	CLA	a	307	-	-	12/39/115/115	-
32	LMG	2	301	-	-	12/36/56/70	0/1/1/1
25	CLA	A	830	1	-	14/39/115/115	-
25	CLA	A	818	1	-	17/39/115/115	-
25	CLA	R	612	-	-	13/33/109/115	-
25	CLA	S	314	-	-	22/39/115/115	-
33	CHL	S	309	-	-	6/25/101/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	I	201	25	-	7/29/63/63	0/2/2/2
25	CLA	5	313	-	-	8/29/105/115	-
25	CLA	B	836	-	-	17/39/115/115	-
33	CHL	4	305	-	-	5/23/99/117	-
35	XAT	P	616	-	-	4/31/93/93	0/4/4/4
33	CHL	R	606	-	-	8/22/98/117	-
25	CLA	a	313	-	-	6/17/93/115	-
27	LHG	P	618	-	-	12/53/53/53	-
25	CLA	8	311	27	-	7/17/93/115	-
25	CLA	4	303	-	-	9/21/97/115	-
32	LMG	1	619	27	-	15/41/61/70	0/1/1/1
34	LUT	S	316	-	-	5/29/67/67	0/2/2/2
34	LUT	a	315	25	-	4/29/67/67	0/2/2/2
25	CLA	3	308	-	-	14/39/115/115	-
25	CLA	A	835	-	-	8/23/99/115	-
25	CLA	2	308	-	-	6/13/89/115	-
33	CHL	3	306	-	-	9/26/102/117	-
25	CLA	8	303	-	-	10/36/112/115	-
25	CLA	2	312	-	-	14/39/115/115	-
25	CLA	7	301	-	-	16/39/115/115	-
25	CLA	B	825	2	-	15/39/115/115	-
25	CLA	T	608	-	-	12/39/115/115	-
25	CLA	a	308	16	-	7/33/109/115	-
25	CLA	B	837	2	-	17/39/115/115	-
25	CLA	1	605	-	-	2/24/100/115	-
25	CLA	G	202	-	-	5/17/93/115	-
25	CLA	5	324	-	-	19/39/115/115	-
36	NEX	T	616	-	-	7/27/83/83	0/3/3/3
25	CLA	2	307	-	-	8/21/97/115	-
25	CLA	A	829	-	-	12/39/115/115	-
25	CLA	S	311	-	-	9/33/109/115	-
28	BCR	L	208	-	-	2/29/63/63	0/2/2/2
25	CLA	P	613	-	-	11/31/107/115	-
25	CLA	1	613	16	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CHL	S	306	-	-	11/20/96/117	-
34	LUT	7	315	-	-	2/29/67/67	0/2/2/2
33	CHL	4	306	-	-	6/23/99/117	-
33	CHL	T	601	-	-	9/22/98/117	-
25	CLA	O	201	-	-	8/10/86/115	-
25	CLA	2	304	-	-	18/39/115/115	-
25	CLA	R	604	-	-	7/21/97/115	-
25	CLA	B	801	-	-	14/39/115/115	-
32	LMG	J	107	-	-	18/50/70/70	0/1/1/1
28	BCR	B	842	-	-	6/29/63/63	0/2/2/2
25	CLA	U	312	-	-	16/39/115/115	-
25	CLA	B	824	2	-	19/39/115/115	-
27	LHG	Q	617	-	-	13/53/53/53	-
34	LUT	1	616	25	-	4/29/67/67	0/2/2/2
33	CHL	P	607	-	-	10/25/101/117	-
34	LUT	Q	614	-	-	0/29/67/67	0/2/2/2
25	CLA	5	312	-	-	7/24/100/115	-
25	CLA	R	611	-	-	11/33/109/115	-
33	CHL	T	604	14	-	4/20/96/117	-
34	LUT	Q	615	-	-	2/29/67/67	0/2/2/2
25	CLA	6	609	-	-	10/21/97/115	-
28	BCR	4	321	-	-	7/29/63/63	0/2/2/2
25	CLA	A	834	1	-	11/15/91/115	-
28	BCR	F	803	-	-	2/29/63/63	0/2/2/2
33	CHL	P	601	-	-	8/23/99/117	-
33	CHL	9	306	-	-	5/12/88/117	-
25	CLA	a	301	-	-	12/39/115/115	-
25	CLA	8	313	-	-	13/39/115/115	-
25	CLA	8	302	23	-	15/39/115/115	-
25	CLA	6	614	-	-	5/15/91/115	-
25	CLA	A	832	1	-	15/39/115/115	-
25	CLA	L	206	-	-	6/12/88/115	-
25	CLA	L	209	-	-	6/10/86/115	-
33	CHL	Q	608	25	-	16/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	3	319	-	-	6/29/63/63	0/2/2/2
34	LUT	a	314	-	-	2/29/67/67	0/2/2/2
25	CLA	P	602	-	-	7/39/115/115	-
25	CLA	6	611	27	-	8/27/103/115	-
27	LHG	S	319	-	-	10/53/53/53	-
25	CLA	K	203	-	-	8/17/93/115	-
25	CLA	6	616	21,27	-	6/17/93/115	-
33	CHL	R	607	-	-	10/25/101/117	-
35	XAT	Q	616	-	-	4/31/93/93	0/4/4/4
25	CLA	T	602	-	-	7/39/115/115	-
25	CLA	7	303	-	-	9/29/105/115	-
25	CLA	A	826	-	-	6/39/115/115	-
25	CLA	H	202	-	-	4/10/86/115	-
25	CLA	B	811	-	-	17/39/115/115	-
33	CHL	P	622	-	-	9/26/102/117	-
25	CLA	9	311	24	-	2/15/91/115	-
25	CLA	R	603	33	-	13/39/115/115	-
34	LUT	P	614	-	-	0/29/67/67	0/2/2/2
25	CLA	9	304	-	-	6/17/93/115	-
25	CLA	A	810	1	-	13/39/115/115	-
25	CLA	4	310	19	-	10/24/100/115	-
25	CLA	5	315	20	-	8/17/93/115	-
25	CLA	B	823	-	-	5/39/115/115	-
25	CLA	B	830	2	-	16/39/115/115	-
25	CLA	B	803	2	-	5/15/91/115	-
25	CLA	4	313	19	-	2/10/86/115	-
25	CLA	K	202	-	-	5/15/91/115	-
25	CLA	A	813	1	-	4/26/102/115	-
25	CLA	6	610	-	-	10/33/109/115	-
33	CHL	T	607	-	-	6/25/101/117	-
25	CLA	2	314	-	-	7/17/93/115	-
33	CHL	7	305	-	-	12/27/103/117	-
25	CLA	A	802	25	-	8/39/115/115	-
25	CLA	P	603	33	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	303	17	-	15/39/115/115	-
33	CHL	S	307	-	-	6/22/98/117	-
25	CLA	A	839	1,25	-	13/39/115/115	-
28	BCR	F	801	-	-	4/29/63/63	0/2/2/2
25	CLA	A	817	-	-	5/30/106/115	-
25	CLA	6	613	-	-	11/29/105/115	-
33	CHL	S	308	-	-	7/25/101/117	-
33	CHL	Q	605	14	-	2/12/88/117	-
25	CLA	A	819	1	-	14/39/115/115	-
25	CLA	A	840	-	-	17/39/115/115	-
25	CLA	B	814	2	-	9/27/103/115	-
25	CLA	A	831	1	-	10/21/97/115	-
25	CLA	a	302	16	-	10/30/106/115	-
25	CLA	H	201	-	-	8/17/93/115	-
25	CLA	A	851	-	-	16/39/115/115	-
25	CLA	F	802	-	-	5/15/91/115	-
27	LHG	a	317	25	-	17/47/47/53	-
36	NEX	P	617	-	-	7/27/83/83	0/3/3/3
25	CLA	5	314	-	-	7/15/91/115	-
36	NEX	U	316	-	-	7/27/83/83	0/3/3/3
25	CLA	A	827	-	-	7/39/115/115	-
25	CLA	Q	602	-	-	7/39/115/115	-
28	BCR	A	846	-	-	2/29/63/63	0/2/2/2
25	CLA	T	612	-	-	11/19/95/115	-
25	CLA	T	609	-	-	14/33/109/115	-
25	CLA	5	311	-	-	10/27/103/115	-
33	CHL	T	606	-	-	7/15/91/117	-
25	CLA	B	816	2	-	13/33/109/115	-
25	CLA	3	310	-	-	7/17/93/115	-
25	CLA	Q	612	-	-	13/33/109/115	-
27	LHG	A	852	25	-	24/49/49/53	-
25	CLA	2	306	17	-	2/10/86/115	-
28	BCR	A	848	-	-	6/29/63/63	0/2/2/2
33	CHL	9	307	-	-	6/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	K	205	-	-	8/15/91/115	-
28	BCR	5	323	-	-	8/29/63/63	0/2/2/2
33	CHL	S	310	15	-	7/25/101/117	-
25	CLA	Q	611	-	-	9/33/109/115	-
33	CHL	Q	606	-	-	7/22/98/117	-
25	CLA	9	301	-	-	5/25/101/115	-
25	CLA	a	309	27	-	10/39/115/115	-
34	LUT	T	613	-	-	0/29/67/67	0/2/2/2
35	XAT	P	620	-	-	4/31/93/93	0/4/4/4
25	CLA	P	610	-	-	9/33/109/115	-
25	CLA	U	303	-	-	13/39/115/115	-
33	CHL	5	308	-	-	7/23/99/117	-
25	CLA	A	801	-	-	13/39/115/115	-
25	CLA	5	303	-	-	13/39/115/115	-
28	BCR	O	205	-	-	4/29/63/63	0/2/2/2
34	LUT	a	316	25	-	6/29/67/67	0/2/2/2
25	CLA	B	818	2	-	11/29/105/115	-
25	CLA	3	302	-	-	8/39/115/115	-
28	BCR	B	841	-	-	4/29/63/63	0/2/2/2
25	CLA	A	833	1	-	0/21/97/115	-
25	CLA	9	308	-	-	6/21/97/115	-
34	LUT	U	314	-	-	0/29/67/67	0/2/2/2
27	LHG	T	617	-	-	12/53/53/53	-
28	BCR	B	844	-	-	2/29/63/63	0/2/2/2
25	CLA	7	302	-	-	5/17/93/115	-
33	CHL	R	609	25	-	16/41/117/117	-
32	LMG	7	319	-	-	13/31/51/70	0/1/1/1
25	CLA	U	302	-	-	8/39/115/115	-
25	CLA	3	313	-	-	5/17/93/115	-
25	CLA	R	610	-	-	12/38/114/115	-
25	CLA	B	809	2,28	-	15/39/115/115	-
25	CLA	5	319	-	-	10/17/93/115	-
28	BCR	B	845	-	-	4/29/63/63	0/2/2/2
27	LHG	1	618	25	-	15/47/47/53	-
28	BCR	B	840	28	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	312	19	-	4/15/91/115	-
28	BCR	A	847	-	-	2/29/63/63	0/2/2/2
25	CLA	A	838	1	-	14/39/115/115	-
25	CLA	B	807	-	-	13/39/115/115	-
25	CLA	T	603	-	-	8/21/97/115	-
25	CLA	Q	604	-	-	8/21/97/115	-
34	LUT	4	315	-	-	1/29/67/67	0/2/2/2
25	CLA	1	603	16	-	12/39/115/115	-
25	CLA	R	613	-	-	17/39/115/115	-
25	CLA	2	305	-	-	9/24/100/115	-
33	CHL	4	322	16,19	-	7/26/102/117	-
25	CLA	8	312	25	-	9/24/100/115	-
25	CLA	A	812	-	-	16/39/115/115	-
25	CLA	A	825	-	-	22/39/115/115	-
25	CLA	S	305	-	-	6/21/97/115	-
34	LUT	3	316	-	-	0/29/67/67	0/2/2/2
25	CLA	J	103	-	-	13/31/107/115	-
25	CLA	a	306	-	-	8/39/115/115	-
25	CLA	B	802	-	-	15/39/115/115	-
25	CLA	a	311	16	-	15/39/115/115	-
25	CLA	Q	609	-	-	11/39/115/115	-
28	BCR	3	318	-	-	8/29/63/63	0/2/2/2
25	CLA	A	804	1	-	11/39/115/115	-
33	CHL	Q	601	-	-	8/23/99/117	-
36	NEX	P	621	-	-	10/27/83/83	0/3/3/3
25	CLA	B	835	2	-	6/18/94/115	-
25	CLA	7	304	-	-	10/12/88/115	-
25	CLA	P	612	-	-	13/33/109/115	-
25	CLA	7	310	-	-	9/24/100/115	-
33	CHL	a	305	-	-	8/20/96/117	-
25	CLA	6	603	-	-	13/39/115/115	-
25	CLA	B	849	-	-	15/39/115/115	-
27	LHG	6	618	25	-	23/53/53/53	-
30	DGD	B	846	-	-	15/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	815	-	-	17/32/108/115	-
34	LUT	4	316	-	-	4/29/67/67	0/2/2/2
25	CLA	1	607	-	-	8/39/115/115	-
25	CLA	A	803	-	-	5/39/115/115	-
25	CLA	8	309	-	-	6/17/93/115	-
25	CLA	8	306	-	-	5/12/88/115	-
25	CLA	L	205	12	-	11/39/115/115	-
25	CLA	9	309	-	-	12/33/109/115	-
33	CHL	U	306	-	-	7/22/98/117	-
28	BCR	4	317	19	-	8/29/63/63	0/2/2/2
25	CLA	S	315	15	-	8/19/95/115	-
25	CLA	9	305	-	-	9/21/97/115	-
28	BCR	8	318	-	-	5/29/63/63	0/2/2/2
25	CLA	H	203	-	-	10/17/93/115	-
25	CLA	A	828	1	-	17/39/115/115	-
33	CHL	6	608	-	-	12/23/99/117	-
25	CLA	A	816	1	-	14/39/115/115	-
28	BCR	6	621	-	-	8/29/63/63	0/2/2/2
25	CLA	7	312	22	-	3/13/89/115	-
25	CLA	S	303	15	-	11/39/115/115	-
32	LMG	6	602	-	-	12/35/55/70	0/1/1/1
29	SF4	C	101	3	-	-	0/6/5/5
25	CLA	2	311	-	-	10/24/100/115	-
25	CLA	5	316	-	-	4/13/89/115	-
25	CLA	2	310	-	-	4/10/86/115	-
25	CLA	3	304	-	-	2/12/88/115	-
25	CLA	1	602	-	-	11/39/115/115	-
25	CLA	A	837	1	-	12/39/115/115	-
27	LHG	P	624	-	-	12/53/53/53	-
28	BCR	J	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	834	2	-	22/39/115/115	-
25	CLA	S	313	-	-	15/33/109/115	-
25	CLA	9	310	24	-	12/21/97/115	-
25	CLA	7	309	27	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	4	318	25	-	20/53/53/53	-
25	CLA	A	853	-	-	17/39/115/115	-
25	CLA	3	307	-	-	9/21/97/115	-
25	CLA	6	623	-	-	15/33/109/115	-
25	CLA	3	303	-	-	10/39/115/115	-
25	CLA	3	305	18	-	14/33/109/115	-
25	CLA	A	806	-	-	19/39/115/115	-
25	CLA	8	314	-	-	9/27/103/115	-
26	PQN	B	839	-	-	3/23/43/43	0/2/2/2
28	BCR	O	204	-	-	5/29/63/63	0/2/2/2
25	CLA	A	842	27	-	13/24/100/115	-
25	CLA	7	306	-	-	4/21/97/115	-
25	CLA	5	309	-	-	12/21/97/115	-
25	CLA	A	808	1	-	13/39/115/115	-
28	BCR	L	207	-	-	8/29/63/63	0/2/2/2
25	CLA	8	315	23	-	7/17/93/115	-
26	PQN	A	841	-	-	6/23/43/43	0/2/2/2
34	LUT	8	316	-	-	1/29/67/67	0/2/2/2
25	CLA	B	805	-	-	16/39/115/115	-
25	CLA	O	203	-	-	0/4/80/115	-
33	CHL	P	619	-	-	10/25/101/117	-
33	CHL	P	609	25	-	16/41/117/117	-
34	LUT	3	315	-	-	0/29/67/67	0/2/2/2
25	CLA	8	308	-	-	6/21/97/115	-
29	SF4	A	850	2,1	-	-	0/6/5/5
25	CLA	A	815	1,27	-	17/33/109/115	-
28	BCR	A	849	-	-	6/29/63/63	0/2/2/2
25	CLA	B	829	-	-	7/20/96/115	-
34	LUT	9	313	-	-	2/29/67/67	0/2/2/2
27	LHG	R	618	-	-	13/53/53/53	-
25	CLA	K	201	1	-	10/23/99/115	-
33	CHL	P	608	-	-	7/15/91/117	-
27	LHG	5	301	-	-	19/49/49/53	-
25	CLA	O	202	-	-	2/6/78/115	-
28	BCR	B	851	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CHL	4	314	19	-	6/14/90/117	-
33	CHL	U	308	-	-	7/15/91/117	-
25	CLA	2	302	17	-	13/17/93/115	-
27	LHG	7	317	25	-	14/41/41/53	-
25	CLA	3	314	-	-	15/29/105/115	-
25	CLA	R	614	-	-	11/19/95/115	-
25	CLA	A	824	-	-	10/27/103/115	-
27	LHG	2	317	-	-	24/53/53/53	-
34	LUT	6	619	-	-	1/29/67/67	0/2/2/2
25	CLA	9	303	-	-	12/33/109/115	-
25	CLA	B	838	-	-	11/39/115/115	-
32	LMG	J	102	-	-	8/35/55/70	0/1/1/1
34	LUT	7	314	-	-	2/29/67/67	0/2/2/2
27	LHG	8	319	25	-	17/53/53/53	-
25	CLA	3	311	-	-	11/27/103/115	-
25	CLA	B	821	2	-	8/33/109/115	-
25	CLA	5	305	-	-	4/21/97/115	-
25	CLA	Q	610	-	-	2/10/82/115	-
25	CLA	U	313	-	-	9/15/91/115	-
32	LMG	H	204	-	-	14/42/62/70	0/1/1/1

All (3923) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	841	PQN	C3-C2	6.71	1.47	1.35
26	B	839	PQN	C3-C2	6.59	1.47	1.35
33	Q	608	CHL	CMC-C2C	5.40	1.56	1.45
33	P	609	CHL	CMC-C2C	5.37	1.56	1.45
33	R	609	CHL	CMC-C2C	5.35	1.56	1.45
33	T	601	CHL	CHD-C1D	5.33	1.48	1.38
33	8	307	CHL	O2D-CGD	5.31	1.46	1.33
33	R	601	CHL	CHD-C1D	5.18	1.48	1.38
33	Q	601	CHL	CHD-C1D	5.18	1.48	1.38
33	U	309	CHL	CHD-C1D	5.18	1.48	1.38
33	4	305	CHL	O2D-CGD	5.17	1.45	1.33
33	P	601	CHL	CHD-C1D	5.17	1.48	1.38
33	T	601	CHL	C2C-C3C	5.16	1.47	1.36
33	P	622	CHL	O2D-CGD	5.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	R	605	CHL	CHD-C1D	5.14	1.48	1.38
33	U	305	CHL	O2D-CGD	5.13	1.45	1.33
33	P	601	CHL	C2C-C3C	5.13	1.47	1.36
33	Q	601	CHL	C2C-C3C	5.13	1.47	1.36
33	T	601	CHL	O2D-CGD	5.11	1.45	1.33
33	R	601	CHL	C2C-C3C	5.11	1.47	1.36
33	U	309	CHL	O2D-CGD	5.10	1.45	1.33
33	Q	601	CHL	O2D-CGD	5.09	1.45	1.33
33	R	601	CHL	O2D-CGD	5.09	1.45	1.33
33	S	302	CHL	O2D-CGD	5.09	1.45	1.33
33	P	622	CHL	CHD-C1D	5.09	1.48	1.38
33	Q	606	CHL	O2D-CGD	5.09	1.45	1.33
33	P	601	CHL	O2D-CGD	5.08	1.45	1.33
33	T	607	CHL	C2C-C3C	5.08	1.47	1.36
33	R	606	CHL	O2D-CGD	5.08	1.45	1.33
33	S	308	CHL	O2D-CGD	5.07	1.45	1.33
33	S	307	CHL	CHD-C1D	5.07	1.48	1.38
33	Q	605	CHL	O2D-CGD	5.06	1.45	1.33
33	S	310	CHL	O2D-CGD	5.06	1.45	1.33
33	U	309	CHL	C2C-C3C	5.06	1.47	1.36
33	S	306	CHL	O2D-CGD	5.05	1.45	1.33
33	T	604	CHL	O2D-CGD	5.05	1.45	1.33
33	P	619	CHL	O2D-CGD	5.05	1.45	1.33
33	4	314	CHL	O2D-CGD	5.04	1.45	1.33
33	P	607	CHL	O2D-CGD	5.04	1.45	1.33
33	9	307	CHL	O2D-CGD	5.03	1.45	1.33
33	S	309	CHL	O2D-CGD	5.03	1.45	1.33
33	T	607	CHL	O2D-CGD	5.03	1.45	1.33
33	R	607	CHL	O2D-CGD	5.01	1.45	1.33
33	6	606	CHL	O2D-CGD	5.01	1.45	1.33
33	R	605	CHL	C2C-C3C	4.98	1.47	1.36
33	4	304	CHL	O2D-CGD	4.97	1.45	1.33
25	a	303	CLA	C2-C3	4.97	1.44	1.33
33	T	607	CHL	CHD-C1D	4.97	1.48	1.38
33	S	307	CHL	O2D-CGD	4.97	1.45	1.33
33	S	306	CHL	CHD-C1D	4.94	1.48	1.38
33	P	606	CHL	O2D-CGD	4.94	1.45	1.33
33	P	605	CHL	O2D-CGD	4.94	1.45	1.33
33	R	608	CHL	O2D-CGD	4.93	1.45	1.33
33	T	605	CHL	O2D-CGD	4.93	1.45	1.33
33	Q	607	CHL	O2D-CGD	4.93	1.45	1.33
33	4	305	CHL	CHD-C1D	4.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	R	605	CHL	O2D-CGD	4.92	1.45	1.33
33	T	606	CHL	O2D-CGD	4.92	1.45	1.33
33	6	607	CHL	O2D-CGD	4.92	1.45	1.33
33	P	608	CHL	O2D-CGD	4.91	1.45	1.33
33	9	306	CHL	C3A-C2A	-4.91	1.49	1.54
33	6	617	CHL	O2D-CGD	4.90	1.45	1.33
33	T	606	CHL	C2C-C3C	4.90	1.47	1.36
33	a	305	CHL	CHD-C1D	4.89	1.47	1.38
33	7	305	CHL	O2D-CGD	4.88	1.45	1.33
33	T	604	CHL	C2C-C3C	4.88	1.47	1.36
33	P	605	CHL	C2C-C3C	4.87	1.47	1.36
33	Q	607	CHL	CHD-C1D	4.87	1.47	1.38
33	U	306	CHL	O2D-CGD	4.87	1.45	1.33
33	U	308	CHL	O2D-CGD	4.87	1.45	1.33
33	P	608	CHL	CHD-C1D	4.86	1.47	1.38
33	R	608	CHL	CHD-C1D	4.86	1.47	1.38
33	U	308	CHL	CHD-C1D	4.86	1.47	1.38
33	U	307	CHL	O2D-CGD	4.86	1.45	1.33
33	9	306	CHL	O2D-CGD	4.86	1.45	1.33
33	S	307	CHL	C2C-C3C	4.86	1.47	1.36
33	S	321	CHL	C2C-C3C	4.85	1.47	1.36
33	U	306	CHL	C2C-C3C	4.85	1.47	1.36
33	4	322	CHL	O2D-CGD	4.85	1.45	1.33
33	5	317	CHL	O2D-CGD	4.84	1.45	1.33
33	S	307	CHL	CHC-C1C	4.83	1.48	1.38
33	U	305	CHL	C2C-C3C	4.83	1.47	1.36
33	U	307	CHL	C2C-C3C	4.82	1.47	1.36
33	a	305	CHL	O2D-CGD	4.80	1.44	1.33
33	T	606	CHL	CHD-C1D	4.79	1.47	1.38
33	Q	605	CHL	C3A-C2A	-4.79	1.50	1.54
33	S	306	CHL	C2C-C3C	4.79	1.47	1.36
33	S	310	CHL	CHD-C1D	4.79	1.47	1.38
33	Q	605	CHL	C2C-C3C	4.76	1.46	1.36
33	Q	605	CHL	CHD-C1D	4.76	1.47	1.38
33	P	606	CHL	C2C-C3C	4.75	1.46	1.36
33	P	619	CHL	CHD-C1D	4.74	1.47	1.38
33	S	321	CHL	CHD-C1D	4.74	1.47	1.38
33	P	606	CHL	CHD-C1D	4.73	1.47	1.38
33	U	307	CHL	CHD-C1D	4.73	1.47	1.38
33	R	607	CHL	CHD-C1D	4.73	1.47	1.38
33	S	309	CHL	C2C-C3C	4.73	1.46	1.36
33	P	607	CHL	CHD-C1D	4.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	617	CHL	CHD-C1D	4.71	1.47	1.38
33	Q	606	CHL	C2C-C3C	4.71	1.46	1.36
33	S	310	CHL	C2C-C3C	4.71	1.46	1.36
33	S	321	CHL	O2D-CGD	4.70	1.44	1.33
33	U	305	CHL	CHD-C1D	4.70	1.47	1.38
33	P	605	CHL	CHD-C1D	4.70	1.47	1.38
33	8	307	CHL	CHD-C1D	4.69	1.47	1.38
33	T	604	CHL	CHD-C1D	4.69	1.47	1.38
33	T	605	CHL	CHD-C1D	4.69	1.47	1.38
33	T	605	CHL	C2C-C3C	4.69	1.46	1.36
33	Q	606	CHL	CHD-C1D	4.69	1.47	1.38
33	1	606	CHL	O2D-CGD	4.68	1.44	1.33
33	U	306	CHL	CHD-C1D	4.68	1.47	1.38
33	U	309	CHL	CHC-C1C	4.67	1.48	1.38
33	R	606	CHL	CHD-C1D	4.66	1.47	1.38
33	4	305	CHL	C2C-C3C	4.66	1.46	1.36
33	P	622	CHL	CHC-C1C	4.66	1.48	1.38
33	S	308	CHL	CHD-C1D	4.66	1.47	1.38
33	Q	607	CHL	C2C-C3C	4.65	1.46	1.36
33	R	606	CHL	C2C-C3C	4.65	1.46	1.36
33	4	305	CHL	CHC-C1C	4.65	1.48	1.38
33	5	307	CHL	O2D-CGD	4.64	1.44	1.33
33	1	606	CHL	C2C-C3C	4.64	1.46	1.36
33	4	314	CHL	CHD-C1D	4.64	1.47	1.38
33	R	608	CHL	C2C-C3C	4.63	1.46	1.36
33	1	606	CHL	CHC-C1C	4.62	1.47	1.38
33	U	308	CHL	C2C-C3C	4.62	1.46	1.36
33	1	606	CHL	CHD-C1D	4.62	1.47	1.38
33	P	608	CHL	C2C-C3C	4.62	1.46	1.36
33	1	601	CHL	O2D-CGD	4.61	1.44	1.33
33	a	305	CHL	C2C-C3C	4.60	1.46	1.36
33	S	309	CHL	CHD-C1D	4.58	1.47	1.38
33	6	608	CHL	O2D-CGD	4.58	1.44	1.33
33	R	605	CHL	O2A-CGA	4.57	1.46	1.30
33	P	619	CHL	C2C-C3C	4.57	1.46	1.36
33	R	601	CHL	CHC-C1C	4.56	1.47	1.38
33	P	607	CHL	C2C-C3C	4.56	1.46	1.36
33	P	601	CHL	CHC-C1C	4.55	1.47	1.38
33	T	601	CHL	CHC-C1C	4.55	1.47	1.38
33	Q	601	CHL	CHC-C1C	4.54	1.47	1.38
33	R	607	CHL	C2C-C3C	4.53	1.46	1.36
33	P	622	CHL	C2C-C3C	4.53	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	307	CHL	CHD-C1D	4.53	1.47	1.38
33	6	607	CHL	C2C-C3C	4.52	1.46	1.36
33	5	307	CHL	CHD-C1D	4.52	1.47	1.38
33	U	305	CHL	O2A-CGA	4.51	1.45	1.30
33	6	606	CHL	O2A-CGA	4.51	1.46	1.33
33	T	607	CHL	CHC-C1C	4.51	1.47	1.38
33	4	322	CHL	C2C-C3C	4.50	1.46	1.36
33	5	307	CHL	C2C-C3C	4.49	1.46	1.36
33	4	304	CHL	CHD-C1D	4.49	1.47	1.38
33	4	306	CHL	O2D-CGD	4.48	1.44	1.33
31	B	850	SQD	O8-S	4.48	1.63	1.47
33	5	308	CHL	O2D-CGD	4.46	1.44	1.33
33	a	305	CHL	CHC-C1C	4.45	1.47	1.38
33	7	305	CHL	CHD-C1D	4.45	1.47	1.38
33	1	606	CHL	O2A-CGA	4.43	1.46	1.33
33	4	306	CHL	O2A-CGA	4.42	1.46	1.33
33	R	605	CHL	CHC-C1C	4.42	1.47	1.38
33	T	605	CHL	O2A-CGA	4.42	1.46	1.33
33	a	305	CHL	O2A-CGA	4.42	1.46	1.33
33	S	308	CHL	C2C-C3C	4.42	1.46	1.36
33	S	302	CHL	C2C-C3C	4.41	1.46	1.36
27	A	852	LHG	O7-C7	4.41	1.46	1.34
25	P	611	CLA	C4B-NB	-4.40	1.32	1.37
33	Q	606	CHL	O2A-CGA	4.38	1.46	1.33
33	6	617	CHL	C2C-C3C	4.38	1.46	1.36
31	B	850	SQD	O48-C23	4.38	1.46	1.33
33	S	302	CHL	CHD-C1D	4.37	1.46	1.38
33	P	605	CHL	O2A-CGA	4.37	1.46	1.33
33	R	606	CHL	CHC-C1C	4.37	1.47	1.38
33	4	306	CHL	CHD-C1D	4.37	1.46	1.38
33	7	305	CHL	O2A-CGA	4.36	1.46	1.33
32	1	619	LMG	O8-C28	4.36	1.46	1.33
27	T	617	LHG	O8-C23	4.36	1.46	1.33
33	U	309	CHL	O2A-CGA	4.35	1.46	1.33
25	P	612	CLA	O2D-CGD	4.35	1.43	1.33
33	P	606	CHL	O2A-CGA	4.35	1.46	1.33
33	S	302	CHL	CHC-C1C	4.35	1.47	1.38
33	4	322	CHL	CHD-C1D	4.34	1.46	1.38
25	P	611	CLA	CHC-C1C	4.34	1.47	1.38
25	R	612	CLA	O2D-CGD	4.33	1.43	1.33
33	5	317	CHL	C2C-C3C	4.33	1.46	1.36
33	6	608	CHL	CHD-C1D	4.33	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Q	601	CHL	O2A-CGA	4.33	1.46	1.33
33	4	305	CHL	O2A-CGA	4.33	1.46	1.33
33	8	307	CHL	C2C-C3C	4.33	1.46	1.36
33	6	606	CHL	CHD-C1D	4.33	1.46	1.38
33	9	306	CHL	CHD-C1D	4.33	1.46	1.38
32	6	602	LMG	O8-C28	4.33	1.46	1.33
33	6	608	CHL	O2A-CGA	4.32	1.46	1.33
33	9	307	CHL	C2C-C3C	4.32	1.46	1.36
33	P	601	CHL	O2A-CGA	4.32	1.46	1.33
33	4	314	CHL	C2C-C3C	4.32	1.46	1.36
33	T	601	CHL	O2A-CGA	4.32	1.46	1.33
33	R	601	CHL	O2A-CGA	4.31	1.45	1.33
33	S	307	CHL	O2A-CGA	4.31	1.45	1.33
33	U	306	CHL	O2A-CGA	4.31	1.45	1.33
33	9	307	CHL	O2A-CGA	4.31	1.45	1.33
33	T	607	CHL	O2A-CGA	4.30	1.45	1.33
33	T	604	CHL	CHC-C1C	4.30	1.47	1.38
33	4	304	CHL	C3A-C2A	-4.30	1.50	1.54
25	T	610	CLA	C1D-ND	4.29	1.43	1.37
33	5	308	CHL	O2A-CGA	4.28	1.45	1.33
32	2	301	LMG	O8-C28	4.28	1.45	1.33
25	R	603	CLA	C1D-ND	4.28	1.43	1.37
33	5	307	CHL	O2A-CGA	4.27	1.45	1.33
33	S	310	CHL	CHC-C1C	4.27	1.47	1.38
33	U	307	CHL	CHC-C1C	4.27	1.47	1.38
27	S	319	LHG	O8-C23	4.26	1.45	1.33
33	5	317	CHL	CHD-C1D	4.26	1.46	1.38
33	S	308	CHL	O2A-CGA	4.26	1.45	1.33
27	P	624	LHG	O8-C23	4.26	1.45	1.33
33	T	606	CHL	CHC-C1C	4.25	1.47	1.38
33	U	306	CHL	CHC-C1C	4.25	1.47	1.38
33	S	310	CHL	O2A-CGA	4.25	1.45	1.33
33	S	302	CHL	O2A-CGA	4.25	1.45	1.33
33	1	601	CHL	C2C-C3C	4.25	1.45	1.36
33	8	307	CHL	CHC-C1C	4.25	1.47	1.38
33	Q	605	CHL	CHC-C1C	4.25	1.47	1.38
33	P	619	CHL	CHC-C1C	4.24	1.47	1.38
27	P	618	LHG	O8-C23	4.24	1.45	1.33
33	U	309	CHL	CHC-C4B	4.24	1.48	1.39
32	7	319	LMG	O7-C10	4.24	1.46	1.34
33	U	308	CHL	CHC-C1C	4.24	1.47	1.38
33	S	321	CHL	CHC-C1C	4.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	309	CHL	O2A-CGA	4.23	1.45	1.33
33	U	307	CHL	O2A-CGA	4.23	1.45	1.33
33	T	604	CHL	O2A-CGA	4.23	1.45	1.33
33	Q	606	CHL	CHC-C1C	4.23	1.47	1.38
33	3	306	CHL	O2D-CGD	4.23	1.43	1.33
33	P	606	CHL	CHC-C1C	4.23	1.47	1.38
33	S	308	CHL	CHC-C1C	4.23	1.47	1.38
33	7	305	CHL	C2C-C3C	4.23	1.45	1.36
33	Q	607	CHL	CHC-C1C	4.23	1.47	1.38
33	6	607	CHL	O2A-CGA	4.22	1.45	1.33
33	9	306	CHL	C2C-C3C	4.22	1.45	1.36
32	J	107	LMG	O8-C28	4.22	1.45	1.33
32	7	318	LMG	O8-C28	4.22	1.45	1.33
33	P	607	CHL	CHC-C1C	4.22	1.47	1.38
33	P	608	CHL	CHC-C1C	4.22	1.47	1.38
33	6	608	CHL	CHC-C1C	4.21	1.47	1.38
33	1	601	CHL	CHD-C1D	4.21	1.46	1.38
27	R	618	LHG	O7-C7	4.21	1.46	1.34
33	8	307	CHL	O2A-CGA	4.21	1.45	1.33
33	P	619	CHL	O2A-CGA	4.21	1.45	1.33
33	R	608	CHL	CHC-C1C	4.21	1.47	1.38
32	7	319	LMG	O8-C28	4.21	1.45	1.33
27	A	844	LHG	O8-C23	4.20	1.45	1.33
33	6	607	CHL	CHD-C1D	4.20	1.46	1.38
33	3	306	CHL	O2A-CGA	4.20	1.45	1.33
33	3	306	CHL	CHD-C1D	4.20	1.46	1.38
33	P	622	CHL	O2A-CGA	4.19	1.45	1.33
32	J	107	LMG	O7-C10	4.19	1.46	1.34
33	R	607	CHL	CHC-C1C	4.18	1.47	1.38
27	4	318	LHG	O8-C23	4.18	1.45	1.33
33	P	607	CHL	O2A-CGA	4.18	1.45	1.33
33	S	306	CHL	O2A-CGA	4.18	1.45	1.33
33	9	307	CHL	CHC-C1C	4.18	1.47	1.38
33	7	305	CHL	CHC-C1C	4.18	1.47	1.38
33	4	304	CHL	C2C-C3C	4.18	1.45	1.36
33	R	607	CHL	O2A-CGA	4.18	1.45	1.33
33	S	307	CHL	CHC-C4B	4.17	1.48	1.39
32	2	301	LMG	O7-C10	4.17	1.46	1.34
32	4	320	LMG	O8-C28	4.16	1.45	1.33
33	U	305	CHL	CHC-C1C	4.16	1.47	1.38
33	S	321	CHL	O2A-CGA	4.16	1.45	1.33
25	Q	610	CLA	C1D-ND	4.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	829	CLA	C4D-ND	-4.14	1.32	1.37
30	B	848	DGD	O1G-C1A	4.14	1.45	1.33
33	P	605	CHL	CHC-C1C	4.14	1.46	1.38
32	7	318	LMG	O7-C10	4.14	1.46	1.34
32	H	204	LMG	O8-C28	4.13	1.45	1.33
27	Q	617	LHG	O8-C23	4.13	1.45	1.33
33	5	308	CHL	CHD-C1D	4.13	1.46	1.38
33	6	607	CHL	CHC-C1C	4.12	1.46	1.38
33	S	309	CHL	CHC-C1C	4.12	1.46	1.38
27	P	624	LHG	O7-C7	4.12	1.45	1.34
33	5	307	CHL	CHC-C1C	4.12	1.46	1.38
27	4	319	LHG	O8-C23	4.11	1.45	1.33
32	1	619	LMG	O7-C10	4.11	1.45	1.34
33	R	601	CHL	CHC-C4B	4.11	1.48	1.39
27	R	618	LHG	O8-C23	4.11	1.45	1.33
33	T	605	CHL	CHC-C1C	4.10	1.46	1.38
33	Q	601	CHL	CHC-C4B	4.09	1.48	1.39
25	R	611	CLA	C1D-ND	4.09	1.42	1.37
33	P	601	CHL	CHC-C4B	4.09	1.48	1.39
27	Q	617	LHG	O7-C7	4.09	1.45	1.34
33	R	605	CHL	CHC-C4B	4.09	1.48	1.39
31	B	850	SQD	O47-C7	4.08	1.45	1.34
27	B	847	LHG	O7-C7	4.07	1.45	1.34
27	8	319	LHG	O7-C7	4.07	1.45	1.34
27	5	301	LHG	O7-C7	4.07	1.45	1.34
25	A	814	CLA	C4D-ND	-4.07	1.32	1.37
27	4	318	LHG	O7-C7	4.07	1.45	1.34
33	4	306	CHL	C2C-C3C	4.07	1.45	1.36
33	4	304	CHL	CHC-C1C	4.07	1.46	1.38
33	4	305	CHL	CHC-C4B	4.07	1.48	1.39
33	T	601	CHL	CHC-C4B	4.06	1.48	1.39
27	8	319	LHG	O8-C23	4.06	1.45	1.33
27	5	301	LHG	O8-C23	4.06	1.45	1.33
25	Q	611	CLA	C1D-ND	4.06	1.42	1.37
33	6	617	CHL	CHC-C1C	4.06	1.46	1.38
27	P	618	LHG	O7-C7	4.05	1.45	1.34
32	J	104	LMG	O8-C28	4.04	1.45	1.33
25	B	811	CLA	C4D-ND	-4.04	1.32	1.37
32	J	102	LMG	O8-C28	4.03	1.45	1.33
27	1	618	LHG	O8-C23	4.03	1.45	1.33
32	H	204	LMG	O7-C10	4.03	1.45	1.34
25	A	806	CLA	C4D-ND	-4.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	P	601	CHL	CHD-C4C	4.03	1.48	1.39
27	6	618	LHG	O8-C23	4.03	1.45	1.33
33	Q	601	CHL	CHD-C4C	4.03	1.48	1.39
25	A	825	CLA	C4D-ND	-4.02	1.32	1.37
33	R	606	CHL	O2A-CGA	4.02	1.45	1.33
32	4	320	LMG	O7-C10	4.01	1.45	1.34
33	R	601	CHL	CHD-C4C	4.01	1.48	1.39
27	5	321	LHG	O8-C23	4.01	1.45	1.33
30	B	846	DGD	O1G-C1A	4.01	1.45	1.33
33	4	322	CHL	O2A-CGA	4.01	1.45	1.33
25	Q	618	CLA	C1D-ND	4.01	1.42	1.37
33	4	306	CHL	CHC-C1C	4.00	1.46	1.38
33	5	308	CHL	CHC-C1C	4.00	1.46	1.38
33	9	306	CHL	CHC-C1C	4.00	1.46	1.38
33	1	606	CHL	CHC-C4B	4.00	1.48	1.39
27	S	319	LHG	O7-C7	4.00	1.45	1.34
27	T	617	LHG	O7-C7	4.00	1.45	1.34
33	S	302	CHL	CHC-C4B	3.99	1.48	1.39
33	a	305	CHL	CHC-C4B	3.99	1.48	1.39
25	B	837	CLA	C4D-ND	-3.99	1.32	1.37
33	4	314	CHL	CHC-C1C	3.99	1.46	1.38
27	2	317	LHG	O8-C23	3.99	1.45	1.33
33	1	601	CHL	O2A-CGA	3.99	1.45	1.33
33	6	606	CHL	C2C-C3C	3.98	1.45	1.36
33	T	601	CHL	CHD-C4C	3.98	1.48	1.39
25	T	609	CLA	C1D-ND	3.98	1.42	1.37
25	A	802	CLA	C4D-ND	-3.98	1.32	1.37
27	A	843	LHG	O8-C23	3.98	1.45	1.33
27	a	317	LHG	O8-C23	3.98	1.45	1.33
30	B	848	DGD	O2G-C1B	3.98	1.45	1.34
25	A	803	CLA	C4D-ND	-3.97	1.32	1.37
33	5	317	CHL	CHC-C1C	3.97	1.46	1.38
25	6	610	CLA	C1D-ND	3.97	1.42	1.37
32	6	602	LMG	O7-C10	3.97	1.45	1.34
32	J	104	LMG	O7-C10	3.97	1.45	1.34
27	B	847	LHG	O8-C23	3.96	1.44	1.33
33	4	322	CHL	CHC-C1C	3.96	1.46	1.38
33	U	309	CHL	CHD-C4C	3.96	1.48	1.39
25	R	610	CLA	C1D-ND	3.95	1.42	1.37
25	R	614	CLA	C1D-ND	3.94	1.42	1.37
25	B	823	CLA	C4D-ND	-3.94	1.32	1.37
33	R	605	CHL	CHD-C4C	3.93	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	T	607	CHL	CHC-C4B	3.93	1.48	1.39
27	4	319	LHG	O7-C7	3.92	1.45	1.34
25	S	314	CLA	C1D-ND	3.92	1.42	1.37
33	U	306	CHL	CHC-C4B	3.92	1.48	1.39
25	P	613	CLA	C1D-ND	3.92	1.42	1.37
33	S	310	CHL	CHC-C4B	3.91	1.48	1.39
33	R	607	CHL	CHC-C4B	3.91	1.48	1.39
25	R	613	CLA	C1D-ND	3.91	1.42	1.37
25	S	313	CLA	C1D-ND	3.90	1.42	1.37
27	2	317	LHG	O7-C7	3.90	1.45	1.34
33	S	321	CHL	CHC-C4B	3.90	1.48	1.39
33	R	606	CHL	CHC-C4B	3.90	1.48	1.39
25	U	302	CLA	C1D-ND	3.90	1.42	1.37
25	B	825	CLA	C4D-ND	-3.90	1.32	1.37
25	3	307	CLA	C4D-ND	-3.89	1.32	1.37
25	B	833	CLA	C4D-ND	-3.89	1.32	1.37
25	Q	611	CLA	C4D-ND	-3.89	1.32	1.37
25	A	826	CLA	C4D-ND	-3.89	1.32	1.37
25	P	611	CLA	C3A-C2A	-3.89	1.50	1.54
25	B	809	CLA	C4D-ND	-3.89	1.32	1.37
33	P	607	CHL	CHC-C4B	3.89	1.48	1.39
27	5	321	LHG	O7-C7	3.89	1.45	1.34
25	R	602	CLA	C1D-ND	3.88	1.42	1.37
33	P	622	CHL	CHB-C1B	3.88	1.48	1.39
25	B	826	CLA	C4D-ND	-3.88	1.32	1.37
25	B	804	CLA	C4D-ND	-3.88	1.32	1.37
33	P	619	CHL	CHC-C4B	3.88	1.48	1.39
33	U	307	CHL	CHC-C4B	3.88	1.48	1.39
25	Q	613	CLA	C1D-ND	3.88	1.42	1.37
33	8	307	CHL	CHC-C4B	3.87	1.48	1.39
33	9	307	CHL	CHC-C4B	3.87	1.48	1.39
27	A	843	LHG	O7-C7	3.87	1.45	1.34
25	B	808	CLA	C4D-ND	-3.87	1.32	1.37
33	6	606	CHL	CHC-C1C	3.87	1.46	1.38
25	A	823	CLA	C4D-ND	-3.86	1.32	1.37
33	1	601	CHL	CHC-C1C	3.86	1.46	1.38
25	B	815	CLA	C4D-ND	-3.86	1.32	1.37
25	3	320	CLA	C4D-ND	-3.86	1.32	1.37
33	S	307	CHL	CHD-C4C	3.86	1.48	1.39
25	A	801	CLA	C4D-ND	-3.86	1.32	1.37
33	S	308	CHL	CHC-C4B	3.85	1.48	1.39
25	3	303	CLA	C4D-ND	-3.84	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	T	606	CHL	CHC-C4B	3.84	1.48	1.39
25	B	829	CLA	C4D-ND	-3.84	1.32	1.37
25	3	313	CLA	C4D-ND	-3.84	1.32	1.37
33	6	608	CHL	CHC-C4B	3.84	1.48	1.39
25	A	820	CLA	C4D-ND	-3.84	1.32	1.37
25	Q	602	CLA	C1D-ND	3.84	1.42	1.37
27	A	852	LHG	O8-C23	3.84	1.44	1.33
25	T	611	CLA	C1D-ND	3.84	1.42	1.37
33	U	305	CHL	OBD-CAD	3.83	1.29	1.22
25	5	313	CLA	C1D-ND	3.83	1.42	1.37
33	P	606	CHL	CHC-C4B	3.83	1.48	1.39
33	T	607	CHL	CHD-C4C	3.83	1.48	1.39
25	U	312	CLA	C1D-ND	3.83	1.42	1.37
25	T	602	CLA	C1D-ND	3.83	1.42	1.37
32	J	102	LMG	O7-C10	3.82	1.45	1.34
25	U	311	CLA	C4D-ND	-3.82	1.32	1.37
25	L	206	CLA	C4D-ND	-3.82	1.32	1.37
33	U	305	CHL	CHC-C4B	3.82	1.48	1.39
25	7	308	CLA	C4D-ND	-3.82	1.32	1.37
25	B	802	CLA	C4D-ND	-3.82	1.32	1.37
33	Q	606	CHL	CHC-C4B	3.81	1.48	1.39
33	6	617	CHL	CHD-C4C	3.81	1.47	1.39
25	T	612	CLA	C1D-ND	3.81	1.42	1.37
27	7	317	LHG	O7-C7	3.81	1.45	1.34
25	Q	609	CLA	C1D-ND	3.81	1.42	1.37
25	U	310	CLA	C1D-ND	3.81	1.42	1.37
27	a	317	LHG	O7-C7	3.81	1.45	1.34
25	5	303	CLA	C4D-ND	-3.81	1.32	1.37
33	4	305	CHL	CHD-C4C	3.81	1.47	1.39
33	U	308	CHL	CHC-C4B	3.80	1.47	1.39
33	6	608	CHL	C2C-C3C	3.80	1.44	1.36
33	S	306	CHL	CHC-C4B	3.80	1.47	1.39
33	Q	605	CHL	CHC-C4B	3.80	1.47	1.39
33	S	309	CHL	CHC-C4B	3.80	1.47	1.39
33	Q	607	CHL	CHC-C4B	3.79	1.47	1.39
25	S	312	CLA	C1D-ND	3.79	1.42	1.37
25	B	827	CLA	C4D-ND	-3.79	1.32	1.37
33	3	306	CHL	C2C-C3C	3.79	1.44	1.36
33	S	306	CHL	CHC-C1C	3.78	1.46	1.38
25	Q	612	CLA	C1D-ND	3.78	1.42	1.37
25	U	311	CLA	CAD-C3D	-3.78	1.43	1.50
33	3	306	CHL	CHC-C1C	3.78	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	T	606	CHL	CHD-C4C	3.78	1.47	1.39
33	P	622	CHL	CHC-C4B	3.78	1.47	1.39
25	L	205	CLA	C4D-ND	-3.78	1.32	1.37
33	T	604	CHL	CHC-C4B	3.78	1.47	1.39
25	U	303	CLA	C1D-ND	3.78	1.42	1.37
25	3	301	CLA	C4D-ND	-3.78	1.32	1.37
25	U	313	CLA	C1D-ND	3.77	1.42	1.37
33	P	608	CHL	CHC-C4B	3.77	1.47	1.39
33	R	607	CHL	OBD-CAD	3.76	1.29	1.22
27	1	618	LHG	O7-C7	3.76	1.44	1.34
33	P	622	CHL	CHD-C4C	3.76	1.47	1.39
25	P	604	CLA	C1D-ND	3.76	1.42	1.37
33	T	605	CHL	CHC-C4B	3.76	1.47	1.39
25	8	303	CLA	C4D-ND	-3.75	1.32	1.37
33	R	608	CHL	CHC-C4B	3.75	1.47	1.39
33	T	601	CHL	OBD-CAD	3.75	1.28	1.22
25	S	320	CLA	C1D-ND	3.75	1.42	1.37
25	7	302	CLA	C4D-ND	-3.75	1.32	1.37
25	A	835	CLA	C4D-ND	-3.75	1.32	1.37
25	T	603	CLA	C1D-ND	3.74	1.42	1.37
33	P	605	CHL	OBD-CAD	3.74	1.28	1.22
33	a	305	CHL	CHD-C4C	3.74	1.47	1.39
25	3	308	CLA	C4D-ND	-3.74	1.32	1.37
33	U	307	CHL	CHD-C4C	3.74	1.47	1.39
25	A	804	CLA	C4D-ND	-3.74	1.32	1.37
25	B	805	CLA	C4D-ND	-3.74	1.32	1.37
33	P	608	CHL	CHD-C4C	3.74	1.47	1.39
33	T	604	CHL	OBD-CAD	3.74	1.28	1.22
33	Q	605	CHL	OBD-CAD	3.74	1.28	1.22
25	Q	603	CLA	C1D-ND	3.74	1.42	1.37
33	P	607	CHL	OBD-CAD	3.73	1.28	1.22
33	R	608	CHL	CHD-C4C	3.73	1.47	1.39
27	7	317	LHG	O8-C23	3.73	1.44	1.33
33	U	308	CHL	CHD-C4C	3.73	1.47	1.39
25	4	301	CLA	C4D-ND	-3.73	1.32	1.37
25	U	304	CLA	C1D-ND	3.73	1.42	1.37
27	A	844	LHG	O7-C7	3.73	1.44	1.34
25	7	313	CLA	C4D-ND	-3.73	1.32	1.37
33	R	601	CHL	CHB-C1B	3.73	1.47	1.39
26	B	839	PQN	C10-C5	3.73	1.46	1.40
25	S	304	CLA	C1D-ND	3.73	1.42	1.37
33	T	601	CHL	CHB-C1B	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	P	605	CHL	CHC-C4B	3.72	1.47	1.39
33	P	601	CHL	CHB-C1B	3.72	1.47	1.39
33	9	306	CHL	CHC-C4B	3.72	1.47	1.39
33	Q	601	CHL	CHB-C1B	3.72	1.47	1.39
33	5	317	CHL	CHC-C4B	3.72	1.47	1.39
33	P	619	CHL	OBD-CAD	3.72	1.28	1.22
25	A	842	CLA	C4D-ND	-3.72	1.32	1.37
25	L	201	CLA	C4D-ND	-3.71	1.32	1.37
25	7	306	CLA	C4D-ND	-3.71	1.32	1.37
25	A	805	CLA	C4D-ND	-3.71	1.32	1.37
33	U	307	CHL	OBD-CAD	3.71	1.28	1.22
33	Q	607	CHL	CHD-C4C	3.71	1.47	1.39
25	A	838	CLA	C4D-ND	-3.71	1.32	1.37
25	B	824	CLA	C4D-ND	-3.71	1.32	1.37
33	S	308	CHL	OBD-CAD	3.71	1.28	1.22
25	2	302	CLA	C4D-ND	-3.71	1.32	1.37
25	6	620	CLA	C4D-ND	-3.71	1.32	1.37
25	A	832	CLA	C4D-ND	-3.71	1.32	1.37
33	T	607	CHL	CHB-C1B	3.70	1.47	1.39
25	B	836	CLA	C4D-ND	-3.70	1.32	1.37
27	6	618	LHG	O7-C7	3.70	1.44	1.34
25	H	205	CLA	C4D-ND	-3.70	1.32	1.37
33	P	606	CHL	CHD-C4C	3.70	1.47	1.39
33	U	308	CHL	OBD-CAD	3.70	1.28	1.22
25	5	305	CLA	C4D-ND	-3.70	1.32	1.37
33	4	314	CHL	OBD-CAD	3.69	1.28	1.22
25	S	303	CLA	C4B-NB	3.69	1.42	1.37
25	A	813	CLA	C4D-ND	-3.69	1.32	1.37
25	B	810	CLA	C4D-ND	-3.69	1.32	1.37
33	3	306	CHL	C1D-ND	-3.69	1.33	1.37
33	U	305	CHL	CHD-C4C	3.68	1.47	1.39
25	6	603	CLA	C4D-ND	-3.68	1.32	1.37
25	A	833	CLA	C4D-ND	-3.68	1.32	1.37
33	S	310	CHL	CHD-C4C	3.68	1.47	1.39
33	Q	605	CHL	CHD-C4C	3.68	1.47	1.39
33	S	321	CHL	CHD-C4C	3.68	1.47	1.39
26	A	841	PQN	C10-C5	3.67	1.46	1.40
25	9	303	CLA	C4D-ND	-3.67	1.32	1.37
33	5	308	CHL	CHC-C4B	3.67	1.47	1.39
25	K	205	CLA	C1D-ND	3.67	1.42	1.37
25	A	819	CLA	C4D-ND	-3.67	1.32	1.37
25	7	304	CLA	C4D-ND	-3.67	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Q	604	CLA	C1D-ND	3.67	1.42	1.37
25	5	316	CLA	C4D-ND	-3.67	1.32	1.37
33	6	617	CHL	CHC-C4B	3.67	1.47	1.39
25	A	839	CLA	C4D-ND	-3.66	1.32	1.37
25	B	817	CLA	C4D-ND	-3.66	1.32	1.37
25	P	602	CLA	C1D-ND	3.66	1.42	1.37
33	S	306	CHL	CHD-C4C	3.66	1.47	1.39
33	5	308	CHL	C2C-C3C	3.66	1.44	1.36
33	S	321	CHL	OBD-CAD	3.66	1.28	1.22
25	Q	613	CLA	C4B-NB	3.66	1.42	1.37
33	U	309	CHL	OBD-CAD	3.66	1.28	1.22
33	7	305	CHL	CHC-C4B	3.66	1.47	1.39
25	B	838	CLA	C4D-ND	-3.66	1.32	1.37
33	U	309	CHL	CHB-C1B	3.65	1.47	1.39
33	R	605	CHL	OBD-CAD	3.65	1.28	1.22
25	4	309	CLA	C1D-ND	3.65	1.42	1.37
25	A	840	CLA	C4D-ND	-3.65	1.32	1.37
25	a	302	CLA	C1D-ND	3.65	1.42	1.37
25	A	851	CLA	C4D-ND	-3.65	1.32	1.37
33	U	306	CHL	OBD-CAD	3.65	1.28	1.22
33	R	601	CHL	OBD-CAD	3.64	1.28	1.22
33	Q	606	CHL	CHD-C4C	3.64	1.47	1.39
25	5	309	CLA	C4D-ND	-3.64	1.32	1.37
30	B	846	DGD	O2G-C1B	3.64	1.44	1.34
33	P	601	CHL	OBD-CAD	3.64	1.28	1.22
33	P	622	CHL	OBD-CAD	3.64	1.28	1.22
33	4	314	CHL	CHD-C4C	3.64	1.47	1.39
25	A	807	CLA	C4D-ND	-3.63	1.32	1.37
25	A	822	CLA	C4D-ND	-3.63	1.32	1.37
25	K	204	CLA	C1D-ND	3.63	1.42	1.37
25	1	612	CLA	OBD-CAD	3.63	1.28	1.22
33	T	606	CHL	OBD-CAD	3.63	1.28	1.22
25	8	305	CLA	C4D-ND	-3.63	1.32	1.37
25	P	610	CLA	C1D-ND	3.63	1.42	1.37
25	3	314	CLA	C4D-ND	-3.63	1.32	1.37
33	Q	606	CHL	OBD-CAD	3.63	1.28	1.22
25	8	310	CLA	C4D-ND	-3.63	1.32	1.37
25	2	310	CLA	C1D-ND	3.63	1.42	1.37
25	B	822	CLA	C4D-ND	-3.63	1.32	1.37
25	B	835	CLA	C4D-ND	-3.63	1.32	1.37
33	R	606	CHL	CHD-C4C	3.62	1.47	1.39
36	R	617	NEX	C7-C8	-3.62	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	809	CLA	C4D-ND	-3.62	1.32	1.37
33	4	304	CHL	CHC-C4B	3.62	1.47	1.39
33	1	601	CHL	C1D-ND	-3.62	1.33	1.37
25	a	312	CLA	C1D-ND	3.61	1.42	1.37
25	5	310	CLA	C1D-ND	3.61	1.42	1.37
33	5	307	CHL	CHC-C4B	3.61	1.47	1.39
25	5	315	CLA	C4D-ND	-3.61	1.32	1.37
33	4	322	CHL	CHC-C4B	3.61	1.47	1.39
25	S	305	CLA	C1D-ND	3.61	1.42	1.37
33	1	606	CHL	CHD-C4C	3.60	1.47	1.39
33	T	604	CHL	CHD-C4C	3.60	1.47	1.39
33	Q	601	CHL	OBD-CAD	3.60	1.28	1.22
33	S	307	CHL	OBD-CAD	3.60	1.28	1.22
25	7	310	CLA	C4D-ND	-3.60	1.32	1.37
25	S	311	CLA	C1D-ND	3.60	1.42	1.37
25	9	301	CLA	C4D-ND	-3.60	1.32	1.37
33	4	305	CHL	OBD-CAD	3.60	1.28	1.22
36	P	617	NEX	C7-C8	-3.60	1.26	1.32
33	R	608	CHL	OBD-CAD	3.59	1.28	1.22
25	7	301	CLA	C4D-ND	-3.59	1.32	1.37
25	9	304	CLA	C4D-ND	-3.59	1.32	1.37
33	T	605	CHL	CHD-C4C	3.59	1.47	1.39
33	U	306	CHL	CHD-C4C	3.59	1.47	1.39
25	R	610	CLA	C4B-NB	3.59	1.42	1.37
25	A	827	CLA	C4D-ND	-3.59	1.32	1.37
25	5	314	CLA	C1D-ND	3.59	1.42	1.37
25	B	828	CLA	C4D-ND	-3.58	1.32	1.37
25	B	812	CLA	C4D-ND	-3.58	1.32	1.37
33	6	606	CHL	CHC-C4B	3.58	1.47	1.39
25	B	821	CLA	C4D-ND	-3.58	1.32	1.37
25	a	309	CLA	C1D-ND	3.58	1.42	1.37
33	4	314	CHL	CHC-C4B	3.58	1.47	1.39
33	S	306	CHL	OBD-CAD	3.58	1.28	1.22
25	F	802	CLA	C4D-ND	-3.58	1.32	1.37
33	P	608	CHL	OBD-CAD	3.57	1.28	1.22
25	6	616	CLA	C4D-ND	-3.57	1.32	1.37
33	4	304	CHL	OBD-CAD	3.57	1.28	1.22
25	7	311	CLA	C4D-ND	-3.57	1.32	1.37
25	8	304	CLA	C4D-ND	-3.57	1.32	1.37
25	2	302	CLA	C1D-ND	3.56	1.42	1.37
25	2	311	CLA	C1D-ND	3.56	1.42	1.37
25	9	302	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	607	CLA	C4D-ND	-3.56	1.32	1.37
25	H	201	CLA	C4D-ND	-3.56	1.32	1.37
33	4	306	CHL	CHD-C4C	3.56	1.47	1.39
25	7	312	CLA	C1D-ND	3.56	1.42	1.37
33	6	607	CHL	CHC-C4B	3.56	1.47	1.39
25	1	602	CLA	C4D-ND	-3.56	1.32	1.37
25	a	310	CLA	C1D-ND	3.56	1.42	1.37
25	R	603	CLA	C4B-NB	3.55	1.42	1.37
33	S	308	CHL	CHD-C4C	3.55	1.47	1.39
25	A	828	CLA	C4D-ND	-3.55	1.32	1.37
33	Q	607	CHL	OBD-CAD	3.55	1.28	1.22
36	U	301	NEX	C7-C8	-3.55	1.26	1.32
25	2	311	CLA	C4D-ND	-3.55	1.32	1.37
25	8	306	CLA	C4D-ND	-3.55	1.32	1.37
25	A	815	CLA	C1D-ND	3.55	1.42	1.37
25	B	801	CLA	C4D-ND	-3.55	1.32	1.37
25	B	803	CLA	C4D-ND	-3.55	1.32	1.37
33	5	317	CHL	OBD-CAD	3.55	1.28	1.22
25	A	811	CLA	C4D-ND	-3.55	1.32	1.37
25	7	303	CLA	C4D-ND	-3.55	1.32	1.37
25	5	304	CLA	C1D-ND	3.55	1.42	1.37
25	A	837	CLA	C4D-ND	-3.55	1.32	1.37
25	7	309	CLA	C4D-ND	-3.55	1.32	1.37
25	A	824	CLA	C4D-ND	-3.54	1.32	1.37
25	B	834	CLA	C4D-ND	-3.54	1.32	1.37
25	B	830	CLA	C4D-ND	-3.54	1.32	1.37
25	T	608	CLA	C1D-ND	3.54	1.42	1.37
25	Q	612	CLA	C4B-NB	3.54	1.42	1.37
25	4	313	CLA	C1D-ND	3.54	1.42	1.37
33	T	605	CHL	OBD-CAD	3.54	1.28	1.22
33	a	305	CHL	CHB-C1B	3.54	1.47	1.39
25	2	313	CLA	C4D-ND	-3.54	1.32	1.37
25	B	820	CLA	C4D-ND	-3.54	1.32	1.37
33	S	309	CHL	CHD-C4C	3.54	1.47	1.39
25	B	807	CLA	C4D-ND	-3.54	1.32	1.37
25	S	315	CLA	C1D-ND	3.54	1.42	1.37
25	A	834	CLA	C4D-ND	-3.53	1.32	1.37
33	1	601	CHL	CHC-C4B	3.53	1.47	1.39
25	a	301	CLA	C1D-ND	3.53	1.42	1.37
33	P	622	CHL	C3D-C2D	3.53	1.48	1.39
33	P	605	CHL	CHD-C4C	3.53	1.47	1.39
36	U	316	NEX	C7-C8	-3.53	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	302	CLA	C4D-ND	-3.53	1.32	1.37
25	6	604	CLA	C4D-ND	-3.53	1.32	1.37
33	R	607	CHL	CHB-C1B	3.52	1.47	1.39
33	5	308	CHL	C1D-ND	-3.52	1.33	1.37
33	T	601	CHL	C3D-C2D	3.52	1.48	1.39
33	9	306	CHL	OBD-CAD	3.52	1.28	1.22
25	6	612	CLA	C4B-NB	3.52	1.42	1.37
33	6	617	CHL	OBD-CAD	3.52	1.28	1.22
25	6	613	CLA	C1D-ND	3.52	1.42	1.37
25	5	304	CLA	C4D-ND	-3.52	1.32	1.37
33	R	609	CHL	O2D-CGD	3.52	1.41	1.33
33	9	307	CHL	CHD-C4C	3.52	1.47	1.39
33	Q	601	CHL	C3D-C2D	3.52	1.48	1.39
25	B	814	CLA	C4D-ND	-3.51	1.32	1.37
25	2	309	CLA	C4D-ND	-3.51	1.32	1.37
33	P	601	CHL	C3D-C2D	3.51	1.48	1.39
33	S	310	CHL	OBD-CAD	3.51	1.28	1.22
25	R	604	CLA	C4B-NB	3.51	1.42	1.37
25	Q	603	CLA	C4B-NB	3.50	1.42	1.37
25	B	831	CLA	C4D-ND	-3.50	1.32	1.37
25	A	812	CLA	C4D-ND	-3.50	1.32	1.37
36	T	616	NEX	C7-C8	-3.50	1.26	1.32
25	S	303	CLA	C4D-ND	-3.50	1.32	1.37
25	2	304	CLA	C4D-ND	-3.50	1.32	1.37
33	S	310	CHL	CHB-C1B	3.50	1.47	1.39
33	P	609	CHL	O2D-CGD	3.50	1.41	1.33
25	Q	618	CLA	C4D-ND	-3.50	1.32	1.37
25	a	311	CLA	C1D-ND	3.50	1.42	1.37
33	R	601	CHL	C3D-C2D	3.49	1.48	1.39
25	S	301	CLA	C1D-ND	3.49	1.42	1.37
25	5	319	CLA	C1D-ND	3.49	1.42	1.37
33	8	307	CHL	CHD-C4C	3.49	1.47	1.39
25	L	209	CLA	C4D-ND	-3.49	1.32	1.37
33	1	606	CHL	CHB-C1B	3.49	1.47	1.39
25	6	615	CLA	C4D-ND	-3.49	1.32	1.37
33	4	306	CHL	CHC-C4B	3.48	1.47	1.39
33	S	307	CHL	CHB-C1B	3.48	1.47	1.39
33	P	606	CHL	OBD-CAD	3.48	1.28	1.22
33	Q	608	CHL	O2D-CGD	3.48	1.41	1.33
25	6	623	CLA	C1D-ND	3.48	1.42	1.37
25	3	304	CLA	C4D-ND	-3.48	1.32	1.37
33	P	607	CHL	CHB-C1B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	849	CLA	C4D-ND	-3.48	1.32	1.37
25	8	312	CLA	C4D-ND	-3.48	1.32	1.37
25	A	821	CLA	C4D-ND	-3.48	1.32	1.37
25	4	310	CLA	C1D-ND	3.47	1.42	1.37
33	U	309	CHL	C3D-C2D	3.47	1.48	1.39
25	8	308	CLA	C4D-ND	-3.47	1.32	1.37
25	P	611	CLA	C1D-ND	3.47	1.42	1.37
33	a	305	CHL	OBD-CAD	3.47	1.28	1.22
25	T	610	CLA	C4B-NB	3.47	1.42	1.37
25	6	614	CLA	C4D-ND	-3.47	1.32	1.37
25	K	203	CLA	C4D-ND	-3.47	1.32	1.37
33	P	619	CHL	CHB-C1B	3.47	1.47	1.39
33	P	607	CHL	CHD-C4C	3.47	1.47	1.39
25	1	613	CLA	C4D-ND	-3.47	1.32	1.37
25	P	611	CLA	C1C-NC	-3.46	1.32	1.37
25	G	202	CLA	C1D-ND	3.46	1.42	1.37
25	O	203	CLA	C1D-ND	3.46	1.42	1.37
25	R	602	CLA	C4B-NB	3.46	1.42	1.37
25	7	312	CLA	C4D-ND	-3.46	1.32	1.37
25	4	303	CLA	C4D-ND	-3.46	1.32	1.37
33	R	606	CHL	OBD-CAD	3.46	1.28	1.22
25	A	853	CLA	C4D-ND	-3.46	1.32	1.37
25	J	105	CLA	C4D-ND	-3.45	1.32	1.37
25	8	313	CLA	C4D-ND	-3.45	1.32	1.37
25	P	603	CLA	C1D-ND	3.45	1.42	1.37
25	9	301	CLA	CAB-C3B	-3.45	1.43	1.50
25	2	314	CLA	C4D-ND	-3.45	1.32	1.37
25	2	307	CLA	C4D-ND	-3.45	1.33	1.37
33	Q	606	CHL	CHB-C1B	3.45	1.47	1.39
25	1	610	CLA	C4D-ND	-3.45	1.33	1.37
25	a	313	CLA	C1D-ND	3.45	1.42	1.37
25	Q	604	CLA	C4B-NB	3.45	1.42	1.37
33	4	306	CHL	C1D-ND	-3.45	1.33	1.37
33	4	322	CHL	C1D-ND	-3.45	1.33	1.37
33	4	304	CHL	CHB-C1B	3.45	1.47	1.39
25	6	609	CLA	C4D-ND	-3.45	1.33	1.37
25	6	612	CLA	C1D-ND	3.44	1.42	1.37
25	9	311	CLA	C1D-ND	3.44	1.42	1.37
25	A	830	CLA	C4D-ND	-3.44	1.33	1.37
33	P	619	CHL	CHD-C4C	3.44	1.47	1.39
25	L	202	CLA	C4D-ND	-3.44	1.33	1.37
25	5	324	CLA	C4D-ND	-3.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	808	CLA	C4D-ND	-3.44	1.33	1.37
25	3	310	CLA	C4D-ND	-3.44	1.33	1.37
25	8	315	CLA	C4D-ND	-3.44	1.33	1.37
25	Q	602	CLA	C4B-NB	3.44	1.42	1.37
25	2	314	CLA	C1D-ND	3.44	1.42	1.37
25	1	614	CLA	C4D-ND	-3.44	1.33	1.37
25	4	311	CLA	C1D-ND	3.44	1.42	1.37
33	U	307	CHL	CHB-C1B	3.44	1.47	1.39
25	4	308	CLA	C4D-ND	-3.44	1.33	1.37
33	R	607	CHL	CHD-C4C	3.43	1.47	1.39
25	6	611	CLA	C1D-ND	3.43	1.42	1.37
33	T	607	CHL	OBD-CAD	3.43	1.28	1.22
25	K	204	CLA	C4B-NB	3.43	1.42	1.37
33	4	322	CHL	OBD-CAD	3.43	1.28	1.22
25	A	831	CLA	C4D-ND	-3.43	1.33	1.37
25	U	302	CLA	C4B-NB	3.43	1.42	1.37
25	B	830	CLA	C1D-ND	3.43	1.42	1.37
25	B	806	CLA	C4D-ND	-3.43	1.33	1.37
25	3	312	CLA	C4D-ND	-3.43	1.33	1.37
25	5	311	CLA	C4D-ND	-3.42	1.33	1.37
25	H	202	CLA	C4D-ND	-3.42	1.33	1.37
25	3	305	CLA	C4D-ND	-3.42	1.33	1.37
25	9	309	CLA	C4D-ND	-3.42	1.33	1.37
25	3	311	CLA	C4D-ND	-3.42	1.33	1.37
25	8	309	CLA	C4D-ND	-3.42	1.33	1.37
33	S	306	CHL	C3D-C2D	3.42	1.48	1.39
25	a	303	CLA	O2A-CGA	3.42	1.43	1.33
25	4	302	CLA	C1D-ND	3.42	1.42	1.37
25	a	306	CLA	C1D-ND	3.42	1.42	1.37
25	K	201	CLA	C4D-ND	-3.42	1.33	1.37
25	A	817	CLA	C4D-ND	-3.41	1.33	1.37
25	B	832	CLA	C4D-ND	-3.41	1.33	1.37
25	K	202	CLA	C1D-ND	3.41	1.42	1.37
25	6	611	CLA	C4D-ND	-3.41	1.33	1.37
25	9	310	CLA	C1D-ND	3.41	1.42	1.37
33	S	321	CHL	CHB-C1B	3.41	1.47	1.39
33	9	307	CHL	CHB-C1B	3.41	1.47	1.39
25	6	610	CLA	C4D-ND	-3.40	1.33	1.37
25	2	310	CLA	C4D-ND	-3.40	1.33	1.37
25	a	306	CLA	C4D-ND	-3.40	1.33	1.37
25	5	310	CLA	C4D-ND	-3.40	1.33	1.37
25	9	311	CLA	C4D-ND	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	305	CLA	C1D-ND	3.40	1.42	1.37
25	A	836	CLA	C4D-ND	-3.40	1.33	1.37
25	U	310	CLA	C4B-NB	3.40	1.42	1.37
25	9	308	CLA	C1D-ND	3.40	1.42	1.37
25	A	810	CLA	C4D-ND	-3.39	1.33	1.37
25	2	303	CLA	C4D-ND	-3.39	1.33	1.37
33	3	306	CHL	CHC-C4B	3.39	1.47	1.39
25	9	309	CLA	C1D-ND	3.39	1.42	1.37
25	3	312	CLA	C1D-ND	3.39	1.41	1.37
25	6	615	CLA	C1D-ND	3.39	1.41	1.37
25	6	604	CLA	C1D-ND	3.39	1.41	1.37
25	6	616	CLA	C1D-ND	3.38	1.41	1.37
33	6	608	CHL	C1D-ND	-3.38	1.33	1.37
25	5	312	CLA	C1D-ND	3.38	1.41	1.37
25	5	315	CLA	C1D-ND	3.38	1.41	1.37
33	R	606	CHL	C3D-C2D	3.38	1.48	1.39
25	4	307	CLA	C4D-ND	-3.38	1.33	1.37
25	5	314	CLA	C4D-ND	-3.38	1.33	1.37
33	4	305	CHL	CHB-C1B	3.38	1.47	1.39
33	5	317	CHL	CHD-C4C	3.38	1.46	1.39
25	1	604	CLA	C4D-ND	-3.38	1.33	1.37
25	8	302	CLA	C4D-ND	-3.38	1.33	1.37
25	9	305	CLA	C1D-ND	3.37	1.41	1.37
25	5	312	CLA	C4D-ND	-3.37	1.33	1.37
33	U	308	CHL	C3D-C2D	3.37	1.48	1.39
25	B	816	CLA	C4D-ND	-3.37	1.33	1.37
33	6	606	CHL	CHB-C1B	3.37	1.47	1.39
33	S	302	CHL	CHD-C4C	3.37	1.46	1.39
25	4	307	CLA	C1D-ND	3.37	1.41	1.37
25	7	307	CLA	C4D-ND	-3.37	1.33	1.37
25	8	314	CLA	C4D-ND	-3.37	1.33	1.37
25	S	313	CLA	C4B-NB	3.37	1.41	1.37
25	5	302	CLA	C1D-ND	3.37	1.41	1.37
25	4	302	CLA	C4B-NB	3.36	1.41	1.37
25	9	311	CLA	C4B-NB	3.36	1.41	1.37
25	a	307	CLA	C1D-ND	3.36	1.41	1.37
25	O	202	CLA	C4D-ND	-3.36	1.33	1.37
25	a	310	CLA	C4B-NB	3.36	1.41	1.37
25	2	308	CLA	C4D-ND	-3.36	1.33	1.37
25	6	605	CLA	C4D-ND	-3.36	1.33	1.37
25	2	305	CLA	C4D-ND	-3.36	1.33	1.37
25	J	105	CLA	C1D-ND	3.36	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	813	CLA	C4D-ND	-3.36	1.33	1.37
25	6	601	CLA	C1D-ND	3.36	1.41	1.37
33	6	606	CHL	OBD-CAD	3.35	1.28	1.22
25	B	819	CLA	C4D-ND	-3.35	1.33	1.37
25	8	311	CLA	C4D-ND	-3.35	1.33	1.37
33	1	606	CHL	OBD-CAD	3.35	1.28	1.22
33	4	305	CHL	C3D-C2D	3.35	1.48	1.39
25	6	603	CLA	C1D-ND	3.35	1.41	1.37
25	2	303	CLA	C1D-ND	3.35	1.41	1.37
25	U	303	CLA	C4B-NB	3.35	1.41	1.37
25	5	306	CLA	C4D-ND	-3.35	1.33	1.37
25	J	103	CLA	C4D-ND	-3.34	1.33	1.37
25	1	608	CLA	C4D-ND	-3.34	1.33	1.37
25	a	312	CLA	C4D-ND	-3.34	1.33	1.37
25	H	203	CLA	C4D-ND	-3.34	1.33	1.37
33	7	305	CHL	CHD-C4C	3.34	1.46	1.39
33	S	309	CHL	OBD-CAD	3.34	1.28	1.22
33	8	307	CHL	CHB-C1B	3.34	1.46	1.39
33	6	607	CHL	OBD-CAD	3.33	1.28	1.22
25	K	203	CLA	C1D-ND	3.33	1.41	1.37
25	U	312	CLA	C4B-NB	3.33	1.41	1.37
33	9	306	CHL	CHB-C1B	3.33	1.46	1.39
25	A	818	CLA	C4D-ND	-3.32	1.33	1.37
25	A	815	CLA	C4D-ND	-3.32	1.33	1.37
25	a	304	CLA	C4B-NB	3.32	1.41	1.37
33	T	606	CHL	C3D-C2D	3.32	1.48	1.39
25	H	202	CLA	C1D-ND	3.32	1.41	1.37
25	A	816	CLA	C4D-ND	-3.31	1.33	1.37
25	O	203	CLA	CAB-C3B	-3.31	1.43	1.50
25	G	202	CLA	C4D-ND	-3.31	1.33	1.37
25	P	603	CLA	C4B-NB	3.31	1.41	1.37
25	3	302	CLA	C1D-ND	3.31	1.41	1.37
25	6	612	CLA	C4D-ND	-3.31	1.33	1.37
25	2	307	CLA	C1D-ND	3.31	1.41	1.37
33	S	310	CHL	C3D-C2D	3.31	1.48	1.39
33	Q	606	CHL	C3D-C2D	3.31	1.48	1.39
25	F	802	CLA	C1D-ND	3.31	1.41	1.37
25	3	311	CLA	C1D-ND	3.31	1.41	1.37
25	B	818	CLA	C4D-ND	-3.31	1.33	1.37
33	6	606	CHL	CHD-C4C	3.30	1.46	1.39
33	T	604	CHL	C3D-C2D	3.30	1.48	1.39
33	S	302	CHL	CHB-C1B	3.30	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	611	CLA	C4B-NB	3.30	1.41	1.37
25	a	311	CLA	C4D-ND	-3.30	1.33	1.37
33	S	307	CHL	C3D-C2D	3.30	1.48	1.39
33	P	606	CHL	CHB-C1B	3.30	1.46	1.39
25	K	202	CLA	C4D-ND	-3.30	1.33	1.37
25	O	201	CLA	C4D-ND	-3.30	1.33	1.37
25	R	604	CLA	C1D-ND	3.30	1.41	1.37
33	5	307	CHL	CHD-C4C	3.30	1.46	1.39
25	S	304	CLA	C4B-NB	3.30	1.41	1.37
25	B	816	CLA	C1D-ND	3.30	1.41	1.37
25	T	602	CLA	C4B-NB	3.30	1.41	1.37
25	U	311	CLA	C4B-NB	3.30	1.41	1.37
33	U	305	CHL	C3D-C2D	3.30	1.48	1.39
33	6	608	CHL	OBD-CAD	3.30	1.28	1.22
33	S	308	CHL	CHB-C1B	3.30	1.46	1.39
25	4	313	CLA	C4D-ND	-3.29	1.33	1.37
33	4	306	CHL	OBD-CAD	3.29	1.28	1.22
33	5	308	CHL	OBD-CAD	3.29	1.28	1.22
25	1	605	CLA	C4D-ND	-3.29	1.33	1.37
33	6	608	CHL	CHD-C4C	3.29	1.46	1.39
25	a	304	CLA	C1D-ND	3.29	1.41	1.37
33	7	305	CHL	OBD-CAD	3.29	1.28	1.22
33	T	607	CHL	C3D-C2D	3.29	1.48	1.39
25	a	309	CLA	C4D-ND	-3.29	1.33	1.37
25	H	203	CLA	C1D-ND	3.29	1.41	1.37
25	a	313	CLA	C4D-ND	-3.29	1.33	1.37
25	4	303	CLA	C1D-ND	3.28	1.41	1.37
25	9	308	CLA	C4D-ND	-3.28	1.33	1.37
25	O	201	CLA	C1D-ND	3.28	1.41	1.37
25	1	603	CLA	C4D-ND	-3.28	1.33	1.37
33	1	606	CHL	C1D-ND	-3.28	1.33	1.37
33	Q	605	CHL	C3D-C2D	3.28	1.48	1.39
25	2	306	CLA	C4B-NB	3.28	1.41	1.37
25	3	309	CLA	C4D-ND	-3.28	1.33	1.37
25	3	310	CLA	C1D-ND	3.28	1.41	1.37
25	G	201	CLA	C4D-ND	-3.28	1.33	1.37
25	A	838	CLA	C1D-ND	3.27	1.41	1.37
25	Q	609	CLA	C4B-NB	3.27	1.41	1.37
25	8	306	CLA	C1D-ND	3.27	1.41	1.37
33	6	607	CHL	C1D-ND	-3.27	1.33	1.37
33	9	307	CHL	OBD-CAD	3.27	1.28	1.22
33	4	314	CHL	C3D-C2D	3.27	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	U	306	CHL	CHB-C1B	3.27	1.46	1.39
25	8	312	CLA	C1D-ND	3.27	1.41	1.37
25	G	201	CLA	C1D-ND	3.26	1.41	1.37
25	J	103	CLA	C1D-ND	3.26	1.41	1.37
25	A	810	CLA	C1D-ND	3.26	1.41	1.37
25	1	610	CLA	C1D-ND	3.26	1.41	1.37
25	a	304	CLA	C4D-ND	-3.26	1.33	1.37
25	2	313	CLA	C1D-ND	3.26	1.41	1.37
25	4	310	CLA	C4B-NB	3.26	1.41	1.37
33	4	304	CHL	CHD-C4C	3.26	1.46	1.39
33	4	306	CHL	CHB-C1B	3.26	1.46	1.39
25	A	808	CLA	C1D-ND	3.26	1.41	1.37
33	S	309	CHL	CHB-C1B	3.26	1.46	1.39
33	U	307	CHL	C3D-C2D	3.26	1.48	1.39
25	4	310	CLA	C4D-ND	-3.25	1.33	1.37
33	4	305	CHL	MG-NA	-3.25	1.98	2.06
33	9	306	CHL	CHD-C4C	3.25	1.46	1.39
25	5	316	CLA	C1D-ND	3.25	1.41	1.37
33	6	608	CHL	CHB-C1B	3.25	1.46	1.39
33	U	306	CHL	C3D-C2D	3.25	1.48	1.39
25	1	613	CLA	C1D-ND	3.25	1.41	1.37
25	A	812	CLA	C1D-ND	3.24	1.41	1.37
25	L	209	CLA	C1D-ND	3.24	1.41	1.37
33	4	322	CHL	CHD-C4C	3.23	1.46	1.39
25	1	611	CLA	C1D-ND	3.23	1.41	1.37
25	8	302	CLA	C1D-ND	3.23	1.41	1.37
33	5	307	CHL	OBD-CAD	3.23	1.28	1.22
25	4	309	CLA	C4D-ND	-3.23	1.33	1.37
25	B	832	CLA	C1D-ND	3.23	1.41	1.37
25	R	610	CLA	C3B-C4B	3.23	1.50	1.42
25	a	301	CLA	C4B-NB	3.23	1.41	1.37
33	T	605	CHL	C3D-C2D	3.22	1.47	1.39
25	T	612	CLA	C4B-NB	3.22	1.41	1.37
25	3	309	CLA	C1D-ND	3.22	1.41	1.37
33	3	306	CHL	OBD-CAD	3.22	1.28	1.22
25	a	307	CLA	C4D-ND	-3.22	1.33	1.37
25	B	834	CLA	C1D-ND	3.22	1.41	1.37
25	S	305	CLA	C4B-NB	3.22	1.41	1.37
33	8	307	CHL	OBD-CAD	3.22	1.28	1.22
25	8	315	CLA	C1D-ND	3.22	1.41	1.37
33	9	307	CHL	C3D-C2D	3.22	1.47	1.39
33	9	306	CHL	C1D-ND	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	305	CHL	C3D-C2D	3.22	1.47	1.39
25	2	306	CLA	C4D-ND	-3.22	1.33	1.37
25	P	612	CLA	O1D-CGD	3.22	1.29	1.21
33	T	605	CHL	CHB-C1B	3.21	1.46	1.39
25	P	613	CLA	C4B-NB	3.21	1.41	1.37
25	4	312	CLA	C4D-ND	-3.21	1.33	1.37
25	1	605	CLA	C4B-NB	3.21	1.41	1.37
33	P	605	CHL	C3D-C2D	3.21	1.47	1.39
33	R	606	CHL	CHB-C1B	3.21	1.46	1.39
33	1	601	CHL	OBD-CAD	3.21	1.28	1.22
33	5	308	CHL	CHD-C4C	3.21	1.46	1.39
25	4	312	CLA	C1D-ND	3.21	1.41	1.37
25	1	605	CLA	C1D-ND	3.21	1.41	1.37
25	O	202	CLA	C1D-ND	3.21	1.41	1.37
25	P	602	CLA	C4B-NB	3.21	1.41	1.37
25	A	840	CLA	C1D-ND	3.21	1.41	1.37
25	S	301	CLA	C4B-NB	3.21	1.41	1.37
33	U	308	CHL	CHB-C1B	3.21	1.46	1.39
25	3	305	CLA	C1D-ND	3.20	1.41	1.37
25	6	613	CLA	C4B-NB	3.20	1.41	1.37
25	P	611	CLA	OBD-CAD	3.20	1.28	1.22
33	Q	605	CHL	CHB-C1B	3.20	1.46	1.39
25	S	314	CLA	C4B-NB	3.20	1.41	1.37
25	S	320	CLA	C4B-NB	3.20	1.41	1.37
25	U	304	CLA	C4B-NB	3.20	1.41	1.37
25	R	612	CLA	O1D-CGD	3.20	1.29	1.21
25	a	307	CLA	C4B-NB	3.20	1.41	1.37
25	O	203	CLA	C4D-ND	-3.20	1.33	1.37
25	P	604	CLA	C4B-NB	3.20	1.41	1.37
25	S	314	CLA	C4D-ND	-3.20	1.33	1.37
25	1	602	CLA	C1D-ND	3.20	1.41	1.37
33	T	604	CHL	CHB-C1B	3.20	1.46	1.39
33	P	608	CHL	CHB-C1B	3.20	1.46	1.39
25	4	311	CLA	C4D-ND	-3.19	1.33	1.37
25	5	311	CLA	C1D-ND	3.19	1.41	1.37
33	4	304	CHL	C1D-ND	-3.19	1.33	1.37
25	R	614	CLA	C4B-NB	3.19	1.41	1.37
25	8	311	CLA	C1D-ND	3.19	1.41	1.37
25	1	614	CLA	C1D-ND	3.19	1.41	1.37
33	9	307	CHL	C1D-ND	-3.19	1.33	1.37
25	H	201	CLA	C1D-ND	3.19	1.41	1.37
33	S	321	CHL	C3D-C2D	3.18	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	603	CLA	C4B-NB	3.18	1.41	1.37
33	S	302	CHL	OBD-CAD	3.18	1.28	1.22
25	8	308	CLA	C1D-ND	3.18	1.41	1.37
33	S	302	CHL	C3D-C2D	3.18	1.47	1.39
25	3	301	CLA	C1D-ND	3.18	1.41	1.37
33	P	622	CHL	MG-NA	-3.18	1.98	2.06
25	4	307	CLA	C4B-NB	3.18	1.41	1.37
25	B	817	CLA	C1D-ND	3.18	1.41	1.37
33	6	607	CHL	CHD-C4C	3.17	1.46	1.39
25	A	816	CLA	C1D-ND	3.17	1.41	1.37
25	P	610	CLA	C4B-NB	3.17	1.41	1.37
33	R	608	CHL	CHB-C1B	3.17	1.46	1.39
25	7	308	CLA	C1D-ND	3.17	1.41	1.37
33	5	308	CHL	CHB-C1B	3.17	1.46	1.39
25	5	312	CLA	C4B-NB	3.17	1.41	1.37
33	1	601	CHL	CHD-C4C	3.17	1.46	1.39
33	1	606	CHL	C3D-C2D	3.17	1.47	1.39
33	S	308	CHL	C3D-C2D	3.17	1.47	1.39
25	4	308	CLA	C1D-ND	3.16	1.41	1.37
25	a	304	CLA	C3B-C4B	3.16	1.50	1.42
33	Q	607	CHL	CHB-C1B	3.16	1.46	1.39
25	1	603	CLA	C1D-ND	3.16	1.41	1.37
25	a	303	CLA	C1-C2	3.16	1.58	1.49
25	2	312	CLA	C1D-ND	3.16	1.41	1.37
25	H	205	CLA	C1D-ND	3.16	1.41	1.37
25	2	309	CLA	C1D-ND	3.16	1.41	1.37
33	5	307	CHL	CHB-C1B	3.16	1.46	1.39
25	A	851	CLA	C1D-ND	3.16	1.41	1.37
33	T	606	CHL	CHB-C1B	3.16	1.46	1.39
25	6	601	CLA	C4D-ND	-3.16	1.33	1.37
25	B	801	CLA	C1D-ND	3.16	1.41	1.37
33	P	606	CHL	C3D-C2D	3.16	1.47	1.39
25	P	610	CLA	C4D-ND	-3.15	1.33	1.37
25	9	310	CLA	C4D-ND	-3.15	1.33	1.37
25	9	302	CLA	C4B-NB	3.15	1.41	1.37
33	P	608	CHL	C3D-C2D	3.15	1.47	1.39
33	Q	607	CHL	C3D-C2D	3.15	1.47	1.39
25	S	301	CLA	C4D-ND	-3.15	1.33	1.37
25	2	306	CLA	C1D-ND	3.15	1.41	1.37
25	B	849	CLA	C1D-ND	3.15	1.41	1.37
33	7	305	CHL	C1D-ND	-3.15	1.33	1.37
25	9	310	CLA	C4B-NB	3.14	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	307	CHL	C1D-ND	-3.14	1.33	1.37
33	3	306	CHL	CHD-C4C	3.14	1.46	1.39
25	R	602	CLA	C3B-C4B	3.14	1.50	1.42
33	6	617	CHL	C3D-C2D	3.14	1.47	1.39
33	R	608	CHL	C3D-C2D	3.14	1.47	1.39
33	6	607	CHL	CHB-C1B	3.14	1.46	1.39
33	1	601	CHL	C3D-C2D	3.14	1.47	1.39
25	B	828	CLA	C1D-ND	3.14	1.41	1.37
33	P	609	CHL	MG-NA	3.14	2.13	2.06
33	P	619	CHL	C3D-C2D	3.14	1.47	1.39
25	A	837	CLA	C1D-ND	3.14	1.41	1.37
33	R	609	CHL	MG-NA	3.13	2.13	2.06
25	7	313	CLA	C1D-ND	3.13	1.41	1.37
25	8	310	CLA	C1D-ND	3.13	1.41	1.37
25	a	302	CLA	C4D-ND	-3.13	1.33	1.37
25	1	611	CLA	C4D-ND	-3.13	1.33	1.37
25	5	313	CLA	C4D-ND	-3.13	1.33	1.37
25	3	314	CLA	C1D-ND	3.13	1.41	1.37
25	2	312	CLA	C4D-ND	-3.13	1.33	1.37
25	9	305	CLA	C4D-ND	-3.13	1.33	1.37
33	U	305	CHL	CHB-C1B	3.13	1.46	1.39
25	Q	610	CLA	C4D-ND	-3.13	1.33	1.37
25	a	301	CLA	C4D-ND	-3.13	1.33	1.37
25	8	305	CLA	C1D-ND	3.13	1.41	1.37
33	P	607	CHL	C3D-C2D	3.13	1.47	1.39
25	A	811	CLA	C1D-ND	3.13	1.41	1.37
25	9	304	CLA	C1D-ND	3.13	1.41	1.37
25	T	608	CLA	C4D-ND	-3.12	1.33	1.37
25	S	311	CLA	C4B-NB	3.12	1.41	1.37
25	7	311	CLA	C1D-ND	3.12	1.41	1.37
33	P	605	CHL	CHB-C1B	3.12	1.46	1.39
25	2	305	CLA	C4B-NB	3.12	1.41	1.37
33	R	607	CHL	C3D-C2D	3.12	1.47	1.39
25	A	817	CLA	C1D-ND	3.12	1.41	1.37
25	R	603	CLA	C3B-C4B	3.12	1.50	1.42
25	7	301	CLA	C1D-ND	3.12	1.41	1.37
25	A	830	CLA	C1D-ND	3.12	1.41	1.37
25	S	315	CLA	C4D-ND	-3.11	1.33	1.37
25	2	308	CLA	C1D-ND	3.11	1.41	1.37
33	Q	608	CHL	MG-NA	3.11	2.13	2.06
33	4	305	CHL	C1D-ND	-3.11	1.34	1.37
25	5	319	CLA	C4D-ND	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	831	CLA	C1D-ND	3.11	1.41	1.37
25	S	304	CLA	C4D-ND	-3.11	1.33	1.37
25	B	821	CLA	C1D-ND	3.11	1.41	1.37
25	R	611	CLA	C4D-ND	-3.11	1.33	1.37
25	R	614	CLA	C4D-ND	-3.10	1.33	1.37
25	6	612	CLA	C3B-C4B	3.10	1.50	1.42
33	8	307	CHL	C3D-C2D	3.10	1.47	1.39
25	B	838	CLA	C1D-ND	3.10	1.41	1.37
25	4	302	CLA	C4D-ND	-3.10	1.33	1.37
33	P	601	CHL	MG-NA	-3.10	1.98	2.06
25	B	820	CLA	C1D-ND	3.10	1.41	1.37
25	A	814	CLA	C1D-ND	3.10	1.41	1.37
33	R	601	CHL	MG-NA	-3.10	1.98	2.06
25	B	814	CLA	C1D-ND	3.09	1.41	1.37
25	K	205	CLA	C4B-NB	3.09	1.41	1.37
25	P	604	CLA	C4D-ND	-3.09	1.33	1.37
33	4	322	CHL	C3D-C2D	3.09	1.47	1.39
25	B	811	CLA	C1D-ND	3.09	1.41	1.37
25	2	304	CLA	C1D-ND	3.09	1.41	1.37
25	2	313	CLA	C4B-NB	3.09	1.41	1.37
25	T	608	CLA	C4B-NB	3.09	1.41	1.37
25	A	804	CLA	C1D-ND	3.09	1.41	1.37
25	B	818	CLA	C1D-ND	3.09	1.41	1.37
25	S	305	CLA	C4D-ND	-3.09	1.33	1.37
33	Q	601	CHL	MG-NA	-3.08	1.98	2.06
25	3	304	CLA	C1D-ND	3.08	1.41	1.37
33	4	314	CHL	C1D-ND	-3.08	1.34	1.37
33	7	305	CHL	CHB-C1B	3.08	1.46	1.39
25	4	313	CLA	C4B-NB	3.08	1.41	1.37
25	R	613	CLA	C4B-NB	3.08	1.41	1.37
33	5	317	CHL	C1D-ND	-3.08	1.34	1.37
25	a	309	CLA	C4B-NB	3.08	1.41	1.37
25	8	304	CLA	C1D-ND	3.08	1.41	1.37
25	a	313	CLA	C4B-NB	3.08	1.41	1.37
33	6	617	CHL	CHB-C1B	3.07	1.46	1.39
25	9	302	CLA	C4D-ND	-3.07	1.33	1.37
25	A	836	CLA	C1D-ND	3.07	1.41	1.37
25	a	303	CLA	C4D-ND	-3.07	1.33	1.37
33	4	304	CHL	C3D-C2D	3.07	1.47	1.39
25	Q	613	CLA	C4D-ND	-3.07	1.33	1.37
25	9	303	CLA	C1D-ND	3.07	1.41	1.37
25	9	305	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	604	CLA	C4D-ND	-3.07	1.33	1.37
33	5	307	CHL	MG-NA	-3.06	1.99	2.06
25	Q	611	CLA	C4B-NB	3.06	1.41	1.37
25	2	314	CLA	C4B-NB	3.06	1.41	1.37
33	R	605	CHL	C3D-C2D	3.06	1.47	1.39
25	7	306	CLA	C1D-ND	3.06	1.41	1.37
25	Q	602	CLA	C3B-C4B	3.06	1.49	1.42
25	4	310	CLA	C3B-C4B	3.06	1.49	1.42
25	7	302	CLA	C1D-ND	3.06	1.41	1.37
25	A	853	CLA	C1D-ND	3.06	1.41	1.37
25	8	309	CLA	C1D-ND	3.05	1.41	1.37
33	P	622	CHL	C1D-ND	-3.05	1.34	1.37
25	4	312	CLA	C4B-NB	3.05	1.41	1.37
25	5	314	CLA	C4B-NB	3.05	1.41	1.37
28	B	845	BCR	C1-C6	-3.05	1.49	1.53
25	a	302	CLA	C4B-NB	3.05	1.41	1.37
25	B	803	CLA	C1D-ND	3.05	1.41	1.37
33	4	314	CHL	CHB-C1B	3.05	1.46	1.39
25	6	614	CLA	C1D-ND	3.05	1.41	1.37
25	P	603	CLA	C4D-ND	-3.05	1.33	1.37
25	1	608	CLA	C1D-ND	3.04	1.41	1.37
25	B	835	CLA	C4B-NB	3.04	1.41	1.37
25	a	312	CLA	C4B-NB	3.04	1.41	1.37
25	P	602	CLA	C3B-C4B	3.04	1.49	1.42
33	T	601	CHL	MG-NA	-3.04	1.99	2.06
33	5	317	CHL	CHB-C1B	3.04	1.46	1.39
25	S	301	CLA	MG-NB	-3.04	1.99	2.05
25	3	304	CLA	C4B-NB	3.03	1.41	1.37
25	8	313	CLA	C1D-ND	3.03	1.41	1.37
25	2	313	CLA	C3B-C4B	3.03	1.49	1.42
33	U	309	CHL	MG-NA	-3.03	1.99	2.06
25	5	302	CLA	C4B-NB	3.03	1.41	1.37
25	7	310	CLA	C1D-ND	3.03	1.41	1.37
25	S	312	CLA	C4D-ND	-3.03	1.33	1.37
25	5	302	CLA	C4D-ND	-3.03	1.33	1.37
25	A	826	CLA	MG-NB	-3.03	1.99	2.05
33	4	306	CHL	C3D-C2D	3.03	1.47	1.39
25	A	828	CLA	C1D-ND	3.02	1.41	1.37
25	G	201	CLA	C4B-NB	3.02	1.41	1.37
25	A	803	CLA	C1D-ND	3.02	1.41	1.37
25	3	312	CLA	C4B-NB	3.02	1.41	1.37
25	T	602	CLA	C3B-C4B	3.02	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	807	CLA	C1D-ND	3.02	1.41	1.37
33	5	317	CHL	C3D-C2D	3.02	1.47	1.39
25	B	835	CLA	C1D-ND	3.02	1.41	1.37
25	K	205	CLA	C4D-ND	-3.01	1.33	1.37
25	6	623	CLA	C4D-ND	-3.01	1.33	1.37
25	A	825	CLA	C1D-ND	3.01	1.41	1.37
25	U	302	CLA	C3B-C4B	3.01	1.49	1.42
33	R	607	CHL	C1D-ND	-3.01	1.34	1.37
25	S	311	CLA	C4D-ND	-3.01	1.33	1.37
25	O	202	CLA	C4B-NB	3.01	1.41	1.37
25	A	801	CLA	C1D-ND	3.01	1.41	1.37
33	P	619	CHL	C1D-ND	-3.01	1.34	1.37
25	U	304	CLA	C4D-ND	-3.01	1.33	1.37
25	A	834	CLA	C1D-ND	3.00	1.41	1.37
25	5	319	CLA	C4B-NB	3.00	1.41	1.37
25	U	313	CLA	C4D-ND	-3.00	1.33	1.37
25	5	309	CLA	C1D-ND	3.00	1.41	1.37
33	R	605	CHL	CHB-C1B	3.00	1.46	1.39
25	T	608	CLA	C3B-C4B	3.00	1.49	1.42
25	8	303	CLA	C1D-ND	3.00	1.41	1.37
33	8	307	CHL	C1D-ND	-3.00	1.34	1.37
33	R	609	CHL	O2A-CGA	3.00	1.42	1.33
28	5	323	BCR	C30-C25	-2.99	1.49	1.53
25	2	304	CLA	C4B-NB	2.99	1.41	1.37
25	P	613	CLA	C4D-ND	-2.99	1.33	1.37
33	Q	608	CHL	O2A-CGA	2.99	1.42	1.33
25	S	312	CLA	C4B-NB	2.99	1.41	1.37
33	P	607	CHL	C1D-ND	-2.99	1.34	1.37
25	3	302	CLA	C3B-C4B	2.99	1.49	1.42
25	Q	604	CLA	C4D-ND	-2.99	1.33	1.37
25	Q	618	CLA	C4B-NB	2.99	1.41	1.37
25	A	803	CLA	MG-NB	-2.99	1.99	2.05
25	R	612	CLA	CMC-C2C	2.99	1.57	1.50
33	6	606	CHL	C3D-C2D	2.99	1.47	1.39
25	A	826	CLA	C1D-ND	2.98	1.41	1.37
33	4	322	CHL	CHB-C1B	2.98	1.46	1.39
33	P	609	CHL	O2A-CGA	2.98	1.42	1.33
25	1	612	CLA	C4B-NB	2.98	1.41	1.37
33	S	309	CHL	C3D-C2D	2.98	1.47	1.39
33	T	601	CHL	C1D-ND	-2.98	1.34	1.37
25	1	611	CLA	C4B-NB	2.98	1.41	1.37
25	T	603	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	202	CLA	C1D-ND	2.97	1.41	1.37
25	a	308	CLA	C3B-C4B	2.97	1.49	1.42
25	B	815	CLA	C1D-ND	2.97	1.41	1.37
33	6	607	CHL	C3D-C2D	2.97	1.47	1.39
25	U	310	CLA	C3B-C4B	2.97	1.49	1.42
25	B	815	CLA	MG-NB	-2.97	1.99	2.05
25	3	302	CLA	C4B-NB	2.97	1.41	1.37
25	3	309	CLA	C4B-NB	2.97	1.41	1.37
25	7	304	CLA	C1D-ND	2.97	1.41	1.37
25	A	806	CLA	MG-NB	-2.97	1.99	2.05
25	2	306	CLA	C3B-C4B	2.96	1.49	1.42
25	R	604	CLA	C3B-C4B	2.96	1.49	1.42
25	R	611	CLA	C3B-C4B	2.96	1.49	1.42
25	A	820	CLA	MG-NB	-2.96	1.99	2.05
25	Q	603	CLA	C3B-C4B	2.96	1.49	1.42
25	a	309	CLA	C3B-C4B	2.96	1.49	1.42
25	B	830	CLA	C4B-NB	2.96	1.41	1.37
25	1	609	CLA	C3B-C4B	2.96	1.49	1.42
25	P	612	CLA	CMC-C2C	2.96	1.57	1.50
25	1	607	CLA	C1D-ND	2.96	1.41	1.37
25	8	306	CLA	C4B-NB	2.96	1.41	1.37
25	5	306	CLA	C1D-ND	2.96	1.41	1.37
25	4	307	CLA	C3B-C4B	2.96	1.49	1.42
25	B	813	CLA	C1D-ND	2.96	1.41	1.37
25	2	302	CLA	C4B-NB	2.96	1.41	1.37
25	S	303	CLA	C1D-ND	2.96	1.41	1.37
25	B	807	CLA	C1D-ND	2.96	1.41	1.37
25	S	313	CLA	C4D-ND	-2.95	1.33	1.37
25	8	309	CLA	C4B-NB	2.95	1.41	1.37
25	A	824	CLA	C1D-ND	2.95	1.41	1.37
25	A	839	CLA	C1D-ND	2.95	1.41	1.37
25	2	312	CLA	C4B-NB	2.95	1.41	1.37
25	3	310	CLA	C4B-NB	2.95	1.41	1.37
25	A	818	CLA	C1D-ND	2.95	1.41	1.37
25	1	604	CLA	CMD-C2D	-2.95	1.44	1.50
25	T	610	CLA	C4D-ND	-2.95	1.33	1.37
25	a	310	CLA	C4D-ND	-2.95	1.33	1.37
25	A	821	CLA	C1D-ND	2.95	1.41	1.37
25	9	309	CLA	C4B-NB	2.95	1.41	1.37
33	6	606	CHL	C1D-ND	-2.95	1.34	1.37
25	6	620	CLA	C1D-ND	2.94	1.41	1.37
25	T	612	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	303	CLA	C1D-ND	2.94	1.41	1.37
25	B	825	CLA	MG-NB	-2.94	2.00	2.05
25	A	836	CLA	C4B-NB	2.94	1.41	1.37
25	9	308	CLA	C4B-NB	2.94	1.41	1.37
25	8	311	CLA	C4B-NB	2.94	1.41	1.37
25	J	103	CLA	C4B-NB	2.94	1.41	1.37
31	B	850	SQD	C6-S	-2.94	1.66	1.77
25	A	813	CLA	C1D-ND	2.94	1.41	1.37
25	K	201	CLA	C1D-ND	2.94	1.41	1.37
25	T	609	CLA	C4B-NB	2.94	1.41	1.37
25	T	609	CLA	C4D-ND	-2.94	1.33	1.37
25	1	614	CLA	C4B-NB	2.94	1.41	1.37
25	5	303	CLA	C1D-ND	2.93	1.41	1.37
25	U	312	CLA	C4D-ND	-2.93	1.33	1.37
25	B	806	CLA	C1D-ND	2.93	1.41	1.37
25	P	611	CLA	C4D-ND	-2.93	1.33	1.37
25	6	613	CLA	C4D-ND	-2.93	1.33	1.37
25	P	611	CLA	CHB-C1B	2.93	1.46	1.39
25	L	206	CLA	C1D-ND	2.93	1.41	1.37
25	B	826	CLA	C1D-ND	2.93	1.41	1.37
25	B	819	CLA	C1D-ND	2.93	1.41	1.37
25	6	609	CLA	C1D-ND	2.93	1.41	1.37
25	6	611	CLA	C3B-C4B	2.93	1.49	1.42
25	1	607	CLA	C4B-NB	2.92	1.41	1.37
25	B	836	CLA	C1D-ND	2.92	1.41	1.37
25	9	301	CLA	C1D-ND	2.92	1.41	1.37
25	A	822	CLA	C1D-ND	2.92	1.41	1.37
25	B	809	CLA	C1D-ND	2.92	1.41	1.37
25	a	306	CLA	C4B-NB	2.92	1.41	1.37
25	U	311	CLA	C2D-C1D	2.92	1.48	1.42
25	Q	609	CLA	C3B-C4B	2.92	1.49	1.42
25	B	822	CLA	C1D-ND	2.92	1.41	1.37
25	B	831	CLA	C1D-ND	2.92	1.41	1.37
33	a	305	CHL	C1D-ND	-2.91	1.34	1.37
25	1	605	CLA	C3B-C4B	2.91	1.49	1.42
33	U	309	CHL	C1D-ND	-2.91	1.34	1.37
33	a	305	CHL	MG-NA	-2.91	1.99	2.06
25	A	825	CLA	MG-NB	-2.91	2.00	2.05
25	B	825	CLA	C1D-ND	2.91	1.41	1.37
25	P	603	CLA	C3B-C4B	2.91	1.49	1.42
25	O	202	CLA	CMD-C2D	-2.91	1.44	1.50
25	6	615	CLA	C3B-C4B	2.91	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	610	CLA	C3B-C4B	2.90	1.49	1.42
25	H	202	CLA	C4B-NB	2.90	1.41	1.37
25	2	308	CLA	C4B-NB	2.90	1.41	1.37
33	1	601	CHL	CHB-C1B	2.90	1.45	1.39
25	Q	609	CLA	C4D-ND	-2.90	1.33	1.37
33	P	608	CHL	C1D-ND	-2.90	1.34	1.37
33	R	608	CHL	C1D-ND	-2.90	1.34	1.37
33	T	607	CHL	C1D-ND	-2.90	1.34	1.37
25	U	310	CLA	C4D-ND	-2.89	1.33	1.37
25	7	307	CLA	C1D-ND	2.89	1.41	1.37
25	8	315	CLA	C4B-NB	2.89	1.41	1.37
25	A	835	CLA	MG-NB	-2.89	2.00	2.05
25	9	304	CLA	C3B-C4B	2.89	1.49	1.42
25	6	604	CLA	C4B-NB	2.89	1.41	1.37
25	Q	612	CLA	C4D-ND	-2.89	1.33	1.37
25	B	812	CLA	C1D-ND	2.89	1.41	1.37
25	4	311	CLA	C4B-NB	2.89	1.41	1.37
25	O	203	CLA	C4B-NB	2.88	1.41	1.37
25	U	303	CLA	C3B-C4B	2.88	1.49	1.42
25	A	822	CLA	MG-NB	-2.88	2.00	2.05
25	S	320	CLA	C3B-C4B	2.88	1.49	1.42
25	S	304	CLA	C3B-C4B	2.88	1.49	1.42
25	T	610	CLA	C3B-C4B	2.88	1.49	1.42
34	5	322	LUT	C1-C6	-2.88	1.49	1.53
25	L	209	CLA	C4B-NB	2.88	1.41	1.37
25	7	309	CLA	C1D-ND	2.88	1.41	1.37
33	3	306	CHL	CHB-C1B	2.88	1.45	1.39
25	Q	611	CLA	C3B-C4B	2.88	1.49	1.42
25	U	312	CLA	C3B-C4B	2.88	1.49	1.42
33	P	605	CHL	C1D-ND	-2.88	1.34	1.37
25	A	816	CLA	C4B-NB	2.88	1.41	1.37
33	5	307	CHL	C3D-C2D	2.88	1.47	1.39
25	8	313	CLA	C4B-NB	2.87	1.41	1.37
25	S	301	CLA	C3B-C4B	2.87	1.49	1.42
25	A	806	CLA	C1D-ND	2.87	1.41	1.37
25	a	311	CLA	C4B-NB	2.87	1.41	1.37
25	2	309	CLA	C4B-NB	2.87	1.41	1.37
25	a	303	CLA	C4B-NB	2.87	1.41	1.37
25	a	307	CLA	C3B-C4B	2.87	1.49	1.42
33	3	306	CHL	MG-NA	-2.87	1.99	2.06
25	A	817	CLA	C4B-NB	2.87	1.41	1.37
25	K	204	CLA	C4D-ND	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	811	CLA	C4B-NB	2.87	1.41	1.37
25	6	616	CLA	C4B-NB	2.86	1.41	1.37
25	5	305	CLA	C1D-ND	2.86	1.41	1.37
25	B	804	CLA	C1D-ND	2.86	1.41	1.37
25	K	203	CLA	C4B-NB	2.86	1.41	1.37
25	B	818	CLA	C4B-NB	2.86	1.41	1.37
25	R	613	CLA	C4D-ND	-2.86	1.33	1.37
25	2	310	CLA	C4B-NB	2.86	1.41	1.37
25	5	303	CLA	MG-NB	-2.86	2.00	2.05
28	4	321	BCR	C30-C25	-2.86	1.49	1.53
25	R	610	CLA	C4D-ND	-2.86	1.33	1.37
25	3	307	CLA	MG-NB	-2.85	2.00	2.05
25	P	604	CLA	C3B-C4B	2.85	1.49	1.42
25	B	810	CLA	MG-NB	-2.85	2.00	2.05
25	R	611	CLA	C4B-NB	2.85	1.41	1.37
33	Q	607	CHL	C1D-ND	-2.85	1.34	1.37
25	3	313	CLA	C1D-ND	2.85	1.41	1.37
25	8	314	CLA	C4B-NB	2.85	1.41	1.37
34	7	314	LUT	C1-C6	-2.85	1.49	1.53
25	A	809	CLA	C1D-ND	2.85	1.41	1.37
25	U	304	CLA	C3B-C4B	2.85	1.49	1.42
25	R	613	CLA	C3B-C4B	2.85	1.49	1.42
25	A	824	CLA	C4B-NB	2.85	1.41	1.37
25	H	201	CLA	C4B-NB	2.85	1.41	1.37
25	B	817	CLA	MG-NB	-2.85	2.00	2.05
25	1	613	CLA	C4B-NB	2.85	1.41	1.37
25	7	303	CLA	C3B-C4B	2.84	1.49	1.42
25	B	824	CLA	C1D-ND	2.84	1.41	1.37
25	1	602	CLA	C4B-NB	2.84	1.41	1.37
25	A	827	CLA	C3B-C4B	2.84	1.49	1.42
25	7	306	CLA	C4B-NB	2.84	1.41	1.37
34	3	316	LUT	C1-C6	-2.84	1.49	1.53
33	P	601	CHL	C1D-ND	-2.84	1.34	1.37
33	1	606	CHL	MG-NA	-2.84	1.99	2.06
25	A	829	CLA	MG-NB	-2.84	2.00	2.05
25	A	830	CLA	CMB-C2B	-2.84	1.44	1.50
25	a	310	CLA	C3B-C4B	2.84	1.49	1.42
25	A	823	CLA	C1D-ND	2.84	1.41	1.37
25	A	801	CLA	MG-NB	-2.84	2.00	2.05
25	1	612	CLA	C4D-ND	-2.84	1.33	1.37
25	a	312	CLA	C3B-C4B	2.84	1.49	1.42
25	6	610	CLA	C4B-NB	2.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	604	CLA	C4B-NB	2.83	1.41	1.37
33	Q	601	CHL	C1D-ND	-2.83	1.34	1.37
25	S	320	CLA	C4D-ND	-2.83	1.33	1.37
25	B	806	CLA	C4B-NB	2.83	1.41	1.37
25	B	827	CLA	CMB-C2B	-2.83	1.44	1.50
25	T	612	CLA	C3B-C4B	2.83	1.49	1.42
25	G	202	CLA	C4B-NB	2.83	1.41	1.37
25	5	324	CLA	C1D-ND	2.83	1.41	1.37
25	A	802	CLA	C1D-ND	2.82	1.41	1.37
25	A	832	CLA	C1D-ND	2.82	1.41	1.37
25	4	302	CLA	C3B-C4B	2.82	1.49	1.42
25	B	832	CLA	C4B-NB	2.82	1.41	1.37
25	3	308	CLA	C1D-ND	2.82	1.41	1.37
25	T	603	CLA	C3B-C4B	2.82	1.49	1.42
25	A	808	CLA	C4B-NB	2.82	1.41	1.37
25	B	811	CLA	MG-NB	-2.82	2.00	2.05
25	B	833	CLA	MG-NB	-2.82	2.00	2.05
25	3	308	CLA	MG-NB	-2.82	2.00	2.05
25	7	312	CLA	C4B-NB	2.82	1.41	1.37
25	A	819	CLA	C1D-ND	2.82	1.41	1.37
33	S	310	CHL	C1D-ND	-2.82	1.34	1.37
25	Q	603	CLA	C4D-ND	-2.82	1.33	1.37
33	R	601	CHL	C1D-ND	-2.82	1.34	1.37
25	R	614	CLA	C3B-C4B	2.82	1.49	1.42
25	P	602	CLA	C4D-ND	-2.82	1.33	1.37
28	B	842	BCR	C30-C25	-2.81	1.49	1.53
25	U	303	CLA	C4D-ND	-2.81	1.33	1.37
25	4	311	CLA	C1B-C2B	2.81	1.49	1.43
25	B	838	CLA	C4B-NB	2.81	1.41	1.37
25	1	608	CLA	C4B-NB	2.81	1.41	1.37
25	P	613	CLA	C3B-C4B	2.81	1.49	1.42
25	2	305	CLA	C3B-C4B	2.81	1.49	1.42
25	A	842	CLA	C1D-ND	2.81	1.41	1.37
25	5	306	CLA	C4B-NB	2.81	1.41	1.37
33	7	305	CHL	C3D-C2D	2.81	1.46	1.39
33	T	607	CHL	MG-NA	-2.81	1.99	2.06
25	7	308	CLA	C3B-C4B	2.81	1.49	1.42
25	T	609	CLA	C3B-C4B	2.80	1.49	1.42
25	3	320	CLA	MG-NB	-2.80	2.00	2.05
25	L	202	CLA	MG-NB	-2.80	2.00	2.05
25	B	837	CLA	C1D-ND	2.80	1.41	1.37
25	3	302	CLA	CMD-C2D	-2.80	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	802	CLA	MG-NB	-2.80	2.00	2.05
25	1	602	CLA	MG-NB	-2.80	2.00	2.05
25	A	827	CLA	C4B-NB	2.80	1.41	1.37
25	A	851	CLA	MG-NB	-2.80	2.00	2.05
25	B	810	CLA	C1D-ND	2.80	1.41	1.37
25	A	804	CLA	MG-NB	-2.80	2.00	2.05
25	O	201	CLA	C4B-NB	2.80	1.41	1.37
34	3	315	LUT	C1-C6	-2.80	1.49	1.53
33	R	606	CHL	C1D-ND	-2.80	1.34	1.37
25	Q	613	CLA	C3B-C4B	2.79	1.49	1.42
33	6	608	CHL	C3D-C2D	2.79	1.46	1.39
25	B	808	CLA	MG-NB	-2.79	2.00	2.05
25	T	611	CLA	C3B-C4B	2.79	1.49	1.42
25	B	805	CLA	C1D-ND	2.79	1.41	1.37
25	1	612	CLA	C1D-ND	2.79	1.41	1.37
25	5	312	CLA	C3B-C4B	2.79	1.49	1.42
25	A	807	CLA	MG-NB	-2.79	2.00	2.05
25	8	314	CLA	C1D-ND	2.79	1.41	1.37
28	L	204	BCR	C1-C6	-2.79	1.49	1.53
25	5	324	CLA	C4B-NB	2.79	1.41	1.37
33	1	601	CHL	C1C-NC	-2.79	1.33	1.37
25	Q	602	CLA	C4D-ND	-2.79	1.33	1.37
25	3	303	CLA	MG-NB	-2.79	2.00	2.05
25	B	829	CLA	MG-NB	-2.78	2.00	2.05
25	A	835	CLA	C1B-NB	-2.78	1.34	1.37
25	B	829	CLA	C1D-ND	2.78	1.41	1.37
25	L	205	CLA	MG-NB	-2.78	2.00	2.05
33	P	606	CHL	C1D-ND	-2.78	1.34	1.37
25	B	814	CLA	MG-NB	-2.78	2.00	2.05
25	Q	610	CLA	C3B-C4B	2.78	1.49	1.42
25	A	830	CLA	C4B-NB	2.78	1.41	1.37
25	T	611	CLA	C4D-ND	-2.78	1.33	1.37
25	4	301	CLA	C1D-ND	2.78	1.41	1.37
25	B	849	CLA	C4B-NB	2.78	1.41	1.37
25	1	609	CLA	C4D-ND	-2.78	1.33	1.37
25	B	826	CLA	CMB-C2B	-2.78	1.44	1.50
28	L	203	BCR	C30-C25	-2.78	1.49	1.53
25	A	853	CLA	C4B-NB	2.78	1.41	1.37
25	Q	604	CLA	C3B-C4B	2.77	1.49	1.42
25	8	310	CLA	MG-NB	-2.77	2.00	2.05
25	A	820	CLA	C1D-ND	2.77	1.41	1.37
25	B	824	CLA	MG-NB	-2.77	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	601	CLA	C4B-NB	2.77	1.41	1.37
25	P	604	CLA	C1B-C2B	2.77	1.49	1.43
25	B	823	CLA	MG-NB	-2.77	2.00	2.05
25	6	603	CLA	MG-NB	-2.77	2.00	2.05
25	a	308	CLA	C1D-ND	2.77	1.41	1.37
33	S	307	CHL	C1D-ND	-2.77	1.34	1.37
25	Q	618	CLA	C3B-C4B	2.77	1.49	1.42
33	S	306	CHL	C4C-C3C	2.77	1.49	1.45
25	B	830	CLA	C3B-C4B	2.77	1.49	1.42
25	5	311	CLA	C4B-NB	2.77	1.41	1.37
25	B	822	CLA	MG-NB	-2.76	2.00	2.05
25	Q	604	CLA	C1B-C2B	2.76	1.49	1.43
25	7	304	CLA	C4B-NB	2.76	1.41	1.37
25	A	819	CLA	MG-NB	-2.76	2.00	2.05
25	U	304	CLA	C1B-C2B	2.76	1.49	1.43
33	8	307	CHL	MG-NA	-2.76	1.99	2.06
25	7	303	CLA	MG-NB	-2.76	2.00	2.05
25	8	303	CLA	MG-NB	-2.76	2.00	2.05
25	9	311	CLA	C3B-C4B	2.76	1.49	1.42
33	T	605	CHL	C1D-ND	-2.76	1.34	1.37
25	B	817	CLA	C4B-NB	2.76	1.41	1.37
25	6	623	CLA	C4B-NB	2.76	1.41	1.37
25	9	310	CLA	C3B-C4B	2.75	1.49	1.42
25	L	206	CLA	MG-NB	-2.75	2.00	2.05
25	B	831	CLA	C4B-NB	2.75	1.41	1.37
33	S	302	CHL	C1D-ND	-2.75	1.34	1.37
25	2	302	CLA	C3B-C4B	2.75	1.49	1.42
33	T	601	CHL	C3B-C4B	2.75	1.49	1.42
33	Q	606	CHL	C1D-ND	-2.75	1.34	1.37
25	B	821	CLA	C4B-NB	2.75	1.41	1.37
25	B	804	CLA	MG-NB	-2.75	2.00	2.05
25	A	802	CLA	MG-NB	-2.75	2.00	2.05
25	S	305	CLA	C3B-C4B	2.75	1.49	1.42
33	S	306	CHL	C1D-ND	-2.75	1.34	1.37
25	9	304	CLA	C4B-NB	2.75	1.41	1.37
25	S	311	CLA	C3B-C4B	2.75	1.49	1.42
25	A	818	CLA	C4B-NB	2.75	1.41	1.37
25	B	833	CLA	C1D-ND	2.75	1.41	1.37
25	7	309	CLA	C4B-NB	2.75	1.41	1.37
25	F	802	CLA	C4B-NB	2.75	1.41	1.37
33	9	307	CHL	MG-NA	-2.75	1.99	2.06
33	T	606	CHL	C1D-ND	-2.74	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	U	302	CLA	C4D-ND	-2.74	1.33	1.37
25	6	605	CLA	C3B-C4B	2.74	1.49	1.42
25	a	303	CLA	CMD-C2D	-2.74	1.45	1.50
25	1	611	CLA	C3B-C4B	2.74	1.49	1.42
25	B	827	CLA	C4B-NB	2.74	1.41	1.37
25	L	201	CLA	C1D-ND	2.74	1.41	1.37
25	A	803	CLA	MG-ND	-2.74	2.00	2.05
25	5	305	CLA	MG-NB	-2.74	2.00	2.05
25	A	819	CLA	CMB-C2B	-2.74	1.45	1.50
25	A	834	CLA	C4B-NB	2.74	1.41	1.37
25	Q	612	CLA	C3B-C4B	2.74	1.49	1.42
25	6	609	CLA	C4B-NB	2.74	1.41	1.37
25	L	201	CLA	MG-NB	-2.74	2.00	2.05
25	9	308	CLA	C3B-C4B	2.73	1.49	1.42
33	1	601	CHL	MG-NA	-2.73	1.99	2.06
25	G	202	CLA	C3B-C4B	2.73	1.49	1.42
25	6	620	CLA	MG-NB	-2.73	2.00	2.05
25	Q	612	CLA	C1B-C2B	2.73	1.49	1.43
25	3	314	CLA	MG-NB	-2.73	2.00	2.05
25	A	805	CLA	C1D-ND	2.73	1.41	1.37
25	B	837	CLA	C4B-NB	2.73	1.41	1.37
25	6	620	CLA	C4B-NB	2.73	1.41	1.37
25	1	610	CLA	C3B-C4B	2.73	1.49	1.42
33	U	309	CHL	C3B-C4B	2.73	1.49	1.42
25	1	602	CLA	C3B-C4B	2.73	1.49	1.42
25	B	821	CLA	CMC-C2C	-2.73	1.45	1.50
25	B	849	CLA	MG-NB	-2.73	2.00	2.05
25	A	833	CLA	C1D-ND	2.73	1.41	1.37
25	1	610	CLA	C4B-NB	2.73	1.41	1.37
25	A	812	CLA	CMB-C2B	-2.73	1.45	1.50
25	A	838	CLA	MG-NB	-2.73	2.00	2.05
25	T	603	CLA	C1B-C2B	2.72	1.49	1.43
25	7	304	CLA	MG-NB	-2.72	2.00	2.05
25	A	827	CLA	C1D-ND	2.72	1.41	1.37
25	A	836	CLA	CMB-C2B	-2.72	1.45	1.50
25	A	839	CLA	C4B-NB	2.72	1.41	1.37
33	S	309	CHL	C1D-ND	-2.72	1.34	1.37
25	a	311	CLA	C1B-C2B	2.72	1.49	1.43
25	5	306	CLA	MG-NB	-2.72	2.00	2.05
25	8	302	CLA	C4B-NB	2.72	1.41	1.37
33	S	306	CHL	CHB-C4A	-2.72	1.31	1.37
25	U	311	CLA	C3B-C4B	2.72	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	315	CLA	C4B-NB	2.72	1.41	1.37
25	a	306	CLA	C3B-C4B	2.72	1.49	1.42
25	S	303	CLA	C3B-C4B	2.72	1.49	1.42
25	7	307	CLA	C4B-NB	2.72	1.41	1.37
25	B	820	CLA	MG-NB	-2.71	2.00	2.05
25	T	602	CLA	C4D-ND	-2.71	1.34	1.37
33	5	308	CHL	C3D-C2D	2.71	1.46	1.39
25	5	315	CLA	C3B-C4B	2.71	1.49	1.42
25	A	829	CLA	C1D-ND	2.71	1.41	1.37
33	P	608	CHL	MG-NA	-2.71	1.99	2.06
25	K	204	CLA	C3B-C4B	2.71	1.49	1.42
25	7	302	CLA	MG-NB	-2.71	2.00	2.05
25	8	304	CLA	MG-NB	-2.71	2.00	2.05
25	1	603	CLA	C4B-NB	2.71	1.41	1.37
25	6	605	CLA	C4B-NB	2.71	1.41	1.37
25	5	305	CLA	C4B-NB	2.71	1.41	1.37
25	A	808	CLA	C3B-C4B	2.71	1.49	1.42
25	8	304	CLA	C4B-NB	2.71	1.41	1.37
25	9	304	CLA	MG-NB	-2.71	2.00	2.05
25	5	309	CLA	MG-NB	-2.70	2.00	2.05
25	L	209	CLA	MG-NB	-2.70	2.00	2.05
33	4	305	CHL	C3B-C4B	2.70	1.49	1.42
25	A	827	CLA	MG-NB	-2.70	2.00	2.05
25	4	310	CLA	CAA-C2A	-2.70	1.49	1.54
33	R	608	CHL	MG-NA	-2.70	1.99	2.06
25	A	809	CLA	C4B-NB	2.70	1.41	1.37
25	4	309	CLA	C4B-NB	2.70	1.41	1.37
25	B	805	CLA	MG-NB	-2.70	2.00	2.05
25	2	303	CLA	C4B-NB	2.70	1.41	1.37
33	5	307	CHL	C1C-NC	-2.70	1.33	1.37
25	A	821	CLA	MG-NB	-2.70	2.00	2.05
25	B	809	CLA	MG-NB	-2.70	2.00	2.05
33	S	309	CHL	C3B-C4B	2.70	1.49	1.42
25	B	802	CLA	C1D-ND	2.69	1.41	1.37
25	6	613	CLA	C3B-C4B	2.69	1.49	1.42
25	B	815	CLA	CMB-C2B	-2.69	1.45	1.50
33	Q	607	CHL	MG-NA	-2.69	1.99	2.06
25	3	307	CLA	C1D-ND	2.69	1.41	1.37
36	U	301	NEX	C1-C6	-2.69	1.50	1.54
25	K	202	CLA	C4B-NB	2.69	1.41	1.37
25	7	303	CLA	C1D-ND	2.69	1.41	1.37
25	A	824	CLA	MG-NB	-2.69	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	604	CLA	MG-NB	-2.69	2.00	2.05
25	O	201	CLA	C3B-C4B	2.69	1.49	1.42
25	B	811	CLA	CMB-C2B	-2.69	1.45	1.50
25	H	203	CLA	C4B-NB	2.69	1.41	1.37
25	B	819	CLA	MG-NB	-2.69	2.00	2.05
33	6	617	CHL	C1D-ND	-2.69	1.34	1.37
25	8	314	CLA	C3B-C4B	2.68	1.49	1.42
25	H	201	CLA	C1B-C2B	2.68	1.49	1.43
25	R	611	CLA	C1B-C2B	2.68	1.49	1.43
33	6	608	CHL	MG-NA	-2.68	1.99	2.06
33	R	601	CHL	C4C-C3C	2.68	1.49	1.45
33	3	306	CHL	C1C-NC	-2.68	1.33	1.37
25	5	310	CLA	MG-NB	-2.68	2.00	2.05
33	T	606	CHL	MG-NA	-2.68	1.99	2.06
25	U	312	CLA	C1B-C2B	2.68	1.49	1.43
25	B	819	CLA	C4B-NB	2.68	1.41	1.37
25	B	823	CLA	C1D-ND	2.68	1.41	1.37
25	6	605	CLA	MG-NB	-2.68	2.00	2.05
25	S	313	CLA	C3B-C4B	2.68	1.49	1.42
25	3	305	CLA	MG-NB	-2.68	2.00	2.05
25	a	308	CLA	C4D-ND	-2.68	1.34	1.37
25	R	613	CLA	C1B-C2B	2.68	1.49	1.43
25	1	603	CLA	MG-NB	-2.68	2.00	2.05
33	Q	606	CHL	C1B-C2B	2.68	1.49	1.43
25	7	303	CLA	C4B-NB	2.68	1.41	1.37
25	7	301	CLA	MG-NB	-2.68	2.00	2.05
25	8	313	CLA	MG-NB	-2.67	2.00	2.05
25	B	804	CLA	C4B-NB	2.67	1.41	1.37
33	9	306	CHL	C3D-C2D	2.67	1.46	1.39
25	5	304	CLA	MG-NB	-2.67	2.00	2.05
25	B	816	CLA	MG-NB	-2.67	2.00	2.05
25	A	805	CLA	CMB-C2B	-2.67	1.45	1.50
25	6	610	CLA	C3B-C4B	2.67	1.49	1.42
25	7	311	CLA	C4B-NB	2.67	1.41	1.37
25	A	815	CLA	MG-NB	-2.67	2.00	2.05
25	A	833	CLA	MG-NB	-2.67	2.00	2.05
25	A	805	CLA	MG-NB	-2.67	2.00	2.05
33	S	306	CHL	CHB-C1B	2.66	1.45	1.39
25	R	602	CLA	C4D-ND	-2.66	1.34	1.37
25	4	312	CLA	C3B-C4B	2.66	1.49	1.42
25	3	313	CLA	MG-NB	-2.66	2.00	2.05
25	8	306	CLA	C3B-C4B	2.66	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	306	CHL	C4D-CHA	2.66	1.47	1.38
25	8	312	CLA	C4B-NB	2.66	1.41	1.37
33	Q	601	CHL	C3B-C4B	2.66	1.49	1.42
25	B	827	CLA	C1D-ND	2.66	1.41	1.37
25	7	313	CLA	C4B-NB	2.66	1.41	1.37
25	5	316	CLA	MG-NB	-2.66	2.00	2.05
25	5	324	CLA	MG-NB	-2.66	2.00	2.05
25	7	308	CLA	MG-NB	-2.66	2.00	2.05
25	B	818	CLA	C3B-C4B	2.66	1.49	1.42
33	P	601	CHL	C3B-C4B	2.66	1.49	1.42
25	B	804	CLA	C3B-C4B	2.66	1.49	1.42
25	3	305	CLA	C4B-NB	2.66	1.41	1.37
25	5	313	CLA	C4B-NB	2.66	1.41	1.37
33	U	306	CHL	C3B-C4B	2.66	1.49	1.42
25	2	314	CLA	C3B-C4B	2.66	1.49	1.42
25	A	831	CLA	CMB-C2B	-2.65	1.45	1.50
25	6	604	CLA	C3B-C4B	2.65	1.49	1.42
25	A	836	CLA	MG-NB	-2.65	2.00	2.05
25	9	303	CLA	MG-NB	-2.65	2.00	2.05
33	P	601	CHL	C4C-C3C	2.65	1.49	1.45
33	S	306	CHL	C4B-NB	-2.65	1.34	1.37
25	5	310	CLA	C3B-C4B	2.65	1.49	1.42
25	A	823	CLA	MG-NB	-2.65	2.00	2.05
33	Q	601	CHL	C4C-C3C	2.65	1.49	1.45
25	B	827	CLA	MG-NB	-2.65	2.00	2.05
33	T	601	CHL	C1B-C2B	2.65	1.49	1.43
33	P	622	CHL	C1C-NC	-2.65	1.33	1.37
25	A	814	CLA	MG-NB	-2.65	2.00	2.05
25	P	613	CLA	C1B-C2B	2.65	1.49	1.43
25	a	302	CLA	C3B-C4B	2.65	1.49	1.42
33	U	305	CHL	C4D-CHA	2.65	1.47	1.38
25	3	301	CLA	MG-NB	-2.64	2.00	2.05
25	8	305	CLA	MG-NB	-2.64	2.00	2.05
33	3	306	CHL	C1B-NB	-2.64	1.34	1.37
25	A	809	CLA	MG-NB	-2.64	2.00	2.05
25	S	304	CLA	C1B-C2B	2.64	1.49	1.43
25	A	826	CLA	C3B-C4B	2.64	1.48	1.42
25	A	840	CLA	C4B-NB	2.64	1.41	1.37
25	5	302	CLA	MG-NB	-2.64	2.00	2.05
25	B	831	CLA	CMB-C2B	-2.64	1.45	1.50
25	1	608	CLA	C3B-C4B	2.64	1.48	1.42
25	A	821	CLA	C4B-NB	2.64	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	615	LUT	C1-C6	-2.64	1.50	1.53
25	S	305	CLA	C1B-C2B	2.64	1.49	1.43
25	a	301	CLA	C3B-C4B	2.64	1.48	1.42
33	Q	601	CHL	C1B-C2B	2.64	1.49	1.43
25	A	812	CLA	C4B-NB	2.64	1.41	1.37
25	A	840	CLA	MG-NB	-2.64	2.00	2.05
25	8	305	CLA	C4B-NB	2.64	1.41	1.37
25	2	312	CLA	C3B-C4B	2.64	1.48	1.42
34	1	616	LUT	C1-C6	-2.63	1.50	1.53
25	B	808	CLA	CMC-C2C	-2.63	1.45	1.50
25	B	813	CLA	C4B-NB	2.63	1.41	1.37
25	6	614	CLA	C4B-NB	2.63	1.41	1.37
25	A	812	CLA	MG-NB	-2.63	2.00	2.05
33	R	601	CHL	C3B-C4B	2.63	1.48	1.42
28	B	841	BCR	C30-C25	-2.63	1.50	1.53
25	1	612	CLA	C1B-C2B	2.63	1.49	1.43
25	A	818	CLA	C3B-C4B	2.63	1.48	1.42
25	7	307	CLA	C3B-C4B	2.63	1.48	1.42
25	A	837	CLA	C4B-NB	2.63	1.41	1.37
25	3	320	CLA	C1D-ND	2.63	1.41	1.37
25	7	310	CLA	C4B-NB	2.63	1.41	1.37
25	B	820	CLA	C4B-NB	2.63	1.41	1.37
33	P	601	CHL	C1B-C2B	2.63	1.49	1.43
33	R	601	CHL	C1B-C2B	2.63	1.49	1.43
25	K	201	CLA	C4B-NB	2.62	1.41	1.37
33	4	304	CHL	MG-NA	-2.62	2.00	2.06
25	A	831	CLA	MG-NB	-2.62	2.00	2.05
25	Q	603	CLA	C1B-C2B	2.62	1.49	1.43
25	A	833	CLA	C4B-NB	2.62	1.41	1.37
25	A	835	CLA	C1D-ND	2.62	1.41	1.37
25	1	607	CLA	C3B-C4B	2.62	1.48	1.42
25	F	802	CLA	MG-NB	-2.62	2.00	2.05
25	4	308	CLA	C3B-C4B	2.62	1.48	1.42
25	S	314	CLA	C1B-C2B	2.62	1.49	1.43
25	6	601	CLA	MG-NB	-2.62	2.00	2.05
33	6	607	CHL	MG-NA	-2.62	2.00	2.06
25	1	613	CLA	C3B-C4B	2.62	1.48	1.42
33	U	305	CHL	C1D-ND	-2.62	1.34	1.37
25	A	810	CLA	MG-NB	-2.62	2.00	2.05
25	B	826	CLA	MG-NB	-2.62	2.00	2.05
25	A	817	CLA	C1B-C2B	2.62	1.49	1.43
25	5	319	CLA	C3B-C4B	2.62	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	205	CLA	C3B-C4B	2.61	1.48	1.42
25	7	301	CLA	CMB-C2B	-2.61	1.45	1.50
25	A	824	CLA	C3B-C4B	2.61	1.48	1.42
33	Q	605	CHL	C4D-CHA	2.61	1.47	1.38
25	A	813	CLA	MG-NB	-2.61	2.00	2.05
25	B	808	CLA	CMD-C2D	-2.61	1.45	1.50
25	9	301	CLA	C4B-NB	2.61	1.41	1.37
25	H	205	CLA	MG-NB	-2.61	2.00	2.05
33	U	308	CHL	C1D-ND	-2.61	1.34	1.37
25	B	837	CLA	MG-NB	-2.61	2.00	2.05
25	8	308	CLA	MG-NB	-2.61	2.00	2.05
25	A	842	CLA	C4B-NB	2.61	1.41	1.37
25	P	603	CLA	C1B-C2B	2.61	1.49	1.43
25	5	309	CLA	CMB-C2B	-2.61	1.45	1.50
25	A	835	CLA	MG-ND	-2.61	2.00	2.05
25	2	304	CLA	MG-NB	-2.61	2.00	2.05
25	B	828	CLA	C4B-NB	2.61	1.41	1.37
25	6	615	CLA	MG-NB	-2.61	2.00	2.05
25	5	314	CLA	C3B-C4B	2.61	1.48	1.42
25	F	802	CLA	C3B-C4B	2.60	1.48	1.42
25	3	312	CLA	C3B-C4B	2.60	1.48	1.42
25	A	811	CLA	CMB-C2B	-2.60	1.45	1.50
25	2	310	CLA	C3B-C4B	2.60	1.48	1.42
25	A	814	CLA	CMC-C2C	-2.60	1.45	1.50
25	A	820	CLA	CMB-C2B	-2.60	1.45	1.50
25	a	308	CLA	CMC-C2C	-2.60	1.45	1.50
25	B	836	CLA	C4B-NB	2.60	1.41	1.37
33	T	601	CHL	C4C-C3C	2.60	1.49	1.45
25	8	309	CLA	C3B-C4B	2.60	1.48	1.42
25	B	822	CLA	C4B-NB	2.60	1.41	1.37
25	A	839	CLA	C3B-C4B	2.60	1.48	1.42
25	7	302	CLA	C3B-C4B	2.60	1.48	1.42
33	T	604	CHL	C4D-CHA	2.60	1.47	1.38
25	B	807	CLA	C4B-NB	2.60	1.41	1.37
25	B	836	CLA	MG-NB	-2.60	2.00	2.05
25	1	603	CLA	C3B-C4B	2.60	1.48	1.42
25	A	832	CLA	MG-NB	-2.60	2.00	2.05
25	7	301	CLA	C4B-NB	2.60	1.41	1.37
25	A	828	CLA	MG-NB	-2.59	2.00	2.05
33	S	308	CHL	C1D-ND	-2.59	1.34	1.37
25	2	308	CLA	C3B-C4B	2.59	1.48	1.42
25	S	312	CLA	C3B-C4B	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	803	BCR	C1-C6	-2.59	1.50	1.53
25	3	311	CLA	C4B-NB	2.59	1.41	1.37
25	8	303	CLA	C4B-NB	2.59	1.41	1.37
25	3	309	CLA	C3B-C4B	2.59	1.48	1.42
25	3	304	CLA	MG-NB	-2.59	2.00	2.05
25	6	605	CLA	CMD-C2D	-2.59	1.45	1.50
25	A	802	CLA	C3B-C4B	2.59	1.48	1.42
25	R	603	CLA	C1B-C2B	2.59	1.49	1.43
25	6	623	CLA	C3B-C4B	2.59	1.48	1.42
25	A	825	CLA	CMD-C2D	-2.59	1.45	1.50
25	1	605	CLA	CMB-C2B	-2.59	1.45	1.50
25	S	303	CLA	C1B-C2B	2.59	1.49	1.43
25	A	806	CLA	CMC-C2C	-2.59	1.45	1.50
25	B	804	CLA	CMB-C2B	-2.59	1.45	1.50
25	9	309	CLA	C1B-C2B	2.59	1.49	1.43
25	K	203	CLA	C3B-C4B	2.59	1.48	1.42
25	O	202	CLA	MG-NB	-2.59	2.00	2.05
25	a	303	CLA	C5-C3	-2.59	1.45	1.51
25	2	307	CLA	C4B-NB	2.59	1.41	1.37
25	B	834	CLA	CMB-C2B	-2.59	1.45	1.50
25	a	313	CLA	C1B-C2B	2.59	1.49	1.43
28	F	801	BCR	C1-C6	-2.59	1.50	1.53
25	B	834	CLA	MG-NB	-2.59	2.00	2.05
33	Q	601	CHL	C4D-CHA	2.59	1.47	1.38
25	4	313	CLA	C3B-C4B	2.59	1.48	1.42
25	1	604	CLA	MG-NB	-2.59	2.00	2.05
25	4	301	CLA	C3B-C4B	2.59	1.48	1.42
25	6	615	CLA	C4B-NB	2.59	1.41	1.37
25	9	303	CLA	C4B-NB	2.59	1.41	1.37
25	A	840	CLA	C3B-C4B	2.59	1.48	1.42
25	1	613	CLA	MG-NB	-2.59	2.00	2.05
25	9	305	CLA	C1B-C2B	2.59	1.49	1.43
25	U	313	CLA	C1B-C2B	2.59	1.49	1.43
25	a	304	CLA	C1B-C2B	2.59	1.49	1.43
25	A	822	CLA	CMB-C2B	-2.59	1.45	1.50
33	P	605	CHL	MG-NA	-2.59	2.00	2.06
33	5	317	CHL	MG-NA	-2.59	2.00	2.06
25	a	303	CLA	C1D-ND	2.59	1.41	1.37
33	S	321	CHL	C1D-ND	-2.59	1.34	1.37
34	7	315	LUT	C1-C6	-2.59	1.50	1.53
25	A	811	CLA	C3B-C4B	2.58	1.48	1.42
25	R	610	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	307	CHL	MG-NA	-2.58	2.00	2.06
25	S	315	CLA	C3B-C4B	2.58	1.48	1.42
25	8	303	CLA	CMC-C2C	-2.58	1.45	1.50
25	Q	613	CLA	C1B-C2B	2.58	1.49	1.43
25	5	311	CLA	MG-NB	-2.58	2.00	2.05
33	R	605	CHL	C3B-C4B	2.58	1.48	1.42
33	S	310	CHL	MG-NA	-2.58	2.00	2.06
33	S	310	CHL	C1B-C2B	2.58	1.49	1.43
25	1	610	CLA	MG-NB	-2.58	2.00	2.05
25	B	816	CLA	CMB-C2B	-2.58	1.45	1.50
25	L	205	CLA	C1D-ND	2.58	1.41	1.37
33	S	307	CHL	C2C-C1C	2.58	1.50	1.44
25	1	611	CLA	MG-NB	-2.58	2.00	2.05
25	A	827	CLA	CMD-C2D	-2.58	1.45	1.50
33	T	607	CHL	C4D-CHA	2.58	1.47	1.38
25	8	315	CLA	C3B-C4B	2.57	1.48	1.42
25	A	834	CLA	MG-NB	-2.57	2.00	2.05
25	B	808	CLA	C1D-ND	2.57	1.40	1.37
25	B	831	CLA	MG-NB	-2.57	2.00	2.05
25	5	306	CLA	CMD-C2D	-2.57	1.45	1.50
25	2	303	CLA	MG-NB	-2.57	2.00	2.05
33	Q	608	CHL	MG-NB	2.57	2.10	2.05
25	B	828	CLA	MG-NB	-2.57	2.00	2.05
25	A	802	CLA	C4B-NB	2.57	1.40	1.37
25	J	105	CLA	C4B-NB	2.57	1.40	1.37
33	R	607	CHL	C1B-C2B	2.57	1.49	1.43
25	B	812	CLA	MG-NB	-2.57	2.00	2.05
25	1	609	CLA	C1D-ND	2.57	1.40	1.37
33	U	306	CHL	C1D-ND	-2.57	1.34	1.37
25	9	309	CLA	C3B-C4B	2.57	1.48	1.42
25	T	611	CLA	C1B-C2B	2.57	1.49	1.43
33	P	609	CHL	MG-NB	2.57	2.10	2.05
25	A	816	CLA	C3B-C4B	2.57	1.48	1.42
25	8	311	CLA	C3B-C4B	2.57	1.48	1.42
33	P	608	CHL	C1B-C2B	2.57	1.49	1.43
25	4	303	CLA	C4B-NB	2.57	1.40	1.37
33	P	601	CHL	C4D-CHA	2.57	1.47	1.38
25	3	310	CLA	C3B-C4B	2.56	1.48	1.42
25	A	821	CLA	CMD-C2D	-2.56	1.45	1.50
25	6	611	CLA	C4B-NB	2.56	1.40	1.37
33	S	321	CHL	MG-NA	-2.56	2.00	2.06
25	T	610	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	308	CLA	C4B-NB	2.56	1.40	1.37
33	R	609	CHL	MG-NB	2.56	2.10	2.05
33	P	619	CHL	C1B-C2B	2.56	1.49	1.43
25	A	823	CLA	C4B-NB	2.56	1.40	1.37
25	7	304	CLA	CMB-C2B	-2.56	1.45	1.50
25	1	612	CLA	CMD-C2D	-2.56	1.45	1.50
25	P	611	CLA	C1B-NB	-2.56	1.34	1.37
33	P	607	CHL	C1B-C2B	2.56	1.49	1.43
25	A	839	CLA	MG-NB	-2.56	2.00	2.05
25	2	302	CLA	MG-NB	-2.56	2.00	2.05
25	3	310	CLA	MG-NB	-2.56	2.00	2.05
25	4	309	CLA	MG-NB	-2.56	2.00	2.05
33	R	601	CHL	C4D-CHA	2.56	1.47	1.38
25	G	201	CLA	C3B-C4B	2.56	1.48	1.42
25	7	306	CLA	C3B-C4B	2.56	1.48	1.42
25	L	209	CLA	C3B-C4B	2.56	1.48	1.42
33	S	302	CHL	C4D-CHA	2.56	1.47	1.38
25	8	302	CLA	MG-NB	-2.56	2.00	2.05
33	Q	607	CHL	C1B-C2B	2.56	1.49	1.43
25	A	819	CLA	C4B-NB	2.56	1.40	1.37
25	J	105	CLA	MG-NB	-2.56	2.00	2.05
25	B	838	CLA	MG-NB	-2.56	2.00	2.05
25	B	810	CLA	C4B-NB	2.56	1.40	1.37
33	U	308	CHL	MG-NA	-2.56	2.00	2.06
25	B	835	CLA	C3B-C4B	2.56	1.48	1.42
25	8	311	CLA	MG-NB	-2.55	2.00	2.05
25	J	103	CLA	C3B-C4B	2.55	1.48	1.42
25	8	315	CLA	MG-NB	-2.55	2.00	2.05
25	S	314	CLA	C3B-C4B	2.55	1.48	1.42
33	P	622	CHL	C4D-CHA	2.55	1.47	1.38
33	7	305	CHL	MG-NA	-2.55	2.00	2.06
25	G	202	CLA	MG-NB	-2.55	2.00	2.05
25	A	814	CLA	CMD-C2D	-2.55	1.45	1.50
25	A	832	CLA	CMD-C2D	-2.55	1.45	1.50
25	B	828	CLA	CMB-C2B	-2.55	1.45	1.50
25	4	301	CLA	MG-NB	-2.55	2.00	2.05
33	T	607	CHL	C1B-C2B	2.55	1.49	1.43
25	8	310	CLA	C3B-C4B	2.55	1.48	1.42
25	B	808	CLA	C4B-NB	2.55	1.40	1.37
33	U	307	CHL	C1B-C2B	2.55	1.49	1.43
25	A	807	CLA	C4B-NB	2.55	1.40	1.37
25	Q	611	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	806	CLA	CMD-C2D	-2.55	1.45	1.50
25	7	311	CLA	MG-NB	-2.55	2.00	2.05
25	B	815	CLA	C4B-NB	2.55	1.40	1.37
25	2	309	CLA	C3B-C4B	2.55	1.48	1.42
28	L	204	BCR	C30-C25	-2.55	1.50	1.53
33	S	307	CHL	C3B-C4B	2.55	1.48	1.42
33	Q	608	CHL	C2-C3	2.55	1.39	1.33
25	O	203	CLA	CMD-C2D	-2.55	1.45	1.50
25	1	611	CLA	CMD-C2D	-2.55	1.45	1.50
25	A	817	CLA	MG-NB	-2.55	2.00	2.05
33	T	604	CHL	C1D-ND	-2.55	1.34	1.37
25	B	810	CLA	CMB-C2B	-2.55	1.45	1.50
25	B	826	CLA	CMD-C2D	-2.55	1.45	1.50
33	U	307	CHL	C1D-ND	-2.55	1.34	1.37
25	a	310	CLA	C1B-C2B	2.55	1.49	1.43
33	U	309	CHL	C1B-C2B	2.54	1.49	1.43
33	T	607	CHL	C4C-C3C	2.54	1.49	1.45
33	R	608	CHL	C1B-C2B	2.54	1.49	1.43
33	T	601	CHL	C4D-CHA	2.54	1.47	1.38
34	6	619	LUT	C1-C6	-2.54	1.50	1.53
25	A	813	CLA	CMB-C2B	-2.54	1.45	1.50
25	B	803	CLA	C4B-NB	2.54	1.40	1.37
25	4	301	CLA	C4B-NB	2.54	1.40	1.37
33	T	605	CHL	C3B-C4B	2.54	1.48	1.42
25	B	820	CLA	C1B-C2B	2.54	1.49	1.43
25	B	832	CLA	MG-NB	-2.54	2.00	2.05
25	K	201	CLA	C3B-C4B	2.54	1.48	1.42
25	2	303	CLA	C3B-C4B	2.54	1.48	1.42
25	6	611	CLA	C1B-C2B	2.54	1.49	1.43
25	A	836	CLA	CMD-C2D	-2.54	1.45	1.50
25	A	806	CLA	CMB-C2B	-2.54	1.45	1.50
25	a	303	CLA	C3B-C4B	2.54	1.48	1.42
25	7	313	CLA	MG-NB	-2.54	2.00	2.05
25	U	310	CLA	C1B-C2B	2.54	1.49	1.43
33	Q	605	CHL	C3B-C4B	2.54	1.48	1.42
33	R	605	CHL	C4D-CHA	2.54	1.47	1.38
33	P	609	CHL	C2-C3	2.54	1.39	1.33
25	B	806	CLA	MG-NB	-2.54	2.00	2.05
25	K	201	CLA	MG-NB	-2.54	2.00	2.05
25	A	835	CLA	CMC-C2C	-2.53	1.45	1.50
25	A	810	CLA	C4B-NB	2.53	1.40	1.37
25	8	312	CLA	MG-NB	-2.53	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	R	606	CHL	C3B-C4B	2.53	1.48	1.42
25	9	308	CLA	CMD-C2D	-2.53	1.45	1.50
25	S	313	CLA	C1B-C2B	2.53	1.49	1.43
28	B	840	BCR	C1-C6	-2.53	1.50	1.53
25	B	831	CLA	C3B-C4B	2.53	1.48	1.42
25	1	604	CLA	MG-ND	-2.53	2.00	2.05
25	2	311	CLA	C4B-NB	2.53	1.40	1.37
25	6	616	CLA	C3B-C4B	2.53	1.48	1.42
25	2	309	CLA	MG-NB	-2.53	2.00	2.05
25	R	603	CLA	C4D-ND	-2.53	1.34	1.37
25	U	303	CLA	C1B-C2B	2.53	1.49	1.43
33	T	606	CHL	C3B-C4B	2.53	1.48	1.42
25	A	805	CLA	CMD-C2D	-2.53	1.45	1.50
25	J	105	CLA	C3B-C4B	2.53	1.48	1.42
25	4	302	CLA	C1B-C2B	2.53	1.49	1.43
25	6	603	CLA	CMB-C2B	-2.53	1.45	1.50
25	6	614	CLA	MG-NB	-2.53	2.00	2.05
33	4	304	CHL	C1C-NC	-2.53	1.34	1.37
33	6	607	CHL	C1C-NC	-2.53	1.34	1.37
25	1	614	CLA	C1B-C2B	2.53	1.49	1.43
33	U	305	CHL	C1B-C2B	2.53	1.49	1.43
25	B	834	CLA	C4B-NB	2.53	1.40	1.37
25	a	308	CLA	C1B-C2B	2.53	1.49	1.43
25	B	810	CLA	C3B-C4B	2.53	1.48	1.42
25	A	804	CLA	C3B-C4B	2.53	1.48	1.42
25	B	815	CLA	MG-ND	-2.53	2.00	2.05
25	7	301	CLA	CMD-C2D	-2.53	1.45	1.50
25	B	801	CLA	MG-NB	-2.53	2.00	2.05
25	H	203	CLA	MG-NB	-2.53	2.00	2.05
25	K	203	CLA	MG-NB	-2.53	2.00	2.05
25	7	310	CLA	MG-NB	-2.53	2.00	2.05
33	S	308	CHL	C3B-C4B	2.52	1.48	1.42
25	7	312	CLA	MG-NB	-2.52	2.00	2.05
25	U	311	CLA	C1B-C2B	2.52	1.49	1.43
28	A	846	BCR	C1-C6	-2.52	1.50	1.53
25	A	838	CLA	C3B-C4B	2.52	1.48	1.42
25	A	813	CLA	CMD-C2D	-2.52	1.45	1.50
25	A	829	CLA	CMB-C2B	-2.52	1.45	1.50
25	8	303	CLA	CMB-C2B	-2.52	1.45	1.50
25	B	804	CLA	CMD-C2D	-2.52	1.45	1.50
25	B	833	CLA	MG-ND	-2.52	2.00	2.05
25	3	314	CLA	C4B-NB	2.52	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	805	CLA	C3B-C4B	2.52	1.48	1.42
33	U	308	CHL	C1B-C2B	2.52	1.49	1.43
33	P	607	CHL	MG-NA	-2.52	2.00	2.06
25	5	311	CLA	C3B-C4B	2.52	1.48	1.42
25	8	312	CLA	C3B-C4B	2.52	1.48	1.42
33	R	609	CHL	C2-C3	2.52	1.39	1.33
34	5	318	LUT	C1-C6	-2.52	1.50	1.53
33	Q	606	CHL	C4C-C3C	2.52	1.49	1.45
25	A	817	CLA	C3B-C4B	2.52	1.48	1.42
25	2	304	CLA	C3B-C4B	2.52	1.48	1.42
25	B	824	CLA	CMD-C2D	-2.52	1.45	1.50
33	3	306	CHL	CHB-C4A	-2.52	1.31	1.37
33	4	322	CHL	C1C-NC	-2.52	1.34	1.37
25	B	821	CLA	C3B-C4B	2.52	1.48	1.42
25	3	304	CLA	C3B-C4B	2.52	1.48	1.42
25	4	309	CLA	C3B-C4B	2.52	1.48	1.42
25	6	613	CLA	C1B-C2B	2.52	1.49	1.43
25	B	829	CLA	C4B-NB	2.52	1.40	1.37
25	A	818	CLA	CMD-C2D	-2.52	1.45	1.50
25	B	809	CLA	C4B-NB	2.52	1.40	1.37
25	S	320	CLA	C1B-C2B	2.51	1.49	1.43
25	A	805	CLA	C4B-NB	2.51	1.40	1.37
25	L	202	CLA	CMB-C2B	-2.51	1.45	1.50
25	6	601	CLA	C3B-C4B	2.51	1.48	1.42
33	S	321	CHL	C1B-C2B	2.51	1.49	1.43
25	B	823	CLA	MG-ND	-2.51	2.00	2.05
25	B	801	CLA	CMC-C2C	-2.51	1.45	1.50
25	B	810	CLA	CMD-C2D	-2.51	1.45	1.50
25	B	822	CLA	CMD-C2D	-2.51	1.45	1.50
25	B	812	CLA	CMC-C2C	-2.51	1.45	1.50
33	4	306	CHL	MG-NA	-2.51	2.00	2.06
25	A	837	CLA	MG-NB	-2.51	2.00	2.05
25	K	202	CLA	MG-NB	-2.51	2.00	2.05
25	U	313	CLA	MG-NB	-2.51	2.00	2.05
25	8	312	CLA	C1B-C2B	2.51	1.49	1.43
33	P	622	CHL	C3B-C4B	2.51	1.48	1.42
25	H	201	CLA	MG-NB	-2.51	2.00	2.05
33	U	307	CHL	C3B-C4B	2.51	1.48	1.42
28	G	203	BCR	C1-C6	-2.51	1.50	1.53
33	T	606	CHL	C1B-C2B	2.51	1.49	1.43
25	A	851	CLA	C3B-C4B	2.51	1.48	1.42
25	L	206	CLA	C4B-NB	2.51	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	302	CLA	C4B-NB	2.51	1.40	1.37
25	P	610	CLA	C1B-C2B	2.51	1.49	1.43
25	S	311	CLA	C1B-C2B	2.51	1.49	1.43
33	P	619	CHL	MG-NA	-2.51	2.00	2.06
33	U	309	CHL	C4D-CHA	2.51	1.47	1.38
25	6	612	CLA	CMD-C2D	-2.50	1.45	1.50
25	5	315	CLA	C4B-NB	2.50	1.40	1.37
25	2	307	CLA	MG-NB	-2.50	2.00	2.05
25	6	614	CLA	C3B-C4B	2.50	1.48	1.42
25	7	312	CLA	C3B-C4B	2.50	1.48	1.42
25	A	808	CLA	CMB-C2B	-2.50	1.45	1.50
25	3	308	CLA	C3B-C4B	2.50	1.48	1.42
33	T	604	CHL	C1B-C2B	2.50	1.49	1.43
25	4	303	CLA	MG-NB	-2.50	2.00	2.05
25	2	310	CLA	MG-NB	-2.50	2.00	2.05
25	H	202	CLA	MG-NB	-2.50	2.00	2.05
25	a	313	CLA	MG-NB	-2.50	2.00	2.05
33	R	605	CHL	C1B-C2B	2.50	1.49	1.43
25	A	804	CLA	CMD-C2D	-2.50	1.45	1.50
25	B	801	CLA	CMD-C2D	-2.50	1.45	1.50
25	6	609	CLA	MG-NB	-2.50	2.00	2.05
25	8	304	CLA	C3B-C4B	2.50	1.48	1.42
25	A	827	CLA	CMB-C2B	-2.50	1.45	1.50
25	B	824	CLA	CMB-C2B	-2.50	1.45	1.50
25	A	821	CLA	CMB-C2B	-2.50	1.45	1.50
25	B	823	CLA	CMD-C2D	-2.50	1.45	1.50
25	H	202	CLA	C3B-C4B	2.50	1.48	1.42
25	5	304	CLA	C3B-C4B	2.50	1.48	1.42
25	a	306	CLA	C1B-C2B	2.50	1.49	1.43
25	6	605	CLA	C1D-ND	2.50	1.40	1.37
33	T	607	CHL	C3B-C4B	2.50	1.48	1.42
25	8	310	CLA	CMB-C2B	-2.50	1.45	1.50
28	B	844	BCR	C30-C25	-2.50	1.50	1.53
25	A	824	CLA	CMB-C2B	-2.50	1.45	1.50
25	1	609	CLA	CMD-C2D	-2.50	1.45	1.50
25	B	802	CLA	C3B-C4B	2.50	1.48	1.42
33	4	314	CHL	MG-NA	-2.49	2.00	2.06
25	U	313	CLA	C4B-NB	2.49	1.40	1.37
25	B	825	CLA	MG-ND	-2.49	2.00	2.05
33	6	617	CHL	MG-NA	-2.49	2.00	2.06
25	L	201	CLA	CMB-C2B	-2.49	1.45	1.50
25	B	812	CLA	CMD-C2D	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	311	CLA	CMD-C2D	-2.49	1.45	1.50
25	A	838	CLA	C4B-NB	2.49	1.40	1.37
25	K	204	CLA	C1B-C2B	2.49	1.49	1.43
33	S	307	CHL	C1B-C2B	2.49	1.49	1.43
28	B	844	BCR	C1-C6	-2.49	1.50	1.53
25	A	819	CLA	CMD-C2D	-2.49	1.45	1.50
25	7	307	CLA	CMD-C2D	-2.49	1.45	1.50
25	A	816	CLA	MG-NB	-2.49	2.00	2.05
25	B	827	CLA	CMD-C2D	-2.49	1.45	1.50
25	B	803	CLA	MG-NB	-2.49	2.00	2.05
25	B	801	CLA	CMB-C2B	-2.49	1.45	1.50
25	3	303	CLA	CMC-C2C	-2.49	1.45	1.50
25	B	838	CLA	C3B-C4B	2.49	1.48	1.42
25	5	313	CLA	CMD-C2D	-2.49	1.45	1.50
25	4	312	CLA	C1B-C2B	2.49	1.49	1.43
25	B	829	CLA	MG-ND	-2.49	2.00	2.05
25	6	611	CLA	MG-NB	-2.49	2.00	2.05
25	B	831	CLA	CMD-C2D	-2.49	1.45	1.50
25	B	849	CLA	C3B-C4B	2.49	1.48	1.42
25	6	623	CLA	MG-NB	-2.49	2.00	2.05
25	A	825	CLA	CMB-C2B	-2.49	1.45	1.50
25	A	839	CLA	CMD-C2D	-2.49	1.45	1.50
25	4	308	CLA	CMC-C2C	-2.49	1.45	1.50
25	5	302	CLA	C1B-C2B	2.49	1.49	1.43
25	5	316	CLA	CMC-C2C	-2.49	1.45	1.50
25	A	853	CLA	C3B-C4B	2.49	1.48	1.42
25	A	840	CLA	CMC-C2C	-2.49	1.45	1.50
25	2	311	CLA	C3B-C4B	2.49	1.48	1.42
33	U	307	CHL	C4C-C3C	2.49	1.49	1.45
25	A	815	CLA	C3B-C4B	2.49	1.48	1.42
25	A	820	CLA	C1B-NB	-2.48	1.34	1.37
25	B	823	CLA	C1B-NB	-2.48	1.34	1.37
25	5	309	CLA	C4B-NB	2.48	1.40	1.37
25	a	313	CLA	C3B-C4B	2.48	1.48	1.42
25	4	311	CLA	C3B-C4B	2.48	1.48	1.42
33	P	622	CHL	C1B-C2B	2.48	1.49	1.43
33	R	607	CHL	MG-NA	-2.48	2.00	2.06
33	4	304	CHL	C1B-C2B	2.48	1.49	1.43
25	A	801	CLA	CMD-C2D	-2.48	1.45	1.50
33	U	305	CHL	C3B-C4B	2.48	1.48	1.42
25	9	301	CLA	MG-NB	-2.48	2.00	2.05
25	A	831	CLA	C4B-NB	2.48	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	802	CLA	CMC-C2C	-2.48	1.45	1.50
25	J	105	CLA	C1B-C2B	2.48	1.49	1.43
33	R	608	CHL	C4C-C3C	2.48	1.49	1.45
28	A	849	BCR	C1-C6	-2.48	1.50	1.53
25	7	309	CLA	CMD-C2D	-2.48	1.45	1.50
25	A	807	CLA	CMD-C2D	-2.48	1.45	1.50
25	B	818	CLA	CMD-C2D	-2.48	1.45	1.50
33	P	605	CHL	C4C-C3C	2.48	1.49	1.45
25	A	826	CLA	CMD-C2D	-2.48	1.45	1.50
25	O	202	CLA	C1B-C2B	2.48	1.49	1.43
25	4	313	CLA	C1B-C2B	2.48	1.49	1.43
25	B	835	CLA	CMD-C2D	-2.48	1.45	1.50
25	A	830	CLA	MG-NB	-2.48	2.00	2.05
25	7	307	CLA	MG-NB	-2.48	2.00	2.05
25	A	835	CLA	CMB-C2B	-2.48	1.45	1.50
25	B	806	CLA	CMB-C2B	-2.48	1.45	1.50
25	A	825	CLA	MG-ND	-2.48	2.00	2.05
25	H	205	CLA	CMD-C2D	-2.48	1.45	1.50
25	B	814	CLA	CMB-C2B	-2.48	1.45	1.50
25	B	835	CLA	CMB-C2B	-2.48	1.45	1.50
33	U	306	CHL	C4D-CHA	2.48	1.47	1.38
33	Q	605	CHL	C1D-ND	-2.48	1.34	1.37
25	1	608	CLA	MG-NB	-2.48	2.00	2.05
25	B	821	CLA	MG-NB	-2.47	2.00	2.05
33	S	302	CHL	C3B-C4B	2.47	1.48	1.42
25	B	833	CLA	C1B-NB	-2.47	1.34	1.37
25	9	301	CLA	CMD-C2D	-2.47	1.45	1.50
33	9	306	CHL	C1C-NC	-2.47	1.34	1.37
25	4	303	CLA	C3B-C4B	2.47	1.48	1.42
25	3	307	CLA	CMD-C2D	-2.47	1.45	1.50
25	K	202	CLA	C3B-C4B	2.47	1.48	1.42
33	9	306	CHL	C3B-C4B	2.47	1.48	1.42
25	B	814	CLA	C4B-NB	2.47	1.40	1.37
25	2	304	CLA	CMD-C2D	-2.47	1.45	1.50
33	3	306	CHL	C3D-C2D	2.47	1.45	1.39
25	A	820	CLA	CMD-C2D	-2.47	1.45	1.50
25	B	816	CLA	CMD-C2D	-2.47	1.45	1.50
33	S	308	CHL	C4D-CHA	2.47	1.47	1.38
33	T	604	CHL	C3B-C4B	2.47	1.48	1.42
25	2	305	CLA	C1B-C2B	2.47	1.49	1.43
25	B	816	CLA	C3B-C4B	2.47	1.48	1.42
33	S	309	CHL	C4D-CHA	2.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	T	605	CHL	C1B-C2B	2.47	1.49	1.43
25	H	205	CLA	C4B-NB	2.47	1.40	1.37
25	A	818	CLA	MG-NB	-2.47	2.00	2.05
33	U	305	CHL	C4C-C3C	2.47	1.49	1.45
25	9	303	CLA	C3B-C4B	2.47	1.48	1.42
33	4	322	CHL	MG-NA	-2.47	2.00	2.06
25	A	807	CLA	CMB-C2B	-2.47	1.45	1.50
25	7	310	CLA	CMD-C2D	-2.47	1.45	1.50
25	A	853	CLA	MG-NB	-2.47	2.00	2.05
25	6	616	CLA	MG-NB	-2.47	2.00	2.05
33	Q	606	CHL	C4D-CHA	2.47	1.47	1.38
33	4	305	CHL	C4D-CHA	2.47	1.47	1.38
33	Q	607	CHL	C4C-C3C	2.47	1.49	1.45
25	B	812	CLA	C4B-NB	2.47	1.40	1.37
25	R	604	CLA	C1B-C2B	2.47	1.49	1.43
25	8	315	CLA	C1B-C2B	2.47	1.49	1.43
25	3	303	CLA	CMD-C2D	-2.47	1.45	1.50
25	B	834	CLA	C3B-C4B	2.47	1.48	1.42
25	T	612	CLA	C1B-C2B	2.47	1.49	1.43
25	B	802	CLA	MG-ND	-2.47	2.00	2.05
25	2	311	CLA	MG-NB	-2.47	2.00	2.05
25	1	610	CLA	CMD-C2D	-2.47	1.45	1.50
25	A	811	CLA	MG-NB	-2.46	2.00	2.05
25	A	837	CLA	CMD-C2D	-2.46	1.45	1.50
25	3	320	CLA	CMD-C2D	-2.46	1.45	1.50
25	8	314	CLA	C1B-C2B	2.46	1.49	1.43
25	A	826	CLA	MG-ND	-2.46	2.00	2.05
25	B	818	CLA	MG-NB	-2.46	2.00	2.05
25	A	819	CLA	CMC-C2C	-2.46	1.45	1.50
25	B	814	CLA	CMC-C2C	-2.46	1.45	1.50
25	L	201	CLA	CMD-C2D	-2.46	1.45	1.50
25	1	604	CLA	C1D-ND	2.46	1.40	1.37
25	Q	618	CLA	MG-NB	-2.46	2.00	2.05
25	A	823	CLA	CMB-C2B	-2.46	1.45	1.50
25	A	833	CLA	CMB-C2B	-2.46	1.45	1.50
25	5	312	CLA	MG-NB	-2.46	2.00	2.05
25	1	614	CLA	C3B-C4B	2.46	1.48	1.42
25	B	802	CLA	CMD-C2D	-2.46	1.45	1.50
28	J	101	BCR	C30-C25	-2.46	1.50	1.53
25	2	307	CLA	C1B-C2B	2.46	1.49	1.43
25	A	851	CLA	CMC-C2C	-2.46	1.45	1.50
25	8	303	CLA	CMD-C2D	-2.46	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	302	CHL	C1B-C2B	2.46	1.49	1.43
28	B	842	BCR	C1-C6	-2.46	1.50	1.53
25	9	302	CLA	C3B-C4B	2.46	1.48	1.42
33	S	321	CHL	C3B-C4B	2.46	1.48	1.42
25	1	605	CLA	CMD-C2D	-2.46	1.45	1.50
33	S	309	CHL	C1B-C2B	2.46	1.49	1.43
25	2	310	CLA	C1B-C2B	2.46	1.49	1.43
25	A	811	CLA	CMD-C2D	-2.46	1.45	1.50
25	O	202	CLA	C3B-C4B	2.46	1.48	1.42
25	A	835	CLA	CMD-C2D	-2.46	1.45	1.50
25	B	837	CLA	CMB-C2B	-2.46	1.45	1.50
25	A	804	CLA	C4B-NB	2.46	1.40	1.37
25	7	301	CLA	C1B-NB	-2.46	1.34	1.37
25	A	839	CLA	CMC-C2C	-2.46	1.45	1.50
25	B	832	CLA	CMB-C2B	-2.46	1.45	1.50
33	P	605	CHL	C4D-CHA	2.46	1.47	1.38
25	A	801	CLA	C3B-C4B	2.46	1.48	1.42
25	H	203	CLA	C3B-C4B	2.46	1.48	1.42
25	A	831	CLA	CMD-C2D	-2.46	1.45	1.50
33	5	307	CHL	CHB-C4A	-2.46	1.31	1.37
25	3	313	CLA	C3B-C4B	2.46	1.48	1.42
25	B	837	CLA	C3B-C4B	2.46	1.48	1.42
25	S	312	CLA	C1B-C2B	2.46	1.49	1.43
25	9	305	CLA	C3B-C4B	2.46	1.48	1.42
25	3	314	CLA	C3B-C4B	2.45	1.48	1.42
25	4	308	CLA	C1B-C2B	2.45	1.49	1.43
25	A	832	CLA	CMB-C2B	-2.45	1.45	1.50
25	B	809	CLA	CMB-C2B	-2.45	1.45	1.50
25	6	603	CLA	C1B-NB	-2.45	1.34	1.37
25	5	305	CLA	MG-ND	-2.45	2.00	2.05
33	R	605	CHL	MG-NA	-2.45	2.00	2.06
25	A	833	CLA	CMD-C2D	-2.45	1.45	1.50
25	a	310	CLA	CMD-C2D	-2.45	1.45	1.50
25	5	305	CLA	C1B-C2B	2.45	1.49	1.43
25	1	614	CLA	MG-NB	-2.45	2.00	2.05
25	B	812	CLA	C3B-C4B	2.45	1.48	1.42
25	7	306	CLA	MG-NB	-2.45	2.00	2.05
25	B	834	CLA	CMD-C2D	-2.45	1.45	1.50
25	L	206	CLA	CMC-C2C	-2.45	1.45	1.50
25	R	614	CLA	C1B-C2B	2.45	1.49	1.43
25	8	306	CLA	C1B-C2B	2.45	1.49	1.43
25	A	815	CLA	CMC-C2C	-2.45	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	307	CHL	C4D-CHA	2.45	1.47	1.38
25	A	812	CLA	CMD-C2D	-2.45	1.45	1.50
25	7	306	CLA	CMB-C2B	-2.45	1.45	1.50
25	8	306	CLA	MG-NB	-2.45	2.00	2.05
25	3	312	CLA	MG-NB	-2.45	2.00	2.05
25	B	823	CLA	CMB-C2B	-2.45	1.45	1.50
25	S	315	CLA	MG-NB	-2.45	2.00	2.05
25	4	309	CLA	C1B-C2B	2.45	1.49	1.43
25	7	308	CLA	CMB-C2B	-2.45	1.45	1.50
25	L	205	CLA	MG-ND	-2.45	2.00	2.05
33	S	310	CHL	C3B-C4B	2.45	1.48	1.42
25	L	209	CLA	MG-ND	-2.45	2.00	2.05
25	B	826	CLA	C3B-C4B	2.45	1.48	1.42
25	6	623	CLA	C1B-C2B	2.44	1.49	1.43
33	P	605	CHL	C3B-C4B	2.44	1.48	1.42
25	B	805	CLA	CMC-C2C	-2.44	1.45	1.50
25	B	820	CLA	CMD-C2D	-2.44	1.45	1.50
25	6	609	CLA	CMB-C2B	-2.44	1.45	1.50
25	6	614	CLA	CMB-C2B	-2.44	1.45	1.50
25	B	805	CLA	C4B-NB	2.44	1.40	1.37
25	B	833	CLA	CMB-C2B	-2.44	1.45	1.50
25	3	304	CLA	CMD-C2D	-2.44	1.45	1.50
25	9	301	CLA	CMB-C2B	-2.44	1.45	1.50
25	3	305	CLA	C3B-C4B	2.44	1.48	1.42
25	A	821	CLA	C1B-NB	-2.44	1.34	1.37
25	B	830	CLA	CMB-C2B	-2.44	1.45	1.50
25	B	818	CLA	CMB-C2B	-2.44	1.45	1.50
33	P	608	CHL	C4C-C3C	2.44	1.49	1.45
25	2	308	CLA	C1B-C2B	2.44	1.49	1.43
25	a	308	CLA	CMD-C2D	-2.44	1.45	1.50
33	U	307	CHL	MG-NA	-2.44	2.00	2.06
25	B	835	CLA	MG-NB	-2.44	2.00	2.05
25	6	610	CLA	MG-NB	-2.44	2.00	2.05
25	9	309	CLA	MG-NB	-2.44	2.00	2.05
25	A	840	CLA	CMB-C2B	-2.44	1.45	1.50
33	T	605	CHL	C4D-CHA	2.44	1.47	1.38
25	5	324	CLA	C3B-C4B	2.44	1.48	1.42
25	3	320	CLA	CMB-C2B	-2.44	1.45	1.50
25	5	316	CLA	CMB-C2B	-2.44	1.45	1.50
25	2	308	CLA	MG-NB	-2.44	2.00	2.05
25	K	205	CLA	C1B-C2B	2.44	1.49	1.43
25	8	314	CLA	MG-NB	-2.44	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	304	CLA	C1B-C2B	2.44	1.49	1.43
25	B	813	CLA	MG-NB	-2.44	2.01	2.05
25	7	309	CLA	MG-NB	-2.44	2.01	2.05
25	B	828	CLA	C3B-C4B	2.44	1.48	1.42
25	3	311	CLA	C3B-C4B	2.44	1.48	1.42
33	8	307	CHL	C3B-C4B	2.44	1.48	1.42
25	9	308	CLA	MG-NB	-2.44	2.01	2.05
25	Q	609	CLA	C1B-C2B	2.44	1.49	1.43
25	A	842	CLA	CMD-C2D	-2.44	1.45	1.50
25	1	604	CLA	CMB-C2B	-2.44	1.45	1.50
25	6	609	CLA	C3B-C4B	2.44	1.48	1.42
25	1	609	CLA	C1B-NB	-2.44	1.34	1.37
25	8	310	CLA	C4B-NB	2.44	1.40	1.37
25	A	818	CLA	CMC-C2C	-2.44	1.45	1.50
25	K	205	CLA	MG-NB	-2.44	2.01	2.05
25	3	307	CLA	CMB-C2B	-2.44	1.45	1.50
25	B	807	CLA	CMD-C2D	-2.44	1.45	1.50
33	4	304	CHL	C4D-CHA	2.44	1.47	1.38
25	A	809	CLA	C3B-C4B	2.43	1.48	1.42
25	A	825	CLA	CMC-C2C	-2.43	1.45	1.50
25	A	840	CLA	CMD-C2D	-2.43	1.45	1.50
25	4	308	CLA	MG-NB	-2.43	2.01	2.05
25	A	820	CLA	CMC-C2C	-2.43	1.45	1.50
34	9	313	LUT	C1-C6	-2.43	1.50	1.53
25	A	814	CLA	C1B-NB	-2.43	1.34	1.37
25	B	808	CLA	MG-ND	-2.43	2.01	2.05
25	a	303	CLA	MG-ND	-2.43	2.01	2.05
33	1	601	CHL	CHB-C4A	-2.43	1.31	1.37
25	A	802	CLA	CMD-C2D	-2.43	1.45	1.50
25	6	601	CLA	C1B-C2B	2.43	1.49	1.43
25	L	205	CLA	CMD-C2D	-2.43	1.45	1.50
25	6	609	CLA	CMD-C2D	-2.43	1.45	1.50
25	A	810	CLA	CMD-C2D	-2.43	1.45	1.50
25	H	202	CLA	CMD-C2D	-2.43	1.45	1.50
25	7	313	CLA	C3B-C4B	2.43	1.48	1.42
25	3	309	CLA	MG-NB	-2.43	2.01	2.05
33	8	307	CHL	C1B-C2B	2.43	1.49	1.43
33	Q	605	CHL	C4C-C3C	2.43	1.49	1.45
25	J	103	CLA	MG-NB	-2.43	2.01	2.05
28	7	316	BCR	C1-C6	-2.43	1.50	1.53
25	9	303	CLA	CMC-C2C	-2.43	1.45	1.50
33	Q	605	CHL	C1B-C2B	2.43	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	T	605	CHL	MG-NA	-2.43	2.00	2.06
25	7	311	CLA	CMD-C2D	-2.43	1.45	1.50
33	5	317	CHL	C1C-NC	-2.43	1.34	1.37
25	8	309	CLA	C1B-C2B	2.43	1.49	1.43
25	5	303	CLA	CMD-C2D	-2.43	1.45	1.50
25	B	816	CLA	C4B-NB	2.43	1.40	1.37
25	a	303	CLA	MG-NB	-2.43	2.01	2.05
33	S	308	CHL	C1B-C2B	2.43	1.49	1.43
25	B	833	CLA	CMD-C2D	-2.43	1.45	1.50
33	Q	606	CHL	C3B-C4B	2.43	1.48	1.42
25	8	303	CLA	MG-ND	-2.43	2.01	2.05
25	O	203	CLA	C1B-C2B	2.43	1.49	1.43
25	3	301	CLA	CMB-C2B	-2.43	1.45	1.50
25	A	837	CLA	C3B-C4B	2.43	1.48	1.42
25	6	620	CLA	C3B-C4B	2.43	1.48	1.42
33	4	305	CHL	C1B-C2B	2.43	1.49	1.43
25	3	303	CLA	CMB-C2B	-2.43	1.45	1.50
25	2	309	CLA	CMD-C2D	-2.43	1.45	1.50
28	L	208	BCR	C1-C6	-2.43	1.50	1.53
33	4	305	CHL	C1C-NC	-2.43	1.34	1.37
25	T	609	CLA	C1B-C2B	2.43	1.49	1.43
33	T	606	CHL	C4C-C3C	2.43	1.49	1.45
25	O	203	CLA	MG-NB	-2.43	2.01	2.05
33	S	309	CHL	MG-NA	-2.43	2.00	2.06
28	A	849	BCR	C30-C25	-2.43	1.50	1.53
25	B	805	CLA	CMD-C2D	-2.42	1.45	1.50
25	8	305	CLA	C3B-C4B	2.42	1.48	1.42
25	5	302	CLA	CMD-C2D	-2.42	1.45	1.50
25	B	836	CLA	C3B-C4B	2.42	1.48	1.42
25	H	205	CLA	C3B-C4B	2.42	1.48	1.42
33	U	306	CHL	C1B-C2B	2.42	1.49	1.43
25	O	201	CLA	MG-NB	-2.42	2.01	2.05
25	7	301	CLA	CMC-C2C	-2.42	1.45	1.50
25	B	824	CLA	C3B-C4B	2.42	1.48	1.42
25	a	312	CLA	MG-NB	-2.42	2.01	2.05
33	R	605	CHL	C4C-C3C	2.42	1.49	1.45
25	6	610	CLA	C1B-C2B	2.42	1.49	1.43
25	B	821	CLA	C1B-C2B	2.42	1.49	1.43
25	6	611	CLA	CMD-C2D	-2.42	1.45	1.50
25	A	801	CLA	CMC-C2C	-2.42	1.45	1.50
25	5	315	CLA	MG-NB	-2.42	2.01	2.05
25	3	301	CLA	C4B-NB	2.42	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	307	CLA	MG-NB	-2.42	2.01	2.05
33	P	606	CHL	C1B-C2B	2.42	1.49	1.43
33	8	307	CHL	C4D-CHA	2.42	1.47	1.38
33	T	604	CHL	C4C-C3C	2.42	1.49	1.45
25	B	826	CLA	C4B-NB	2.42	1.40	1.37
33	a	305	CHL	C1C-NC	-2.42	1.34	1.37
25	8	305	CLA	CMB-C2B	-2.42	1.45	1.50
33	P	619	CHL	C3B-C4B	2.42	1.48	1.42
25	A	808	CLA	MG-NB	-2.42	2.01	2.05
28	F	803	BCR	C30-C25	-2.42	1.50	1.53
25	6	603	CLA	C4B-NB	2.42	1.40	1.37
25	P	602	CLA	C1B-C2B	2.42	1.49	1.43
25	S	303	CLA	CMD-C2D	-2.42	1.45	1.50
25	T	608	CLA	C1B-C2B	2.42	1.49	1.43
25	A	822	CLA	CMC-C2C	-2.42	1.45	1.50
33	U	308	CHL	C4D-CHA	2.42	1.47	1.38
25	B	806	CLA	CMD-C2D	-2.42	1.45	1.50
25	8	314	CLA	CMD-C2D	-2.42	1.45	1.50
25	a	311	CLA	C3B-C4B	2.42	1.48	1.42
25	A	814	CLA	CMB-C2B	-2.42	1.45	1.50
25	6	612	CLA	CHC-C1C	2.42	1.43	1.38
25	A	823	CLA	MG-ND	-2.42	2.01	2.05
25	B	803	CLA	CMD-C2D	-2.42	1.45	1.50
25	B	804	CLA	CMC-C2C	-2.42	1.45	1.50
25	3	314	CLA	CMB-C2B	-2.42	1.45	1.50
25	3	313	CLA	C4B-NB	2.42	1.40	1.37
25	A	851	CLA	MG-ND	-2.42	2.01	2.05
25	5	306	CLA	C3B-C4B	2.42	1.48	1.42
25	B	811	CLA	CMD-C2D	-2.42	1.45	1.50
25	K	201	CLA	CMB-C2B	-2.42	1.45	1.50
25	8	302	CLA	CMD-C2D	-2.42	1.45	1.50
25	8	302	CLA	C1B-C2B	2.41	1.48	1.43
33	U	308	CHL	C4C-C3C	2.41	1.49	1.45
25	7	303	CLA	CMD-C2D	-2.41	1.45	1.50
25	A	834	CLA	C3B-C4B	2.41	1.48	1.42
25	Q	610	CLA	C4B-NB	2.41	1.40	1.37
25	2	303	CLA	CMD-C2D	-2.41	1.45	1.50
25	2	311	CLA	C1B-C2B	2.41	1.48	1.43
34	8	317	LUT	C1-C6	-2.41	1.50	1.53
33	4	306	CHL	C4D-CHA	2.41	1.47	1.38
25	A	818	CLA	C1B-C2B	2.41	1.48	1.43
25	A	823	CLA	C3B-C4B	2.41	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	313	CLA	C3B-C4B	2.41	1.48	1.42
28	A	854	BCR	C1-C6	-2.41	1.50	1.53
25	3	310	CLA	C1B-C2B	2.41	1.48	1.43
25	A	828	CLA	CMD-C2D	-2.41	1.45	1.50
25	A	813	CLA	C4B-NB	2.41	1.40	1.37
25	A	842	CLA	CMB-C2B	-2.41	1.45	1.50
25	B	803	CLA	CMB-C2B	-2.41	1.45	1.50
25	A	801	CLA	CMB-C2B	-2.41	1.45	1.50
25	A	815	CLA	CMB-C2B	-2.41	1.45	1.50
25	B	836	CLA	CMB-C2B	-2.41	1.45	1.50
25	B	837	CLA	CMD-C2D	-2.41	1.45	1.50
25	B	824	CLA	C1B-NB	-2.41	1.34	1.37
25	B	838	CLA	CMB-C2B	-2.41	1.45	1.50
33	6	617	CHL	C4D-CHA	2.41	1.47	1.38
33	a	305	CHL	C4D-CHA	2.41	1.47	1.38
25	4	312	CLA	CMD-C2D	-2.41	1.45	1.50
25	A	820	CLA	MG-ND	-2.41	2.01	2.05
25	B	803	CLA	C3B-C4B	2.41	1.48	1.42
25	7	304	CLA	C3B-C4B	2.41	1.48	1.42
33	P	607	CHL	C3B-C4B	2.41	1.48	1.42
25	A	823	CLA	CMD-C2D	-2.41	1.45	1.50
33	P	608	CHL	C3B-C4B	2.40	1.48	1.42
25	9	301	CLA	C4B-C3B	2.40	1.48	1.43
25	A	829	CLA	CMC-C2C	-2.40	1.45	1.50
25	3	304	CLA	CMB-C2B	-2.40	1.45	1.50
25	A	807	CLA	CMC-C2C	-2.40	1.45	1.50
25	A	828	CLA	CMC-C2C	-2.40	1.45	1.50
25	B	828	CLA	CMD-C2D	-2.40	1.45	1.50
25	a	301	CLA	CMB-C2B	-2.40	1.45	1.50
25	1	602	CLA	C1B-C2B	2.40	1.48	1.43
25	B	807	CLA	CMC-C2C	-2.40	1.45	1.50
33	U	307	CHL	C4D-CHA	2.40	1.46	1.38
25	5	304	CLA	C4B-NB	2.40	1.40	1.37
25	B	819	CLA	C3B-C4B	2.40	1.48	1.42
28	L	207	BCR	C30-C25	-2.40	1.50	1.53
25	A	809	CLA	CMD-C2D	-2.40	1.45	1.50
25	1	607	CLA	MG-NB	-2.40	2.01	2.05
33	S	310	CHL	C2C-C1C	2.40	1.49	1.44
25	B	830	CLA	CMD-C2D	-2.40	1.45	1.50
33	R	608	CHL	C3B-C4B	2.40	1.48	1.42
25	B	827	CLA	MG-ND	-2.40	2.01	2.05
33	P	605	CHL	CAA-C2A	-2.40	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	846	BCR	C30-C25	-2.40	1.50	1.53
25	8	313	CLA	C3B-C4B	2.40	1.48	1.42
25	A	830	CLA	CMD-C2D	-2.40	1.45	1.50
25	a	303	CLA	CMB-C2B	-2.40	1.45	1.50
25	A	828	CLA	C1B-C2B	2.40	1.48	1.43
25	L	209	CLA	C1B-C2B	2.40	1.48	1.43
25	B	813	CLA	CMB-C2B	-2.40	1.45	1.50
25	4	301	CLA	CMB-C2B	-2.40	1.45	1.50
25	A	834	CLA	CMB-C2B	-2.40	1.45	1.50
25	A	837	CLA	CMB-C2B	-2.40	1.45	1.50
25	3	302	CLA	CMB-C2B	-2.40	1.45	1.50
25	3	309	CLA	C1B-C2B	2.40	1.48	1.43
25	A	842	CLA	MG-NB	-2.40	2.01	2.05
25	2	314	CLA	MG-NB	-2.40	2.01	2.05
25	3	320	CLA	MG-ND	-2.40	2.01	2.05
33	Q	607	CHL	C3B-C4B	2.39	1.48	1.42
25	5	303	CLA	CMC-C2C	-2.39	1.45	1.50
25	3	320	CLA	C3B-C4B	2.39	1.48	1.42
25	R	611	CLA	MG-NB	-2.39	2.01	2.05
25	B	823	CLA	CMC-C2C	-2.39	1.45	1.50
34	4	315	LUT	C1-C6	-2.39	1.50	1.53
33	T	606	CHL	C4D-CHA	2.39	1.46	1.38
25	B	808	CLA	CMB-C2B	-2.39	1.45	1.50
25	A	815	CLA	C4B-NB	2.39	1.40	1.37
25	A	829	CLA	CMD-C2D	-2.39	1.45	1.50
25	A	810	CLA	CMB-C2B	-2.39	1.45	1.50
33	6	606	CHL	MG-NA	-2.39	2.00	2.06
33	P	606	CHL	C3B-C4B	2.39	1.48	1.42
25	1	605	CLA	MG-NB	-2.39	2.01	2.05
33	S	310	CHL	C4C-C3C	2.39	1.49	1.45
33	R	607	CHL	C3B-C4B	2.39	1.48	1.42
25	A	802	CLA	CMC-C2C	-2.39	1.45	1.50
25	B	801	CLA	C4B-NB	2.39	1.40	1.37
25	3	301	CLA	CMC-C2C	-2.39	1.45	1.50
33	P	606	CHL	C4D-CHA	2.39	1.46	1.38
34	8	316	LUT	C1-C6	-2.39	1.50	1.53
25	2	306	CLA	CMB-C2B	-2.39	1.45	1.50
25	K	201	CLA	CMD-C2D	-2.39	1.45	1.50
25	3	304	CLA	CMC-C2C	-2.39	1.45	1.50
25	a	312	CLA	C1B-C2B	2.39	1.48	1.43
25	B	830	CLA	MG-NB	-2.39	2.01	2.05
25	A	808	CLA	CMD-C2D	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	311	CLA	CMD-C2D	-2.39	1.45	1.50
25	R	610	CLA	CHC-C1C	2.39	1.43	1.38
25	A	802	CLA	CMB-C2B	-2.39	1.45	1.50
25	A	851	CLA	CMB-C2B	-2.39	1.45	1.50
25	7	302	CLA	CMB-C2B	-2.39	1.45	1.50
25	A	822	CLA	C4B-NB	2.39	1.40	1.37
25	A	851	CLA	C4B-NB	2.39	1.40	1.37
25	1	607	CLA	CMB-C2B	-2.39	1.45	1.50
25	U	302	CLA	CHC-C1C	2.39	1.43	1.38
25	7	310	CLA	C3B-C4B	2.39	1.48	1.42
25	1	611	CLA	CMB-C2B	-2.39	1.45	1.50
25	A	822	CLA	MG-ND	-2.39	2.01	2.05
25	Q	610	CLA	MG-NB	-2.39	2.01	2.05
25	7	309	CLA	C3B-C4B	2.39	1.48	1.42
25	L	206	CLA	MG-ND	-2.39	2.01	2.05
25	a	304	CLA	MG-NB	-2.39	2.01	2.05
33	9	307	CHL	C4D-CHA	2.39	1.46	1.38
25	B	832	CLA	C3B-C4B	2.39	1.48	1.42
25	8	302	CLA	C3B-C4B	2.39	1.48	1.42
25	5	319	CLA	MG-NB	-2.38	2.01	2.05
33	T	604	CHL	MG-NA	-2.38	2.00	2.06
25	A	822	CLA	CMD-C2D	-2.38	1.45	1.50
33	9	306	CHL	MG-NA	-2.38	2.00	2.06
25	3	313	CLA	CMD-C2D	-2.38	1.45	1.50
33	6	607	CHL	C4D-CHA	2.38	1.46	1.38
25	5	324	CLA	CMB-C2B	-2.38	1.45	1.50
25	6	603	CLA	CMC-C2C	-2.38	1.45	1.50
25	R	612	CLA	C2-C3	2.38	1.38	1.33
25	B	825	CLA	CMD-C2D	-2.38	1.45	1.50
25	B	805	CLA	C1B-NB	-2.38	1.34	1.37
25	A	826	CLA	CMC-C2C	-2.38	1.45	1.50
25	B	809	CLA	CMD-C2D	-2.38	1.45	1.50
25	T	602	CLA	C1B-C2B	2.38	1.48	1.43
25	B	826	CLA	MG-ND	-2.38	2.01	2.05
25	B	817	CLA	CMC-C2C	-2.38	1.45	1.50
25	A	832	CLA	C3B-C4B	2.38	1.48	1.42
33	6	606	CHL	C3B-C4B	2.38	1.48	1.42
25	B	824	CLA	CMC-C2C	-2.38	1.45	1.50
25	4	312	CLA	MG-NB	-2.38	2.01	2.05
25	A	821	CLA	C3B-C4B	2.38	1.48	1.42
25	B	817	CLA	CMB-C2B	-2.38	1.45	1.50
25	A	829	CLA	C1B-NB	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	307	CHL	C1B-C2B	2.38	1.48	1.43
25	P	612	CLA	O2A-CGA	2.38	1.40	1.33
25	1	603	CLA	CMD-C2D	-2.38	1.45	1.50
25	7	308	CLA	CMD-C2D	-2.38	1.45	1.50
33	P	622	CHL	C4C-C3C	2.38	1.49	1.45
33	6	617	CHL	C1B-C2B	2.38	1.48	1.43
33	U	309	CHL	C2C-C1C	2.38	1.49	1.44
25	9	303	CLA	CMD-C2D	-2.38	1.45	1.50
33	P	605	CHL	C1B-C2B	2.38	1.48	1.43
25	B	811	CLA	CMC-C2C	-2.38	1.45	1.50
25	B	836	CLA	CMD-C2D	-2.38	1.45	1.50
25	6	614	CLA	CMD-C2D	-2.38	1.45	1.50
25	6	620	CLA	C1B-C2B	2.38	1.48	1.43
25	A	828	CLA	C4B-NB	2.38	1.40	1.37
30	B	848	DGD	O3G-C1D	2.37	1.44	1.40
33	4	306	CHL	C1B-C2B	2.37	1.48	1.43
25	A	817	CLA	CMB-C2B	-2.37	1.45	1.50
25	9	305	CLA	CMB-C2B	-2.37	1.45	1.50
25	A	817	CLA	CMD-C2D	-2.37	1.45	1.50
25	4	301	CLA	CMD-C2D	-2.37	1.45	1.50
25	8	314	CLA	CMB-C2B	-2.37	1.45	1.50
25	3	303	CLA	MG-ND	-2.37	2.01	2.05
25	7	304	CLA	C1B-C2B	2.37	1.48	1.43
25	A	809	CLA	CMC-C2C	-2.37	1.45	1.50
25	1	610	CLA	CMB-C2B	-2.37	1.45	1.50
25	1	612	CLA	CMC-C2C	-2.37	1.45	1.50
25	A	827	CLA	CMC-C2C	-2.37	1.45	1.50
25	B	807	CLA	CMB-C2B	-2.37	1.45	1.50
33	1	606	CHL	C4D-CHA	2.37	1.46	1.38
25	2	309	CLA	C1B-C2B	2.37	1.48	1.43
25	B	822	CLA	CMB-C2B	-2.37	1.45	1.50
25	8	304	CLA	CMB-C2B	-2.37	1.45	1.50
33	S	307	CHL	C4C-C3C	2.37	1.49	1.45
33	6	606	CHL	C4D-CHA	2.37	1.46	1.38
25	A	813	CLA	C3B-C4B	2.37	1.48	1.42
25	a	307	CLA	C1B-C2B	2.37	1.48	1.43
25	1	612	CLA	CMB-C2B	-2.37	1.45	1.50
25	O	201	CLA	C1B-C2B	2.37	1.48	1.43
25	5	309	CLA	CMD-C2D	-2.37	1.45	1.50
25	B	807	CLA	MG-NB	-2.37	2.01	2.05
25	A	819	CLA	C1B-NB	-2.37	1.34	1.37
25	B	814	CLA	CMD-C2D	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	303	CLA	C1B-C2B	2.37	1.48	1.43
25	L	206	CLA	CMD-C2D	-2.37	1.45	1.50
25	1	609	CLA	CMC-C2C	-2.37	1.45	1.50
25	7	308	CLA	C4B-NB	2.37	1.40	1.37
25	Q	618	CLA	C2A-C1A	2.37	1.54	1.51
33	4	314	CHL	C4D-CHA	2.37	1.46	1.38
25	A	842	CLA	C1B-C2B	2.37	1.48	1.43
25	B	819	CLA	CMB-C2B	-2.37	1.45	1.50
25	A	827	CLA	C1B-NB	-2.37	1.34	1.37
33	R	606	CHL	C4C-C3C	2.37	1.49	1.45
25	5	319	CLA	CMB-C2B	-2.36	1.45	1.50
33	a	305	CHL	C3B-C4B	2.36	1.48	1.42
25	A	829	CLA	C4B-NB	2.36	1.40	1.37
25	B	805	CLA	CMB-C2B	-2.36	1.45	1.50
25	1	608	CLA	CMD-C2D	-2.36	1.45	1.50
25	5	303	CLA	MG-ND	-2.36	2.01	2.05
25	2	314	CLA	C1B-C2B	2.36	1.48	1.43
25	B	812	CLA	CMB-C2B	-2.36	1.45	1.50
25	7	311	CLA	C1B-C2B	2.36	1.48	1.43
25	9	302	CLA	C1B-C2B	2.36	1.48	1.43
25	6	610	CLA	CMC-C2C	-2.36	1.45	1.50
25	S	315	CLA	C1B-C2B	2.36	1.48	1.43
25	A	809	CLA	MG-ND	-2.36	2.01	2.05
25	5	314	CLA	MG-NB	-2.36	2.01	2.05
33	a	305	CHL	C1B-C2B	2.36	1.48	1.43
25	B	814	CLA	C1B-NB	-2.36	1.34	1.37
25	8	312	CLA	CMD-C2D	-2.36	1.45	1.50
25	8	313	CLA	CMB-C2B	-2.36	1.45	1.50
33	R	605	CHL	CHB-C4A	-2.36	1.32	1.37
25	B	801	CLA	C3B-C4B	2.36	1.48	1.42
25	A	809	CLA	CMB-C2B	-2.36	1.45	1.50
25	Q	602	CLA	C1B-C2B	2.36	1.48	1.43
25	A	816	CLA	CMD-C2D	-2.36	1.45	1.50
25	a	306	CLA	MG-NB	-2.36	2.01	2.05
25	A	833	CLA	CMC-C2C	-2.36	1.45	1.50
25	3	308	CLA	CMD-C2D	-2.36	1.45	1.50
25	6	604	CLA	C1B-C2B	2.36	1.48	1.43
25	3	320	CLA	C1B-NB	-2.36	1.34	1.37
33	9	307	CHL	C3B-C4B	2.36	1.48	1.42
25	1	607	CLA	CMD-C2D	-2.36	1.45	1.50
25	3	308	CLA	CMB-C2B	-2.36	1.45	1.50
25	2	303	CLA	CMB-C2B	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	U	302	CLA	C1B-C2B	2.36	1.48	1.43
33	U	308	CHL	C3B-C4B	2.36	1.48	1.42
25	5	313	CLA	CMB-C2B	-2.36	1.45	1.50
33	R	608	CHL	C4D-CHA	2.36	1.46	1.38
25	H	201	CLA	CMC-C2C	-2.36	1.45	1.50
33	Q	605	CHL	MG-NA	-2.36	2.00	2.06
33	5	308	CHL	MG-NA	-2.36	2.00	2.06
25	A	804	CLA	CMB-C2B	-2.35	1.45	1.50
25	A	853	CLA	CMB-C2B	-2.35	1.45	1.50
25	J	103	CLA	CMD-C2D	-2.35	1.45	1.50
25	8	313	CLA	CMD-C2D	-2.35	1.45	1.50
25	A	833	CLA	C3B-C4B	2.35	1.48	1.42
25	A	815	CLA	C1B-NB	-2.35	1.34	1.37
25	A	831	CLA	C1B-NB	-2.35	1.34	1.37
25	5	316	CLA	C3B-C4B	2.35	1.48	1.42
33	Q	606	CHL	C2C-C1C	2.35	1.49	1.44
25	A	803	CLA	CMB-C2B	-2.35	1.45	1.50
25	P	612	CLA	C2-C3	2.35	1.38	1.33
25	Q	611	CLA	MG-NB	-2.35	2.01	2.05
25	a	309	CLA	C1B-C2B	2.35	1.48	1.43
33	U	309	CHL	C4C-C3C	2.35	1.49	1.45
25	A	817	CLA	CMC-C2C	-2.35	1.45	1.50
25	B	826	CLA	CMC-C2C	-2.35	1.45	1.50
34	3	316	LUT	C22-C21	-2.35	1.51	1.54
25	a	302	CLA	MG-NB	-2.35	2.01	2.05
33	6	617	CHL	C4C-C3C	2.35	1.49	1.45
25	5	312	CLA	CMD-C2D	-2.35	1.45	1.50
25	U	311	CLA	MG-NB	-2.35	2.01	2.05
25	8	308	CLA	C1B-C2B	2.35	1.48	1.43
25	2	308	CLA	CMB-C2B	-2.35	1.45	1.50
25	7	311	CLA	C3B-C4B	2.35	1.48	1.42
25	R	612	CLA	O2A-CGA	2.35	1.40	1.33
25	A	830	CLA	CMC-C2C	-2.35	1.45	1.50
33	Q	607	CHL	C4D-CHA	2.35	1.46	1.38
25	7	306	CLA	CMD-C2D	-2.35	1.45	1.50
25	A	851	CLA	C1B-C2B	2.35	1.48	1.43
25	B	822	CLA	MG-ND	-2.35	2.01	2.05
25	K	201	CLA	CMC-C2C	-2.35	1.45	1.50
25	B	826	CLA	C1B-NB	-2.35	1.34	1.37
25	3	310	CLA	CMD-C2D	-2.35	1.45	1.50
25	K	202	CLA	CMD-C2D	-2.35	1.45	1.50
25	2	308	CLA	CMD-C2D	-2.35	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	613	CLA	CMD-C2D	-2.35	1.45	1.50
25	7	313	CLA	CMD-C2D	-2.35	1.45	1.50
25	9	311	CLA	C1B-C2B	2.35	1.48	1.43
25	5	316	CLA	C4B-NB	2.35	1.40	1.37
34	2	316	LUT	C1-C6	-2.35	1.50	1.53
25	G	201	CLA	C1B-C2B	2.35	1.48	1.43
25	B	805	CLA	MG-ND	-2.35	2.01	2.05
25	Q	602	CLA	CHC-C1C	2.34	1.43	1.38
25	7	310	CLA	C1B-C2B	2.34	1.48	1.43
25	A	815	CLA	CMD-C2D	-2.34	1.45	1.50
25	4	308	CLA	CMB-C2B	-2.34	1.45	1.50
25	B	815	CLA	CMC-C2C	-2.34	1.45	1.50
25	7	301	CLA	MG-ND	-2.34	2.01	2.05
25	U	310	CLA	CHC-C1C	2.34	1.43	1.38
33	P	606	CHL	C2C-C1C	2.34	1.49	1.44
25	3	307	CLA	C3B-C4B	2.34	1.48	1.42
25	2	303	CLA	C1B-C2B	2.34	1.48	1.43
33	P	608	CHL	C4D-CHA	2.34	1.46	1.38
33	1	606	CHL	C1B-C2B	2.34	1.48	1.43
25	R	602	CLA	CHC-C1C	2.34	1.43	1.38
25	1	614	CLA	CMD-C2D	-2.34	1.45	1.50
25	6	612	CLA	CMB-C2B	-2.34	1.45	1.50
33	6	607	CHL	C1B-C2B	2.34	1.48	1.43
25	B	849	CLA	CMB-C2B	-2.34	1.45	1.50
25	8	309	CLA	MG-NB	-2.34	2.01	2.05
25	B	802	CLA	C4B-NB	2.34	1.40	1.37
25	A	838	CLA	CMB-C2B	-2.34	1.45	1.50
33	6	606	CHL	C1C-NC	-2.34	1.34	1.37
25	3	305	CLA	C1B-C2B	2.34	1.48	1.43
25	B	825	CLA	CMB-C2B	-2.34	1.45	1.50
25	7	303	CLA	CMC-C2C	-2.34	1.45	1.50
25	8	305	CLA	CMD-C2D	-2.34	1.45	1.50
25	3	302	CLA	MG-NB	-2.34	2.01	2.05
25	3	301	CLA	CMD-C2D	-2.34	1.45	1.50
25	B	823	CLA	C3B-C4B	2.34	1.48	1.42
25	7	302	CLA	MG-ND	-2.34	2.01	2.05
28	I	201	BCR	C1-C6	-2.34	1.50	1.53
25	B	824	CLA	MG-ND	-2.34	2.01	2.05
25	B	813	CLA	CMD-C2D	-2.34	1.45	1.50
25	7	312	CLA	CMD-C2D	-2.34	1.45	1.50
25	9	304	CLA	CMB-C2B	-2.34	1.45	1.50
25	5	309	CLA	CMC-C2C	-2.34	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	311	CLA	CMB-C2B	-2.34	1.45	1.50
33	P	606	CHL	C4C-C3C	2.34	1.49	1.45
25	B	832	CLA	CMD-C2D	-2.34	1.45	1.50
25	A	853	CLA	CMD-C2D	-2.34	1.45	1.50
25	7	302	CLA	CMC-C2C	-2.34	1.45	1.50
25	H	202	CLA	C1B-C2B	2.34	1.48	1.43
25	3	312	CLA	C1B-C2B	2.34	1.48	1.43
25	H	205	CLA	C1B-C2B	2.33	1.48	1.43
25	2	312	CLA	CMB-C2B	-2.33	1.45	1.50
25	7	312	CLA	CMB-C2B	-2.33	1.45	1.50
25	A	829	CLA	C3B-C4B	2.33	1.48	1.42
33	6	606	CHL	C1B-C2B	2.33	1.48	1.43
25	B	817	CLA	C3B-C4B	2.33	1.48	1.42
25	B	838	CLA	CMC-C2C	-2.33	1.45	1.50
33	R	607	CHL	C4D-CHA	2.33	1.46	1.38
33	P	606	CHL	MG-NA	-2.33	2.00	2.06
25	O	203	CLA	CMC-C2C	-2.33	1.45	1.50
25	5	305	CLA	CMB-C2B	-2.33	1.45	1.50
33	U	305	CHL	MG-NA	-2.33	2.00	2.06
33	U	306	CHL	C4C-C3C	2.33	1.49	1.45
25	H	203	CLA	CMB-C2B	-2.33	1.45	1.50
25	A	836	CLA	C3B-C4B	2.33	1.48	1.42
25	S	312	CLA	MG-NB	-2.33	2.01	2.05
25	B	802	CLA	C1B-NB	-2.33	1.34	1.37
33	Q	607	CHL	CHB-C4A	-2.33	1.32	1.37
25	R	603	CLA	CHC-C1C	2.33	1.43	1.38
25	T	609	CLA	CHC-C1C	2.33	1.43	1.38
25	A	839	CLA	CMB-C2B	-2.33	1.45	1.50
25	8	308	CLA	C3B-C4B	2.33	1.48	1.42
25	2	313	CLA	MG-NB	-2.33	2.01	2.05
25	A	821	CLA	CMC-C2C	-2.33	1.45	1.50
25	9	310	CLA	CHC-C1C	2.33	1.43	1.38
25	5	313	CLA	C1B-C2B	2.33	1.48	1.43
33	9	307	CHL	C1C-NC	-2.33	1.34	1.37
25	B	821	CLA	CMB-C2B	-2.33	1.45	1.50
25	8	308	CLA	CMD-C2D	-2.33	1.45	1.50
25	8	311	CLA	C1B-C2B	2.33	1.48	1.43
25	A	807	CLA	MG-ND	-2.33	2.01	2.05
25	L	201	CLA	C1B-NB	-2.33	1.34	1.37
33	4	322	CHL	CHB-C4A	-2.33	1.32	1.37
25	G	202	CLA	CMB-C2B	-2.33	1.45	1.50
25	B	805	CLA	C3B-C4B	2.33	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	827	CLA	C3B-C4B	2.33	1.48	1.42
25	3	308	CLA	CMC-C2C	-2.33	1.45	1.50
25	A	807	CLA	C1B-NB	-2.33	1.34	1.37
33	P	607	CHL	C4C-C3C	2.33	1.49	1.45
25	8	304	CLA	CMD-C2D	-2.33	1.45	1.50
25	F	802	CLA	CMB-C2B	-2.32	1.45	1.50
33	P	608	CHL	CHB-C4A	-2.32	1.32	1.37
33	P	607	CHL	C4D-CHA	2.32	1.46	1.38
25	6	605	CLA	MG-ND	-2.32	2.01	2.05
25	3	311	CLA	MG-NB	-2.32	2.01	2.05
25	A	838	CLA	CMD-C2D	-2.32	1.45	1.50
33	S	310	CHL	C4D-CHA	2.32	1.46	1.38
25	1	602	CLA	CMB-C2B	-2.32	1.45	1.50
25	3	304	CLA	C1B-C2B	2.32	1.48	1.43
25	5	316	CLA	CMD-C2D	-2.32	1.45	1.50
25	7	309	CLA	CMC-C2C	-2.32	1.45	1.50
25	B	829	CLA	CMD-C2D	-2.32	1.45	1.50
25	4	313	CLA	MG-NB	-2.32	2.01	2.05
33	R	608	CHL	CHB-C4A	-2.32	1.32	1.37
25	9	304	CLA	CMD-C2D	-2.32	1.45	1.50
25	1	608	CLA	C1B-C2B	2.32	1.48	1.43
33	P	619	CHL	C4C-C3C	2.32	1.49	1.45
33	P	619	CHL	C4D-CHA	2.32	1.46	1.38
25	L	202	CLA	C4B-NB	2.32	1.40	1.37
25	A	834	CLA	CMD-C2D	-2.32	1.45	1.50
33	Q	605	CHL	C2C-C1C	2.32	1.49	1.44
25	L	201	CLA	MG-ND	-2.32	2.01	2.05
25	3	314	CLA	MG-ND	-2.32	2.01	2.05
25	L	205	CLA	CMB-C2B	-2.32	1.45	1.50
25	A	819	CLA	MG-ND	-2.32	2.01	2.05
25	J	103	CLA	CMB-C2B	-2.32	1.45	1.50
25	A	834	CLA	C1B-C2B	2.32	1.48	1.43
25	B	812	CLA	MG-ND	-2.32	2.01	2.05
25	5	312	CLA	C1B-C2B	2.32	1.48	1.43
25	a	302	CLA	C1B-C2B	2.32	1.48	1.43
25	3	307	CLA	C4B-NB	2.32	1.40	1.37
25	4	302	CLA	MG-NB	-2.32	2.01	2.05
25	1	611	CLA	CMC-C2C	-2.32	1.45	1.50
33	T	605	CHL	C4C-C3C	2.32	1.49	1.45
25	B	835	CLA	CMC-C2C	-2.32	1.45	1.50
25	A	826	CLA	CMB-C2B	-2.31	1.45	1.50
33	S	309	CHL	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	305	CHL	CHB-C4A	-2.31	1.32	1.37
25	R	604	CLA	CHC-C1C	2.31	1.43	1.38
25	B	829	CLA	CMB-C2B	-2.31	1.45	1.50
25	8	309	CLA	CMD-C2D	-2.31	1.45	1.50
25	2	313	CLA	C1B-C2B	2.31	1.48	1.43
25	B	837	CLA	CMC-C2C	-2.31	1.45	1.50
25	B	830	CLA	CMC-C2C	-2.31	1.45	1.50
25	2	305	CLA	CMB-C2B	-2.31	1.45	1.50
25	P	612	CLA	MG-NC	2.31	2.11	2.06
25	5	309	CLA	C3B-C4B	2.31	1.48	1.42
25	L	202	CLA	CMD-C2D	-2.31	1.45	1.50
25	8	306	CLA	CMD-C2D	-2.31	1.45	1.50
33	S	309	CHL	C2C-C1C	2.31	1.49	1.44
33	R	606	CHL	C4D-CHA	2.31	1.46	1.38
25	A	804	CLA	CMC-C2C	-2.31	1.45	1.50
25	4	303	CLA	CMB-C2B	-2.31	1.45	1.50
25	A	824	CLA	CMC-C2C	-2.31	1.45	1.50
25	H	202	CLA	CMB-C2B	-2.31	1.45	1.50
33	7	305	CHL	C1C-NC	-2.31	1.34	1.37
25	7	302	CLA	CMD-C2D	-2.31	1.45	1.50
33	S	308	CHL	MG-NA	-2.31	2.00	2.06
25	A	816	CLA	CMB-C2B	-2.31	1.45	1.50
33	S	306	CHL	C2C-C1C	2.31	1.49	1.44
33	S	321	CHL	C4C-C3C	2.31	1.49	1.45
25	1	613	CLA	CMB-C2B	-2.31	1.45	1.50
25	B	821	CLA	CMD-C2D	-2.31	1.45	1.50
25	B	813	CLA	CMC-C2C	-2.31	1.45	1.50
25	4	310	CLA	CMD-C2D	-2.31	1.45	1.50
33	R	607	CHL	C4C-C3C	2.31	1.49	1.45
25	5	314	CLA	C1B-C2B	2.31	1.48	1.43
25	B	849	CLA	CMD-C2D	-2.31	1.45	1.50
25	a	307	CLA	CMD-C2D	-2.31	1.45	1.50
25	A	829	CLA	MG-ND	-2.31	2.01	2.05
25	Q	618	CLA	C1B-C2B	2.31	1.48	1.43
25	Q	612	CLA	CHC-C1C	2.31	1.43	1.38
33	5	308	CHL	CHB-C4A	-2.31	1.32	1.37
28	B	845	BCR	C30-C25	-2.30	1.50	1.53
25	2	312	CLA	MG-NB	-2.30	2.01	2.05
25	O	202	CLA	CMB-C2B	-2.30	1.45	1.50
25	2	314	CLA	CMC-C2C	-2.30	1.45	1.50
25	6	616	CLA	CMB-C2B	-2.30	1.45	1.50
25	8	315	CLA	CMD-C2D	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	308	CHL	C4D-CHA	2.30	1.46	1.38
25	B	825	CLA	CMC-C2C	-2.30	1.45	1.50
25	4	309	CLA	CMD-C2D	-2.30	1.45	1.50
25	B	829	CLA	C1B-C2B	2.30	1.48	1.43
25	B	817	CLA	CMD-C2D	-2.30	1.45	1.50
25	B	818	CLA	CMC-C2C	-2.30	1.45	1.50
25	L	202	CLA	C1B-NB	-2.30	1.35	1.37
25	8	303	CLA	C1B-NB	-2.30	1.35	1.37
25	B	833	CLA	CMC-C2C	-2.30	1.45	1.50
25	B	814	CLA	MG-ND	-2.30	2.01	2.05
25	5	304	CLA	CMD-C2D	-2.30	1.45	1.50
25	A	833	CLA	MG-ND	-2.30	2.01	2.05
25	B	834	CLA	CMC-C2C	-2.30	1.45	1.50
25	3	308	CLA	MG-ND	-2.30	2.01	2.05
25	4	301	CLA	CMC-C2C	-2.30	1.45	1.50
25	A	807	CLA	C3B-C4B	2.30	1.48	1.42
25	A	813	CLA	MG-ND	-2.30	2.01	2.05
25	5	315	CLA	CMD-C2D	-2.30	1.45	1.50
33	R	606	CHL	MG-NA	-2.30	2.00	2.06
33	P	622	CHL	C1B-NB	-2.30	1.35	1.37
33	4	314	CHL	C1B-C2B	2.30	1.48	1.43
25	L	205	CLA	C1B-C2B	2.30	1.48	1.43
25	5	305	CLA	CMC-C2C	-2.30	1.45	1.50
25	7	303	CLA	CMB-C2B	-2.30	1.45	1.50
25	7	307	CLA	C1B-C2B	2.30	1.48	1.43
25	3	303	CLA	C3B-C4B	2.30	1.48	1.42
25	G	201	CLA	MG-NB	-2.30	2.01	2.05
28	3	318	BCR	C30-C25	-2.30	1.50	1.53
33	U	306	CHL	MG-NA	-2.30	2.00	2.06
25	8	308	CLA	CMB-C2B	-2.30	1.45	1.50
25	A	813	CLA	C1B-NB	-2.30	1.35	1.37
25	1	604	CLA	C3B-C4B	2.30	1.48	1.42
33	4	304	CHL	C3B-C4B	2.30	1.48	1.42
25	J	105	CLA	CMD-C2D	-2.30	1.45	1.50
25	L	201	CLA	C4B-NB	2.30	1.40	1.37
25	3	311	CLA	CMB-C2B	-2.30	1.45	1.50
25	B	807	CLA	C1B-C2B	2.30	1.48	1.43
28	B	851	BCR	C1-C6	-2.30	1.50	1.53
25	A	851	CLA	CMD-C2D	-2.30	1.45	1.50
25	A	806	CLA	MG-ND	-2.30	2.01	2.05
25	3	314	CLA	CMD-C2D	-2.30	1.45	1.50
25	A	832	CLA	CMC-C2C	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	305	CLA	CMD-C2D	-2.30	1.45	1.50
25	8	310	CLA	MG-ND	-2.29	2.01	2.05
33	T	607	CHL	C2C-C1C	2.29	1.49	1.44
25	A	816	CLA	CMC-C2C	-2.29	1.45	1.50
33	S	302	CHL	MG-NA	-2.29	2.00	2.06
25	9	311	CLA	CMC-C2C	-2.29	1.45	1.50
25	2	312	CLA	C1B-C2B	2.29	1.48	1.43
25	6	612	CLA	MG-NB	-2.29	2.01	2.05
25	L	206	CLA	CMB-C2B	-2.29	1.45	1.50
25	S	305	CLA	MG-NB	-2.29	2.01	2.05
25	5	306	CLA	C1B-C2B	2.29	1.48	1.43
33	S	308	CHL	C2C-C1C	2.29	1.49	1.44
25	J	103	CLA	CMC-C2C	-2.29	1.45	1.50
25	A	812	CLA	CMC-C2C	-2.29	1.45	1.50
25	A	835	CLA	C3B-C4B	2.29	1.48	1.42
25	7	303	CLA	MG-ND	-2.29	2.01	2.05
33	R	605	CHL	C2C-C1C	2.29	1.49	1.44
25	B	803	CLA	CMC-C2C	-2.29	1.45	1.50
25	2	310	CLA	CMD-C2D	-2.29	1.45	1.50
25	2	312	CLA	CMC-C2C	-2.29	1.45	1.50
25	A	803	CLA	CMC-C2C	-2.29	1.45	1.50
25	a	308	CLA	C1B-NB	-2.29	1.35	1.37
25	L	202	CLA	MG-ND	-2.29	2.01	2.05
25	9	303	CLA	CMB-C2B	-2.29	1.45	1.50
25	5	312	CLA	CMB-C2B	-2.29	1.45	1.50
25	1	602	CLA	CMD-C2D	-2.29	1.46	1.50
25	6	604	CLA	CMD-C2D	-2.29	1.46	1.50
25	7	304	CLA	CMD-C2D	-2.29	1.46	1.50
33	T	605	CHL	C2C-C1C	2.29	1.49	1.44
25	a	309	CLA	MG-NB	-2.29	2.01	2.05
25	8	309	CLA	CMB-C2B	-2.29	1.46	1.50
33	1	601	CHL	C4D-CHA	2.29	1.46	1.38
34	5	322	LUT	C22-C21	-2.28	1.51	1.54
25	2	306	CLA	C1B-C2B	2.28	1.48	1.43
25	B	824	CLA	C4B-NB	2.28	1.40	1.37
25	K	202	CLA	C1B-C2B	2.28	1.48	1.43
25	7	306	CLA	CMC-C2C	-2.28	1.46	1.50
25	3	301	CLA	MG-ND	-2.28	2.01	2.05
25	3	307	CLA	MG-ND	-2.28	2.01	2.05
25	R	612	CLA	MG-NC	2.28	2.11	2.06
25	F	802	CLA	CMC-C2C	-2.28	1.46	1.50
25	A	813	CLA	CMC-C2C	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	201	CLA	C1B-C2B	2.28	1.48	1.43
33	4	322	CHL	C4D-CHA	2.28	1.46	1.38
25	B	819	CLA	C1B-NB	-2.28	1.35	1.37
25	2	311	CLA	CMC-C2C	-2.28	1.46	1.50
25	7	307	CLA	CMB-C2B	-2.28	1.46	1.50
25	A	831	CLA	C3B-C4B	2.28	1.48	1.42
25	8	308	CLA	CMC-C2C	-2.28	1.46	1.50
25	7	313	CLA	C1B-C2B	2.28	1.48	1.43
25	2	305	CLA	MG-NB	-2.28	2.01	2.05
25	9	301	CLA	CMC-C2C	-2.28	1.46	1.50
25	a	301	CLA	CMD-C2D	-2.28	1.46	1.50
25	3	301	CLA	C1B-C2B	2.28	1.48	1.43
25	A	827	CLA	MG-ND	-2.28	2.01	2.05
25	B	819	CLA	CMD-C2D	-2.28	1.46	1.50
25	2	311	CLA	CMB-C2B	-2.28	1.46	1.50
25	a	303	CLA	O2A-C1	2.28	1.52	1.46
25	B	810	CLA	CMC-C2C	-2.28	1.46	1.50
33	3	306	CHL	C3B-C4B	2.28	1.48	1.42
33	6	608	CHL	CHB-C4A	-2.28	1.32	1.37
25	A	823	CLA	CMC-C2C	-2.28	1.46	1.50
25	5	314	CLA	CMD-C2D	-2.28	1.46	1.50
25	7	303	CLA	C1B-NB	-2.28	1.35	1.37
25	5	311	CLA	CMB-C2B	-2.28	1.46	1.50
25	Q	618	CLA	CHC-C1C	2.28	1.43	1.38
25	2	303	CLA	CMC-C2C	-2.28	1.46	1.50
25	5	309	CLA	MG-ND	-2.28	2.01	2.05
25	A	836	CLA	C1B-NB	-2.28	1.35	1.37
25	1	607	CLA	C1B-C2B	2.28	1.48	1.43
25	A	804	CLA	MG-ND	-2.28	2.01	2.05
25	A	821	CLA	MG-ND	-2.28	2.01	2.05
33	7	305	CHL	C4D-CHA	2.27	1.46	1.38
25	7	310	CLA	CMB-C2B	-2.27	1.46	1.50
25	A	805	CLA	MG-ND	-2.27	2.01	2.05
33	S	302	CHL	C2C-C1C	2.27	1.49	1.44
25	6	620	CLA	MG-ND	-2.27	2.01	2.05
25	3	313	CLA	CMB-C2B	-2.27	1.46	1.50
25	7	312	CLA	CMC-C2C	-2.27	1.46	1.50
34	1	615	LUT	C22-C21	-2.27	1.51	1.54
25	3	314	CLA	CMC-C2C	-2.27	1.46	1.50
25	7	309	CLA	CMB-C2B	-2.27	1.46	1.50
25	8	312	CLA	CMC-C2C	-2.27	1.46	1.50
33	S	321	CHL	C4D-CHA	2.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	H	201	CLA	CMD-C2D	-2.27	1.46	1.50
25	H	201	CLA	C3B-C4B	2.27	1.48	1.42
25	B	802	CLA	CMB-C2B	-2.27	1.46	1.50
25	3	308	CLA	C4B-NB	2.27	1.40	1.37
25	L	201	CLA	CMC-C2C	-2.27	1.46	1.50
25	1	609	CLA	CMB-C2B	-2.27	1.46	1.50
25	A	812	CLA	C3B-C4B	2.27	1.48	1.42
25	9	310	CLA	MG-NB	-2.27	2.01	2.05
25	K	203	CLA	CMD-C2D	-2.27	1.46	1.50
25	6	616	CLA	C1B-C2B	2.27	1.48	1.43
33	T	606	CHL	CHB-C4A	-2.27	1.32	1.37
25	G	201	CLA	CMB-C2B	-2.27	1.46	1.50
25	6	605	CLA	CMB-C2B	-2.27	1.46	1.50
25	B	820	CLA	CMB-C2B	-2.27	1.46	1.50
25	8	310	CLA	CMD-C2D	-2.27	1.46	1.50
25	A	822	CLA	C3B-C4B	2.27	1.48	1.42
25	P	610	CLA	CHC-C1C	2.27	1.43	1.38
25	A	839	CLA	MG-ND	-2.27	2.01	2.05
25	a	301	CLA	MG-NB	-2.27	2.01	2.05
25	6	610	CLA	CMB-C2B	-2.27	1.46	1.50
25	7	304	CLA	CMC-C2C	-2.27	1.46	1.50
25	7	309	CLA	MG-ND	-2.27	2.01	2.05
25	1	612	CLA	C3B-C4B	2.27	1.48	1.42
25	A	825	CLA	C1B-NB	-2.27	1.35	1.37
25	B	806	CLA	C1B-C2B	2.27	1.48	1.43
25	L	206	CLA	C3B-C4B	2.27	1.48	1.42
25	5	311	CLA	MG-ND	-2.27	2.01	2.05
25	B	809	CLA	C3B-C4B	2.27	1.48	1.42
25	H	205	CLA	CMC-C2C	-2.27	1.46	1.50
25	2	312	CLA	CMD-C2D	-2.27	1.46	1.50
25	A	840	CLA	C1B-C2B	2.27	1.48	1.43
25	7	308	CLA	CMC-C2C	-2.27	1.46	1.50
33	4	306	CHL	CHB-C4A	-2.27	1.32	1.37
25	A	818	CLA	CMB-C2B	-2.27	1.46	1.50
25	K	203	CLA	CMB-C2B	-2.27	1.46	1.50
25	6	620	CLA	CMD-C2D	-2.27	1.46	1.50
25	3	313	CLA	C1B-C2B	2.27	1.48	1.43
33	6	607	CHL	CHB-C4A	-2.26	1.32	1.37
33	5	317	CHL	C4D-CHA	2.26	1.46	1.38
25	B	815	CLA	CMD-C2D	-2.26	1.46	1.50
25	5	305	CLA	CMD-C2D	-2.26	1.46	1.50
25	7	307	CLA	MG-ND	-2.26	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	838	CLA	CMD-C2D	-2.26	1.46	1.50
25	A	810	CLA	CMC-C2C	-2.26	1.46	1.50
25	4	310	CLA	MG-NB	-2.26	2.01	2.05
33	R	608	CHL	C2C-C1C	2.26	1.49	1.44
25	4	311	CLA	MG-NB	-2.26	2.01	2.05
25	1	603	CLA	C1B-C2B	2.26	1.48	1.43
33	U	308	CHL	C2C-C1C	2.26	1.49	1.44
25	2	307	CLA	C3B-C4B	2.26	1.48	1.42
25	5	319	CLA	CMD-C2D	-2.26	1.46	1.50
25	B	829	CLA	C3B-C4B	2.26	1.48	1.42
25	3	309	CLA	CMD-C2D	-2.26	1.46	1.50
25	7	307	CLA	CMC-C2C	-2.26	1.46	1.50
25	B	814	CLA	C3B-C4B	2.26	1.48	1.42
25	B	832	CLA	CMC-C2C	-2.26	1.46	1.50
25	7	304	CLA	MG-ND	-2.26	2.01	2.05
33	Q	608	CHL	MG-NC	2.26	2.11	2.06
25	A	806	CLA	C1B-NB	-2.26	1.35	1.37
33	4	314	CHL	C4C-C3C	2.26	1.48	1.45
25	1	613	CLA	C1B-C2B	2.26	1.48	1.43
25	A	853	CLA	CMC-C2C	-2.26	1.46	1.50
25	4	307	CLA	C1B-C2B	2.26	1.48	1.43
25	Q	613	CLA	CHC-C1C	2.26	1.43	1.38
25	3	302	CLA	CMC-C2C	-2.26	1.46	1.50
25	4	307	CLA	CMD-C2D	-2.26	1.46	1.50
25	A	803	CLA	C1B-C2B	2.26	1.48	1.43
25	5	315	CLA	CMC-C2C	-2.26	1.46	1.50
25	2	302	CLA	CMB-C2B	-2.26	1.46	1.50
33	4	314	CHL	CHB-C4A	-2.26	1.32	1.37
25	3	303	CLA	C4B-NB	2.26	1.40	1.37
25	3	311	CLA	C1B-C2B	2.26	1.48	1.43
25	1	603	CLA	CMB-C2B	-2.26	1.46	1.50
25	Q	609	CLA	CHC-C1C	2.26	1.43	1.38
25	G	201	CLA	CHC-C1C	2.25	1.43	1.38
33	8	307	CHL	C3D-C4D	-2.25	1.39	1.44
25	L	205	CLA	CMC-C2C	-2.25	1.46	1.50
25	6	616	CLA	CMD-C2D	-2.25	1.46	1.50
25	1	611	CLA	C1B-C2B	2.25	1.48	1.43
25	1	609	CLA	C1B-C2B	2.25	1.48	1.43
25	A	825	CLA	C4B-NB	2.25	1.40	1.37
25	1	608	CLA	CMB-C2B	-2.25	1.46	1.50
25	4	307	CLA	CMB-C2B	-2.25	1.46	1.50
25	8	312	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	312	CLA	CMC-C2C	-2.25	1.46	1.50
33	7	305	CHL	C1B-NB	-2.25	1.35	1.37
25	a	307	CLA	CMB-C2B	-2.25	1.46	1.50
25	2	311	CLA	CMD-C2D	-2.25	1.46	1.50
25	6	615	CLA	CMD-C2D	-2.25	1.46	1.50
25	a	313	CLA	CMD-C2D	-2.25	1.46	1.50
33	4	314	CHL	C3B-C4B	2.25	1.48	1.42
25	A	828	CLA	CMB-C2B	-2.25	1.46	1.50
25	5	306	CLA	CMB-C2B	-2.25	1.46	1.50
28	A	847	BCR	C30-C25	-2.25	1.50	1.53
25	R	602	CLA	C1B-C2B	2.25	1.48	1.43
25	a	302	CLA	CMC-C2C	-2.25	1.46	1.50
25	A	830	CLA	MG-ND	-2.25	2.01	2.05
25	A	842	CLA	CMC-C2C	-2.25	1.46	1.50
25	B	816	CLA	CMC-C2C	-2.25	1.46	1.50
25	B	803	CLA	MG-ND	-2.25	2.01	2.05
25	S	311	CLA	MG-NB	-2.25	2.01	2.05
25	9	310	CLA	CMD-C2D	-2.25	1.46	1.50
33	S	308	CHL	C4C-C3C	2.25	1.48	1.45
33	6	608	CHL	C1C-NC	-2.25	1.34	1.37
25	B	809	CLA	CMC-C2C	-2.25	1.46	1.50
25	7	310	CLA	CMC-C2C	-2.25	1.46	1.50
25	5	324	CLA	MG-ND	-2.25	2.01	2.05
25	2	308	CLA	CMC-C2C	-2.25	1.46	1.50
25	L	202	CLA	C1B-C2B	2.25	1.48	1.43
25	5	310	CLA	CMC-C2C	-2.25	1.46	1.50
25	B	813	CLA	MG-ND	-2.25	2.01	2.05
34	2	315	LUT	C1-C6	-2.25	1.50	1.53
25	B	837	CLA	MG-ND	-2.25	2.01	2.05
25	6	609	CLA	MG-ND	-2.25	2.01	2.05
25	a	301	CLA	C1B-C2B	2.25	1.48	1.43
25	R	612	CLA	MG-ND	-2.25	2.01	2.05
25	A	802	CLA	C1B-C2B	2.24	1.48	1.43
25	2	307	CLA	CMB-C2B	-2.24	1.46	1.50
25	B	812	CLA	C1B-C2B	2.24	1.48	1.43
33	U	308	CHL	CHB-C4A	-2.24	1.32	1.37
25	6	609	CLA	C1B-C2B	2.24	1.48	1.43
25	K	204	CLA	CMD-C2D	-2.24	1.46	1.50
25	9	302	CLA	MG-NB	-2.24	2.01	2.05
33	8	307	CHL	C1C-NC	-2.24	1.34	1.37
25	B	806	CLA	CMC-C2C	-2.24	1.46	1.50
25	2	313	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	806	CLA	C3B-C4B	2.24	1.48	1.42
25	9	310	CLA	C1B-C2B	2.24	1.48	1.43
25	A	811	CLA	CMC-C2C	-2.24	1.46	1.50
25	8	311	CLA	CMB-C2B	-2.24	1.46	1.50
25	a	302	CLA	CMB-C2B	-2.24	1.46	1.50
25	a	302	CLA	CMD-C2D	-2.24	1.46	1.50
25	T	609	CLA	MG-NB	-2.24	2.01	2.05
25	5	324	CLA	CMD-C2D	-2.24	1.46	1.50
25	5	315	CLA	C1B-C2B	2.24	1.48	1.43
25	A	840	CLA	MG-ND	-2.24	2.01	2.05
33	R	606	CHL	C1B-C2B	2.24	1.48	1.43
25	A	803	CLA	CMD-C2D	-2.24	1.46	1.50
25	9	308	CLA	C1B-C2B	2.24	1.48	1.43
25	H	201	CLA	CMB-C2B	-2.24	1.46	1.50
25	4	302	CLA	CMD-C2D	-2.24	1.46	1.50
25	5	311	CLA	CMC-C2C	-2.24	1.46	1.50
25	A	814	CLA	C4B-NB	2.24	1.40	1.37
25	4	308	CLA	C4B-NB	2.24	1.40	1.37
25	B	827	CLA	CMC-C2C	-2.24	1.46	1.50
25	1	608	CLA	CMC-C2C	-2.24	1.46	1.50
33	9	306	CHL	C4D-CHA	2.24	1.46	1.38
25	A	853	CLA	C1B-C2B	2.24	1.48	1.43
25	3	311	CLA	CMD-C2D	-2.24	1.46	1.50
25	a	301	CLA	CMC-C2C	-2.24	1.46	1.50
25	A	825	CLA	C3B-C4B	2.24	1.48	1.42
25	B	817	CLA	MG-ND	-2.24	2.01	2.05
25	F	802	CLA	CMD-C2D	-2.24	1.46	1.50
25	5	304	CLA	CMB-C2B	-2.24	1.46	1.50
25	4	311	CLA	CMD-C2D	-2.24	1.46	1.50
25	6	603	CLA	MG-ND	-2.24	2.01	2.05
25	8	313	CLA	C1B-C2B	2.24	1.48	1.43
25	6	601	CLA	CMC-C2C	-2.24	1.46	1.50
28	B	851	BCR	C30-C25	-2.23	1.50	1.53
25	A	814	CLA	MG-ND	-2.23	2.01	2.05
33	R	609	CHL	MG-NC	2.23	2.11	2.06
25	S	301	CLA	MG-ND	-2.23	2.01	2.05
25	8	303	CLA	C3B-C4B	2.23	1.48	1.42
28	B	841	BCR	C1-C6	-2.23	1.50	1.53
25	B	804	CLA	C1B-NB	-2.23	1.35	1.37
25	3	307	CLA	CMC-C2C	-2.23	1.46	1.50
34	1	616	LUT	C22-C21	-2.23	1.51	1.54
25	A	833	CLA	C1B-C2B	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	301	CLA	C3B-C4B	2.23	1.48	1.42
25	5	312	CLA	CHC-C1C	2.23	1.43	1.38
25	P	612	CLA	MG-ND	-2.23	2.01	2.05
25	6	610	CLA	CMD-C2D	-2.23	1.46	1.50
25	B	819	CLA	CMC-C2C	-2.23	1.46	1.50
25	2	306	CLA	CMD-C2D	-2.23	1.46	1.50
25	4	310	CLA	CHC-C1C	2.23	1.43	1.38
25	H	203	CLA	CMD-C2D	-2.23	1.46	1.50
25	2	302	CLA	CMC-C2C	-2.23	1.46	1.50
25	A	835	CLA	C4B-NB	2.23	1.40	1.37
25	B	823	CLA	C4B-NB	2.23	1.40	1.37
25	3	305	CLA	CMD-C2D	-2.23	1.46	1.50
25	2	304	CLA	CMB-C2B	-2.23	1.46	1.50
25	K	201	CLA	MG-ND	-2.23	2.01	2.05
25	6	604	CLA	CMB-C2B	-2.23	1.46	1.50
25	7	302	CLA	C1B-C2B	2.23	1.48	1.43
25	a	309	CLA	CMD-C2D	-2.23	1.46	1.50
25	A	836	CLA	CMC-C2C	-2.23	1.46	1.50
33	P	609	CHL	MG-NC	2.23	2.11	2.06
25	4	301	CLA	C1B-NB	-2.23	1.35	1.37
33	6	617	CHL	CHB-C4A	-2.23	1.32	1.37
25	S	303	CLA	CHC-C1C	2.23	1.43	1.38
33	Q	605	CHL	CHB-C4A	-2.22	1.32	1.37
25	4	313	CLA	CMD-C2D	-2.22	1.46	1.50
25	A	823	CLA	C1B-NB	-2.22	1.35	1.37
25	A	832	CLA	C4B-NB	2.22	1.40	1.37
25	2	302	CLA	CHC-C1C	2.22	1.43	1.38
25	4	312	CLA	CHC-C1C	2.22	1.43	1.38
25	H	205	CLA	MG-ND	-2.22	2.01	2.05
25	T	611	CLA	CHC-C1C	2.22	1.43	1.38
25	a	311	CLA	CMC-C2C	-2.22	1.46	1.50
25	O	203	CLA	C4B-C3B	2.22	1.48	1.43
25	5	313	CLA	C1D-C2D	2.22	1.49	1.45
25	2	314	CLA	CMB-C2B	-2.22	1.46	1.50
25	a	310	CLA	CHC-C1C	2.22	1.43	1.38
33	3	306	CHL	C3D-C4D	-2.22	1.39	1.44
25	B	808	CLA	C3B-C4B	2.22	1.48	1.42
28	J	106	BCR	C1-C6	-2.22	1.50	1.53
33	P	608	CHL	C2C-C1C	2.22	1.49	1.44
25	B	837	CLA	C1B-C2B	2.22	1.48	1.43
25	A	824	CLA	CMD-C2D	-2.22	1.46	1.50
25	6	611	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	814	CLA	C3B-C4B	2.22	1.48	1.42
25	S	303	CLA	MG-NB	-2.22	2.01	2.05
33	T	604	CHL	C2C-C1C	2.22	1.49	1.44
25	K	205	CLA	CMB-C2B	-2.22	1.46	1.50
25	T	608	CLA	CHC-C1C	2.22	1.43	1.38
25	4	303	CLA	C1B-C2B	2.22	1.48	1.43
25	1	602	CLA	CMC-C2C	-2.22	1.46	1.50
25	9	309	CLA	CMD-C2D	-2.22	1.46	1.50
25	P	602	CLA	CHC-C1C	2.22	1.43	1.38
33	5	317	CHL	CHB-C4A	-2.22	1.32	1.37
25	B	811	CLA	C4B-NB	2.22	1.40	1.37
25	A	808	CLA	CMC-C2C	-2.22	1.46	1.50
25	L	202	CLA	C3B-C4B	2.22	1.48	1.42
25	K	202	CLA	CMB-C2B	-2.22	1.46	1.50
25	2	308	CLA	MG-ND	-2.22	2.01	2.05
25	1	605	CLA	CMC-C2C	-2.22	1.46	1.50
25	A	830	CLA	C3B-C4B	2.22	1.48	1.42
25	A	822	CLA	C1B-NB	-2.22	1.35	1.37
25	5	305	CLA	C1B-NB	-2.22	1.35	1.37
25	H	202	CLA	CMC-C2C	-2.22	1.46	1.50
25	B	832	CLA	MG-ND	-2.22	2.01	2.05
25	B	815	CLA	C1B-NB	-2.22	1.35	1.37
25	6	613	CLA	CMB-C2B	-2.22	1.46	1.50
25	5	324	CLA	C1B-C2B	2.22	1.48	1.43
25	B	810	CLA	MG-ND	-2.22	2.01	2.05
33	Q	606	CHL	MG-NA	-2.22	2.01	2.06
25	A	801	CLA	MG-ND	-2.22	2.01	2.05
28	B	845	BCR	C21-C22	-2.22	1.32	1.35
25	B	836	CLA	CMC-C2C	-2.22	1.46	1.50
25	6	623	CLA	CMD-C2D	-2.22	1.46	1.50
25	a	304	CLA	CMD-C2D	-2.22	1.46	1.50
25	A	810	CLA	MG-ND	-2.21	2.01	2.05
25	B	819	CLA	MG-ND	-2.21	2.01	2.05
25	A	810	CLA	C1B-C2B	2.21	1.48	1.43
25	3	312	CLA	CMB-C2B	-2.21	1.46	1.50
25	7	313	CLA	CMB-C2B	-2.21	1.46	1.50
25	B	811	CLA	MG-ND	-2.21	2.01	2.05
25	7	310	CLA	MG-ND	-2.21	2.01	2.05
25	8	304	CLA	CMC-C2C	-2.21	1.46	1.50
25	L	205	CLA	C1B-NB	-2.21	1.35	1.37
25	K	203	CLA	C1B-C2B	2.21	1.48	1.43
25	Q	604	CLA	CHC-C1C	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	849	CLA	CMC-C2C	-2.21	1.46	1.50
25	8	313	CLA	CMC-C2C	-2.21	1.46	1.50
28	B	843	BCR	C30-C25	-2.21	1.50	1.53
25	A	805	CLA	CMC-C2C	-2.21	1.46	1.50
25	8	305	CLA	CMC-C2C	-2.21	1.46	1.50
25	a	309	CLA	CHC-C1C	2.21	1.43	1.38
25	5	313	CLA	CMC-C2C	-2.21	1.46	1.50
25	A	831	CLA	CMC-C2C	-2.21	1.46	1.50
25	1	603	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	832	CLA	C1B-C2B	2.21	1.48	1.43
25	B	822	CLA	C1B-C2B	2.21	1.48	1.43
25	2	310	CLA	CMB-C2B	-2.21	1.46	1.50
33	1	606	CHL	C2C-C1C	2.21	1.49	1.44
25	F	802	CLA	C1B-C2B	2.21	1.48	1.43
25	8	302	CLA	CMB-C2B	-2.21	1.46	1.50
25	a	306	CLA	CMD-C2D	-2.21	1.46	1.50
25	B	809	CLA	C1B-C2B	2.21	1.48	1.43
25	A	819	CLA	C3B-C4B	2.21	1.47	1.42
33	U	305	CHL	CHB-C4A	-2.21	1.32	1.37
33	Q	601	CHL	C2C-C1C	2.21	1.49	1.44
25	5	303	CLA	CMB-C2B	-2.21	1.46	1.50
33	R	601	CHL	C1C-NC	-2.21	1.34	1.37
25	6	603	CLA	CMD-C2D	-2.21	1.46	1.50
25	B	813	CLA	C1B-NB	-2.21	1.35	1.37
25	B	834	CLA	C1B-NB	-2.21	1.35	1.37
25	1	609	CLA	CHC-C1C	2.21	1.43	1.38
25	S	314	CLA	MG-NB	-2.20	2.01	2.05
25	9	311	CLA	CMB-C2B	-2.20	1.46	1.50
25	6	603	CLA	C3B-C4B	2.20	1.47	1.42
25	8	310	CLA	C1B-C2B	2.20	1.48	1.43
25	B	807	CLA	C3B-C4B	2.20	1.47	1.42
33	U	306	CHL	C2C-C1C	2.20	1.49	1.44
25	1	613	CLA	CMD-C2D	-2.20	1.46	1.50
25	3	310	CLA	CMB-C2B	-2.20	1.46	1.50
25	5	302	CLA	CMB-C2B	-2.20	1.46	1.50
25	B	825	CLA	C1B-C2B	2.20	1.48	1.43
25	5	315	CLA	CMB-C2B	-2.20	1.46	1.50
25	A	830	CLA	C1B-C2B	2.20	1.48	1.43
25	B	822	CLA	C3B-C4B	2.20	1.47	1.42
33	S	302	CHL	CHB-C4A	-2.20	1.32	1.37
25	5	304	CLA	MG-ND	-2.20	2.01	2.05
25	A	824	CLA	C1B-NB	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	8	317	LUT	C22-C21	-2.20	1.52	1.54
25	9	305	CLA	MG-NB	-2.20	2.01	2.05
25	4	307	CLA	CHC-C1C	2.20	1.43	1.38
25	a	311	CLA	MG-NB	-2.20	2.01	2.05
25	Q	603	CLA	CHC-C1C	2.20	1.43	1.38
25	6	612	CLA	C1B-C2B	2.20	1.48	1.43
25	3	301	CLA	C3B-C4B	2.20	1.47	1.42
25	6	615	CLA	CMB-C2B	-2.20	1.46	1.50
25	3	320	CLA	CMC-C2C	-2.20	1.46	1.50
25	1	607	CLA	CMC-C2C	-2.20	1.46	1.50
25	P	603	CLA	CHC-C1C	2.20	1.43	1.38
25	B	836	CLA	C1B-C2B	2.20	1.48	1.43
25	A	837	CLA	CMC-C2C	-2.20	1.46	1.50
25	3	311	CLA	CMC-C2C	-2.20	1.46	1.50
25	O	203	CLA	CMB-C2B	-2.20	1.46	1.50
25	B	849	CLA	MG-ND	-2.20	2.01	2.05
25	5	305	CLA	C3B-C4B	2.20	1.47	1.42
33	T	606	CHL	C2C-C1C	2.20	1.49	1.44
25	A	808	CLA	C1B-C2B	2.20	1.48	1.43
25	Q	610	CLA	C1B-C2B	2.20	1.48	1.43
33	Q	607	CHL	C2C-C1C	2.20	1.49	1.44
25	1	610	CLA	MG-ND	-2.20	2.01	2.05
25	A	834	CLA	CMC-C2C	-2.19	1.46	1.50
25	B	817	CLA	C1B-C2B	2.19	1.48	1.43
25	5	313	CLA	MG-NB	-2.19	2.01	2.05
25	H	203	CLA	CMC-C2C	-2.19	1.46	1.50
25	5	304	CLA	C1B-C2B	2.19	1.48	1.43
25	9	310	CLA	CMB-C2B	-2.19	1.46	1.50
25	L	209	CLA	CMD-C2D	-2.19	1.46	1.50
33	5	307	CHL	C4D-CHA	2.19	1.46	1.38
25	A	815	CLA	C1B-C2B	2.19	1.48	1.43
25	9	305	CLA	CMC-C2C	-2.19	1.46	1.50
25	T	612	CLA	MG-NB	-2.19	2.01	2.05
25	B	822	CLA	CMC-C2C	-2.19	1.46	1.50
25	T	602	CLA	CHC-C1C	2.19	1.43	1.38
33	4	306	CHL	C2C-C1C	2.19	1.49	1.44
25	L	206	CLA	C1B-C2B	2.19	1.48	1.43
25	B	808	CLA	C1B-C2B	2.19	1.48	1.43
25	G	202	CLA	CMD-C2D	-2.19	1.46	1.50
25	3	313	CLA	CMC-C2C	-2.19	1.46	1.50
25	3	313	CLA	MG-ND	-2.19	2.01	2.05
25	Q	610	CLA	CHC-C1C	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	301	CLA	C1B-C2B	2.19	1.48	1.43
33	Q	601	CHL	C1C-NC	-2.19	1.34	1.37
25	a	308	CLA	C4B-NB	2.19	1.40	1.37
25	6	612	CLA	CMC-C2C	-2.19	1.46	1.50
25	2	309	CLA	MG-ND	-2.19	2.01	2.05
33	T	601	CHL	C1C-NC	-2.19	1.34	1.37
33	6	606	CHL	C1B-NB	-2.19	1.35	1.37
25	1	614	CLA	MG-ND	-2.19	2.01	2.05
28	J	106	BCR	C30-C25	-2.19	1.50	1.53
33	P	601	CHL	C2C-C1C	2.19	1.49	1.44
25	5	314	CLA	CMB-C2B	-2.19	1.46	1.50
25	7	313	CLA	MG-ND	-2.19	2.01	2.05
25	2	306	CLA	CMC-C2C	-2.19	1.46	1.50
25	A	820	CLA	C3B-C4B	2.19	1.47	1.42
25	R	611	CLA	CHC-C1C	2.19	1.43	1.38
25	P	610	CLA	MG-NB	-2.19	2.01	2.05
33	P	601	CHL	C1C-NC	-2.19	1.34	1.37
25	B	820	CLA	MG-ND	-2.19	2.01	2.05
25	P	611	CLA	CHC-C4B	2.19	1.44	1.39
25	6	620	CLA	CMB-C2B	-2.19	1.46	1.50
25	A	832	CLA	C1B-NB	-2.18	1.35	1.37
25	P	602	CLA	MG-NB	-2.18	2.01	2.05
33	6	607	CHL	C3B-C4B	2.18	1.47	1.42
25	3	310	CLA	CMC-C2C	-2.18	1.46	1.50
25	6	615	CLA	CMC-C2C	-2.18	1.46	1.50
25	8	306	CLA	CMB-C2B	-2.18	1.46	1.50
25	S	320	CLA	CHC-C1C	2.18	1.43	1.38
25	3	303	CLA	C1B-C2B	2.18	1.48	1.43
25	L	209	CLA	CMB-C2B	-2.18	1.46	1.50
25	5	311	CLA	C1B-C2B	2.18	1.48	1.43
25	O	201	CLA	CMB-C2B	-2.18	1.46	1.50
25	6	601	CLA	CMD-C2D	-2.18	1.46	1.50
25	9	308	CLA	CMC-C2C	-2.18	1.46	1.50
25	6	603	CLA	C1B-C2B	2.18	1.48	1.43
25	A	853	CLA	MG-ND	-2.18	2.01	2.05
25	3	312	CLA	CMC-C2C	-2.18	1.46	1.50
25	B	831	CLA	CMC-C2C	-2.18	1.46	1.50
25	H	205	CLA	CMB-C2B	-2.18	1.46	1.50
25	L	202	CLA	CMC-C2C	-2.18	1.46	1.50
25	A	809	CLA	C1B-NB	-2.18	1.35	1.37
33	U	305	CHL	C2C-C1C	2.18	1.49	1.44
28	I	201	BCR	C30-C25	-2.18	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	311	CLA	CMC-C2C	-2.18	1.46	1.50
25	9	304	CLA	MG-ND	-2.18	2.01	2.05
25	1	608	CLA	CHC-C1C	2.18	1.43	1.38
25	2	305	CLA	CMD-C2D	-2.18	1.46	1.50
25	1	613	CLA	MG-ND	-2.18	2.01	2.05
25	3	305	CLA	CMB-C2B	-2.18	1.46	1.50
25	A	805	CLA	C1B-NB	-2.18	1.35	1.37
25	5	303	CLA	C4B-NB	2.18	1.40	1.37
25	9	309	CLA	CMB-C2B	-2.18	1.46	1.50
33	T	607	CHL	C1C-NC	-2.18	1.34	1.37
33	5	308	CHL	C2C-C1C	2.18	1.49	1.44
25	2	314	CLA	CMD-C2D	-2.18	1.46	1.50
25	4	310	CLA	CMC-C2C	-2.18	1.46	1.50
25	5	304	CLA	CMC-C2C	-2.18	1.46	1.50
25	S	311	CLA	CHC-C1C	2.18	1.42	1.38
25	3	303	CLA	C1B-NB	-2.18	1.35	1.37
25	3	308	CLA	C1B-NB	-2.18	1.35	1.37
25	B	833	CLA	C1B-C2B	2.18	1.48	1.43
25	8	315	CLA	CMC-C2C	-2.18	1.46	1.50
25	7	301	CLA	C1B-C2B	2.18	1.48	1.43
25	7	312	CLA	C1B-C2B	2.18	1.48	1.43
33	9	306	CHL	C1B-C2B	2.18	1.48	1.43
25	B	820	CLA	CMC-C2C	-2.18	1.46	1.50
25	3	312	CLA	CMD-C2D	-2.18	1.46	1.50
25	2	310	CLA	CHC-C1C	2.18	1.42	1.38
28	F	801	BCR	C30-C25	-2.18	1.50	1.53
25	A	820	CLA	CAC-C3C	-2.18	1.45	1.51
25	H	203	CLA	C1B-C2B	2.18	1.48	1.43
25	5	310	CLA	C1B-C2B	2.18	1.48	1.43
25	U	312	CLA	CHC-C1C	2.18	1.42	1.38
25	6	620	CLA	CMC-C2C	-2.17	1.46	1.50
33	T	604	CHL	CHB-C4A	-2.17	1.32	1.37
25	a	311	CLA	CMD-C2D	-2.17	1.46	1.50
25	4	302	CLA	CMB-C2B	-2.17	1.46	1.50
25	8	311	CLA	MG-ND	-2.17	2.01	2.05
25	O	202	CLA	CMC-C2C	-2.17	1.46	1.50
25	B	828	CLA	C1B-C2B	2.17	1.48	1.43
25	4	309	CLA	MG-ND	-2.17	2.01	2.05
33	7	305	CHL	C1B-C2B	2.17	1.48	1.43
33	4	305	CHL	C1B-NB	-2.17	1.35	1.37
25	a	301	CLA	CHC-C1C	2.17	1.42	1.38
25	2	305	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	314	LUT	C1-C6	-2.17	1.50	1.53
25	B	803	CLA	CHC-C1C	2.17	1.42	1.38
25	5	310	CLA	CMB-C2B	-2.17	1.46	1.50
25	L	201	CLA	C1B-C2B	2.17	1.48	1.43
28	O	204	BCR	C1-C6	-2.17	1.50	1.53
25	9	308	CLA	CMB-C2B	-2.17	1.46	1.50
25	B	811	CLA	C1B-NB	-2.17	1.35	1.37
33	1	606	CHL	C1C-NC	-2.17	1.34	1.37
25	4	307	CLA	MG-NB	-2.17	2.01	2.05
25	9	311	CLA	MG-NB	-2.17	2.01	2.05
25	7	311	CLA	CMC-C2C	-2.17	1.46	1.50
33	P	605	CHL	CHB-C4A	-2.17	1.32	1.37
33	4	322	CHL	C4C-C3C	2.17	1.48	1.45
25	L	201	CLA	C3B-C4B	2.17	1.47	1.42
25	7	308	CLA	MG-ND	-2.17	2.01	2.05
28	L	207	BCR	C1-C6	-2.16	1.50	1.53
33	R	601	CHL	C2C-C1C	2.16	1.49	1.44
25	7	308	CLA	C1B-NB	-2.16	1.35	1.37
33	4	322	CHL	C3B-C4B	2.16	1.47	1.42
25	2	302	CLA	CMD-C2D	-2.16	1.46	1.50
25	5	302	CLA	CMC-C2C	-2.16	1.46	1.50
25	6	613	CLA	CMC-C2C	-2.16	1.46	1.50
25	A	839	CLA	C1B-C2B	2.16	1.48	1.43
33	6	617	CHL	C3B-C4B	2.16	1.47	1.42
25	4	312	CLA	CMB-C2B	-2.16	1.46	1.50
25	2	304	CLA	MG-ND	-2.16	2.01	2.05
25	2	313	CLA	CMC-C2C	-2.16	1.46	1.50
25	2	313	CLA	CMD-C2D	-2.16	1.46	1.50
25	a	310	CLA	MG-NB	-2.16	2.01	2.05
25	A	806	CLA	C3B-C4B	2.16	1.47	1.42
25	1	605	CLA	C1B-C2B	2.16	1.48	1.43
33	R	605	CHL	C1D-ND	-2.16	1.35	1.37
33	6	617	CHL	C2C-C1C	2.16	1.49	1.44
25	U	311	CLA	CMC-C2C	-2.16	1.46	1.50
25	A	826	CLA	C1B-C2B	2.16	1.48	1.43
25	B	802	CLA	C1B-C2B	2.16	1.48	1.43
25	T	612	CLA	CHC-C1C	2.16	1.42	1.38
25	B	836	CLA	MG-ND	-2.16	2.01	2.05
25	8	304	CLA	MG-ND	-2.16	2.01	2.05
33	1	601	CHL	C4B-NB	-2.16	1.35	1.37
25	8	304	CLA	C1B-C2B	2.16	1.48	1.43
25	U	303	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	303	CLA	CMD-C2D	-2.16	1.46	1.50
25	A	804	CLA	C1B-NB	-2.16	1.35	1.37
25	B	813	CLA	C3B-C4B	2.16	1.47	1.42
25	1	604	CLA	C1B-C2B	2.16	1.48	1.43
25	4	308	CLA	CMD-C2D	-2.16	1.46	1.50
25	9	303	CLA	MG-ND	-2.16	2.01	2.05
25	8	315	CLA	CMB-C2B	-2.16	1.46	1.50
25	a	311	CLA	CMB-C2B	-2.16	1.46	1.50
25	A	822	CLA	C1B-C2B	2.16	1.48	1.43
25	R	614	CLA	MG-NB	-2.15	2.01	2.05
25	B	808	CLA	C1B-NB	-2.15	1.35	1.37
25	Q	613	CLA	CMC-C2C	-2.15	1.46	1.50
25	8	306	CLA	CMC-C2C	-2.15	1.46	1.50
25	B	831	CLA	C1B-C2B	2.15	1.48	1.43
25	5	324	CLA	C1B-NB	-2.15	1.35	1.37
33	T	605	CHL	CHB-C4A	-2.15	1.32	1.37
25	B	834	CLA	MG-ND	-2.15	2.01	2.05
25	A	838	CLA	MG-ND	-2.15	2.01	2.05
25	B	819	CLA	C1B-C2B	2.15	1.48	1.43
25	6	614	CLA	C1B-C2B	2.15	1.48	1.43
25	2	307	CLA	CMD-C2D	-2.15	1.46	1.50
25	2	306	CLA	MG-NB	-2.15	2.01	2.05
30	B	848	DGD	O5D-C1E	2.15	1.43	1.40
25	9	311	CLA	CHC-C1C	2.15	1.42	1.38
25	S	304	CLA	CMD-C2D	-2.15	1.46	1.50
33	P	605	CHL	C2C-C1C	2.15	1.49	1.44
25	B	821	CLA	MG-ND	-2.15	2.01	2.05
25	5	306	CLA	MG-ND	-2.15	2.01	2.05
25	a	306	CLA	CMC-C2C	-2.15	1.46	1.50
25	6	604	CLA	CMC-C2C	-2.15	1.46	1.50
25	R	602	CLA	CMB-C2B	-2.15	1.46	1.50
25	B	835	CLA	CHC-C1C	2.15	1.42	1.38
33	5	308	CHL	C1C-NC	-2.15	1.34	1.37
25	a	312	CLA	CMD-C2D	-2.15	1.46	1.50
25	B	830	CLA	CHC-C1C	2.15	1.42	1.38
33	4	305	CHL	C2C-C1C	2.15	1.49	1.44
33	4	305	CHL	C4C-C3C	2.15	1.48	1.45
33	8	307	CHL	CHB-C4A	-2.15	1.32	1.37
25	B	829	CLA	CMC-C2C	-2.15	1.46	1.50
25	2	304	CLA	CMC-C2C	-2.15	1.46	1.50
25	B	825	CLA	C4B-NB	2.15	1.40	1.37
25	A	810	CLA	C3B-C4B	2.15	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	201	CLA	CMD-C2D	-2.15	1.46	1.50
33	U	307	CHL	C2C-C1C	2.15	1.49	1.44
25	A	816	CLA	CHC-C1C	2.14	1.42	1.38
25	A	832	CLA	MG-ND	-2.14	2.01	2.05
25	8	310	CLA	CMC-C2C	-2.14	1.46	1.50
25	J	103	CLA	C1B-C2B	2.14	1.48	1.43
25	5	316	CLA	C1B-NB	-2.14	1.35	1.37
28	3	317	BCR	C1-C6	-2.14	1.50	1.53
25	L	205	CLA	C4B-NB	2.14	1.40	1.37
25	F	802	CLA	MG-ND	-2.14	2.01	2.05
25	A	803	CLA	C3B-C4B	2.14	1.47	1.42
25	4	301	CLA	MG-ND	-2.14	2.01	2.05
33	7	305	CHL	C3B-C4B	2.14	1.47	1.42
25	B	809	CLA	MG-ND	-2.14	2.01	2.05
25	K	202	CLA	CMC-C2C	-2.14	1.46	1.50
25	A	826	CLA	C4B-NB	2.14	1.40	1.37
33	R	606	CHL	C2C-C1C	2.14	1.49	1.44
25	8	311	CLA	CMC-C2C	-2.14	1.46	1.50
35	Q	616	XAT	O24-C25	-2.14	1.43	1.46
25	4	308	CLA	MG-ND	-2.14	2.01	2.05
25	6	614	CLA	CMC-C2C	-2.14	1.46	1.50
25	2	309	CLA	CHC-C1C	2.14	1.42	1.38
33	9	306	CHL	CHB-C4A	-2.14	1.32	1.37
25	T	608	CLA	MG-NB	-2.14	2.01	2.05
25	S	303	CLA	CMC-C2C	-2.14	1.46	1.50
25	B	804	CLA	MG-ND	-2.14	2.01	2.05
25	G	202	CLA	CMC-C2C	-2.14	1.46	1.50
25	3	309	CLA	CMB-C2B	-2.14	1.46	1.50
25	6	616	CLA	CMC-C2C	-2.14	1.46	1.50
25	A	828	CLA	C3B-C4B	2.14	1.47	1.42
25	a	310	CLA	CMB-C2B	-2.14	1.46	1.50
25	6	614	CLA	MG-ND	-2.14	2.01	2.05
25	A	828	CLA	MG-ND	-2.14	2.01	2.05
33	4	322	CHL	C1B-C2B	2.14	1.48	1.43
25	A	820	CLA	C4B-NB	2.14	1.40	1.37
33	R	606	CHL	CHB-C4A	-2.14	1.32	1.37
25	7	306	CLA	MG-ND	-2.14	2.01	2.05
25	a	303	CLA	O1A-CGA	2.13	1.28	1.22
25	B	806	CLA	MG-ND	-2.13	2.01	2.05
25	3	302	CLA	MG-ND	-2.13	2.01	2.05
25	A	832	CLA	C1B-C2B	2.13	1.48	1.43
25	1	610	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	805	CLA	C1B-C2B	2.13	1.48	1.43
33	6	608	CHL	C4D-CHA	2.13	1.46	1.38
25	K	204	CLA	MG-NB	-2.13	2.01	2.05
33	1	606	CHL	C3B-C4B	2.13	1.47	1.42
25	5	310	CLA	CMD-C2D	-2.13	1.46	1.50
25	5	316	CLA	C1B-C2B	2.13	1.48	1.43
34	3	315	LUT	C22-C21	-2.13	1.52	1.54
25	5	303	CLA	C3B-C4B	2.13	1.47	1.42
25	5	319	CLA	C1B-C2B	2.13	1.48	1.43
25	A	837	CLA	MG-ND	-2.13	2.01	2.05
25	a	312	CLA	CMC-C2C	-2.13	1.46	1.50
25	A	833	CLA	C1B-NB	-2.13	1.35	1.37
25	B	838	CLA	C1B-C2B	2.13	1.48	1.43
25	B	820	CLA	C3B-C4B	2.13	1.47	1.42
28	3	317	BCR	C30-C25	-2.13	1.50	1.53
25	J	105	CLA	CMB-C2B	-2.13	1.46	1.50
25	8	302	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	828	CLA	CMC-C2C	-2.13	1.46	1.50
25	K	203	CLA	MG-ND	-2.13	2.01	2.05
33	6	608	CHL	C2C-C1C	2.13	1.49	1.44
25	A	812	CLA	MG-ND	-2.13	2.01	2.05
28	A	848	BCR	C1-C6	-2.13	1.50	1.53
33	4	306	CHL	C1B-NB	-2.13	1.35	1.37
25	B	805	CLA	CAC-C3C	-2.13	1.45	1.51
25	1	609	CLA	CAC-C3C	-2.13	1.45	1.51
33	S	321	CHL	C1C-NC	-2.13	1.34	1.37
25	A	807	CLA	CAC-C3C	-2.13	1.45	1.51
33	P	607	CHL	C2C-C1C	2.13	1.49	1.44
34	9	312	LUT	C22-C21	-2.12	1.52	1.54
25	B	831	CLA	MG-ND	-2.12	2.01	2.05
25	5	309	CLA	C1B-NB	-2.12	1.35	1.37
25	2	313	CLA	CMB-C2B	-2.12	1.46	1.50
25	9	311	CLA	CMD-C2D	-2.12	1.46	1.50
28	B	843	BCR	C1-C6	-2.12	1.50	1.53
33	S	306	CHL	MG-NA	-2.12	2.01	2.06
25	2	309	CLA	CMB-C2B	-2.12	1.46	1.50
25	A	801	CLA	C4B-NB	2.12	1.40	1.37
25	B	814	CLA	C1B-C2B	2.12	1.48	1.43
25	A	802	CLA	CAA-C2A	-2.12	1.50	1.54
25	1	614	CLA	CMC-C2C	-2.12	1.46	1.50
25	8	308	CLA	MG-ND	-2.12	2.01	2.05
33	P	619	CHL	C2C-C1C	2.12	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	9	307	CHL	C1B-NB	-2.12	1.35	1.37
25	A	842	CLA	C3B-C4B	2.12	1.47	1.42
25	P	613	CLA	MG-NB	-2.12	2.01	2.05
33	5	308	CHL	C1B-NB	-2.12	1.35	1.37
25	6	623	CLA	CMB-C2B	-2.12	1.46	1.50
25	a	309	CLA	CMB-C2B	-2.12	1.46	1.50
25	4	310	CLA	CMB-C2B	-2.12	1.46	1.50
25	A	824	CLA	C1B-C2B	2.12	1.48	1.43
25	T	602	CLA	MG-NB	-2.12	2.01	2.05
25	4	310	CLA	C1B-NB	-2.12	1.35	1.37
25	B	801	CLA	C1B-C2B	2.12	1.48	1.43
25	3	308	CLA	C1B-C2B	2.12	1.48	1.43
34	Q	615	LUT	C1-C6	-2.12	1.50	1.53
25	3	307	CLA	C1B-C2B	2.12	1.48	1.43
25	2	303	CLA	C1B-NB	-2.12	1.35	1.37
25	6	604	CLA	MG-ND	-2.12	2.01	2.05
33	6	608	CHL	C3B-C4B	2.12	1.47	1.42
33	1	601	CHL	C1B-NB	-2.12	1.35	1.37
25	7	309	CLA	C1B-C2B	2.12	1.48	1.43
25	A	831	CLA	MG-ND	-2.12	2.01	2.05
25	A	838	CLA	C1B-C2B	2.12	1.48	1.43
25	R	610	CLA	CMC-C2C	-2.12	1.46	1.50
25	S	313	CLA	CHC-C1C	2.12	1.42	1.38
25	A	834	CLA	MG-ND	-2.12	2.01	2.05
25	Q	611	CLA	CHC-C1C	2.11	1.42	1.38
25	7	303	CLA	CHC-C1C	2.11	1.42	1.38
25	B	818	CLA	MG-ND	-2.11	2.01	2.05
25	R	604	CLA	MG-NB	-2.11	2.01	2.05
25	A	853	CLA	CHC-C1C	2.11	1.42	1.38
25	3	314	CLA	C1B-C2B	2.11	1.48	1.43
25	6	601	CLA	CMB-C2B	-2.11	1.46	1.50
25	R	613	CLA	MG-NB	-2.11	2.01	2.05
25	a	302	CLA	CHC-C1C	2.11	1.42	1.38
25	A	809	CLA	C1B-C2B	2.11	1.48	1.43
25	a	312	CLA	CMB-C2B	-2.11	1.46	1.50
25	6	605	CLA	C1B-NB	-2.11	1.35	1.37
25	J	103	CLA	MG-ND	-2.11	2.01	2.05
25	8	305	CLA	C1B-C2B	2.11	1.48	1.43
25	S	315	CLA	CMD-C2D	-2.11	1.46	1.50
28	4	321	BCR	C1-C6	-2.11	1.50	1.53
25	1	614	CLA	CMB-C2B	-2.11	1.46	1.50
25	B	818	CLA	C1B-C2B	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	305	CLA	CMC-C2C	-2.11	1.46	1.50
25	6	623	CLA	CMC-C2C	-2.11	1.46	1.50
33	P	605	CHL	C1C-NC	-2.11	1.34	1.37
25	O	202	CLA	MG-ND	-2.11	2.01	2.05
25	A	838	CLA	CMC-C2C	-2.11	1.46	1.50
33	5	307	CHL	C1B-C2B	2.11	1.48	1.43
25	a	313	CLA	CMC-C2C	-2.11	1.46	1.50
25	5	302	CLA	MG-ND	-2.11	2.01	2.05
25	2	309	CLA	CMC-C2C	-2.11	1.46	1.50
25	3	320	CLA	C4B-NB	2.11	1.40	1.37
25	S	313	CLA	MG-NB	-2.11	2.01	2.05
25	8	309	CLA	CMC-C2C	-2.11	1.46	1.50
33	S	302	CHL	C4C-C3C	2.11	1.48	1.45
25	a	304	CLA	CMC-C2C	-2.11	1.46	1.50
25	A	842	CLA	MG-ND	-2.11	2.01	2.05
25	8	305	CLA	MG-ND	-2.11	2.01	2.05
25	7	308	CLA	CHC-C1C	2.11	1.42	1.38
25	Q	613	CLA	MG-NB	-2.11	2.01	2.05
25	O	201	CLA	CMD-C2D	-2.11	1.46	1.50
25	B	828	CLA	MG-ND	-2.11	2.01	2.05
25	9	310	CLA	CMC-C2C	-2.11	1.46	1.50
25	8	306	CLA	CHC-C1C	2.11	1.42	1.38
25	5	303	CLA	C1B-NB	-2.11	1.35	1.37
25	A	824	CLA	MG-ND	-2.11	2.01	2.05
25	B	833	CLA	C3B-C4B	2.11	1.47	1.42
25	9	309	CLA	CMC-C2C	-2.11	1.46	1.50
33	R	607	CHL	C2C-C1C	2.10	1.49	1.44
25	S	315	CLA	CHC-C1C	2.10	1.42	1.38
25	6	613	CLA	CHC-C1C	2.10	1.42	1.38
25	5	309	CLA	C1B-C2B	2.10	1.48	1.43
33	5	317	CHL	C1B-C2B	2.10	1.48	1.43
25	2	307	CLA	MG-ND	-2.10	2.01	2.05
25	5	316	CLA	MG-ND	-2.10	2.01	2.05
25	7	313	CLA	CMC-C2C	-2.10	1.46	1.50
33	4	306	CHL	C3B-C4B	2.10	1.47	1.42
25	B	827	CLA	C1B-NB	-2.10	1.35	1.37
25	B	832	CLA	C1B-NB	-2.10	1.35	1.37
34	4	316	LUT	C1-C6	-2.10	1.50	1.53
25	B	830	CLA	C1B-C2B	2.10	1.48	1.43
25	Q	611	CLA	CMB-C2B	-2.10	1.46	1.50
25	5	302	CLA	C3B-C4B	2.10	1.47	1.42
25	5	303	CLA	CAC-C3C	-2.10	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	302	CLA	CHC-C1C	2.10	1.42	1.38
25	B	849	CLA	C1B-C2B	2.10	1.48	1.43
25	7	306	CLA	C1B-C2B	2.10	1.48	1.43
25	B	825	CLA	C1B-NB	-2.10	1.35	1.37
33	4	314	CHL	C1B-NB	-2.10	1.35	1.37
33	5	307	CHL	C4B-NB	-2.10	1.35	1.37
33	5	308	CHL	C3B-C4B	2.10	1.47	1.42
25	a	307	CLA	CMC-C2C	-2.10	1.46	1.50
25	8	314	CLA	MG-ND	-2.10	2.01	2.05
25	9	303	CLA	C1B-NB	-2.10	1.35	1.37
25	1	613	CLA	CMC-C2C	-2.10	1.46	1.50
25	1	608	CLA	MG-ND	-2.10	2.01	2.05
25	S	312	CLA	CMD-C2D	-2.10	1.46	1.50
25	A	805	CLA	CHC-C1C	2.10	1.42	1.38
28	A	847	BCR	C21-C22	-2.10	1.33	1.35
25	K	201	CLA	C1B-NB	-2.10	1.35	1.37
25	2	302	CLA	C1B-C2B	2.09	1.48	1.43
25	K	202	CLA	MG-ND	-2.09	2.01	2.05
28	L	208	BCR	C30-C25	-2.09	1.50	1.53
33	S	309	CHL	CHB-C4A	-2.09	1.32	1.37
25	6	613	CLA	MG-NB	-2.09	2.01	2.05
25	5	303	CLA	C1B-C2B	2.09	1.48	1.43
25	B	830	CLA	C1B-NB	-2.09	1.35	1.37
25	4	301	CLA	CHC-C1C	2.09	1.42	1.38
34	6	622	LUT	C22-C21	-2.09	1.52	1.54
25	Q	610	CLA	CMB-C2B	-2.09	1.46	1.50
25	S	320	CLA	CMD-C2D	-2.09	1.46	1.50
28	3	319	BCR	C30-C25	-2.09	1.50	1.53
25	B	813	CLA	C1B-C2B	2.09	1.48	1.43
33	3	306	CHL	C4D-CHA	2.09	1.45	1.38
25	A	827	CLA	CHC-C1C	2.09	1.42	1.38
25	T	608	CLA	CMB-C2B	-2.09	1.46	1.50
33	T	601	CHL	C2C-C1C	2.09	1.49	1.44
25	1	603	CLA	MG-ND	-2.09	2.01	2.05
25	5	314	CLA	CMC-C2C	-2.09	1.46	1.50
33	U	306	CHL	CHB-C4A	-2.09	1.32	1.37
25	A	811	CLA	C1B-C2B	2.09	1.48	1.43
25	A	813	CLA	C1B-C2B	2.09	1.48	1.43
25	3	311	CLA	C1B-NB	-2.09	1.35	1.37
25	A	810	CLA	C1B-NB	-2.09	1.35	1.37
25	S	304	CLA	MG-NB	-2.09	2.01	2.05
25	T	603	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	315	CLA	CMB-C2B	-2.08	1.46	1.50
25	B	838	CLA	MG-ND	-2.08	2.01	2.05
25	P	613	CLA	CHC-C1C	2.08	1.42	1.38
28	6	621	BCR	C30-C25	-2.08	1.50	1.53
33	P	606	CHL	CHB-C4A	-2.08	1.32	1.37
25	K	204	CLA	CMB-C2B	-2.08	1.46	1.50
25	J	105	CLA	CMC-C2C	-2.08	1.46	1.50
25	2	302	CLA	MG-ND	-2.08	2.01	2.05
35	P	623	XAT	C22-C21	-2.08	1.51	1.54
25	A	837	CLA	C1B-C2B	2.08	1.48	1.43
25	Q	618	CLA	C3D-C4D	2.08	1.48	1.44
25	H	203	CLA	MG-ND	-2.08	2.01	2.05
25	4	303	CLA	MG-ND	-2.08	2.01	2.05
25	8	302	CLA	MG-ND	-2.08	2.01	2.05
25	4	309	CLA	CMB-C2B	-2.08	1.46	1.50
25	7	309	CLA	C1B-NB	-2.08	1.35	1.37
33	6	607	CHL	C1B-NB	-2.08	1.35	1.37
25	2	311	CLA	MG-ND	-2.08	2.01	2.05
28	O	205	BCR	C1-C6	-2.08	1.50	1.53
25	a	307	CLA	CHC-C1C	2.08	1.42	1.38
25	P	603	CLA	MG-NB	-2.08	2.01	2.05
25	5	319	CLA	MG-ND	-2.08	2.01	2.05
25	S	303	CLA	CMB-C2B	-2.08	1.46	1.50
25	T	610	CLA	CMC-C2C	-2.08	1.46	1.50
25	J	105	CLA	MG-ND	-2.08	2.01	2.05
25	8	313	CLA	MG-ND	-2.08	2.01	2.05
25	L	206	CLA	C1B-NB	-2.08	1.35	1.37
25	Q	611	CLA	CMC-C2C	-2.08	1.46	1.50
25	B	816	CLA	MG-ND	-2.08	2.01	2.05
25	B	836	CLA	C1B-NB	-2.08	1.35	1.37
25	A	815	CLA	MG-ND	-2.08	2.01	2.05
25	5	310	CLA	MG-ND	-2.08	2.01	2.05
33	1	601	CHL	C3B-C4B	2.08	1.47	1.42
25	S	301	CLA	CMD-C2D	-2.07	1.46	1.50
25	5	310	CLA	C1B-NB	-2.07	1.35	1.37
25	B	801	CLA	MG-ND	-2.07	2.01	2.05
25	O	202	CLA	CHC-C1C	2.07	1.42	1.38
25	A	826	CLA	C1B-NB	-2.07	1.35	1.37
25	4	313	CLA	CMB-C2B	-2.07	1.46	1.50
25	8	314	CLA	CMC-C2C	-2.07	1.46	1.50
25	R	613	CLA	CHC-C1C	2.07	1.42	1.38
25	8	305	CLA	C1B-NB	-2.07	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	610	CLA	C1B-C2B	2.07	1.48	1.43
25	2	314	CLA	MG-ND	-2.07	2.01	2.05
33	R	606	CHL	C1C-NC	-2.07	1.34	1.37
25	4	307	CLA	CMC-C2C	-2.07	1.46	1.50
25	a	308	CLA	CHC-C1C	2.07	1.42	1.38
33	S	321	CHL	C2C-C1C	2.07	1.49	1.44
25	6	601	CLA	MG-ND	-2.07	2.01	2.05
25	U	313	CLA	C3B-C4B	2.07	1.47	1.42
33	6	607	CHL	C4C-C3C	2.07	1.48	1.45
25	O	201	CLA	CMC-C2C	-2.07	1.46	1.50
25	4	302	CLA	CMC-C2C	-2.07	1.46	1.50
25	A	801	CLA	C1B-NB	-2.07	1.35	1.37
25	5	302	CLA	C1B-NB	-2.07	1.35	1.37
25	3	309	CLA	CMC-C2C	-2.07	1.46	1.50
25	a	303	CLA	CHC-C1C	2.07	1.42	1.38
25	B	809	CLA	C1B-NB	-2.07	1.35	1.37
25	2	306	CLA	C1B-NB	-2.07	1.35	1.37
33	9	307	CHL	CHB-C4A	-2.07	1.32	1.37
25	8	303	CLA	CAC-C3C	-2.07	1.45	1.51
25	1	609	CLA	C1A-CHA	-2.07	1.34	1.43
25	P	613	CLA	CMB-C2B	-2.07	1.46	1.50
25	U	312	CLA	MG-NB	-2.07	2.01	2.05
25	6	605	CLA	C1B-C2B	2.07	1.48	1.43
25	U	304	CLA	MG-NB	-2.07	2.01	2.05
25	Q	609	CLA	MG-NB	-2.07	2.01	2.05
25	9	304	CLA	CMC-C2C	-2.07	1.46	1.50
25	K	204	CLA	MG-ND	-2.07	2.01	2.05
25	7	312	CLA	MG-ND	-2.07	2.01	2.05
25	7	309	CLA	CHC-C1C	2.07	1.42	1.38
33	1	606	CHL	C4B-NB	-2.07	1.35	1.37
25	U	303	CLA	MG-NB	-2.07	2.01	2.05
25	S	304	CLA	CMB-C2B	-2.07	1.46	1.50
25	1	602	CLA	MG-ND	-2.06	2.01	2.05
25	K	205	CLA	CMC-C2C	-2.06	1.46	1.50
25	P	603	CLA	CMD-C2D	-2.06	1.46	1.50
25	T	611	CLA	CMB-C2B	-2.06	1.46	1.50
25	3	320	CLA	C1B-C2B	2.06	1.48	1.43
25	K	205	CLA	CMD-C2D	-2.06	1.46	1.50
25	B	811	CLA	C3B-C4B	2.06	1.47	1.42
25	K	202	CLA	C1B-NB	-2.06	1.35	1.37
25	5	310	CLA	C4B-NB	2.06	1.40	1.37
25	R	604	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	807	CLA	MG-ND	-2.06	2.01	2.05
25	9	302	CLA	CMD-C2D	-2.06	1.46	1.50
25	B	815	CLA	C3B-C4B	2.06	1.47	1.42
25	8	303	CLA	C1B-C2B	2.06	1.48	1.43
33	5	308	CHL	C1B-C2B	2.06	1.48	1.43
25	U	311	CLA	CHC-C1C	2.06	1.42	1.38
25	B	835	CLA	MG-ND	-2.06	2.01	2.05
25	8	315	CLA	MG-ND	-2.06	2.01	2.05
25	6	615	CLA	C1B-C2B	2.06	1.48	1.43
33	a	305	CHL	C2C-C1C	2.06	1.49	1.44
33	5	307	CHL	C3D-C4D	-2.06	1.39	1.44
33	9	306	CHL	C2C-C1C	2.06	1.49	1.44
25	S	304	CLA	CHC-C1C	2.06	1.42	1.38
25	8	311	CLA	C1B-NB	-2.06	1.35	1.37
25	B	821	CLA	CHC-C1C	2.06	1.42	1.38
33	S	308	CHL	CHB-C4A	-2.06	1.32	1.37
25	3	309	CLA	MG-ND	-2.06	2.01	2.05
33	7	305	CHL	C4C-C3C	2.06	1.48	1.45
25	P	604	CLA	MG-NB	-2.06	2.01	2.05
33	6	608	CHL	C1B-C2B	2.06	1.48	1.43
25	3	313	CLA	C1B-NB	-2.06	1.35	1.37
25	a	306	CLA	CHC-C1C	2.06	1.42	1.38
25	A	816	CLA	C1B-C2B	2.06	1.48	1.43
33	Q	608	CHL	O1D-CGD	2.06	1.26	1.21
25	U	313	CLA	CMD-C2D	-2.05	1.46	1.50
25	6	609	CLA	C1B-NB	-2.05	1.35	1.37
33	4	322	CHL	C4B-NB	-2.05	1.35	1.37
25	S	314	CLA	CHC-C1C	2.05	1.42	1.38
25	6	615	CLA	CHC-C1C	2.05	1.42	1.38
25	1	604	CLA	C1B-NB	-2.05	1.35	1.37
25	A	802	CLA	MG-ND	-2.05	2.01	2.05
33	5	307	CHL	C4C-C3C	2.05	1.48	1.45
25	8	312	CLA	C1B-NB	-2.05	1.35	1.37
25	A	831	CLA	C1B-C2B	2.05	1.48	1.43
25	A	808	CLA	CHC-C1C	2.05	1.42	1.38
33	5	317	CHL	C2C-C1C	2.05	1.49	1.44
25	P	604	CLA	CMB-C2B	-2.05	1.46	1.50
25	K	203	CLA	CHC-C1C	2.05	1.42	1.38
33	5	307	CHL	C3B-C4B	2.05	1.47	1.42
25	U	310	CLA	MG-NB	-2.05	2.01	2.05
25	A	829	CLA	C1B-C2B	2.05	1.48	1.43
28	5	323	BCR	C1-C6	-2.05	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Q	607	CHL	C1C-NC	-2.05	1.34	1.37
25	Q	603	CLA	CMD-C2D	-2.05	1.46	1.50
25	Q	602	CLA	MG-NB	-2.05	2.01	2.05
33	T	605	CHL	C1C-NC	-2.05	1.34	1.37
25	R	610	CLA	CMB-C2B	-2.05	1.46	1.50
33	4	305	CHL	CHB-C4A	-2.05	1.32	1.37
25	5	306	CLA	CMC-C2C	-2.05	1.46	1.50
25	G	202	CLA	CHC-C1C	2.04	1.42	1.38
33	a	305	CHL	C4C-C3C	2.04	1.48	1.45
33	5	317	CHL	C3B-C4B	2.04	1.47	1.42
25	Q	618	CLA	CMB-C2B	-2.04	1.46	1.50
33	9	306	CHL	C3D-C4D	-2.04	1.39	1.44
25	A	809	CLA	CHC-C1C	2.04	1.42	1.38
25	K	203	CLA	CMC-C2C	-2.04	1.46	1.50
25	3	307	CLA	C1B-NB	-2.04	1.35	1.37
25	a	310	CLA	CMC-C2C	-2.04	1.46	1.50
25	B	804	CLA	C1B-C2B	2.04	1.48	1.43
25	T	603	CLA	CMB-C2B	-2.04	1.46	1.50
25	a	313	CLA	CMB-C2B	-2.04	1.46	1.50
25	A	806	CLA	C4B-NB	2.04	1.40	1.37
25	7	304	CLA	C1B-NB	-2.04	1.35	1.37
33	8	307	CHL	C1B-NB	-2.04	1.35	1.37
25	4	303	CLA	CHC-C1C	2.04	1.42	1.38
25	P	604	CLA	CHC-C1C	2.04	1.42	1.38
25	L	209	CLA	CMC-C2C	-2.04	1.46	1.50
34	9	312	LUT	C1-C6	-2.04	1.51	1.53
25	A	823	CLA	C1B-C2B	2.04	1.48	1.43
25	K	204	CLA	CHC-C1C	2.04	1.42	1.38
25	1	603	CLA	C1B-NB	-2.04	1.35	1.37
25	5	324	CLA	CHC-C1C	2.04	1.42	1.38
25	a	308	CLA	CMB-C2B	-2.04	1.46	1.50
33	9	307	CHL	C4C-C3C	2.04	1.48	1.45
25	5	314	CLA	MG-ND	-2.03	2.01	2.05
25	4	311	CLA	CMB-C2B	-2.03	1.46	1.50
25	a	306	CLA	CMB-C2B	-2.03	1.46	1.50
33	R	605	CHL	CMC-C2C	2.03	1.49	1.45
34	4	316	LUT	C22-C21	-2.03	1.52	1.54
25	1	611	CLA	CHC-C1C	2.03	1.42	1.38
25	6	604	CLA	C1B-NB	-2.03	1.35	1.37
33	U	309	CHL	C1C-NC	-2.03	1.34	1.37
25	9	301	CLA	MG-ND	-2.03	2.01	2.05
33	1	601	CHL	C1B-C2B	2.03	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	7	305	CHL	C2C-C1C	2.03	1.48	1.44
25	T	610	CLA	CMB-C2B	-2.03	1.46	1.50
28	O	204	BCR	C30-C25	-2.03	1.51	1.53
25	a	303	CLA	CMC-C2C	-2.03	1.46	1.50
25	R	602	CLA	MG-NB	-2.03	2.01	2.05
25	R	614	CLA	CHC-C1C	2.03	1.42	1.38
33	1	606	CHL	C4C-C3C	2.03	1.48	1.45
34	7	315	LUT	C22-C21	-2.03	1.52	1.54
25	Q	602	CLA	CMD-C2D	-2.03	1.46	1.50
25	3	305	CLA	MG-ND	-2.03	2.01	2.05
25	P	604	CLA	CMD-C2D	-2.03	1.46	1.50
25	4	303	CLA	CMC-C2C	-2.03	1.46	1.50
33	P	607	CHL	C1C-NC	-2.03	1.34	1.37
25	B	838	CLA	C1B-NB	-2.03	1.35	1.37
25	3	304	CLA	MG-ND	-2.03	2.01	2.05
25	3	310	CLA	MG-ND	-2.03	2.01	2.05
25	3	302	CLA	CHC-C1C	2.03	1.42	1.38
28	5	320	BCR	C1-C6	-2.03	1.51	1.53
25	B	834	CLA	C1B-C2B	2.03	1.48	1.43
25	P	610	CLA	CMD-C2D	-2.03	1.46	1.50
32	4	320	LMG	O1-C1	2.03	1.43	1.40
25	B	838	CLA	CHC-C1C	2.03	1.42	1.38
33	S	321	CHL	CHB-C4A	-2.03	1.32	1.37
33	4	314	CHL	C1C-NC	-2.03	1.34	1.37
25	7	311	CLA	MG-ND	-2.03	2.01	2.05
25	B	835	CLA	C1B-C2B	2.03	1.48	1.43
25	U	302	CLA	MG-NB	-2.03	2.01	2.05
25	Q	612	CLA	CMC-C2C	-2.03	1.46	1.50
25	T	602	CLA	CMD-C2D	-2.03	1.46	1.50
25	3	320	CLA	CAC-C3C	-2.03	1.45	1.51
25	P	610	CLA	CMB-C2B	-2.03	1.46	1.50
25	O	201	CLA	CHC-C1C	2.03	1.42	1.38
33	R	609	CHL	O1D-CGD	2.03	1.26	1.21
33	P	609	CHL	O1D-CGD	2.03	1.26	1.21
25	B	829	CLA	C1B-NB	-2.03	1.35	1.37
25	S	301	CLA	CMB-C2B	-2.02	1.46	1.50
25	1	609	CLA	MG-NB	-2.02	2.01	2.05
33	S	302	CHL	C1C-NC	-2.02	1.34	1.37
25	1	604	CLA	CHC-C1C	2.02	1.42	1.38
25	S	315	CLA	MG-ND	-2.02	2.01	2.05
25	7	312	CLA	CHC-C1C	2.02	1.42	1.38
25	A	806	CLA	C1B-C2B	2.02	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	604	CLA	CMC-C2C	-2.02	1.46	1.50
25	6	611	CLA	CMC-C2C	-2.02	1.46	1.50
25	a	304	CLA	CHC-C1C	2.02	1.42	1.38
33	5	308	CHL	C3A-C2A	-2.02	1.48	1.54
25	2	303	CLA	MG-ND	-2.02	2.01	2.05
25	4	310	CLA	MG-ND	-2.02	2.01	2.05
25	F	802	CLA	CHC-C1C	2.02	1.42	1.38
25	B	830	CLA	MG-ND	-2.02	2.01	2.05
25	6	615	CLA	MG-ND	-2.02	2.01	2.05
25	1	609	CLA	C4B-NB	2.02	1.40	1.37
25	5	306	CLA	C1B-NB	-2.02	1.35	1.37
25	7	311	CLA	C1B-NB	-2.02	1.35	1.37
25	Q	604	CLA	CMD-C2D	-2.02	1.46	1.50
25	A	802	CLA	CHC-C1C	2.02	1.42	1.38
33	P	608	CHL	C1C-NC	-2.02	1.34	1.37
25	B	833	CLA	C4B-NB	2.02	1.40	1.37
25	U	302	CLA	CMD-C2D	-2.02	1.46	1.50
25	9	302	CLA	CMB-C2B	-2.02	1.46	1.50
25	9	301	CLA	C1B-C2B	2.02	1.48	1.43
28	A	845	BCR	C1-C6	-2.02	1.51	1.53
25	R	604	CLA	C3C-C2C	2.02	1.41	1.36
33	1	606	CHL	C1B-NB	-2.02	1.35	1.37
33	P	619	CHL	C1C-NC	-2.02	1.34	1.37
25	U	304	CLA	CHC-C1C	2.02	1.42	1.38
25	S	305	CLA	CMD-C2D	-2.02	1.46	1.50
25	S	311	CLA	CMB-C2B	-2.02	1.46	1.50
25	B	823	CLA	C1B-C2B	2.02	1.48	1.43
25	Q	609	CLA	CMB-C2B	-2.02	1.46	1.50
25	S	313	CLA	CMD-C2D	-2.02	1.46	1.50
25	A	851	CLA	C1B-NB	-2.02	1.35	1.37
25	T	609	CLA	CMB-C2B	-2.02	1.46	1.50
25	S	305	CLA	CHC-C1C	2.02	1.42	1.38
33	R	607	CHL	C1C-NC	-2.02	1.34	1.37
25	1	611	CLA	MG-ND	-2.02	2.01	2.05
25	3	309	CLA	CHC-C1C	2.02	1.42	1.38
33	5	317	CHL	C4B-NB	-2.02	1.35	1.37
25	S	311	CLA	CMD-C2D	-2.02	1.46	1.50
25	8	309	CLA	CHC-C1C	2.01	1.42	1.38
25	A	812	CLA	C1B-NB	-2.01	1.35	1.37
25	S	320	CLA	MG-NB	-2.01	2.01	2.05
32	7	319	LMG	O1-C1	2.01	1.43	1.40
25	H	201	CLA	MG-ND	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	604	CLA	CMC-C2C	-2.01	1.46	1.50
30	B	846	DGD	O2G-C2G	-2.01	1.41	1.46
25	2	310	CLA	MG-ND	-2.01	2.01	2.05
25	5	319	CLA	CHC-C1C	2.01	1.42	1.38
25	T	610	CLA	MG-NB	-2.01	2.01	2.05
25	S	312	CLA	CMB-C2B	-2.01	1.46	1.50
25	S	314	CLA	CMC-C2C	-2.01	1.46	1.50
25	G	201	CLA	MG-ND	-2.01	2.01	2.05
25	a	312	CLA	CHC-C1C	2.01	1.42	1.38
34	5	318	LUT	C22-C21	-2.01	1.52	1.54
34	a	314	LUT	C22-C21	-2.01	1.52	1.54
25	P	611	CLA	MG-NB	-2.01	2.01	2.05
25	T	611	CLA	MG-NB	-2.01	2.01	2.05
27	A	844	LHG	O7-C5	-2.01	1.41	1.46
25	5	310	CLA	CAC-C3C	-2.01	1.46	1.51
33	6	617	CHL	C1B-NB	-2.01	1.35	1.37
25	B	816	CLA	CAC-C3C	-2.01	1.46	1.51
28	8	318	BCR	C30-C25	-2.01	1.51	1.53
25	B	828	CLA	C1B-NB	-2.01	1.35	1.37
25	A	836	CLA	MG-ND	-2.01	2.01	2.05
25	A	836	CLA	C1B-C2B	2.01	1.48	1.43
25	B	824	CLA	C1B-C2B	2.01	1.48	1.43
25	8	314	CLA	CHC-C1C	2.01	1.42	1.38
25	K	203	CLA	C1B-NB	-2.01	1.35	1.37
25	5	313	CLA	C1B-NB	-2.01	1.35	1.37
25	1	612	CLA	C3D-C4D	2.01	1.48	1.44
25	H	205	CLA	C1B-NB	-2.01	1.35	1.37
25	U	303	CLA	CMD-C2D	-2.01	1.46	1.50
25	A	811	CLA	MG-ND	-2.01	2.01	2.05
33	7	305	CHL	C3D-C4D	-2.01	1.39	1.44
25	7	308	CLA	C1B-C2B	2.01	1.48	1.43
25	6	609	CLA	CMC-C2C	-2.01	1.46	1.50
25	K	202	CLA	CHC-C1C	2.01	1.42	1.38
34	7	314	LUT	C22-C21	-2.00	1.52	1.54
25	A	814	CLA	CAA-C2A	-2.00	1.50	1.54
25	U	302	CLA	CMB-C2B	-2.00	1.46	1.50
25	A	820	CLA	C1B-C2B	2.00	1.48	1.43
25	4	313	CLA	CMC-C2C	-2.00	1.46	1.50
25	a	309	CLA	CMC-C2C	-2.00	1.46	1.50
25	U	304	CLA	C3C-C2C	2.00	1.41	1.36
35	S	318	XAT	O24-C25	-2.00	1.43	1.46
25	U	312	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	608	CLA	CMD-C2D	-2.00	1.46	1.50
25	8	308	CLA	CAC-C3C	-2.00	1.46	1.51
25	Q	604	CLA	MG-NB	-2.00	2.01	2.05

All (5047) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	303	CLA	C1-C2-C3	16.98	155.41	126.04
25	1	612	CLA	C4A-NA-C1A	13.26	112.67	106.71
36	P	621	NEX	C16-C1-C6	12.24	121.42	110.47
25	a	303	CLA	C4-C3-C5	-10.98	96.79	115.27
33	S	306	CHL	C2B-C1B-NB	10.73	117.43	110.23
33	P	605	CHL	C2B-C1B-NB	10.49	117.26	110.23
33	R	605	CHL	C2B-C1B-NB	10.45	117.24	110.23
33	R	609	CHL	C4A-NA-C1A	10.42	111.39	106.71
33	T	606	CHL	C2B-C1B-NB	10.38	117.19	110.23
33	Q	608	CHL	C4A-NA-C1A	10.38	111.37	106.71
33	6	617	CHL	C2B-C1B-NB	10.37	117.19	110.23
25	a	303	CLA	O2A-C1-C2	10.37	135.89	108.64
33	Q	605	CHL	C2B-C1B-NB	10.36	117.18	110.23
33	P	609	CHL	C4A-NA-C1A	10.35	111.36	106.71
33	U	305	CHL	C2B-C1B-NB	10.33	117.16	110.23
33	4	322	CHL	C2B-C1B-NB	10.29	117.13	110.23
33	T	604	CHL	C2B-C1B-NB	10.25	117.10	110.23
33	1	601	CHL	C2B-C1B-NB	10.16	117.04	110.23
33	U	306	CHL	C2B-C1B-NB	10.13	117.02	110.23
33	5	317	CHL	C2B-C1B-NB	10.10	117.00	110.23
33	Q	607	CHL	C2B-C1B-NB	10.09	117.00	110.23
33	P	608	CHL	C2B-C1B-NB	10.09	117.00	110.23
33	U	308	CHL	C2B-C1B-NB	10.08	116.99	110.23
33	S	309	CHL	C2B-C1B-NB	10.08	116.99	110.23
33	R	608	CHL	C2B-C1B-NB	10.05	116.97	110.23
33	4	314	CHL	C2B-C1B-NB	10.02	116.95	110.23
33	Q	606	CHL	C2B-C1B-NB	10.01	116.94	110.23
33	S	308	CHL	C2B-C1B-NB	9.97	116.92	110.23
33	4	306	CHL	C2B-C1B-NB	9.93	116.89	110.23
33	P	606	CHL	C2B-C1B-NB	9.91	116.87	110.23
33	T	605	CHL	C2B-C1B-NB	9.87	116.85	110.23
33	S	302	CHL	C2B-C1B-NB	9.77	116.78	110.23
33	6	607	CHL	C2B-C1B-NB	9.76	116.78	110.23
33	3	306	CHL	C2B-C1B-NB	9.71	116.74	110.23
33	R	606	CHL	C2B-C1B-NB	9.69	116.73	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	323	BCR	C16-C17-C18	-9.68	113.50	127.31
33	P	619	CHL	C2B-C1B-NB	9.63	116.69	110.23
33	S	321	CHL	C2B-C1B-NB	9.63	116.69	110.23
33	5	308	CHL	C2B-C1B-NB	9.63	116.69	110.23
33	R	607	CHL	C2B-C1B-NB	9.62	116.68	110.23
33	7	305	CHL	C2B-C1B-NB	9.59	116.66	110.23
33	P	607	CHL	C2B-C1B-NB	9.58	116.66	110.23
33	U	307	CHL	C2B-C1B-NB	9.58	116.65	110.23
25	a	303	CLA	C4-C3-C2	9.52	148.10	123.68
33	9	306	CHL	C2B-C1B-NB	9.33	116.49	110.23
33	6	606	CHL	C2B-C1B-NB	9.33	116.48	110.23
33	6	608	CHL	C2B-C1B-NB	9.32	116.48	110.23
33	8	307	CHL	C2B-C1B-NB	9.19	116.39	110.23
33	S	310	CHL	C2B-C1B-NB	9.16	116.37	110.23
33	S	307	CHL	C2B-C1B-NB	9.05	116.30	110.23
36	R	617	NEX	O24-C25-C24	9.03	120.16	113.38
33	4	304	CHL	C2B-C1B-NB	9.02	116.28	110.23
33	5	307	CHL	C2B-C1B-NB	9.01	116.27	110.23
33	9	307	CHL	C2B-C1B-NB	8.86	116.17	110.23
35	S	318	XAT	O24-C25-C24	8.82	120.00	113.38
33	4	305	CHL	C2B-C1B-NB	8.78	116.12	110.23
25	P	612	CLA	C4A-NA-C1A	8.76	110.64	106.71
36	U	301	NEX	O24-C25-C24	8.71	119.92	113.38
25	a	311	CLA	C4A-NA-C1A	8.71	110.62	106.71
33	a	305	CHL	C2B-C1B-NB	8.58	115.98	110.23
35	P	623	XAT	O4-C5-C4	8.52	119.78	113.38
25	R	612	CLA	C4A-NA-C1A	8.51	110.53	106.71
33	6	608	CHL	C4D-CHA-C1A	-8.50	110.90	121.25
33	8	307	CHL	C4D-CHA-C1A	-8.48	110.92	121.25
33	T	601	CHL	C2B-C1B-NB	8.38	115.85	110.23
33	1	606	CHL	C2B-C1B-NB	8.38	115.85	110.23
33	T	607	CHL	C2B-C1B-NB	8.35	115.83	110.23
33	U	309	CHL	C2B-C1B-NB	8.35	115.83	110.23
33	Q	601	CHL	C2B-C1B-NB	8.35	115.83	110.23
33	P	601	CHL	C2B-C1B-NB	8.34	115.83	110.23
36	T	616	NEX	O24-C25-C24	8.32	119.63	113.38
35	Q	616	XAT	O4-C5-C4	8.29	119.61	113.38
33	P	605	CHL	C4D-CHA-C1A	-8.29	111.16	121.25
35	T	615	XAT	O4-C5-C4	8.27	119.59	113.38
33	R	601	CHL	C2B-C1B-NB	8.25	115.76	110.23
25	B	807	CLA	C4A-NA-C1A	8.19	110.39	106.71
33	P	622	CHL	C2C-C3C-C4C	-8.18	100.66	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	8	307	CHL	O2D-CGD-CBD	8.15	125.75	111.27
33	S	309	CHL	C4D-CHA-C1A	-8.12	111.37	121.25
33	5	308	CHL	C4D-CHA-C1A	-8.12	111.37	121.25
33	S	302	CHL	C2C-C3C-C4C	-8.10	100.72	106.49
36	P	617	NEX	O24-C25-C24	8.09	119.46	113.38
35	P	616	XAT	O24-C25-C24	8.01	119.40	113.38
33	Q	605	CHL	C4D-CHA-C1A	-7.98	111.53	121.25
33	5	307	CHL	CMD-C2D-C1D	7.98	138.78	124.71
33	6	607	CHL	C2C-C3C-C4C	-7.98	100.80	106.49
28	5	323	BCR	C11-C10-C9	-7.97	115.94	127.31
35	P	620	XAT	O4-C5-C4	7.97	119.37	113.38
33	4	322	CHL	C2C-C3C-C4C	-7.96	100.82	106.49
35	P	623	XAT	O24-C25-C24	7.96	119.36	113.38
28	4	321	BCR	C7-C8-C9	-7.95	114.22	126.23
28	B	840	BCR	C7-C8-C9	-7.95	114.22	126.23
33	R	605	CHL	C4D-CHA-C1A	-7.94	111.59	121.25
33	S	302	CHL	C4D-CHA-C1A	-7.92	111.61	121.25
33	9	306	CHL	CMD-C2D-C1D	7.88	138.61	124.71
25	a	308	CLA	C4A-NA-C1A	7.87	110.24	106.71
35	T	615	XAT	O24-C25-C24	7.82	119.25	113.38
33	6	608	CHL	C2C-C3C-C4C	-7.81	100.92	106.49
36	U	316	NEX	O24-C25-C24	7.81	119.25	113.38
33	3	306	CHL	CMD-C2D-C1D	7.81	138.47	124.71
33	T	604	CHL	C4D-CHA-C1A	-7.79	111.77	121.25
33	3	306	CHL	C4D-CHA-C1A	-7.78	111.78	121.25
35	P	616	XAT	O4-C5-C4	7.77	119.22	113.38
33	P	619	CHL	C4D-CHA-C1A	-7.74	111.82	121.25
28	5	323	BCR	C7-C8-C9	-7.74	114.53	126.23
33	P	607	CHL	C4D-CHA-C1A	-7.74	111.83	121.25
25	B	837	CLA	C4A-NA-C1A	7.74	110.18	106.71
33	R	607	CHL	C4D-CHA-C1A	-7.72	111.85	121.25
25	A	834	CLA	C4A-NA-C1A	7.72	110.18	106.71
33	U	305	CHL	C4D-CHA-C1A	-7.69	111.89	121.25
25	4	311	CLA	C4A-NA-C1A	7.68	110.16	106.71
33	6	608	CHL	CMD-C2D-C1D	7.68	138.25	124.71
33	9	307	CHL	C4D-CHA-C1A	-7.66	111.92	121.25
25	A	842	CLA	C4A-NA-C1A	7.64	110.14	106.71
33	T	607	CHL	C4D-CHA-C1A	-7.63	111.96	121.25
33	7	305	CHL	CMD-C2D-C1D	7.63	138.16	124.71
33	6	606	CHL	C4D-CHA-C1A	-7.62	111.97	121.25
25	8	308	CLA	C4A-NA-C1A	7.59	110.12	106.71
25	1	609	CLA	C4A-NA-C1A	7.58	110.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Q	606	CHL	C4D-CHA-C1A	-7.58	112.02	121.25
33	1	601	CHL	C2C-C3C-C4C	-7.58	101.09	106.49
33	S	307	CHL	C4D-CHA-C1A	-7.58	112.03	121.25
33	S	308	CHL	C4D-CHA-C1A	-7.58	112.03	121.25
33	S	310	CHL	C4D-CHA-C1A	-7.54	112.08	121.25
33	4	306	CHL	C4D-CHA-C1A	-7.53	112.09	121.25
33	8	307	CHL	CMD-C2D-C1D	7.52	137.97	124.71
33	R	605	CHL	CMD-C2D-C1D	7.51	137.96	124.71
33	6	617	CHL	C4D-CHA-C1A	-7.51	112.11	121.25
25	B	803	CLA	C4A-NA-C1A	7.50	110.08	106.71
33	S	309	CHL	CMD-C2D-C1D	7.49	137.92	124.71
33	P	619	CHL	CMD-C2D-C1D	7.49	137.91	124.71
33	7	305	CHL	C4D-CHA-C1A	-7.49	112.14	121.25
33	T	606	CHL	C4D-CHA-C1A	-7.48	112.14	121.25
33	S	321	CHL	CMD-C2D-C1D	7.47	137.88	124.71
33	R	607	CHL	CMD-C2D-C1D	7.47	137.88	124.71
25	Q	604	CLA	C4A-NA-C1A	7.47	110.06	106.71
33	P	607	CHL	CMD-C2D-C1D	7.47	137.87	124.71
35	P	620	XAT	O24-C25-C24	7.46	118.99	113.38
33	Q	605	CHL	CMD-C2D-C1D	7.44	137.82	124.71
33	U	307	CHL	CMD-C2D-C1D	7.41	137.78	124.71
33	9	307	CHL	C2C-C3C-C4C	-7.41	101.21	106.49
33	T	601	CHL	C4D-CHA-C1A	-7.41	112.24	121.25
33	P	606	CHL	CMD-C2D-C1D	7.40	137.76	124.71
28	J	106	BCR	C20-C21-C22	-7.40	116.75	127.31
33	S	307	CHL	CMD-C2D-C1D	7.40	137.76	124.71
33	T	607	CHL	CMD-C2D-C1D	7.40	137.75	124.71
28	K	206	BCR	C16-C17-C18	-7.38	116.77	127.31
33	S	308	CHL	CMD-C2D-C1D	7.38	137.72	124.71
33	P	622	CHL	C4D-CHA-C1A	-7.38	112.27	121.25
33	4	305	CHL	C4D-CHA-C1A	-7.38	112.27	121.25
33	P	622	CHL	C2B-C1B-NB	7.37	115.18	110.23
33	4	322	CHL	C4D-CHA-C1A	-7.37	112.27	121.25
33	U	307	CHL	C4D-CHA-C1A	-7.37	112.28	121.25
25	7	311	CLA	C4A-NA-C1A	7.36	110.02	106.71
25	6	613	CLA	C4A-NA-C1A	7.35	110.01	106.71
25	Q	603	CLA	C4A-NA-C1A	7.35	110.01	106.71
33	6	617	CHL	CMD-C2D-C1D	7.35	137.66	124.71
25	B	820	CLA	C4A-NA-C1A	7.35	110.01	106.71
33	4	305	CHL	CMD-C2D-C1D	7.35	137.66	124.71
33	P	606	CHL	C4D-CHA-C1A	-7.34	112.32	121.25
33	5	307	CHL	C2C-C3C-C4C	-7.34	101.26	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	811	CLA	C4A-NA-C1A	7.33	110.00	106.71
33	U	306	CHL	CMD-C2D-C1D	7.33	137.63	124.71
33	Q	601	CHL	C4D-CHA-C1A	-7.32	112.33	121.25
33	Q	607	CHL	C4D-CHA-C1A	-7.32	112.34	121.25
33	P	608	CHL	C4D-CHA-C1A	-7.32	112.34	121.25
33	P	608	CHL	CMD-C2D-C1D	7.32	137.60	124.71
33	Q	607	CHL	CMD-C2D-C1D	7.31	137.60	124.71
33	R	608	CHL	C4D-CHA-C1A	-7.31	112.35	121.25
35	Q	616	XAT	O24-C25-C24	7.31	118.87	113.38
33	T	605	CHL	C4D-CHA-C1A	-7.31	112.36	121.25
33	P	605	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
33	R	608	CHL	CMD-C2D-C1D	7.30	137.58	124.71
25	9	309	CLA	C4A-NA-C1A	7.30	109.99	106.71
33	9	306	CHL	C4D-CHA-C1A	-7.30	112.37	121.25
33	R	601	CHL	C4D-CHA-C1A	-7.29	112.37	121.25
33	P	601	CHL	C4D-CHA-C1A	-7.29	112.37	121.25
25	7	310	CLA	C4A-NA-C1A	7.29	109.98	106.71
33	6	606	CHL	CMD-C2D-C1D	7.29	137.55	124.71
33	9	306	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
25	5	313	CLA	C4A-NA-C1A	7.28	109.98	106.71
25	A	828	CLA	C4A-NA-C1A	7.27	109.97	106.71
25	2	304	CLA	C4A-NA-C1A	7.27	109.97	106.71
33	5	308	CHL	CMD-C2D-C1D	7.27	137.52	124.71
28	B	842	BCR	C24-C23-C22	-7.27	115.25	126.23
33	1	606	CHL	CMD-C2D-C1D	7.27	137.52	124.71
25	9	305	CLA	C4A-NA-C1A	7.26	109.97	106.71
28	O	205	BCR	C7-C8-C9	-7.26	115.26	126.23
33	T	604	CHL	CMD-C2D-C1D	7.26	137.51	124.71
33	T	605	CHL	CMD-C2D-C1D	7.26	137.51	124.71
33	T	606	CHL	CMD-C2D-C1D	7.26	137.50	124.71
33	a	305	CHL	CMD-C2D-C1D	7.25	137.49	124.71
25	2	306	CLA	C4A-NA-C1A	7.25	109.97	106.71
33	5	317	CHL	C4D-CHA-C1A	-7.24	112.44	121.25
33	U	308	CHL	CMD-C2D-C1D	7.24	137.47	124.71
25	K	204	CLA	C4A-NA-C1A	7.23	109.96	106.71
33	4	314	CHL	CMD-C2D-C1D	7.22	137.43	124.71
33	4	304	CHL	C4D-CHA-C1A	-7.21	112.48	121.25
33	R	606	CHL	C4D-CHA-C1A	-7.20	112.48	121.25
33	4	314	CHL	C4D-CHA-C1A	-7.19	112.50	121.25
25	2	312	CLA	C4A-NA-C1A	7.19	109.94	106.71
25	3	311	CLA	C4A-NA-C1A	7.19	109.94	106.71
25	6	623	CLA	C4A-NA-C1A	7.19	109.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	S	306	CHL	C3B-C2B-C1B	-7.19	98.48	107.16
33	U	308	CHL	C4D-CHA-C1A	-7.19	112.50	121.25
33	Q	601	CHL	CMD-C2D-C1D	7.17	137.36	124.71
33	P	601	CHL	CMD-C2D-C1D	7.17	137.35	124.71
25	A	821	CLA	C4A-NA-C1A	7.17	109.93	106.71
25	T	603	CLA	C4A-NA-C1A	7.16	109.93	106.71
33	R	601	CHL	CMD-C2D-C1D	7.16	137.34	124.71
33	U	306	CHL	C4D-CHA-C1A	-7.15	112.54	121.25
33	5	308	CHL	C2C-C3C-C4C	-7.14	101.40	106.49
25	A	830	CLA	C4A-NA-C1A	7.14	109.92	106.71
25	8	312	CLA	C4A-NA-C1A	7.14	109.92	106.71
33	1	606	CHL	C4D-CHA-C1A	-7.13	112.57	121.25
33	Q	606	CHL	CMD-C2D-C1D	7.13	137.28	124.71
25	3	314	CLA	C4A-NA-C1A	7.13	109.91	106.71
25	B	802	CLA	C4A-NA-C1A	7.12	109.91	106.71
25	R	604	CLA	C4A-NA-C1A	7.12	109.91	106.71
33	U	305	CHL	CMD-C2D-C1D	7.12	137.26	124.71
25	A	822	CLA	C4A-NA-C1A	7.12	109.91	106.71
33	P	605	CHL	CMD-C2D-C1D	7.11	137.25	124.71
33	U	309	CHL	C4D-CHA-C1A	-7.11	112.60	121.25
25	P	604	CLA	C4A-NA-C1A	7.10	109.90	106.71
33	6	607	CHL	C4D-CHA-C1A	-7.09	112.62	121.25
25	A	839	CLA	C4A-NA-C1A	7.09	109.89	106.71
33	U	309	CHL	CMD-C2D-C1D	7.08	137.19	124.71
25	L	209	CLA	C4A-NA-C1A	7.08	109.89	106.71
33	7	305	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
33	S	306	CHL	CMD-C2D-C1D	7.07	137.18	124.71
25	K	201	CLA	C4A-NA-C1A	7.06	109.88	106.71
25	P	603	CLA	C4A-NA-C1A	7.06	109.88	106.71
33	5	317	CHL	CMD-C2D-C1D	7.05	137.15	124.71
25	A	806	CLA	C4A-NA-C1A	7.04	109.87	106.71
25	S	320	CLA	C4A-NA-C1A	7.04	109.87	106.71
33	S	302	CHL	CMD-C2D-C1D	7.04	137.12	124.71
33	1	601	CHL	C4D-CHA-C1A	-7.04	112.68	121.25
25	B	818	CLA	C4A-NA-C1A	7.03	109.87	106.71
33	6	607	CHL	CMD-C2D-C1D	7.03	137.10	124.71
25	1	607	CLA	C4A-NA-C1A	7.02	109.86	106.71
33	T	601	CHL	CMD-C2D-C1D	7.02	137.09	124.71
25	L	202	CLA	C4A-NA-C1A	7.02	109.86	106.71
25	B	832	CLA	C4A-NA-C1A	7.02	109.86	106.71
25	6	616	CLA	C4A-NA-C1A	7.01	109.86	106.71
25	2	305	CLA	C4A-NA-C1A	6.99	109.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	317	CHL	C2C-C3C-C4C	-6.98	101.51	106.49
25	U	303	CLA	C4A-NA-C1A	6.98	109.84	106.71
25	A	837	CLA	C4A-NA-C1A	6.97	109.84	106.71
36	P	621	NEX	C38-C25-C26	-6.95	110.62	122.26
33	5	307	CHL	C4D-CHA-C1A	-6.95	112.80	121.25
25	A	829	CLA	C4A-NA-C1A	6.94	109.83	106.71
33	4	306	CHL	CMD-C2D-C1D	6.94	136.95	124.71
33	P	622	CHL	CMD-C2D-C1D	6.93	136.92	124.71
33	T	604	CHL	C2C-C3C-C4C	-6.92	101.55	106.49
25	U	304	CLA	C4A-NA-C1A	6.92	109.82	106.71
33	R	606	CHL	CMD-C2D-C1D	6.92	136.91	124.71
25	A	810	CLA	C4A-NA-C1A	6.91	109.81	106.71
25	3	303	CLA	C4A-NA-C1A	6.91	109.81	106.71
25	K	205	CLA	C4A-NA-C1A	6.91	109.81	106.71
25	B	816	CLA	C4A-NA-C1A	6.91	109.81	106.71
25	L	206	CLA	C4A-NA-C1A	6.91	109.81	106.71
33	9	307	CHL	CMD-C2D-C1D	6.90	136.88	124.71
33	U	305	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
33	U	307	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
25	5	303	CLA	C4A-NA-C1A	6.90	109.81	106.71
25	5	305	CLA	C4A-NA-C1A	6.90	109.81	106.71
25	3	301	CLA	C4A-NA-C1A	6.90	109.81	106.71
28	I	201	BCR	C20-C21-C22	-6.90	117.46	127.31
25	A	818	CLA	C4A-NA-C1A	6.89	109.80	106.71
25	B	831	CLA	C4A-NA-C1A	6.88	109.80	106.71
33	S	310	CHL	CMD-C2D-C1D	6.87	136.82	124.71
25	B	811	CLA	C4A-NA-C1A	6.87	109.79	106.71
25	B	834	CLA	C4A-NA-C1A	6.86	109.79	106.71
25	U	312	CLA	C4A-NA-C1A	6.85	109.79	106.71
25	A	802	CLA	C4A-NA-C1A	6.84	109.78	106.71
25	B	805	CLA	C4A-NA-C1A	6.82	109.77	106.71
33	4	304	CHL	C2C-C3C-C4C	-6.82	101.63	106.49
25	5	316	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	H	202	CLA	C4A-NA-C1A	6.81	109.77	106.71
33	S	321	CHL	C2C-C3C-C4C	-6.81	101.64	106.49
33	a	305	CHL	C4D-CHA-C1A	-6.81	112.97	121.25
33	Q	605	CHL	C2C-C3C-C4C	-6.80	101.64	106.49
33	Q	606	CHL	C2C-C3C-C4C	-6.80	101.64	106.49
33	a	305	CHL	C2C-C3C-C4C	-6.80	101.64	106.49
25	R	613	CLA	C4A-NA-C1A	6.79	109.76	106.71
25	S	303	CLA	C4A-NA-C1A	6.79	109.76	106.71
33	R	606	CHL	C2C-C3C-C4C	-6.78	101.65	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	306	CLA	C4A-NA-C1A	6.77	109.75	106.71
25	B	819	CLA	C4A-NA-C1A	6.77	109.75	106.71
33	4	304	CHL	CMD-C2D-C1D	6.76	136.62	124.71
25	A	823	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	A	833	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	B	825	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	P	613	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	H	205	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	3	320	CLA	C4A-NA-C1A	6.75	109.74	106.71
33	S	321	CHL	C4D-CHA-C1A	-6.74	113.04	121.25
25	8	313	CLA	C4A-NA-C1A	6.74	109.74	106.71
25	B	821	CLA	C4A-NA-C1A	6.73	109.73	106.71
25	8	315	CLA	C4A-NA-C1A	6.73	109.73	106.71
25	6	601	CLA	C4A-NA-C1A	6.72	109.73	106.71
36	R	617	NEX	C38-C25-C26	-6.72	110.99	122.26
28	3	319	BCR	C11-C10-C9	-6.72	117.71	127.31
25	B	814	CLA	C4A-NA-C1A	6.72	109.73	106.71
25	4	303	CLA	C4A-NA-C1A	6.72	109.73	106.71
28	B	841	BCR	C7-C8-C9	-6.71	116.09	126.23
25	S	314	CLA	C4A-NA-C1A	6.71	109.72	106.71
25	6	604	CLA	C4A-NA-C1A	6.69	109.72	106.71
25	1	614	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	6	605	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	S	304	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	6	614	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	4	301	CLA	C4A-NA-C1A	6.68	109.71	106.71
25	J	105	CLA	C4A-NA-C1A	6.68	109.71	106.71
36	U	301	NEX	C17-C1-C6	-6.68	104.50	110.47
25	9	310	CLA	C4A-NA-C1A	6.68	109.71	106.71
25	B	836	CLA	C4A-NA-C1A	6.66	109.70	106.71
33	8	307	CHL	C2C-C3C-C4C	-6.66	101.74	106.49
25	L	201	CLA	C4A-NA-C1A	6.66	109.70	106.71
33	U	306	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
25	6	610	CLA	C4A-NA-C1A	6.65	109.69	106.71
25	A	832	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	7	307	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	B	804	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	A	840	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	B	813	CLA	C4A-NA-C1A	6.63	109.69	106.71
33	S	306	CHL	C4D-CHA-C1A	-6.62	113.19	121.25
25	J	103	CLA	C4A-NA-C1A	6.61	109.68	106.71
25	a	303	CLA	C4A-NA-C1A	6.61	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	201	CLA	C4A-NA-C1A	6.61	109.68	106.71
35	P	616	XAT	C18-C5-C6	-6.60	111.19	122.26
28	F	801	BCR	C24-C23-C22	-6.60	116.26	126.23
25	A	831	CLA	C4A-NA-C1A	6.60	109.67	106.71
36	U	316	NEX	C38-C25-C26	-6.60	111.20	122.26
25	A	816	CLA	C4A-NA-C1A	6.60	109.67	106.71
25	A	817	CLA	C4A-NA-C1A	6.59	109.67	106.71
25	a	313	CLA	C4A-NA-C1A	6.59	109.67	106.71
28	4	321	BCR	C24-C23-C22	-6.58	116.29	126.23
36	U	301	NEX	C35-C34-C33	-6.58	117.92	127.31
25	Q	612	CLA	C4A-NA-C1A	6.56	109.66	106.71
25	5	304	CLA	C4A-NA-C1A	6.56	109.65	106.71
25	a	310	CLA	C4A-NA-C1A	6.55	109.65	106.71
25	Q	610	CLA	C4A-NA-C1A	6.55	109.65	106.71
33	S	308	CHL	C2C-C3C-C4C	-6.54	101.83	106.49
36	U	301	NEX	C38-C25-C26	-6.54	111.30	122.26
33	S	310	CHL	C2C-C3C-C4C	-6.54	101.83	106.49
25	B	828	CLA	C4A-NA-C1A	6.54	109.64	106.71
25	A	805	CLA	C4A-NA-C1A	6.53	109.64	106.71
36	U	316	NEX	C35-C34-C33	-6.52	118.00	127.31
25	A	838	CLA	C4A-NA-C1A	6.52	109.64	106.71
33	T	601	CHL	C2C-C3C-C4C	-6.51	101.84	106.49
35	P	620	XAT	C38-C25-C26	-6.51	111.35	122.26
36	P	617	NEX	C38-C25-C26	-6.51	111.35	122.26
25	B	809	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	P	611	CLA	CMD-C2D-C1D	6.51	136.18	124.71
33	T	605	CHL	C2C-C3C-C4C	-6.50	101.85	106.49
25	T	611	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	9	308	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	5	315	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	8	309	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	A	836	CLA	C4A-NA-C1A	6.49	109.62	106.71
25	A	809	CLA	C4A-NA-C1A	6.49	109.62	106.71
25	2	311	CLA	C4A-NA-C1A	6.48	109.62	106.71
25	5	312	CLA	C4A-NA-C1A	6.48	109.62	106.71
33	P	606	CHL	C2C-C3C-C4C	-6.47	101.88	106.49
25	O	203	CLA	C4A-NA-C1A	6.47	109.61	106.71
25	7	301	CLA	C4A-NA-C1A	6.46	109.61	106.71
25	U	313	CLA	C4A-NA-C1A	6.45	109.61	106.71
25	B	833	CLA	C4A-NA-C1A	6.45	109.61	106.71
25	S	312	CLA	C4A-NA-C1A	6.45	109.61	106.71
25	6	603	CLA	C4A-NA-C1A	6.45	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	S	309	CHL	C2C-C3C-C4C	-6.44	101.90	106.49
25	9	301	CLA	C4A-NA-C1A	6.44	109.60	106.71
36	U	301	NEX	C15-C14-C13	-6.43	118.13	127.31
25	8	306	CLA	C4A-NA-C1A	6.43	109.60	106.71
36	T	616	NEX	C38-C25-C26	-6.43	111.49	122.26
25	B	810	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	3	310	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	7	302	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	K	202	CLA	C4A-NA-C1A	6.42	109.59	106.71
25	3	308	CLA	C4A-NA-C1A	6.42	109.59	106.71
36	T	616	NEX	C35-C34-C33	-6.42	118.15	127.31
25	B	829	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	H	201	CLA	C4A-NA-C1A	6.41	109.59	106.71
33	P	601	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
33	R	601	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
25	6	609	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	8	314	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	S	305	CLA	C4A-NA-C1A	6.40	109.58	106.71
25	7	308	CLA	C4A-NA-C1A	6.40	109.58	106.71
33	Q	607	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
33	T	607	CHL	C2C-C3C-C4C	-6.40	101.93	106.49
25	4	312	CLA	C4A-NA-C1A	6.40	109.58	106.71
25	O	201	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	A	813	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	2	310	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	5	306	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	2	302	CLA	C4A-NA-C1A	6.39	109.58	106.71
28	I	201	BCR	C24-C23-C22	-6.39	116.58	126.23
25	B	827	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	3	305	CLA	C4A-NA-C1A	6.39	109.58	106.71
33	U	308	CHL	C2C-C3C-C4C	-6.39	101.94	106.49
33	Q	601	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
35	T	615	XAT	C38-C25-C26	-6.38	111.56	122.26
33	R	608	CHL	C2C-C3C-C4C	-6.38	101.94	106.49
28	5	323	BCR	C23-C22-C21	-6.38	109.15	118.94
33	U	309	CHL	C2C-C3C-C4C	-6.37	101.94	106.49
25	1	611	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	8	303	CLA	C4A-NA-C1A	6.37	109.57	106.71
35	S	318	XAT	O4-C5-C4	6.37	118.17	113.38
33	P	607	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
25	S	313	CLA	C4A-NA-C1A	6.37	109.57	106.71
36	P	617	NEX	C35-C34-C33	-6.36	118.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	P	608	CHL	C2C-C3C-C4C	-6.36	101.95	106.49
35	T	615	XAT	C18-C5-C6	-6.36	111.60	122.26
25	T	608	CLA	C4A-NA-C1A	6.36	109.56	106.71
25	6	615	CLA	C4A-NA-C1A	6.36	109.56	106.71
25	8	310	CLA	C4A-NA-C1A	6.36	109.56	106.71
33	9	306	CHL	CHD-C4C-C3C	-6.35	115.50	124.84
25	T	610	CLA	C4A-NA-C1A	6.35	109.56	106.71
33	P	619	CHL	C2C-C3C-C4C	-6.35	101.96	106.49
25	R	614	CLA	C4A-NA-C1A	6.35	109.56	106.71
28	B	851	BCR	C16-C17-C18	-6.35	118.25	127.31
25	H	203	CLA	C4A-NA-C1A	6.35	109.56	106.71
36	P	621	NEX	O24-C25-C24	6.35	118.15	113.38
33	S	306	CHL	C2C-C3C-C4C	-6.34	101.97	106.49
35	P	620	XAT	C18-C5-C6	-6.34	111.64	122.26
25	A	820	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	4	313	CLA	C4A-NA-C1A	6.33	109.55	106.71
34	a	316	LUT	C15-C14-C13	-6.33	118.27	127.31
35	Q	616	XAT	C38-C25-C26	-6.33	111.65	122.26
25	4	302	CLA	C4A-NA-C1A	6.33	109.55	106.71
35	P	623	XAT	C31-C30-C29	-6.33	118.28	127.31
33	T	606	CHL	C2C-C3C-C4C	-6.33	101.98	106.49
25	3	313	CLA	C4A-NA-C1A	6.33	109.55	106.71
33	4	314	CHL	C2C-C3C-C4C	-6.32	101.98	106.49
35	P	623	XAT	C18-C5-C6	-6.32	111.66	122.26
35	S	318	XAT	C38-C25-C26	-6.32	111.67	122.26
33	R	607	CHL	C2C-C3C-C4C	-6.32	101.99	106.49
25	B	806	CLA	C4A-NA-C1A	6.31	109.55	106.71
28	O	204	BCR	C3-C4-C5	-6.31	102.81	114.08
25	8	304	CLA	C4A-NA-C1A	6.31	109.54	106.71
28	O	205	BCR	C11-C10-C9	-6.30	118.31	127.31
25	9	304	CLA	C4A-NA-C1A	6.30	109.54	106.71
36	P	617	NEX	C15-C14-C13	-6.29	118.34	127.31
35	P	616	XAT	C38-C25-C26	-6.29	111.72	122.26
33	1	606	CHL	C2C-C3C-C4C	-6.29	102.01	106.49
28	3	318	BCR	C20-C21-C22	-6.28	118.35	127.31
33	P	622	CHL	OMC-CMC-C2C	-6.28	111.49	125.69
25	4	308	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	A	807	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	3	304	CLA	C4A-NA-C1A	6.27	109.53	106.71
25	A	808	CLA	C4A-NA-C1A	6.27	109.52	106.71
25	B	817	CLA	C4A-NA-C1A	6.26	109.52	106.71
35	Q	616	XAT	C18-C5-C6	-6.26	111.77	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	307	CLA	C4A-NA-C1A	6.26	109.52	106.71
25	L	205	CLA	C4A-NA-C1A	6.25	109.52	106.71
25	1	605	CLA	C4A-NA-C1A	6.24	109.51	106.71
36	R	617	NEX	C35-C34-C33	-6.24	118.41	127.31
35	S	318	XAT	C18-C5-C6	-6.23	111.81	122.26
25	G	202	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	9	302	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	R	603	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	7	306	CLA	C4A-NA-C1A	6.23	109.51	106.71
33	6	617	CHL	C2C-C3C-C4C	-6.23	102.05	106.49
25	3	302	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	7	313	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	3	307	CLA	C4A-NA-C1A	6.22	109.50	106.71
33	6	606	CHL	C2C-C3C-C4C	-6.21	102.06	106.49
33	3	306	CHL	C2C-C3C-C4C	-6.21	102.06	106.49
25	2	307	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	B	849	CLA	C4A-NA-C1A	6.20	109.49	106.71
25	S	315	CLA	C4A-NA-C1A	6.20	109.49	106.71
36	U	316	NEX	C15-C14-C13	-6.20	118.47	127.31
36	R	617	NEX	C15-C14-C13	-6.19	118.48	127.31
28	3	318	BCR	C11-C10-C9	-6.19	118.48	127.31
25	B	826	CLA	C4A-NA-C1A	6.19	109.49	106.71
25	A	815	CLA	C4A-NA-C1A	6.18	109.49	106.71
33	4	305	CHL	C2C-C3C-C4C	-6.18	102.08	106.49
25	T	612	CLA	C4A-NA-C1A	6.18	109.48	106.71
25	1	602	CLA	C4A-NA-C1A	6.18	109.48	106.71
25	5	319	CLA	C4A-NA-C1A	6.17	109.48	106.71
35	P	623	XAT	C38-C25-C26	-6.14	111.97	122.26
35	P	616	XAT	C31-C30-C29	-6.14	118.55	127.31
36	P	621	NEX	C15-C14-C13	-6.13	118.57	127.31
25	4	310	CLA	C4A-NA-C1A	6.12	109.46	106.71
36	T	616	NEX	C15-C14-C13	-6.11	118.59	127.31
33	6	608	CHL	CHD-C4C-C3C	-6.11	115.86	124.84
25	B	838	CLA	C4A-NA-C1A	6.11	109.45	106.71
33	S	302	CHL	CHD-C4C-C3C	-6.10	115.87	124.84
25	3	312	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	2	308	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	A	814	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	5	302	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	a	302	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	Q	609	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	8	305	CLA	C4A-NA-C1A	6.08	109.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	804	CLA	C4A-NA-C1A	6.07	109.44	106.71
25	A	824	CLA	C4A-NA-C1A	6.07	109.43	106.71
28	I	201	BCR	C16-C17-C18	-6.06	118.66	127.31
34	1	617	LUT	C15-C14-C13	-6.06	118.66	127.31
33	3	306	CHL	CHD-C4C-C3C	-6.06	115.93	124.84
25	U	310	CLA	C4A-NA-C1A	6.05	109.43	106.71
25	a	301	CLA	C4A-NA-C1A	6.05	109.42	106.71
35	P	620	XAT	C31-C30-C29	-6.04	118.69	127.31
33	R	605	CHL	C2C-C3C-C4C	-6.03	102.19	106.49
25	A	819	CLA	C4A-NA-C1A	6.03	109.42	106.71
25	P	610	CLA	C4A-NA-C1A	6.02	109.41	106.71
28	4	321	BCR	C11-C10-C9	-6.02	118.72	127.31
28	L	204	BCR	C7-C8-C9	-6.01	117.15	126.23
28	L	203	BCR	C3-C4-C5	-6.01	103.35	114.08
33	S	307	CHL	O2D-CGD-CBD	6.01	121.94	111.27
25	1	604	CLA	C4A-NA-C1A	6.01	109.41	106.71
25	2	313	CLA	C4A-NA-C1A	6.01	109.41	106.71
25	2	314	CLA	C4A-NA-C1A	6.01	109.41	106.71
28	4	317	BCR	C15-C14-C13	-6.00	118.75	127.31
25	5	309	CLA	C4A-NA-C1A	6.00	109.40	106.71
25	A	835	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	B	824	CLA	C4A-NA-C1A	5.99	109.40	106.71
33	1	601	CHL	CHD-C4C-C3C	-5.99	116.04	124.84
25	A	803	CLA	C4A-NA-C1A	5.98	109.40	106.71
25	B	808	CLA	C4A-NA-C1A	5.98	109.40	106.71
28	O	204	BCR	C28-C27-C26	-5.98	103.41	114.08
25	O	202	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	A	853	CLA	C4A-NA-C1A	5.97	109.39	106.71
36	P	621	NEX	C35-C34-C33	-5.97	118.79	127.31
25	5	314	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	6	620	CLA	C4A-NA-C1A	5.96	109.39	106.71
25	K	203	CLA	C4A-NA-C1A	5.96	109.39	106.71
33	5	308	CHL	CHD-C4C-C3C	-5.95	116.09	124.84
33	5	317	CHL	CHD-C4C-C3C	-5.95	116.09	124.84
28	6	621	BCR	C11-C10-C9	-5.95	118.82	127.31
25	5	311	CLA	C4A-NA-C1A	5.95	109.38	106.71
33	4	322	CHL	O2D-CGD-CBD	5.94	121.82	111.27
25	A	812	CLA	C4A-NA-C1A	5.93	109.37	106.71
33	U	308	CHL	C3B-C2B-C1B	-5.93	100.00	107.16
33	S	307	CHL	C2C-C3C-C4C	-5.93	102.26	106.49
33	4	322	CHL	C3B-C2B-C1B	-5.93	100.01	107.16
25	4	310	CLA	CAA-C2A-C3A	-5.93	96.55	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	812	CLA	C4A-NA-C1A	5.93	109.37	106.71
28	3	318	BCR	C7-C8-C9	-5.92	117.29	126.23
33	6	617	CHL	C3B-C2B-C1B	-5.91	100.03	107.16
25	5	324	CLA	C4A-NA-C1A	5.91	109.36	106.71
25	6	612	CLA	C4A-NA-C1A	5.90	109.36	106.71
25	Q	613	CLA	C4A-NA-C1A	5.90	109.36	106.71
35	T	615	XAT	C31-C30-C29	-5.90	118.89	127.31
25	9	303	CLA	C4A-NA-C1A	5.89	109.35	106.71
25	4	307	CLA	C4A-NA-C1A	5.87	109.34	106.71
25	a	304	CLA	C4A-NA-C1A	5.87	109.34	106.71
33	S	321	CHL	O2D-CGD-CBD	5.86	121.68	111.27
33	1	601	CHL	O2D-CGD-CBD	5.86	121.68	111.27
33	T	606	CHL	C3B-C2B-C1B	-5.86	100.09	107.16
25	R	611	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	U	302	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	a	303	CLA	C6-C7-C8	-5.85	97.03	115.92
25	7	312	CLA	C4A-NA-C1A	5.84	109.33	106.71
33	R	605	CHL	C3B-C2B-C1B	-5.83	100.12	107.16
33	4	306	CHL	C3B-C2B-C1B	-5.83	100.12	107.16
25	F	802	CLA	C4A-NA-C1A	5.82	109.32	106.71
25	B	835	CLA	C4A-NA-C1A	5.81	109.32	106.71
25	7	304	CLA	C4A-NA-C1A	5.81	109.32	106.71
33	5	317	CHL	C3B-C2B-C1B	-5.80	100.17	107.16
33	6	606	CHL	CHD-C4C-C3C	-5.80	116.32	124.84
33	P	608	CHL	C3B-C2B-C1B	-5.79	100.17	107.16
25	2	303	CLA	C4A-NA-C1A	5.79	109.31	106.71
33	Q	607	CHL	C3B-C2B-C1B	-5.79	100.18	107.16
33	4	322	CHL	CHD-C4C-C3C	-5.79	116.34	124.84
25	T	609	CLA	C4A-NA-C1A	5.79	109.31	106.71
33	6	607	CHL	CHD-C4C-C3C	-5.78	116.34	124.84
25	R	610	CLA	C4A-NA-C1A	5.78	109.30	106.71
25	5	310	CLA	C4A-NA-C1A	5.78	109.30	106.71
33	R	608	CHL	C3B-C2B-C1B	-5.77	100.19	107.16
25	Q	611	CLA	C4A-NA-C1A	5.77	109.30	106.71
25	B	830	CLA	C4A-NA-C1A	5.76	109.30	106.71
33	Q	606	CHL	C3B-C2B-C1B	-5.75	100.22	107.16
33	P	605	CHL	C3B-C2B-C1B	-5.74	100.23	107.16
25	B	822	CLA	C4A-NA-C1A	5.74	109.29	106.71
28	F	801	BCR	C20-C21-C22	-5.74	119.12	127.31
33	U	305	CHL	C3B-C2B-C1B	-5.73	100.25	107.16
28	F	803	BCR	C11-C10-C9	-5.73	119.14	127.31
25	8	311	CLA	C4A-NA-C1A	5.73	109.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	302	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	A	851	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	1	603	CLA	C4A-NA-C1A	5.71	109.28	106.71
33	S	309	CHL	CHD-C4C-C3C	-5.71	116.44	124.84
33	1	601	CHL	C3B-C2B-C1B	-5.70	100.28	107.16
28	B	841	BCR	C3-C4-C5	-5.69	103.92	114.08
33	Q	605	CHL	C3B-C2B-C1B	-5.69	100.30	107.16
25	S	301	CLA	C4A-NA-C1A	5.69	109.26	106.71
33	4	314	CHL	C3B-C2B-C1B	-5.68	100.30	107.16
25	P	602	CLA	C4A-NA-C1A	5.68	109.26	106.71
25	a	309	CLA	C4A-NA-C1A	5.68	109.26	106.71
33	4	322	CHL	CMD-C2D-C1D	5.68	134.72	124.71
25	H	205	CLA	CAA-C2A-C3A	-5.68	100.07	114.26
33	P	606	CHL	C3B-C2B-C1B	-5.67	100.31	107.16
33	4	306	CHL	CHD-C4C-C3C	-5.67	116.51	124.84
25	9	311	CLA	C4A-NA-C1A	5.67	109.25	106.71
33	S	302	CHL	C3B-C2B-C1B	-5.66	100.33	107.16
33	U	309	CHL	O2D-CGD-CBD	5.66	121.32	111.27
28	3	318	BCR	C19-C18-C17	5.65	127.62	118.94
33	S	307	CHL	C3B-C2B-C1B	-5.65	100.34	107.16
25	Q	618	CLA	C4A-NA-C1A	5.65	109.25	106.71
33	5	317	CHL	C2A-C1A-CHA	-5.64	114.00	123.86
33	S	308	CHL	CHD-C4C-C3C	-5.63	116.57	124.84
28	F	801	BCR	C16-C17-C18	-5.62	119.29	127.31
25	2	309	CLA	C4A-NA-C1A	5.61	109.23	106.71
33	T	604	CHL	C3B-C2B-C1B	-5.61	100.39	107.16
33	4	306	CHL	C2C-C3C-C4C	-5.61	102.49	106.49
25	3	309	CLA	C4A-NA-C1A	5.61	109.23	106.71
33	6	608	CHL	C2A-C1A-CHA	-5.60	114.06	123.86
33	6	608	CHL	C3B-C2B-C1B	-5.60	100.40	107.16
25	6	611	CLA	C4A-NA-C1A	5.60	109.22	106.71
28	7	316	BCR	C28-C27-C26	-5.60	104.08	114.08
28	L	207	BCR	C38-C26-C25	-5.60	118.24	124.53
25	1	608	CLA	C4A-NA-C1A	5.60	109.22	106.71
28	3	319	BCR	C7-C8-C9	-5.59	117.78	126.23
25	P	611	CLA	C2B-C1B-NB	5.58	113.97	110.23
33	1	606	CHL	C3B-C2B-C1B	-5.58	100.43	107.16
25	A	825	CLA	C4A-NA-C1A	5.58	109.21	106.71
25	a	312	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	R	602	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	B	801	CLA	C4A-NA-C1A	5.55	109.20	106.71
25	S	311	CLA	C4A-NA-C1A	5.55	109.20	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	607	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
33	S	321	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
33	P	605	CHL	CHD-C4C-C3C	-5.53	116.71	124.84
33	P	619	CHL	C3B-C2B-C1B	-5.53	100.49	107.16
33	6	607	CHL	C3B-C2B-C1B	-5.52	100.49	107.16
28	6	621	BCR	C38-C26-C25	-5.52	118.33	124.53
33	P	607	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
28	8	318	BCR	C15-C14-C13	-5.51	119.44	127.31
28	J	101	BCR	C38-C26-C25	-5.51	118.34	124.53
25	7	303	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	1	613	CLA	C4A-NA-C1A	5.50	109.18	106.71
25	T	602	CLA	C4A-NA-C1A	5.50	109.18	106.71
33	5	317	CHL	O2D-CGD-CBD	5.50	121.03	111.27
33	S	321	CHL	CHD-C4C-C3C	-5.49	116.77	124.84
33	7	305	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
36	R	617	NEX	C11-C10-C9	-5.49	119.48	127.31
33	7	305	CHL	CHD-C4C-C3C	-5.49	116.78	124.84
33	a	305	CHL	C3B-C2B-C1B	-5.48	100.54	107.16
33	T	605	CHL	C3B-C2B-C1B	-5.48	100.54	107.16
36	U	301	NEX	C11-C10-C9	-5.48	119.49	127.31
33	4	304	CHL	CHD-C4C-C3C	-5.48	116.79	124.84
25	A	826	CLA	C4A-NA-C1A	5.47	109.17	106.71
25	Q	602	CLA	C4A-NA-C1A	5.47	109.17	106.71
28	5	323	BCR	C20-C21-C22	5.47	135.12	127.31
28	B	845	BCR	C20-C21-C22	-5.47	119.50	127.31
33	S	310	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
34	6	619	LUT	C35-C34-C33	-5.47	119.51	127.31
34	1	617	LUT	C31-C30-C29	-5.46	119.52	127.31
35	S	318	XAT	C11-C10-C9	-5.46	119.52	127.31
33	T	604	CHL	CHD-C4C-C3C	-5.46	116.82	124.84
35	Q	616	XAT	C27-C28-C29	-5.45	117.07	125.53
33	U	306	CHL	CHD-C4C-C3C	-5.45	116.83	124.84
25	B	815	CLA	C4A-NA-C1A	5.44	109.15	106.71
33	5	308	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
33	P	606	CHL	CHD-C4C-C3C	-5.43	116.85	124.84
34	a	316	LUT	C31-C30-C29	-5.43	119.56	127.31
33	P	619	CHL	O2D-CGD-CBD	5.43	120.92	111.27
33	U	306	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
33	P	622	CHL	C1D-ND-C4D	5.42	110.19	106.33
33	T	605	CHL	CHD-C4C-C3C	-5.42	116.88	124.84
33	U	309	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
35	Q	616	XAT	C31-C30-C29	-5.41	119.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	O	204	BCR	C24-C23-C22	-5.41	118.06	126.23
28	B	845	BCR	C24-C23-C22	-5.41	118.06	126.23
25	7	309	CLA	C4A-NA-C1A	5.41	109.14	106.71
33	P	607	CHL	O2D-CGD-CBD	5.40	120.87	111.27
33	Q	605	CHL	CHD-C4C-C3C	-5.40	116.91	124.84
33	T	607	CHL	C3B-C2B-C1B	-5.40	100.65	107.16
25	4	309	CLA	C4A-NA-C1A	5.40	109.13	106.71
33	R	607	CHL	O2D-CGD-CBD	5.40	120.86	111.27
33	9	306	CHL	C2A-C1A-CHA	-5.39	114.44	123.85
33	S	308	CHL	C3B-C2B-C1B	-5.39	100.65	107.16
33	U	307	CHL	C3B-C2B-C1B	-5.39	100.66	107.16
28	3	317	BCR	C16-C17-C18	-5.39	119.62	127.31
35	P	623	XAT	C27-C28-C29	-5.38	117.18	125.53
28	G	203	BCR	C24-C23-C22	-5.37	118.13	126.23
28	4	317	BCR	C31-C1-C6	-5.36	101.60	110.30
33	4	305	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
28	B	840	BCR	C16-C17-C18	-5.34	119.69	127.31
35	Q	616	XAT	C15-C14-C13	-5.34	119.69	127.31
28	4	321	BCR	C30-C25-C26	-5.34	115.10	122.61
33	S	309	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
33	5	307	CHL	C3B-C2B-C1B	-5.33	100.72	107.16
25	A	827	CLA	C4A-NA-C1A	5.33	109.10	106.71
33	8	307	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
33	Q	606	CHL	C2A-C1A-CHA	-5.33	114.55	123.86
33	S	310	CHL	C2A-C1A-CHA	-5.32	114.55	123.86
28	K	206	BCR	C28-C27-C26	-5.32	104.57	114.08
33	U	307	CHL	CHD-C4C-C3C	-5.32	117.02	124.84
25	U	311	CLA	C4A-NA-C1A	5.32	109.10	106.71
33	Q	601	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
28	4	317	BCR	C28-C27-C26	-5.30	104.61	114.08
33	U	305	CHL	CHD-C4C-C3C	-5.30	117.05	124.84
25	B	823	CLA	C4A-NA-C1A	5.30	109.09	106.71
33	P	601	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
34	2	315	LUT	C35-C34-C33	-5.29	119.76	127.31
28	3	317	BCR	C28-C27-C26	-5.29	104.63	114.08
33	S	306	CHL	C1D-ND-C4D	5.28	110.09	106.33
33	R	601	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
33	6	617	CHL	C2A-C1A-CHA	-5.26	114.67	123.86
33	S	310	CHL	CHD-C4C-C3C	-5.25	117.12	124.84
35	T	615	XAT	C35-C34-C33	-5.25	119.81	127.31
33	R	606	CHL	CHD-C4C-C3C	-5.25	117.12	124.84
36	U	301	NEX	C27-C28-C29	-5.25	117.39	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	U	308	CHL	CHD-C4C-C3C	-5.24	117.13	124.84
33	4	304	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
34	R	615	LUT	C35-C34-C33	-5.23	119.84	127.31
33	Q	606	CHL	CHD-C4C-C3C	-5.23	117.15	124.84
28	5	320	BCR	C3-C4-C5	-5.23	104.74	114.08
33	T	606	CHL	CHD-C4C-C3C	-5.22	117.16	124.84
33	9	307	CHL	C3B-C2B-C1B	-5.22	100.86	107.16
28	6	621	BCR	C1-C6-C5	-5.21	115.28	122.61
25	a	303	CLA	C1-O2A-CGA	5.21	130.11	116.44
25	R	611	CLA	C6-C5-C3	5.21	127.11	113.45
33	5	307	CHL	CHD-C4C-C3C	-5.20	117.19	124.84
33	6	617	CHL	CHD-C4C-C3C	-5.20	117.20	124.84
33	8	307	CHL	CHD-C4C-C3C	-5.20	117.20	124.84
33	T	601	CHL	C3B-C2B-C1B	-5.20	100.89	107.16
28	G	203	BCR	C16-C17-C18	-5.19	119.90	127.31
36	T	616	NEX	C11-C10-C9	-5.18	119.92	127.31
33	P	619	CHL	CHD-C4C-C3C	-5.18	117.23	124.84
33	T	601	CHL	C1D-ND-C4D	5.18	110.01	106.33
36	U	316	NEX	C11-C10-C9	-5.18	119.92	127.31
33	P	607	CHL	CHD-C4C-C3C	-5.17	117.23	124.84
35	P	616	XAT	C27-C28-C29	-5.17	117.51	125.53
33	T	605	CHL	C2A-C1A-CHA	-5.17	114.82	123.86
28	J	106	BCR	C28-C27-C26	-5.16	104.86	114.08
33	9	307	CHL	CHD-C4C-C3C	-5.16	117.26	124.84
36	P	617	NEX	C11-C10-C9	-5.15	119.96	127.31
28	A	854	BCR	C24-C23-C22	-5.14	118.47	126.23
28	A	848	BCR	C11-C10-C9	-5.14	119.97	127.31
28	G	203	BCR	C20-C21-C22	-5.14	119.97	127.31
33	1	601	CHL	C2A-C1A-CHA	-5.14	114.87	123.86
35	P	620	XAT	C27-C28-C29	-5.14	117.56	125.53
28	A	845	BCR	C28-C27-C26	-5.14	104.90	114.08
27	A	852	LHG	O7-C7-C8	5.14	122.57	111.50
28	A	849	BCR	C20-C21-C22	-5.14	119.98	127.31
33	R	608	CHL	CHD-C4C-C3C	-5.12	117.31	124.84
33	P	607	CHL	C2A-C1A-CHA	-5.12	114.90	123.86
33	R	607	CHL	CHD-C4C-C3C	-5.12	117.31	124.84
33	P	619	CHL	C2A-C1A-CHA	-5.12	114.91	123.86
33	R	607	CHL	C2A-C1A-CHA	-5.12	114.91	123.86
33	P	606	CHL	C2A-C1A-CHA	-5.11	114.92	123.86
36	P	617	NEX	C27-C28-C29	-5.11	117.60	125.53
33	R	606	CHL	C3B-C2B-C1B	-5.10	101.00	107.16
28	B	844	BCR	C24-C23-C22	-5.10	118.53	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	314	LUT	C35-C34-C33	-5.10	120.03	127.31
33	P	608	CHL	CHD-C4C-C3C	-5.10	117.34	124.84
33	Q	607	CHL	CHD-C4C-C3C	-5.10	117.35	124.84
33	U	307	CHL	C2A-C1A-CHA	-5.10	114.95	123.86
33	R	606	CHL	O2D-CGD-CBD	5.09	120.31	111.27
33	S	321	CHL	C2A-C1A-CHA	-5.08	114.97	123.86
25	1	610	CLA	C4A-NA-C1A	5.08	108.99	106.71
35	P	623	XAT	O24-C25-C38	5.07	121.14	115.06
28	A	846	BCR	C16-C17-C18	-5.07	120.07	127.31
28	B	842	BCR	C16-C17-C18	-5.07	120.07	127.31
28	O	204	BCR	C20-C21-C22	-5.07	120.07	127.31
33	1	601	CHL	CMD-C2D-C1D	5.07	133.65	124.71
33	8	307	CHL	C2A-C1A-CHA	-5.07	115.00	123.86
34	a	316	LUT	C35-C34-C33	-5.06	120.09	127.31
35	P	616	XAT	C15-C14-C13	-5.05	120.10	127.31
33	8	307	CHL	OBD-CAD-C3D	-5.05	116.36	128.52
33	Q	606	CHL	O2D-CGD-CBD	5.05	120.24	111.27
28	3	317	BCR	C3-C4-C5	-5.05	105.06	114.08
33	4	314	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
28	L	204	BCR	C16-C17-C18	-5.03	120.14	127.31
28	3	319	BCR	C12-C13-C14	5.02	126.65	118.94
33	9	306	CHL	C3B-C2B-C1B	-5.01	101.11	107.16
33	P	606	CHL	O2D-CGD-CBD	5.01	120.17	111.27
28	3	318	BCR	C24-C23-C22	-5.00	118.67	126.23
33	P	605	CHL	C2A-C1A-CHA	-5.00	115.11	123.86
33	3	306	CHL	C3B-C2B-C1B	-5.00	101.12	107.16
33	T	601	CHL	CHB-C1B-NB	-5.00	118.97	124.26
33	U	309	CHL	C1D-ND-C4D	5.00	109.88	106.33
33	S	309	CHL	C2A-C1A-CHA	-4.99	115.13	123.86
33	P	622	CHL	O2D-CGD-CBD	4.99	120.13	111.27
33	T	607	CHL	O2D-CGD-CBD	4.98	120.13	111.27
35	P	620	XAT	C35-C34-C33	-4.98	120.20	127.31
35	P	616	XAT	C35-C34-C33	-4.98	120.20	127.31
33	4	322	CHL	C2A-C1A-CHA	-4.97	115.16	123.86
33	7	305	CHL	C2A-C1A-CHA	-4.97	115.16	123.86
33	T	601	CHL	O2D-CGD-CBD	4.97	120.09	111.27
36	T	616	NEX	C27-C28-C29	-4.96	117.83	125.53
28	B	840	BCR	C11-C10-C9	-4.96	120.23	127.31
33	a	305	CHL	CHD-C4C-C3C	-4.96	117.55	124.84
33	T	607	CHL	C1D-ND-C4D	4.95	109.85	106.33
33	U	306	CHL	C2A-C1A-CHA	-4.95	115.21	123.86
28	B	845	BCR	C16-C17-C18	-4.95	120.25	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	204	BCR	C33-C5-C6	-4.94	118.98	124.53
34	Q	614	LUT	C7-C8-C9	-4.93	118.78	126.23
28	5	323	BCR	C19-C18-C17	4.93	126.50	118.94
28	A	849	BCR	C7-C8-C9	-4.92	118.81	126.23
25	A	801	CLA	C4A-NA-C1A	4.92	108.92	106.71
35	T	615	XAT	C15-C14-C13	-4.91	120.30	127.31
28	4	321	BCR	C33-C5-C6	-4.90	119.02	124.53
34	1	615	LUT	C35-C34-C33	-4.90	120.32	127.31
28	B	844	BCR	C15-C14-C13	-4.90	120.32	127.31
33	T	605	CHL	O2D-CGD-CBD	4.90	119.97	111.27
35	P	623	XAT	C35-C34-C33	-4.89	120.33	127.31
33	1	606	CHL	CHD-C4C-C3C	-4.89	117.65	124.84
33	S	310	CHL	O2D-CGD-CBD	4.89	119.96	111.27
33	S	308	CHL	C2A-C1A-CHA	-4.89	115.31	123.86
33	R	605	CHL	CHD-C4C-C3C	-4.88	117.66	124.84
33	P	601	CHL	C1D-ND-C4D	4.88	109.80	106.33
34	4	315	LUT	C35-C34-C33	-4.88	120.34	127.31
33	5	308	CHL	C2A-C1A-CHA	-4.88	115.33	123.86
34	P	614	LUT	C35-C34-C33	-4.87	120.35	127.31
33	P	601	CHL	O2D-CGD-CBD	4.87	119.93	111.27
33	U	307	CHL	O2D-CGD-CBD	4.87	119.93	111.27
33	4	305	CHL	O2D-CGD-CBD	4.87	119.93	111.27
33	4	314	CHL	O2D-CGD-CBD	4.87	119.92	111.27
33	6	606	CHL	C3B-C2B-C1B	-4.87	101.29	107.16
33	Q	601	CHL	C1D-ND-C4D	4.86	109.79	106.33
33	R	601	CHL	O2D-CGD-CBD	4.86	119.91	111.27
28	K	206	BCR	C16-C15-C14	-4.86	113.51	123.47
36	P	621	NEX	O24-C25-C38	4.86	120.88	115.06
35	T	615	XAT	C27-C28-C29	-4.86	117.99	125.53
28	3	318	BCR	C20-C19-C18	-4.86	112.77	126.42
33	6	606	CHL	C2A-C1A-CHA	-4.85	115.37	123.86
33	P	601	CHL	CHB-C1B-NB	-4.85	119.12	124.26
33	Q	601	CHL	O2D-CGD-CBD	4.85	119.88	111.27
28	A	848	BCR	C16-C17-C18	-4.84	120.40	127.31
33	T	606	CHL	C2A-C1A-CHA	-4.84	115.40	123.86
33	R	601	CHL	C1D-ND-C4D	4.83	109.76	106.33
33	Q	601	CHL	CHB-C1B-NB	-4.83	119.15	124.26
28	L	208	BCR	C15-C14-C13	-4.82	120.43	127.31
34	T	613	LUT	C35-C34-C33	-4.82	120.43	127.31
33	3	306	CHL	C2A-C1A-CHA	-4.82	115.43	123.86
35	P	623	XAT	C15-C14-C13	-4.82	120.43	127.31
34	S	317	LUT	C31-C30-C29	-4.81	120.44	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	101	BCR	C3-C4-C5	-4.81	105.48	114.08
33	R	601	CHL	CHB-C1B-NB	-4.80	119.17	124.26
34	Q	614	LUT	C35-C34-C33	-4.79	120.48	127.31
33	R	606	CHL	C2A-C1A-CHA	-4.78	115.50	123.86
28	L	204	BCR	C38-C26-C25	-4.78	119.16	124.53
33	Q	607	CHL	C2A-C1A-CHA	-4.77	115.51	123.86
33	6	617	CHL	O2D-CGD-CBD	4.77	119.74	111.27
32	1	619	LMG	O7-C10-C11	4.77	121.77	111.50
33	P	608	CHL	C2A-C1A-CHA	-4.77	115.53	123.86
28	L	203	BCR	C15-C16-C17	-4.77	113.71	123.47
33	6	608	CHL	O2D-CGD-CBD	4.77	119.74	111.27
35	P	620	XAT	C15-C14-C13	-4.76	120.51	127.31
33	R	608	CHL	C2A-C1A-CHA	-4.76	115.53	123.86
33	S	306	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
33	S	307	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
33	U	309	CHL	CHB-C1B-NB	-4.76	119.22	124.26
33	S	308	CHL	O2D-CGD-CBD	4.75	119.71	111.27
33	R	605	CHL	O2D-CGD-CBD	4.75	119.71	111.27
34	T	613	LUT	C7-C8-C9	-4.75	119.06	126.23
35	S	318	XAT	C15-C14-C13	-4.75	120.54	127.31
33	U	309	CHL	CED-O2D-CGD	4.74	126.66	115.94
28	4	321	BCR	C15-C14-C13	-4.73	120.56	127.31
28	8	318	BCR	C28-C27-C26	-4.73	105.64	114.08
33	U	306	CHL	O2D-CGD-CBD	4.73	119.67	111.27
28	A	847	BCR	C16-C17-C18	-4.73	120.56	127.31
33	6	607	CHL	C2A-C1A-CHA	-4.72	115.60	123.86
28	3	317	BCR	C33-C5-C6	-4.72	119.23	124.53
33	4	314	CHL	C2A-C1A-CHA	-4.72	115.61	123.86
32	7	319	LMG	O7-C10-C11	4.71	121.66	111.50
33	4	305	CHL	C1D-ND-C4D	4.71	109.68	106.33
36	U	316	NEX	C27-C28-C29	-4.70	118.24	125.53
33	9	307	CHL	C2A-C1A-CHA	-4.69	115.67	123.86
28	F	803	BCR	C7-C8-C9	-4.69	119.16	126.23
28	A	848	BCR	C15-C14-C13	-4.68	120.63	127.31
33	5	308	CHL	CAC-C3C-C4C	4.68	130.88	124.81
33	S	307	CHL	C2A-C1A-CHA	-4.68	115.68	123.86
33	1	601	CHL	C1-C2-C3	-4.68	117.96	126.04
33	4	306	CHL	C2A-C1A-CHA	-4.67	115.69	123.86
33	T	607	CHL	CHB-C1B-NB	-4.67	119.31	124.26
27	7	317	LHG	O7-C7-C8	4.67	121.56	111.50
33	4	304	CHL	O2D-CGD-CBD	4.66	119.55	111.27
28	L	207	BCR	C11-C10-C9	-4.66	120.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	U	308	CHL	C2A-C1A-CHA	-4.66	115.72	123.86
34	U	314	LUT	C35-C34-C33	-4.65	120.67	127.31
28	A	845	BCR	C16-C17-C18	-4.65	120.68	127.31
28	6	621	BCR	C15-C14-C13	-4.64	120.69	127.31
34	3	315	LUT	C18-C5-C6	-4.63	119.32	124.53
28	B	845	BCR	C33-C5-C6	-4.62	119.33	124.53
28	7	316	BCR	C15-C14-C13	-4.62	120.71	127.31
33	P	622	CHL	CHB-C1B-NB	-4.62	119.36	124.26
28	G	203	BCR	C7-C8-C9	-4.62	119.25	126.23
28	I	201	BCR	C3-C4-C5	-4.62	105.83	114.08
35	Q	616	XAT	C11-C10-C9	-4.61	120.73	127.31
34	1	617	LUT	C35-C34-C33	-4.60	120.75	127.31
28	L	203	BCR	C7-C8-C9	-4.60	119.29	126.23
28	3	318	BCR	C36-C18-C17	-4.60	116.48	122.92
34	a	315	LUT	C7-C8-C9	-4.59	119.30	126.23
25	Q	618	CLA	C2A-C1A-CHA	4.59	129.82	122.71
28	B	841	BCR	C4-C5-C6	-4.59	116.07	122.73
28	O	204	BCR	C16-C17-C18	-4.58	120.78	127.31
27	6	618	LHG	O7-C7-C8	4.57	121.36	111.50
34	a	316	LUT	C1-C6-C5	-4.57	116.18	122.61
28	3	319	BCR	C38-C26-C25	-4.55	119.42	124.53
33	1	606	CHL	C1D-ND-C4D	4.55	109.57	106.33
28	A	854	BCR	C15-C14-C13	-4.55	120.82	127.31
35	P	620	XAT	O24-C25-C38	4.54	120.50	115.06
28	8	318	BCR	C3-C4-C5	-4.54	105.97	114.08
28	A	846	BCR	C11-C10-C9	-4.53	120.85	127.31
35	S	318	XAT	C6-C7-C8	-4.52	116.44	125.99
33	U	309	CHL	CHD-C4C-C3C	-4.52	118.20	124.84
33	5	307	CHL	CMD-C2D-C3D	-4.52	117.22	127.61
25	S	301	CLA	C3B-C4B-NB	-4.51	106.33	110.52
33	4	305	CHL	CHD-C4C-C3C	-4.51	118.22	124.84
28	K	206	BCR	C3-C4-C5	-4.50	106.04	114.08
28	5	320	BCR	C24-C23-C22	-4.50	119.44	126.23
33	4	305	CHL	CHB-C1B-NB	-4.50	119.50	124.26
33	6	606	CHL	O2D-CGD-CBD	4.49	119.25	111.27
28	3	317	BCR	C24-C23-C22	-4.49	119.45	126.23
33	9	307	CHL	O2D-CGD-CBD	4.49	119.25	111.27
33	8	307	CHL	C1D-ND-C4D	4.49	109.52	106.33
33	S	306	CHL	CBB-CAB-C3B	-4.49	105.29	127.62
33	P	622	CHL	C3B-C2B-C1B	-4.48	101.75	107.16
35	S	318	XAT	O4-C5-C18	4.47	120.42	115.06
33	a	305	CHL	CHB-C1B-NB	-4.47	119.53	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	846	DGD	C2G-O2G-C1B	-4.47	106.80	117.79
28	5	323	BCR	C3-C4-C5	-4.46	106.11	114.08
25	P	611	CLA	CMD-C2D-C3D	-4.46	117.36	127.61
33	4	305	CHL	CHD-C1D-ND	-4.45	120.36	124.45
33	Q	601	CHL	CHD-C1D-ND	-4.45	120.37	124.45
28	3	319	BCR	C11-C12-C13	-4.45	113.92	126.42
34	1	616	LUT	C7-C8-C9	-4.45	119.52	126.23
33	R	601	CHL	CHD-C1D-ND	-4.45	120.37	124.45
25	a	303	CLA	C7-C6-C5	-4.44	101.30	113.36
35	T	615	XAT	O24-C25-C38	4.44	120.38	115.06
34	P	615	LUT	C31-C30-C29	-4.44	120.98	127.31
33	7	305	CHL	O2D-CGD-CBD	4.44	119.15	111.27
28	J	106	BCR	C15-C14-C13	-4.43	120.99	127.31
28	3	319	BCR	C35-C13-C14	-4.43	116.72	122.92
33	P	601	CHL	CHD-C1D-ND	-4.43	120.39	124.45
28	3	318	BCR	C12-C13-C14	4.43	125.73	118.94
28	3	319	BCR	C36-C18-C17	-4.43	116.72	122.92
28	F	803	BCR	C38-C26-C25	-4.42	119.56	124.53
33	T	607	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
33	a	305	CHL	C1D-ND-C4D	4.41	109.47	106.33
28	3	317	BCR	C36-C18-C17	-4.41	116.75	122.92
34	8	316	LUT	C35-C34-C33	-4.40	121.03	127.31
28	6	621	BCR	C4-C5-C6	-4.40	116.35	122.73
28	B	841	BCR	C15-C14-C13	-4.40	121.04	127.31
33	4	322	CHL	C1-C2-C3	-4.39	118.44	126.04
28	3	319	BCR	C24-C23-C22	-4.39	119.60	126.23
35	P	616	XAT	O4-C5-C18	4.39	120.31	115.06
28	B	842	BCR	C7-C8-C9	-4.38	119.61	126.23
28	5	323	BCR	C23-C24-C25	-4.38	114.89	127.20
28	A	854	BCR	C28-C27-C26	-4.38	106.26	114.08
33	S	302	CHL	C2A-C1A-CHA	-4.37	116.21	123.86
33	Q	605	CHL	O2D-CGD-CBD	4.37	119.03	111.27
28	5	323	BCR	C21-C20-C19	-4.37	109.59	123.22
33	3	306	CHL	CMD-C2D-C3D	-4.36	117.58	127.61
36	T	616	NEX	O24-C25-C38	4.36	120.28	115.06
33	a	305	CHL	CHD-C1D-ND	-4.36	120.45	124.45
33	Q	605	CHL	C2A-C1A-CHA	-4.35	116.25	123.85
34	P	614	LUT	C7-C8-C9	-4.35	119.66	126.23
27	5	321	LHG	O7-C7-C8	4.35	120.88	111.50
33	1	606	CHL	O2D-CGD-CBD	4.35	119.00	111.27
33	1	606	CHL	CHB-C1B-NB	-4.35	119.66	124.26
33	4	306	CHL	O2D-CGD-CBD	4.33	118.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	322	CHL	C7-C6-C5	-4.33	94.16	112.67
33	P	622	CHL	CHD-C4C-C3C	-4.33	118.48	124.84
28	L	208	BCR	C24-C23-C22	-4.32	119.71	126.23
34	7	315	LUT	C18-C5-C6	-4.31	119.69	124.53
33	9	306	CHL	CMD-C2D-C3D	-4.31	117.70	127.61
28	5	323	BCR	C38-C26-C25	-4.30	119.70	124.53
28	K	206	BCR	C24-C23-C22	-4.30	119.74	126.23
33	7	305	CHL	CMD-C2D-C3D	-4.30	117.72	127.61
28	4	317	BCR	C8-C7-C6	-4.30	115.13	127.20
28	A	848	BCR	C3-C4-C5	-4.30	106.40	114.08
33	6	608	CHL	CAC-C3C-C4C	4.29	130.38	124.81
35	P	616	XAT	C11-C10-C9	-4.29	121.19	127.31
36	P	621	NEX	C11-C10-C9	-4.29	121.19	127.31
35	P	616	XAT	O24-C25-C38	4.28	120.19	115.06
34	2	315	LUT	C18-C5-C6	-4.28	119.72	124.53
28	A	845	BCR	C24-C23-C22	-4.28	119.77	126.23
25	R	611	CLA	C1-C2-C3	4.27	133.43	126.04
35	Q	616	XAT	O4-C5-C18	4.27	120.17	115.06
28	3	319	BCR	C20-C21-C22	-4.27	121.22	127.31
28	3	319	BCR	C19-C18-C17	4.27	125.49	118.94
33	8	307	CHL	CMD-C2D-C3D	-4.27	117.80	127.61
33	9	306	CHL	O2D-CGD-CBD	4.27	118.85	111.27
33	P	619	CHL	CMD-C2D-C3D	-4.27	117.80	127.61
33	S	307	CHL	CMD-C2D-C3D	-4.26	117.80	127.61
36	P	617	NEX	C17-C1-C6	-4.26	106.66	110.47
28	3	318	BCR	C38-C26-C25	-4.26	119.74	124.53
33	S	307	CHL	C1D-ND-C4D	4.26	109.36	106.33
34	Q	615	LUT	C31-C30-C29	-4.26	121.23	127.31
33	U	309	CHL	CHD-C1D-ND	-4.26	120.54	124.45
34	9	312	LUT	C35-C34-C33	-4.26	121.23	127.31
33	P	607	CHL	CMD-C2D-C3D	-4.25	117.83	127.61
33	R	607	CHL	CMD-C2D-C3D	-4.25	117.83	127.61
28	L	207	BCR	C7-C8-C9	-4.25	119.81	126.23
33	9	307	CHL	C1D-ND-C4D	4.25	109.35	106.33
28	B	844	BCR	C7-C8-C9	-4.24	119.82	126.23
33	5	308	CHL	O2D-CGD-CBD	4.24	118.80	111.27
33	4	305	CHL	CMD-C2D-C3D	-4.24	117.86	127.61
33	T	601	CHL	CHD-C1D-ND	-4.24	120.56	124.45
28	J	101	BCR	C33-C5-C6	-4.24	119.77	124.53
35	Q	616	XAT	O24-C25-C38	4.23	120.12	115.06
33	P	605	CHL	O2D-CGD-CBD	4.22	118.77	111.27
32	H	204	LMG	O7-C10-C11	4.22	120.60	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	319	LHG	O7-C7-C8	4.21	120.58	111.50
28	5	320	BCR	C16-C17-C18	-4.21	121.30	127.31
33	T	604	CHL	C2A-C1A-CHA	-4.21	116.50	123.86
34	U	315	LUT	C31-C30-C29	-4.20	121.31	127.31
28	3	317	BCR	C15-C14-C13	-4.20	121.31	127.31
28	A	845	BCR	C15-C14-C13	-4.20	121.31	127.31
25	Q	618	CLA	CBD-CHA-C1A	4.20	133.45	128.50
28	5	323	BCR	C16-C15-C14	-4.20	114.88	123.47
28	A	848	BCR	C7-C8-C9	-4.20	119.90	126.23
28	A	845	BCR	C3-C4-C5	-4.19	106.59	114.08
33	T	606	CHL	O2D-CGD-CBD	4.19	118.72	111.27
28	B	844	BCR	C15-C16-C17	-4.19	114.89	123.47
34	1	617	LUT	C1-C6-C5	-4.19	116.71	122.61
28	A	854	BCR	C16-C17-C18	-4.19	121.33	127.31
25	A	821	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
33	S	306	CHL	O2D-CGD-CBD	4.18	118.69	111.27
28	J	106	BCR	C38-C26-C25	-4.18	119.84	124.53
36	R	617	NEX	C27-C28-C29	-4.18	119.05	125.53
35	T	615	XAT	C11-C10-C9	-4.18	121.35	127.31
33	6	608	CHL	CMD-C2D-C3D	-4.17	118.01	127.61
32	7	318	LMG	O7-C10-C11	4.17	120.49	111.50
33	5	307	CHL	C1-C2-C3	-4.17	120.00	126.75
33	U	307	CHL	CMD-C2D-C3D	-4.17	118.03	127.61
33	5	307	CHL	C2A-C1A-CHA	-4.17	116.58	123.86
35	Q	616	XAT	C6-C7-C8	-4.16	117.19	125.99
33	S	321	CHL	CMD-C2D-C3D	-4.16	118.04	127.61
33	P	622	CHL	CAC-C3C-C4C	4.16	130.21	124.81
28	G	203	BCR	C11-C10-C9	-4.15	121.39	127.31
33	U	305	CHL	O2D-CGD-CBD	4.15	118.64	111.27
33	T	607	CHL	CMD-C2D-C3D	-4.15	118.07	127.61
25	1	609	CLA	CHB-C4A-NA	4.14	130.23	124.51
34	U	314	LUT	C7-C8-C9	-4.14	119.99	126.23
33	8	307	CHL	CHA-C4D-ND	4.13	141.14	132.50
33	T	604	CHL	O2D-CGD-CBD	4.12	118.60	111.27
33	S	309	CHL	CMD-C2D-C3D	-4.12	118.13	127.61
35	P	620	XAT	C11-C10-C9	-4.12	121.43	127.31
28	8	318	BCR	C38-C26-C25	-4.12	119.90	124.53
28	A	847	BCR	C24-C23-C22	-4.12	120.01	126.23
27	A	843	LHG	O7-C7-C8	4.12	120.37	111.50
33	P	605	CHL	CAA-CBA-CGA	-4.12	101.22	113.25
25	6	623	CLA	O2D-CGD-O1D	-4.11	115.79	123.84
33	Q	607	CHL	CMD-C2D-C3D	-4.10	118.19	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	207	BCR	C16-C17-C18	-4.10	121.47	127.31
34	P	614	LUT	C15-C14-C13	-4.09	121.48	127.31
32	2	301	LMG	O7-C10-C11	4.09	120.31	111.50
33	R	605	CHL	CMD-C2D-C3D	-4.09	118.22	127.61
33	R	601	CHL	CMD-C2D-C3D	-4.09	118.22	127.61
33	8	307	CHL	CHB-C1B-NB	-4.08	119.93	124.26
33	P	608	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
33	P	601	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
33	Q	601	CHL	CMD-C2D-C3D	-4.08	118.22	127.61
28	B	842	BCR	C38-C26-C25	-4.08	119.95	124.53
33	5	307	CHL	C1D-ND-C4D	4.08	109.23	106.33
33	R	608	CHL	CMD-C2D-C3D	-4.07	118.24	127.61
28	4	321	BCR	C37-C22-C21	-4.07	117.22	122.92
34	U	314	LUT	C15-C14-C13	-4.07	121.50	127.31
27	2	317	LHG	O7-C7-C8	4.06	120.26	111.50
25	5	313	CLA	CMD-C2D-C1D	4.06	131.87	124.71
33	1	606	CHL	CMD-C2D-C3D	-4.05	118.29	127.61
30	B	846	DGD	O2G-C1B-C2B	4.05	120.23	111.50
28	7	316	BCR	C33-C5-C6	-4.05	119.98	124.53
34	1	616	LUT	C18-C5-C4	4.05	121.86	114.36
32	4	320	LMG	O7-C10-C11	4.05	120.22	111.50
28	A	847	BCR	C20-C21-C22	-4.05	121.54	127.31
28	4	321	BCR	C28-C27-C26	-4.04	106.86	114.08
33	T	601	CHL	CMD-C2D-C3D	-4.04	118.33	127.61
28	J	101	BCR	C20-C21-C22	-4.04	121.55	127.31
33	T	606	CHL	CMD-C2D-C3D	-4.03	118.33	127.61
34	R	616	LUT	C35-C34-C33	-4.03	121.55	127.31
36	U	316	NEX	O24-C25-C38	4.03	119.89	115.06
26	B	839	PQN	C11-C12-C13	-4.03	120.08	126.79
28	3	318	BCR	C33-C5-C6	-4.03	120.00	124.53
33	6	606	CHL	CAC-C3C-C4C	4.03	130.04	124.81
27	1	618	LHG	O7-C7-C8	4.03	120.18	111.50
36	R	617	NEX	O24-C25-C38	4.02	119.88	115.06
33	5	307	CHL	O2D-CGD-CBD	4.02	118.41	111.27
33	P	622	CHL	CHD-C1D-ND	-4.02	120.76	124.45
28	3	318	BCR	C11-C12-C13	-4.02	115.13	126.42
28	O	205	BCR	C38-C26-C25	-4.01	120.02	124.53
25	A	827	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
33	P	606	CHL	CMD-C2D-C3D	-4.01	118.39	127.61
28	L	207	BCR	C15-C14-C13	-4.01	121.59	127.31
33	U	306	CHL	CMD-C2D-C3D	-4.01	118.39	127.61
28	J	106	BCR	C16-C17-C18	-4.00	121.60	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	304	CHL	C2A-C1A-CHA	-4.00	116.86	123.85
33	S	308	CHL	CMD-C2D-C3D	-4.00	118.41	127.61
33	4	304	CHL	C1D-ND-C4D	4.00	109.18	106.33
33	R	601	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
33	P	601	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
33	Q	605	CHL	CMD-C2D-C3D	-3.99	118.43	127.61
27	4	318	LHG	O7-C7-C8	3.99	120.11	111.50
33	Q	601	CHL	CHD-C4C-C3C	-3.98	118.99	124.84
34	R	615	LUT	C15-C14-C13	-3.98	121.63	127.31
33	Q	608	CHL	O2D-CGD-CBD	3.98	118.34	111.27
36	P	617	NEX	O24-C25-C38	3.98	119.83	115.06
35	P	620	XAT	C6-C7-C8	-3.98	117.58	125.99
35	T	615	XAT	C6-C7-C8	-3.98	117.59	125.99
34	R	616	LUT	C31-C30-C29	-3.97	121.64	127.31
33	U	309	CHL	CMD-C2D-C3D	-3.97	118.47	127.61
33	5	307	CHL	CHD-C1D-ND	-3.97	120.80	124.45
33	P	609	CHL	O2D-CGD-CBD	3.97	118.32	111.27
32	J	104	LMG	O7-C10-C11	3.97	120.05	111.50
34	1	615	LUT	C18-C5-C6	-3.96	120.08	124.53
31	B	850	SQD	O47-C7-C8	3.96	120.05	111.50
28	4	317	BCR	C38-C26-C25	-3.96	120.08	124.53
27	8	319	LHG	O7-C7-C8	3.96	120.04	111.50
28	A	847	BCR	C15-C14-C13	-3.96	121.66	127.31
33	R	609	CHL	O2D-CGD-CBD	3.96	118.31	111.27
28	L	208	BCR	C7-C8-C9	-3.96	120.25	126.23
25	1	612	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
33	R	601	CHL	C1-C2-C3	-3.96	120.34	126.75
33	5	308	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
33	U	308	CHL	CMD-C2D-C3D	-3.96	118.50	127.61
33	1	606	CHL	C2A-C1A-CHA	-3.96	116.94	123.86
33	6	617	CHL	CMD-C2D-C3D	-3.96	118.51	127.61
33	Q	601	CHL	C1-C2-C3	-3.95	120.36	126.75
33	S	307	CHL	CHD-C1D-ND	-3.95	120.82	124.45
33	Q	607	CHL	O2D-CGD-CBD	3.95	118.28	111.27
25	1	612	CLA	CHB-C4A-NA	3.95	129.97	124.51
32	6	602	LMG	O7-C10-C11	3.94	120.00	111.50
33	P	601	CHL	C1-C2-C3	-3.94	120.37	126.75
25	a	308	CLA	CHB-C4A-NA	3.94	129.96	124.51
33	P	608	CHL	O2D-CGD-CBD	3.94	118.27	111.27
33	4	304	CHL	CHB-C1B-NB	-3.94	120.09	124.26
28	6	621	BCR	C3-C4-C5	-3.94	107.05	114.08
27	A	844	LHG	O7-C7-C8	3.93	119.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	314	CHL	C1D-ND-C4D	3.93	109.13	106.33
33	a	305	CHL	CMD-C2D-C3D	-3.93	118.57	127.61
28	3	318	BCR	C35-C13-C14	-3.93	117.42	122.92
33	S	302	CHL	CHA-C4D-ND	3.93	140.72	132.50
33	T	601	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
28	L	204	BCR	C15-C14-C13	-3.93	121.70	127.31
34	6	619	LUT	C18-C5-C6	-3.93	120.11	124.53
33	R	608	CHL	O2D-CGD-CBD	3.92	118.24	111.27
33	T	605	CHL	CMD-C2D-C3D	-3.92	118.59	127.61
28	3	317	BCR	C7-C8-C9	-3.92	120.31	126.23
34	2	315	LUT	C21-C26-C27	-3.92	107.75	112.70
33	a	305	CHL	C2A-C1A-CHA	-3.91	117.02	123.86
33	T	607	CHL	CHD-C1D-ND	-3.91	120.86	124.45
34	T	614	LUT	C31-C30-C29	-3.91	121.73	127.31
33	6	607	CHL	O2D-CGD-CBD	3.91	118.21	111.27
35	P	623	XAT	C6-C7-C8	-3.91	117.73	125.99
33	1	606	CHL	CHD-C1D-ND	-3.90	120.87	124.45
28	O	205	BCR	C20-C21-C22	-3.90	121.74	127.31
28	5	323	BCR	C11-C12-C13	-3.90	115.46	126.42
33	S	306	CHL	CMD-C2D-C3D	-3.90	118.64	127.61
25	7	303	CLA	C3B-C4B-NB	-3.89	106.90	110.52
28	I	201	BCR	C28-C27-C26	-3.89	107.12	114.08
27	a	317	LHG	O7-C7-C8	3.89	119.89	111.50
33	6	606	CHL	CHA-C4D-ND	3.89	140.64	132.50
28	B	844	BCR	C33-C5-C6	-3.89	120.16	124.53
33	7	305	CHL	CAC-C3C-C4C	3.89	129.86	124.81
35	P	623	XAT	O4-C5-C18	3.88	119.71	115.06
25	H	202	CLA	CAA-C2A-C3A	-3.88	107.05	116.10
33	T	604	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
33	4	314	CHL	CAC-C3C-C4C	3.88	129.84	124.81
35	P	616	XAT	C6-C7-C8	-3.88	117.80	125.99
35	Q	616	XAT	C26-C27-C28	-3.88	117.80	125.99
33	U	308	CHL	O2D-CGD-CBD	3.88	118.16	111.27
33	4	314	CHL	CMD-C2D-C3D	-3.87	118.71	127.61
28	A	847	BCR	C28-C27-C26	-3.87	107.17	114.08
28	5	320	BCR	C15-C14-C13	-3.86	121.80	127.31
35	Q	616	XAT	C35-C34-C33	-3.86	121.80	127.31
35	T	615	XAT	O4-C5-C18	3.86	119.68	115.06
33	P	622	CHL	CMD-C2D-C3D	-3.86	118.73	127.61
28	A	846	BCR	C3-C4-C5	-3.86	107.19	114.08
33	Q	606	CHL	CMD-C2D-C3D	-3.86	118.74	127.61
28	K	206	BCR	C33-C5-C6	-3.86	120.20	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	842	BCR	C11-C10-C9	-3.86	121.81	127.31
28	B	845	BCR	C28-C27-C26	-3.86	107.19	114.08
33	6	606	CHL	CMB-C2B-C1B	3.85	131.24	125.37
33	S	310	CHL	CMD-C2D-C3D	-3.85	118.75	127.61
35	S	318	XAT	C19-C9-C10	-3.85	117.53	122.92
28	8	301	BCR	C28-C27-C26	-3.85	107.20	114.08
28	B	851	BCR	C20-C21-C22	-3.85	121.81	127.31
28	B	843	BCR	C28-C27-C26	-3.85	107.20	114.08
35	P	623	XAT	C26-C27-C28	-3.84	117.87	125.99
33	S	306	CHL	CHA-C4D-ND	3.84	140.53	132.50
28	L	207	BCR	C20-C21-C22	-3.84	121.83	127.31
25	A	813	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
33	S	306	CHL	C2A-C1A-CHA	-3.83	117.15	123.86
25	A	805	CLA	C3B-C4B-NB	-3.83	106.96	110.52
33	5	308	CHL	CHA-C4D-ND	3.83	140.52	132.50
33	P	605	CHL	CMD-C2D-C3D	-3.83	118.80	127.61
36	P	621	NEX	C5-C6-C1	-3.83	115.89	119.70
33	S	302	CHL	CAC-C3C-C4C	3.83	129.78	124.81
28	F	803	BCR	C15-C14-C13	-3.83	121.85	127.31
28	4	317	BCR	C11-C10-C9	-3.83	121.85	127.31
28	K	206	BCR	C7-C8-C9	-3.83	120.45	126.23
35	P	620	XAT	O4-C5-C18	3.82	119.64	115.06
33	4	304	CHL	CAC-C3C-C4C	3.82	129.77	124.81
25	A	827	CLA	C3B-C4B-NB	-3.82	106.97	110.52
34	T	613	LUT	C15-C14-C13	-3.82	121.85	127.31
25	5	313	CLA	CHD-C1D-ND	-3.82	120.94	124.45
35	S	318	XAT	O24-C25-C38	3.82	119.63	115.06
33	8	307	CHL	C1-C2-C3	-3.82	119.44	126.04
33	4	304	CHL	CMB-C2B-C1B	3.81	131.18	125.37
28	B	840	BCR	C15-C14-C13	-3.81	121.87	127.31
28	5	323	BCR	C37-C22-C23	3.81	124.08	118.08
33	3	306	CHL	CHD-C4C-NC	3.81	130.20	124.20
33	5	308	CHL	C1-C2-C3	-3.81	120.59	126.75
34	3	316	LUT	C18-C5-C6	-3.81	120.25	124.53
33	6	606	CHL	CMD-C2D-C3D	-3.80	118.87	127.61
28	A	846	BCR	C24-C23-C22	-3.80	120.49	126.23
33	7	305	CHL	CHA-C4D-ND	3.80	140.45	132.50
34	4	316	LUT	C18-C5-C6	-3.80	120.26	124.53
33	a	305	CHL	O2D-CGD-CBD	3.79	118.01	111.27
34	a	315	LUT	C18-C5-C4	3.79	121.38	114.36
28	F	803	BCR	C33-C5-C6	-3.79	120.27	124.53
33	S	307	CHL	CHB-C1B-NB	-3.79	120.25	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	841	BCR	C16-C17-C18	-3.79	121.91	127.31
28	B	843	BCR	C21-C20-C19	-3.78	111.41	123.22
25	S	301	CLA	CHB-C1B-NB	3.78	128.26	124.26
33	5	317	CHL	CMD-C2D-C3D	-3.78	118.92	127.61
34	U	315	LUT	C21-C26-C27	-3.78	107.92	112.70
33	U	305	CHL	CMD-C2D-C3D	-3.78	118.92	127.61
34	5	318	LUT	C35-C34-C33	-3.77	121.93	127.31
33	U	305	CHL	C1D-ND-C4D	3.77	109.01	106.33
28	F	801	BCR	C33-C5-C6	-3.77	120.30	124.53
27	S	319	LHG	O7-C7-C8	3.77	119.62	111.50
33	S	321	CHL	CHD-C1D-ND	-3.77	120.99	124.45
34	U	314	LUT	C11-C10-C9	-3.76	121.94	127.31
34	2	316	LUT	C7-C8-C9	-3.76	120.55	126.23
28	B	851	BCR	C33-C5-C6	-3.76	120.30	124.53
28	A	846	BCR	C20-C21-C22	-3.76	121.94	127.31
33	7	305	CHL	C1D-ND-C4D	3.76	109.00	106.33
28	6	621	BCR	C33-C5-C4	3.76	120.83	113.62
28	5	320	BCR	C33-C5-C6	-3.76	120.31	124.53
28	B	841	BCR	C28-C27-C26	-3.75	107.38	114.08
34	S	317	LUT	C15-C14-C13	-3.75	121.96	127.31
33	9	306	CHL	CHD-C4C-NC	3.74	130.10	124.20
25	L	205	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
30	B	848	DGD	C1E-C2E-C3E	3.74	117.79	110.00
34	8	316	LUT	C18-C5-C6	-3.74	120.33	124.53
28	5	323	BCR	C15-C14-C13	-3.74	121.98	127.31
25	A	830	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
33	T	607	CHL	CHA-C4D-ND	3.73	140.31	132.50
34	5	322	LUT	C18-C5-C6	-3.73	120.34	124.53
33	9	306	CHL	CHA-C4D-ND	3.73	140.30	132.50
33	3	306	CHL	CHA-C4D-ND	3.73	140.30	132.50
27	B	847	LHG	O7-C7-C8	3.73	119.54	111.50
34	7	314	LUT	C35-C34-C33	-3.73	121.99	127.31
28	8	301	BCR	C7-C8-C9	-3.73	120.61	126.23
33	S	310	CHL	C4-C3-C5	3.72	120.24	115.98
33	R	605	CHL	C1D-ND-C4D	3.72	108.98	106.33
33	4	314	CHL	CHA-C4D-ND	3.72	140.28	132.50
33	4	322	CHL	CAC-C3C-C4C	3.72	129.64	124.81
33	6	617	CHL	CHD-C1D-ND	-3.72	121.04	124.45
25	T	610	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
34	Q	614	LUT	C15-C14-C13	-3.72	122.01	127.31
33	S	306	CHL	CAC-C3C-C4C	3.72	129.63	124.81
34	S	316	LUT	C35-C34-C33	-3.72	122.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	9	307	CHL	CHA-C4D-ND	3.71	140.27	132.50
33	3	306	CHL	O2D-CGD-CBD	3.71	117.86	111.27
33	6	608	CHL	OMC-CMC-C2C	-3.71	117.31	125.69
33	4	306	CHL	CMD-C2D-C3D	-3.70	119.10	127.61
33	S	309	CHL	CHA-C4D-ND	3.70	140.24	132.50
33	Q	607	CHL	CHD-C1D-ND	-3.70	121.05	124.45
33	4	304	CHL	CHA-C4D-ND	3.70	140.24	132.50
28	B	843	BCR	C15-C14-C13	-3.70	122.03	127.31
33	4	306	CHL	CHD-C4C-NC	3.70	130.03	124.20
25	a	308	CLA	CMA-C3A-C4A	3.70	121.71	111.77
25	a	311	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
33	5	307	CHL	C1D-CHD-C4C	-3.69	118.09	126.06
28	O	204	BCR	C15-C14-C13	-3.69	122.04	127.31
33	P	606	CHL	CHD-C1D-ND	-3.69	121.06	124.45
28	4	321	BCR	C23-C22-C21	3.69	124.61	118.94
30	B	848	DGD	C1D-C2D-C3D	3.69	117.68	110.00
33	9	307	CHL	CMD-C2D-C3D	-3.69	119.13	127.61
32	J	102	LMG	O7-C10-C11	3.69	119.45	111.50
33	6	607	CHL	CMD-C2D-C3D	-3.68	119.14	127.61
34	R	615	LUT	C18-C5-C6	-3.68	120.39	124.53
33	U	307	CHL	CHD-C1D-ND	-3.68	121.07	124.45
33	S	302	CHL	C1D-ND-C4D	3.68	108.95	106.33
28	B	845	BCR	C7-C8-C9	-3.68	120.68	126.23
33	U	305	CHL	CHA-C4D-ND	3.68	140.19	132.50
28	3	319	BCR	C33-C5-C6	-3.68	120.40	124.53
33	9	307	CHL	CAC-C3C-C4C	3.67	129.58	124.81
34	1	617	LUT	C18-C5-C4	3.67	121.16	114.36
33	Q	605	CHL	CHA-C4D-ND	3.67	140.18	132.50
34	2	316	LUT	C18-C5-C6	-3.67	120.41	124.53
25	B	822	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
28	L	204	BCR	C28-C27-C26	-3.67	107.53	114.08
28	A	845	BCR	C33-C5-C6	-3.67	120.41	124.53
33	T	606	CHL	CHD-C1D-ND	-3.67	121.08	124.45
33	U	309	CHL	C2A-C1A-CHA	-3.67	117.45	123.86
25	6	613	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
25	1	609	CLA	CMA-C3A-C4A	3.67	121.62	111.77
25	9	304	CLA	C3B-C4B-NB	-3.66	107.12	110.52
25	P	611	CLA	CHB-C4A-NA	3.66	129.58	124.51
25	B	826	CLA	C3B-C4B-NB	-3.66	107.12	110.52
33	9	306	CHL	CHD-C1D-ND	-3.66	121.09	124.45
33	6	608	CHL	CHA-C4D-ND	3.66	140.16	132.50
33	9	307	CHL	CHB-C1B-NB	-3.66	120.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	849	BCR	C20-C19-C18	-3.66	116.13	126.42
25	A	835	CLA	C3B-C4B-NB	-3.66	107.12	110.52
33	S	309	CHL	C4-C3-C5	3.66	120.16	115.98
25	A	840	CLA	O2D-CGD-O1D	-3.66	116.69	123.84
33	8	307	CHL	C6-C5-C3	-3.66	108.64	114.62
28	8	301	BCR	C3-C4-C5	-3.65	107.55	114.08
33	T	605	CHL	CHD-C1D-ND	-3.65	121.10	124.45
33	R	605	CHL	C2A-C1A-CHA	-3.65	117.47	123.86
33	P	619	CHL	CHA-C4D-ND	3.65	140.14	132.50
33	5	307	CHL	CAC-C3C-C4C	3.65	129.55	124.81
33	6	617	CHL	CHA-C4D-ND	3.65	140.13	132.50
28	J	106	BCR	C37-C22-C21	-3.64	117.82	122.92
28	B	841	BCR	C11-C10-C9	-3.64	122.11	127.31
25	B	810	CLA	C3B-C4B-NB	-3.64	107.14	110.52
33	S	307	CHL	CHA-C4D-ND	3.64	140.12	132.50
33	6	607	CHL	CHB-C1B-NB	-3.64	120.40	124.26
33	P	607	CHL	CHA-C4D-ND	3.64	140.11	132.50
33	4	306	CHL	CHA-C4D-ND	3.64	140.11	132.50
25	5	324	CLA	C3B-C4B-NB	-3.64	107.14	110.52
34	4	315	LUT	C18-C5-C6	-3.64	120.44	124.53
34	Q	615	LUT	C35-C34-C33	-3.64	122.12	127.31
33	T	601	CHL	C2A-C1A-CHA	-3.64	117.50	123.86
34	8	316	LUT	C7-C8-C9	-3.64	120.74	126.23
28	J	101	BCR	C15-C16-C17	-3.63	116.03	123.47
33	P	608	CHL	CHD-C1D-ND	-3.63	121.12	124.45
33	T	607	CHL	OBD-CAD-C3D	-3.63	119.78	128.52
28	5	323	BCR	C34-C9-C10	-3.63	117.84	122.92
33	R	607	CHL	CHA-C4D-ND	3.63	140.09	132.50
33	5	307	CHL	CHA-C4D-ND	3.63	140.09	132.50
33	4	322	CHL	C1D-ND-C4D	3.62	108.91	106.33
28	8	301	BCR	C33-C5-C6	-3.62	120.46	124.53
34	1	616	LUT	C35-C34-C33	-3.62	122.14	127.31
33	S	302	CHL	O2D-CGD-CBD	3.62	117.69	111.27
28	B	851	BCR	C21-C20-C19	-3.62	111.93	123.22
34	7	314	LUT	C18-C5-C6	-3.62	120.47	124.53
33	U	308	CHL	CHD-C1D-ND	-3.61	121.13	124.45
33	4	314	CHL	CHD-C1D-ND	-3.61	121.13	124.45
33	P	605	CHL	CHD-C1D-ND	-3.61	121.13	124.45
28	J	106	BCR	C1-C6-C5	-3.61	117.52	122.61
28	5	323	BCR	C33-C5-C6	-3.61	120.47	124.53
33	1	606	CHL	CHA-C4D-ND	3.61	140.06	132.50
33	Q	606	CHL	CHA-C4D-ND	3.61	140.05	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	605	CHL	CHA-C4D-ND	3.61	140.05	132.50
25	2	302	CLA	C3B-C4B-NB	-3.61	107.17	110.52
28	A	847	BCR	C38-C26-C25	-3.61	120.48	124.53
33	S	309	CHL	O2D-CGD-CBD	3.60	117.67	111.27
33	P	622	CHL	C6-C5-C3	-3.60	108.72	114.62
25	1	612	CLA	C4D-C3D-CAD	3.60	112.34	108.10
28	B	851	BCR	C33-C5-C4	3.60	120.54	113.62
34	U	314	LUT	C21-C26-C27	-3.60	108.15	112.70
33	6	607	CHL	C1D-CHD-C4C	-3.60	118.29	126.06
28	A	849	BCR	C3-C4-C5	-3.60	107.66	114.08
25	A	836	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
33	Q	606	CHL	CHB-C1B-NB	-3.60	120.45	124.26
35	T	615	XAT	C26-C27-C28	-3.59	118.39	125.99
34	T	614	LUT	C15-C14-C13	-3.59	122.18	127.31
33	Q	606	CHL	C3B-C4B-NB	3.59	113.85	110.52
33	6	608	CHL	CHD-C4C-NC	3.59	129.86	124.20
28	B	842	BCR	C33-C5-C6	-3.59	120.50	124.53
33	4	304	CHL	CMD-C2D-C3D	-3.59	119.36	127.61
33	R	608	CHL	CHD-C1D-ND	-3.59	121.16	124.45
28	8	318	BCR	C7-C8-C9	-3.59	120.81	126.23
36	U	301	NEX	O24-C25-C38	3.59	119.35	115.06
28	8	318	BCR	C33-C5-C6	-3.59	120.50	124.53
33	R	607	CHL	CHD-C1D-ND	-3.59	121.16	124.45
33	4	306	CHL	C1D-ND-C4D	3.58	108.88	106.33
34	1	617	LUT	C7-C8-C9	-3.58	120.83	126.23
28	A	846	BCR	C15-C14-C13	-3.58	122.20	127.31
33	6	606	CHL	C3B-C4B-NB	3.58	113.83	110.52
28	B	844	BCR	C3-C4-C5	-3.58	107.69	114.08
33	S	308	CHL	CHA-C4D-ND	3.58	139.98	132.50
33	S	302	CHL	C3C-C4C-NC	3.58	114.58	110.57
28	J	101	BCR	C7-C8-C9	-3.58	120.83	126.23
33	8	307	CHL	O1D-CGD-CBD	-3.57	117.17	124.48
33	T	607	CHL	C2A-C1A-CHA	-3.57	117.61	123.86
33	R	606	CHL	CMD-C2D-C3D	-3.57	119.39	127.61
33	6	606	CHL	CHD-C4C-NC	3.57	129.83	124.20
28	7	316	BCR	C3-C4-C5	-3.57	107.70	114.08
28	F	803	BCR	C3-C4-C5	-3.57	107.70	114.08
33	P	607	CHL	CHD-C1D-ND	-3.57	121.17	124.45
34	8	317	LUT	C7-C8-C9	-3.57	120.84	126.23
25	P	611	CLA	CMA-C3A-C4A	-3.57	102.18	111.77
28	A	849	BCR	C34-C9-C10	-3.57	117.93	122.92
25	a	303	CLA	C6-C5-C3	-3.57	104.10	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	T	604	CHL	CHA-C4D-ND	3.57	139.96	132.50
34	T	613	LUT	C18-C5-C6	-3.56	120.53	124.53
33	U	306	CHL	CHA-C4D-ND	3.56	139.95	132.50
33	P	606	CHL	CHA-C4D-ND	3.56	139.94	132.50
33	P	619	CHL	CHD-C1D-ND	-3.56	121.19	124.45
34	6	622	LUT	C18-C5-C6	-3.56	120.53	124.53
33	P	622	CHL	C2A-C1A-CHA	-3.55	117.64	123.86
28	A	846	BCR	C33-C5-C6	-3.55	120.54	124.53
25	a	308	CLA	O2D-CGD-O1D	-3.55	116.91	123.84
28	B	842	BCR	C15-C14-C13	-3.55	122.25	127.31
28	3	319	BCR	C20-C19-C18	-3.54	116.46	126.42
35	P	620	XAT	C26-C27-C28	-3.54	118.51	125.99
34	S	317	LUT	C31-C32-C33	-3.54	116.47	126.42
33	S	308	CHL	C3B-C4B-NB	3.54	113.80	110.52
33	U	306	CHL	CHD-C1D-ND	-3.54	121.20	124.45
33	5	317	CHL	CHD-C4C-NC	3.54	129.78	124.20
33	T	605	CHL	CHA-C4D-ND	3.54	139.90	132.50
33	U	305	CHL	C2A-C1A-CHA	-3.54	117.68	123.86
33	U	307	CHL	CHA-C4D-ND	3.53	139.89	132.50
27	1	618	LHG	C5-O7-C7	-3.53	109.09	117.79
28	G	203	BCR	C33-C5-C6	-3.53	120.56	124.53
33	T	606	CHL	CHA-C4D-ND	3.53	139.89	132.50
36	T	616	NEX	C17-C1-C6	-3.53	107.31	110.47
33	U	308	CHL	CAC-C3C-C4C	3.53	129.39	124.81
25	B	830	CLA	C3B-C4B-NB	-3.53	107.24	110.52
33	S	309	CHL	CHD-C4C-NC	3.53	129.76	124.20
25	B	815	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
25	A	819	CLA	C3B-C4B-NB	-3.53	107.24	110.52
33	T	604	CHL	C3B-C4B-NB	3.53	113.79	110.52
33	Q	605	CHL	CAA-C2A-C3A	-3.53	107.87	116.10
34	Q	615	LUT	C15-C14-C13	-3.53	122.28	127.31
25	B	803	CLA	C3B-C4B-NB	-3.52	107.25	110.52
33	P	622	CHL	CHA-C4D-ND	3.52	139.87	132.50
34	P	614	LUT	C11-C10-C9	-3.52	122.28	127.31
33	U	305	CHL	C3B-C4B-NB	3.52	113.78	110.52
25	A	842	CLA	CAC-C3C-C2C	3.52	133.55	127.53
25	Q	610	CLA	CBD-CHA-C1A	3.52	132.65	128.50
33	4	305	CHL	CMB-C2B-C1B	3.52	130.73	125.37
36	R	617	NEX	C31-C30-C29	-3.52	122.29	127.31
25	7	309	CLA	CAA-C2A-C3A	-3.52	107.89	116.10
33	5	308	CHL	O2A-CGA-CBA	3.52	122.95	111.91
34	T	613	LUT	C21-C26-C27	-3.52	108.25	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	608	CHL	CHD-C1D-ND	-3.52	121.22	124.45
33	8	307	CHL	CHD-C1D-ND	-3.52	121.22	124.45
33	3	306	CHL	C6-C5-C3	-3.52	108.87	114.62
33	4	322	CHL	CHA-C4D-ND	3.51	139.85	132.50
34	P	614	LUT	C35-C15-C14	-3.51	116.28	123.47
27	5	301	LHG	O7-C7-C8	3.51	119.07	111.50
25	3	320	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
28	I	201	BCR	C33-C5-C4	3.51	120.36	113.62
33	1	601	CHL	C1D-CHD-C4C	-3.51	118.48	126.06
28	L	203	BCR	C38-C26-C25	-3.51	120.59	124.53
27	Q	617	LHG	O7-C7-C8	3.51	119.06	111.50
34	U	314	LUT	C35-C15-C14	-3.51	116.29	123.47
33	S	310	CHL	CAC-C3C-C4C	3.51	129.36	124.81
25	B	834	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
33	6	617	CHL	CAC-C3C-C4C	3.51	129.36	124.81
25	B	815	CLA	C3B-C4B-NB	-3.50	107.27	110.52
33	1	601	CHL	C1D-ND-C4D	3.50	108.82	106.33
34	R	615	LUT	C11-C10-C9	-3.50	122.31	127.31
34	8	316	LUT	C16-C1-C6	-3.50	104.62	110.30
28	4	321	BCR	C3-C4-C5	-3.50	107.83	114.08
33	8	307	CHL	O2D-CGD-O1D	-3.50	117.00	123.84
33	8	307	CHL	CMB-C2B-C1B	3.50	130.70	125.37
33	8	307	CHL	CAC-C3C-C4C	3.50	129.35	124.81
34	T	614	LUT	C35-C34-C33	-3.50	122.32	127.31
33	R	606	CHL	CHA-C4D-ND	3.49	139.81	132.50
28	8	318	BCR	C16-C17-C18	-3.49	122.33	127.31
34	P	615	LUT	C15-C14-C13	-3.49	122.33	127.31
33	T	601	CHL	CHA-C4D-ND	3.49	139.79	132.50
28	I	201	BCR	C11-C10-C9	-3.49	122.34	127.31
33	Q	606	CHL	CAC-C3C-C4C	3.49	129.33	124.81
33	Q	605	CHL	CHD-C1D-ND	-3.48	121.25	124.45
25	A	840	CLA	C3B-C4B-NB	-3.48	107.28	110.52
25	B	804	CLA	C3B-C4B-NB	-3.48	107.28	110.52
33	R	606	CHL	C3B-C4B-NB	3.48	113.75	110.52
33	4	322	CHL	C4-C3-C5	3.48	121.13	115.27
34	4	315	LUT	C15-C14-C13	-3.48	122.34	127.31
33	P	605	CHL	C3B-C4B-NB	3.48	113.75	110.52
28	K	206	BCR	C36-C18-C17	-3.48	118.05	122.92
33	4	306	CHL	C1-C2-C3	-3.48	121.12	126.75
34	R	615	LUT	C7-C8-C9	-3.48	120.98	126.23
33	4	304	CHL	C3B-C4B-NB	3.48	113.74	110.52
34	U	315	LUT	C15-C14-C13	-3.48	122.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	S	316	LUT	C18-C5-C6	-3.48	120.62	124.53
33	U	308	CHL	CHA-C4D-ND	3.48	139.77	132.50
35	S	318	XAT	C26-C27-C28	-3.47	118.65	125.99
33	6	607	CHL	CHA-C4D-ND	3.47	139.77	132.50
36	P	621	NEX	C27-C28-C29	-3.47	120.14	125.53
33	Q	601	CHL	C2A-C1A-CHA	-3.47	117.79	123.86
33	S	302	CHL	CMD-C2D-C3D	-3.47	119.63	127.61
33	R	607	CHL	C3B-C4B-NB	3.47	113.73	110.52
33	T	604	CHL	CHD-C1D-ND	-3.47	121.27	124.45
33	P	608	CHL	CHA-C4D-ND	3.47	139.75	132.50
32	6	602	LMG	C4-C3-C2	3.47	116.88	110.82
34	1	615	LUT	C35-C15-C14	-3.47	116.37	123.47
28	8	301	BCR	C24-C23-C22	-3.47	121.00	126.23
34	7	314	LUT	C7-C8-C9	-3.47	121.00	126.23
33	4	322	CHL	C3C-C4C-NC	3.47	114.46	110.57
33	6	607	CHL	CMB-C2B-C1B	3.47	130.65	125.37
33	P	607	CHL	C3B-C4B-NB	3.47	113.73	110.52
33	P	619	CHL	CAC-C3C-C4C	3.47	129.31	124.81
33	S	308	CHL	CAC-C3C-C4C	3.47	129.31	124.81
33	R	601	CHL	C2A-C1A-CHA	-3.46	117.80	123.86
33	R	605	CHL	CHD-C1D-ND	-3.46	121.27	124.45
33	3	306	CHL	C1D-ND-C4D	3.46	108.80	106.33
34	8	316	LUT	C15-C14-C13	-3.46	122.37	127.31
33	Q	607	CHL	CHA-C4D-ND	3.46	139.74	132.50
33	6	606	CHL	C1D-ND-C4D	3.46	108.79	106.33
33	P	601	CHL	C2A-C1A-CHA	-3.46	117.81	123.86
25	A	824	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
33	Q	607	CHL	C3B-C4B-NB	3.46	113.72	110.52
28	A	846	BCR	C7-C8-C9	-3.46	121.01	126.23
27	a	317	LHG	C5-O7-C7	-3.45	109.28	117.79
35	P	616	XAT	C26-C27-C28	-3.45	118.69	125.99
28	F	803	BCR	C21-C20-C19	-3.45	112.44	123.22
33	P	605	CHL	CHA-C4D-ND	3.45	139.72	132.50
33	4	305	CHL	C2A-C1A-CHA	-3.45	117.82	123.86
34	a	314	LUT	C18-C5-C6	-3.45	120.65	124.53
25	P	611	CLA	C3B-C2B-C1B	-3.45	103.00	107.16
28	F	803	BCR	C15-C16-C17	-3.45	116.41	123.47
33	5	308	CHL	C3C-C4C-NC	3.45	114.44	110.57
33	Q	606	CHL	CHD-C1D-ND	-3.45	121.28	124.45
25	K	201	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
25	5	313	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
25	L	209	CLA	C3B-C4B-NB	-3.45	107.32	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	803	BCR	C1-C6-C5	-3.44	117.76	122.61
33	5	317	CHL	CHA-C4D-ND	3.44	139.70	132.50
33	P	607	CHL	CAC-C3C-C4C	3.44	129.28	124.81
25	A	833	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
25	R	612	CLA	C11-C10-C8	3.44	127.05	115.92
33	Q	605	CHL	C1D-ND-C4D	3.44	108.78	106.33
33	4	322	CHL	C1D-CHD-C4C	-3.44	118.64	126.06
25	U	313	CLA	CHC-C4B-NB	3.44	127.90	124.26
36	R	617	NEX	C17-C1-C6	-3.44	107.39	110.47
33	U	309	CHL	CHA-C4D-ND	3.44	139.69	132.50
32	6	602	LMG	C3-C4-C5	3.44	116.37	110.24
33	R	608	CHL	CHA-C4D-ND	3.44	139.69	132.50
25	A	801	CLA	C3B-C4B-NB	-3.44	107.33	110.52
33	P	619	CHL	C3B-C4B-NB	3.44	113.70	110.52
33	R	605	CHL	CAA-C2A-C3A	-3.43	103.37	112.78
34	8	317	LUT	C18-C5-C6	-3.43	120.67	124.53
33	T	605	CHL	C3B-C4B-NB	3.43	113.70	110.52
28	A	854	BCR	C33-C5-C6	-3.43	120.67	124.53
25	P	612	CLA	C11-C10-C8	3.43	127.01	115.92
33	S	309	CHL	C3B-C4B-NB	3.43	113.70	110.52
25	P	603	CLA	CHB-C4A-NA	3.43	129.25	124.51
28	7	316	BCR	C16-C17-C18	-3.43	122.42	127.31
33	S	321	CHL	CHD-C4C-NC	3.43	129.60	124.20
33	R	608	CHL	CAC-C3C-C4C	3.43	129.25	124.81
28	I	201	BCR	C16-C15-C14	-3.42	116.46	123.47
34	R	616	LUT	C18-C5-C6	-3.42	120.68	124.53
33	1	601	CHL	C3C-C4C-NC	3.42	114.41	110.57
34	R	615	LUT	C35-C15-C14	-3.42	116.46	123.47
33	1	606	CHL	CMB-C2B-C1B	3.42	130.58	125.37
25	4	308	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
33	1	606	CHL	C1D-CHD-C4C	-3.42	118.68	126.06
33	P	608	CHL	C3B-C4B-NB	3.42	113.69	110.52
36	U	301	NEX	C11-C12-C13	-3.42	116.81	126.42
34	4	315	LUT	C7-C8-C9	-3.42	121.07	126.23
33	U	306	CHL	C1D-ND-C4D	3.42	108.76	106.33
25	1	610	CLA	C3B-C4B-NB	-3.42	107.34	110.52
33	6	607	CHL	C3B-C4B-NB	3.42	113.69	110.52
25	P	611	CLA	C4D-CHA-C1A	-3.42	117.09	121.25
28	I	201	BCR	C7-C8-C9	-3.42	121.07	126.23
33	R	606	CHL	CHD-C1D-ND	-3.42	121.31	124.45
25	B	812	CLA	C3B-C4B-NB	-3.41	107.35	110.52
25	B	806	CLA	O2D-CGD-O1D	-3.41	117.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	3	306	CHL	C1-C2-C3	-3.41	120.14	126.04
33	S	308	CHL	CHD-C1D-ND	-3.41	121.32	124.45
27	5	321	LHG	C5-O7-C7	-3.41	109.39	117.79
25	1	613	CLA	O1D-CGD-CBD	3.41	131.46	124.48
25	L	209	CLA	CAA-C2A-C3A	-3.41	108.15	116.10
33	R	608	CHL	C3B-C4B-NB	3.41	113.67	110.52
33	9	306	CHL	C3C-C4C-NC	3.41	114.39	110.57
33	R	607	CHL	CAC-C3C-C4C	3.41	129.23	124.81
28	L	207	BCR	C24-C23-C22	-3.40	121.09	126.23
33	P	608	CHL	CAC-C3C-C4C	3.40	129.23	124.81
33	Q	607	CHL	CAC-C3C-C4C	3.40	129.22	124.81
33	T	604	CHL	CAA-C2A-C3A	-3.40	103.46	112.78
33	U	307	CHL	C3B-C4B-NB	3.40	113.67	110.52
36	P	617	NEX	C31-C30-C29	-3.40	122.45	127.31
28	J	106	BCR	C23-C22-C21	3.40	124.16	118.94
33	6	617	CHL	C3B-C4B-NB	3.40	113.67	110.52
25	A	807	CLA	C3B-C4B-NB	-3.40	107.36	110.52
25	B	801	CLA	C3B-C4B-NB	-3.40	107.36	110.52
28	B	842	BCR	C3-C4-C5	-3.40	108.01	114.08
25	A	806	CLA	C3B-C4B-NB	-3.40	107.36	110.52
25	B	838	CLA	C3B-C4B-NB	-3.40	107.36	110.52
33	4	306	CHL	CHD-C1D-ND	-3.40	121.33	124.45
28	B	841	BCR	C1-C6-C5	-3.39	117.83	122.61
25	a	309	CLA	C3B-C4B-NB	-3.39	107.37	110.52
33	4	305	CHL	CHA-C4D-ND	3.39	139.60	132.50
28	L	208	BCR	C11-C10-C9	-3.39	122.47	127.31
33	1	601	CHL	CHD-C4C-NC	3.39	129.55	124.20
33	a	305	CHL	CHA-C4D-ND	3.39	139.59	132.50
28	F	803	BCR	C11-C12-C13	-3.39	116.89	126.42
25	3	311	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
28	7	316	BCR	C38-C26-C25	-3.39	120.72	124.53
25	R	614	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
28	4	321	BCR	C38-C26-C27	3.39	120.12	113.62
33	Q	607	CHL	CMB-C2B-C1B	3.39	130.53	125.37
34	4	315	LUT	C20-C13-C12	3.39	123.41	118.08
33	S	302	CHL	CHD-C4C-NC	3.39	129.54	124.20
25	2	314	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
33	U	306	CHL	C3B-C4B-NB	3.38	113.66	110.52
33	T	605	CHL	C1D-ND-C4D	3.38	108.74	106.33
28	4	321	BCR	C33-C5-C4	3.38	120.11	113.62
34	5	322	LUT	C3-C4-C5	-3.38	105.12	111.85
33	S	321	CHL	CHA-C4D-ND	3.38	139.56	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Q	615	LUT	C10-C11-C12	-3.37	112.69	123.22
33	P	608	CHL	CMB-C2B-C1B	3.37	130.51	125.37
25	5	302	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
33	S	308	CHL	CHD-C4C-NC	3.37	129.51	124.20
32	J	107	LMG	O7-C10-C11	3.37	118.76	111.50
25	B	816	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
33	5	307	CHL	O2A-CGA-CBA	3.37	122.47	111.91
34	U	315	LUT	C35-C34-C33	-3.37	122.51	127.31
28	B	842	BCR	C33-C5-C4	3.37	120.08	113.62
33	U	308	CHL	C1D-ND-C4D	3.37	108.73	106.33
33	R	608	CHL	CMB-C2B-C1B	3.37	130.50	125.37
25	9	301	CLA	C3B-C4B-NB	-3.37	107.98	110.23
28	A	849	BCR	C10-C11-C12	-3.36	112.72	123.22
36	P	621	NEX	C24-C23-C22	-3.36	104.28	110.77
25	R	611	CLA	C1-O2A-CGA	3.36	125.27	116.44
25	4	310	CLA	CHB-C4A-NA	3.36	129.16	124.51
33	Q	601	CHL	CHA-C4D-ND	3.36	139.53	132.50
34	8	317	LUT	C15-C14-C13	-3.36	122.52	127.31
33	P	601	CHL	CHA-C4D-ND	3.36	139.53	132.50
33	S	310	CHL	CHA-C4D-ND	3.36	139.52	132.50
33	7	305	CHL	CHD-C1D-ND	-3.36	121.37	124.45
33	5	307	CHL	CHC-C1C-NC	3.36	129.29	124.20
36	T	616	NEX	C31-C30-C29	-3.36	122.52	127.31
33	8	307	CHL	C1D-CHD-C4C	-3.36	118.82	126.06
33	Q	606	CHL	C1D-ND-C4D	3.35	108.72	106.33
33	6	607	CHL	C3C-C4C-NC	3.35	114.33	110.57
33	Q	605	CHL	C3B-C4B-NB	3.35	113.63	110.52
28	K	206	BCR	C11-C10-C9	-3.35	122.53	127.31
33	4	306	CHL	CAC-C3C-C4C	3.35	129.16	124.81
33	S	310	CHL	CHD-C1D-ND	-3.35	121.37	124.45
28	8	318	BCR	C23-C24-C25	-3.35	117.79	127.20
28	B	843	BCR	C7-C8-C9	-3.35	121.17	126.23
25	B	807	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
25	4	303	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
33	S	321	CHL	C4A-NA-C1A	-3.35	105.20	106.71
33	R	601	CHL	CHA-C4D-ND	3.35	139.50	132.50
25	6	605	CLA	C3B-C4B-NB	-3.35	107.41	110.52
25	K	204	CLA	CHB-C4A-NA	3.35	129.14	124.51
25	7	312	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
25	A	813	CLA	C3B-C4B-NB	-3.34	107.41	110.52
36	P	617	NEX	C39-C29-C30	-3.34	118.24	122.92
28	L	203	BCR	C20-C21-C22	-3.34	122.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	308	CLA	C3B-C4B-NB	-3.34	107.42	110.52
33	5	308	CHL	CHD-C4C-NC	3.34	129.47	124.20
35	P	623	XAT	C10-C11-C12	-3.34	116.33	124.67
28	F	803	BCR	C33-C5-C4	3.34	120.03	113.62
34	Q	614	LUT	C35-C15-C14	-3.34	116.63	123.47
25	L	201	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
33	T	604	CHL	C1D-ND-C4D	3.34	108.71	106.33
34	9	313	LUT	C35-C34-C33	-3.34	122.55	127.31
25	B	825	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
28	3	318	BCR	C15-C16-C17	-3.34	116.64	123.47
36	P	621	NEX	C26-C27-C28	-3.34	118.94	125.99
28	B	851	BCR	C3-C4-C5	-3.34	108.12	114.08
25	3	309	CLA	CAA-C2A-C3A	-3.34	108.31	116.10
33	P	606	CHL	C1D-ND-C4D	3.33	108.70	106.33
25	A	804	CLA	C3B-C4B-NB	-3.33	107.42	110.52
36	T	616	NEX	C11-C12-C13	-3.33	117.05	126.42
25	7	307	CLA	C3B-C4B-NB	-3.33	107.42	110.52
33	S	321	CHL	C3B-C4B-NB	3.33	113.61	110.52
33	9	307	CHL	CHD-C1D-ND	-3.33	121.39	124.45
25	A	825	CLA	C3B-C4B-NB	-3.33	107.43	110.52
32	J	107	LMG	C7-O1-C1	-3.33	107.24	113.74
28	B	851	BCR	C16-C15-C14	-3.33	116.66	123.47
27	R	618	LHG	O7-C7-C8	3.32	118.67	111.50
33	S	310	CHL	C1D-ND-C4D	3.32	108.70	106.33
33	S	309	CHL	C1-C2-C3	-3.32	120.30	126.04
25	6	612	CLA	C3B-C4B-NB	-3.32	107.43	110.52
28	L	203	BCR	C4-C5-C6	-3.32	117.91	122.73
25	Q	618	CLA	C3B-C4B-NB	-3.32	107.43	110.52
33	9	307	CHL	C1D-CHD-C4C	-3.32	118.89	126.06
25	1	604	CLA	C2D-C1D-ND	-3.32	107.66	110.10
25	O	203	CLA	C3B-C4B-NB	-3.32	108.01	110.23
33	5	317	CHL	CHD-C1D-ND	-3.32	121.40	124.45
36	P	617	NEX	C11-C12-C13	-3.32	117.09	126.42
36	P	621	NEX	C17-C1-C16	3.32	118.71	108.53
33	6	617	CHL	C1D-ND-C4D	3.32	108.69	106.33
28	O	205	BCR	C24-C23-C22	-3.32	121.22	126.23
34	Q	614	LUT	C11-C10-C9	-3.31	122.58	127.31
27	P	624	LHG	O7-C7-C8	3.31	118.64	111.50
34	P	614	LUT	C18-C5-C6	-3.31	120.81	124.53
35	S	318	XAT	C31-C30-C29	-3.31	122.58	127.31
33	4	322	CHL	CBA-CAA-C2A	-3.31	104.09	113.86
28	8	301	BCR	C11-C10-C9	-3.31	122.59	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	P	618	LHG	O7-C7-C8	3.31	118.63	111.50
33	U	309	CHL	OBD-CAD-C3D	-3.31	120.56	128.52
33	R	606	CHL	C1D-ND-C4D	3.31	108.69	106.33
33	5	308	CHL	C1D-ND-C4D	3.31	108.69	106.33
25	5	312	CLA	C3B-C4B-NB	-3.31	107.45	110.52
33	R	605	CHL	O2D-CGD-O1D	-3.30	117.38	123.84
33	1	601	CHL	CHA-C4D-ND	3.30	139.41	132.50
33	T	606	CHL	CHD-C4C-NC	3.30	129.41	124.20
33	3	306	CHL	C3B-C4B-NB	3.30	113.58	110.52
25	5	313	CLA	CHB-C4A-NA	3.30	129.08	124.51
25	a	308	CLA	C3C-C4C-NC	-3.30	106.87	110.57
33	6	608	CHL	C3C-C4C-NC	3.30	114.27	110.57
33	3	306	CHL	CHD-C1D-ND	-3.30	121.42	124.45
33	P	622	CHL	C1D-CHD-C4C	-3.30	118.94	126.06
33	5	307	CHL	CMB-C2B-C1B	3.30	130.39	125.37
28	3	317	BCR	C20-C21-C22	-3.30	122.60	127.31
34	3	315	LUT	C15-C14-C13	-3.30	122.60	127.31
25	B	827	CLA	C3B-C4B-NB	-3.30	107.46	110.52
35	Q	616	XAT	C24-C23-C22	-3.30	104.41	110.77
33	6	607	CHL	CHD-C1D-ND	-3.29	121.43	124.45
34	a	316	LUT	C1-C2-C3	3.29	121.08	113.64
25	B	812	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
30	B	848	DGD	O2G-C1B-C2B	3.29	118.60	111.50
33	S	302	CHL	CMB-C2B-C1B	3.29	130.38	125.37
25	2	313	CLA	CAA-C2A-C3A	-3.29	103.77	112.78
33	T	607	CHL	C4-C3-C5	3.29	119.74	115.98
33	a	305	CHL	C1D-CHD-C4C	-3.29	118.96	126.06
25	A	822	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
33	U	306	CHL	CHD-C4C-NC	3.29	129.38	124.20
25	B	837	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	7	309	CLA	C3B-C4B-NB	-3.29	107.47	110.52
28	O	205	BCR	C34-C9-C10	-3.29	118.32	122.92
33	6	607	CHL	C1D-ND-C4D	3.29	108.67	106.33
33	T	606	CHL	C3B-C4B-NB	3.28	113.56	110.52
28	O	205	BCR	C3-C4-C5	-3.28	108.21	114.08
25	6	615	CLA	C3B-C4B-NB	-3.28	107.47	110.52
36	U	316	NEX	C31-C30-C29	-3.28	122.63	127.31
28	A	849	BCR	C19-C18-C17	3.28	123.98	118.94
34	P	615	LUT	C10-C11-C12	-3.28	112.98	123.22
28	3	318	BCR	C38-C26-C27	3.28	119.92	113.62
25	O	201	CLA	CAA-C2A-C3A	-3.28	108.44	116.10
28	7	316	BCR	C33-C5-C4	3.28	119.92	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	843	BCR	C38-C26-C25	-3.28	120.85	124.53
25	3	307	CLA	C3B-C4B-NB	-3.28	107.47	110.52
34	7	314	LUT	C18-C5-C4	3.28	120.43	114.36
28	5	320	BCR	C38-C26-C25	-3.28	120.85	124.53
25	B	828	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
25	B	837	CLA	C3B-C4B-NB	-3.28	107.48	110.52
25	A	826	CLA	C3B-C4B-NB	-3.27	107.48	110.52
34	6	619	LUT	C15-C14-C13	-3.27	122.64	127.31
25	A	836	CLA	C3B-C4B-NB	-3.27	107.48	110.52
25	A	842	CLA	CAC-C3C-C4C	-3.27	120.57	124.81
34	U	315	LUT	C18-C5-C6	-3.27	120.86	124.53
33	S	309	CHL	CHD-C1D-ND	-3.27	121.45	124.45
28	3	317	BCR	C38-C26-C25	-3.27	120.86	124.53
33	T	605	CHL	CHD-C4C-NC	3.27	129.35	124.20
25	B	810	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
25	6	611	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
25	A	831	CLA	O2D-CGD-O1D	-3.26	117.45	123.84
33	U	308	CHL	CMB-C2B-C1B	3.26	130.34	125.37
34	T	613	LUT	C11-C10-C9	-3.26	122.65	127.31
36	U	316	NEX	C11-C12-C13	-3.26	117.25	126.42
34	T	613	LUT	C35-C15-C14	-3.26	116.79	123.47
33	4	314	CHL	C3B-C4B-NB	3.26	113.54	110.52
28	J	106	BCR	C20-C19-C18	-3.26	117.26	126.42
34	a	315	LUT	C35-C34-C33	-3.26	122.66	127.31
28	I	201	BCR	C33-C5-C6	-3.26	120.87	124.53
25	6	620	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
25	9	310	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
33	6	608	CHL	O2A-CGA-CBA	3.26	122.13	111.91
25	4	311	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
28	B	844	BCR	C11-C10-C9	-3.25	122.67	127.31
33	P	606	CHL	CHD-C4C-NC	3.25	129.33	124.20
28	A	849	BCR	C38-C26-C25	-3.25	120.88	124.53
28	8	301	BCR	C38-C26-C25	-3.25	120.88	124.53
33	6	607	CHL	CHD-C4C-NC	3.25	129.32	124.20
33	4	305	CHL	C1D-CHD-C4C	-3.25	119.05	126.06
25	5	310	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
33	S	302	CHL	CHB-C1B-NB	-3.25	120.82	124.26
34	2	315	LUT	C15-C14-C13	-3.25	122.67	127.31
33	6	607	CHL	CAC-C3C-C4C	3.25	129.02	124.81
35	P	623	XAT	C24-C23-C22	-3.24	104.51	110.77
34	P	614	LUT	C21-C26-C27	-3.24	108.60	112.70
25	B	829	CLA	C3B-C4B-NB	-3.24	107.51	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	304	CHL	CHD-C4C-NC	3.24	129.31	124.20
28	B	844	BCR	C38-C26-C25	-3.24	120.89	124.53
25	5	303	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
34	1	615	LUT	C21-C26-C27	-3.23	108.61	112.70
34	T	614	LUT	C10-C11-C12	-3.23	113.12	123.22
34	2	315	LUT	C7-C8-C9	-3.23	121.35	126.23
25	A	821	CLA	C3B-C4B-NB	-3.23	107.52	110.52
33	6	617	CHL	CHD-C4C-NC	3.23	129.29	124.20
25	7	306	CLA	C3B-C4B-NB	-3.23	107.52	110.52
32	1	619	LMG	C8-O7-C10	-3.23	109.84	117.79
34	Q	614	LUT	C21-C26-C27	-3.23	108.62	112.70
36	U	301	NEX	C4-C3-C2	-3.23	104.54	110.77
33	9	306	CHL	C1D-CHD-C4C	-3.23	119.09	126.06
34	R	616	LUT	C21-C26-C27	-3.23	108.62	112.70
33	U	308	CHL	CHD-C4C-NC	3.23	129.29	124.20
33	4	304	CHL	C1D-CHD-C4C	-3.23	119.10	126.06
33	1	601	CHL	C3B-C4B-NB	3.23	113.51	110.52
28	A	849	BCR	C24-C23-C22	-3.22	121.37	126.23
33	P	605	CHL	CHD-C4C-NC	3.22	129.28	124.20
28	4	321	BCR	C1-C6-C7	3.22	124.89	115.78
28	8	301	BCR	C20-C21-C22	-3.22	122.72	127.31
33	Q	605	CHL	CAC-C3C-C4C	3.22	128.99	124.81
34	U	315	LUT	C8-C7-C6	-3.22	118.17	127.20
25	T	612	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
28	L	208	BCR	C3-C4-C5	-3.22	108.33	114.08
34	S	316	LUT	C18-C5-C4	3.22	120.31	114.36
33	U	307	CHL	CHD-C4C-NC	3.22	129.27	124.20
33	S	307	CHL	CAC-C3C-C4C	3.21	128.98	124.81
25	3	305	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
35	S	318	XAT	C15-C35-C34	-3.21	116.89	123.47
35	Q	616	XAT	C7-C8-C9	-3.21	120.54	125.53
34	R	616	LUT	C8-C7-C6	-3.21	118.19	127.20
34	9	313	LUT	C15-C14-C13	-3.21	122.73	127.31
25	1	605	CLA	C3B-C4B-NB	-3.21	107.54	110.52
28	I	201	BCR	C20-C19-C18	-3.20	117.41	126.42
28	F	803	BCR	C35-C13-C14	-3.20	118.43	122.92
33	4	305	CHL	CAC-C3C-C4C	3.20	128.97	124.81
25	8	310	CLA	C3B-C4B-NB	-3.20	107.54	110.52
33	U	309	CHL	CMB-C2B-C1B	3.20	130.25	125.37
34	R	616	LUT	C15-C14-C13	-3.20	122.74	127.31
33	7	305	CHL	CHD-C4C-NC	3.20	129.25	124.20
33	1	606	CHL	CHD-C4C-NC	3.20	129.25	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	610	CLA	C3B-C4B-NB	-3.20	107.55	110.52
33	P	622	CHL	C1-C2-C3	-3.20	120.51	126.04
34	S	317	LUT	C7-C8-C9	-3.20	121.40	126.23
25	A	828	CLA	C1-C2-C3	-3.20	120.51	126.04
33	5	317	CHL	CMB-C2B-C1B	3.20	130.24	125.37
25	B	801	CLA	C1-C2-C3	-3.20	120.51	126.04
34	R	615	LUT	C21-C26-C27	-3.20	108.66	112.70
34	5	322	LUT	C35-C34-C33	-3.20	122.75	127.31
33	R	609	CHL	CAA-C2A-C3A	-3.19	104.03	112.78
25	8	309	CLA	C3B-C4B-NB	-3.19	107.55	110.52
25	A	809	CLA	C3B-C4B-NB	-3.19	107.55	110.52
25	Q	603	CLA	CHB-C4A-NA	3.19	128.93	124.51
25	B	831	CLA	CAA-CBA-CGA	-3.19	103.92	113.25
28	7	316	BCR	C8-C7-C6	-3.19	118.23	127.20
33	7	305	CHL	CHB-C1B-NB	-3.19	120.88	124.26
34	6	619	LUT	C18-C5-C4	3.19	120.27	114.36
33	7	305	CHL	CMB-C2B-C1B	3.19	130.23	125.37
33	S	302	CHL	C1D-CHD-C4C	-3.19	119.17	126.06
25	A	829	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
33	T	604	CHL	CHD-C4C-NC	3.19	129.23	124.20
33	3	306	CHL	CMB-C2B-C1B	3.19	130.23	125.37
33	P	608	CHL	C1D-ND-C4D	3.19	108.60	106.33
34	U	314	LUT	C18-C5-C6	-3.19	120.95	124.53
33	S	306	CHL	CHD-C1D-ND	-3.19	121.53	124.45
33	9	307	CHL	CMB-C2B-C1B	3.19	130.22	125.37
25	5	311	CLA	C3B-C4B-NB	-3.19	107.56	110.52
25	4	310	CLA	C2A-C1A-CHA	3.19	129.43	123.86
33	5	307	CHL	CHD-C4C-NC	3.19	129.22	124.20
28	O	204	BCR	C33-C5-C4	3.19	119.73	113.62
34	U	315	LUT	C10-C11-C12	-3.18	113.28	123.22
33	S	307	CHL	CMB-C2B-C1B	3.18	130.22	125.37
33	P	619	CHL	C1D-ND-C4D	3.18	108.60	106.33
25	L	209	CLA	CHB-C4A-NA	3.18	128.91	124.51
33	S	310	CHL	CHB-C1B-NB	-3.18	120.89	124.26
33	1	601	CHL	CMB-C2B-C1B	3.18	130.22	125.37
33	U	308	CHL	C3B-C4B-NB	3.18	113.47	110.52
33	6	606	CHL	C1D-CHD-C4C	-3.18	119.19	126.06
25	6	616	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
33	P	609	CHL	CAA-C2A-C3A	-3.18	104.07	112.78
33	Q	608	CHL	CAA-C2A-C3A	-3.18	104.07	112.78
33	R	605	CHL	CHB-C4A-NA	3.18	128.91	124.51
33	U	305	CHL	CHD-C1D-ND	-3.18	121.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	314	CHL	CHD-C4C-NC	3.18	129.21	124.20
34	a	314	LUT	C21-C26-C27	-3.18	108.69	112.70
28	O	205	BCR	C28-C27-C26	-3.18	108.41	114.08
33	9	306	CHL	CAC-C3C-C4C	3.18	128.93	124.81
25	A	811	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
36	P	617	NEX	C35-C15-C14	-3.17	116.97	123.47
33	R	608	CHL	CHD-C4C-NC	3.17	129.20	124.20
33	4	322	CHL	CHD-C4C-NC	3.17	129.20	124.20
33	5	317	CHL	C3C-C4C-NC	3.17	114.13	110.57
25	B	815	CLA	CHB-C1B-NB	3.17	127.62	124.26
25	A	837	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
33	Q	605	CHL	CHD-C4C-NC	3.17	129.20	124.20
33	T	606	CHL	C1D-ND-C4D	3.17	108.59	106.33
33	4	306	CHL	CHB-C1B-NB	-3.17	120.90	124.26
32	J	107	LMG	O6-C1-C2	3.17	117.06	110.35
33	Q	607	CHL	CHD-C4C-NC	3.17	129.19	124.20
34	a	315	LUT	C11-C10-C9	-3.17	122.79	127.31
25	1	613	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
28	B	843	BCR	C24-C23-C22	-3.17	121.45	126.23
33	P	608	CHL	CHD-C4C-NC	3.17	129.19	124.20
25	A	818	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
25	A	853	CLA	C1-C2-C3	-3.16	120.57	126.04
25	B	818	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
36	R	617	NEX	C35-C15-C14	-3.16	117.00	123.47
25	K	204	CLA	C2A-C1A-CHA	3.16	129.39	123.86
33	a	305	CHL	CMB-C2B-C1B	3.16	130.18	125.37
33	6	607	CHL	CHC-C1C-NC	3.16	129.00	124.20
33	8	307	CHL	CHD-C4C-NC	3.16	129.18	124.20
28	G	203	BCR	C38-C26-C25	-3.16	120.98	124.53
33	P	607	CHL	C1D-ND-C4D	3.16	108.58	106.33
25	Q	610	CLA	C2A-C1A-CHA	3.16	127.61	122.71
28	4	317	BCR	C3-C4-C5	-3.16	108.44	114.08
33	S	310	CHL	C1-C2-C3	-3.16	120.58	126.04
34	5	322	LUT	C16-C1-C6	-3.16	105.18	110.30
25	3	312	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
28	O	205	BCR	C15-C16-C17	-3.16	117.01	123.47
25	O	203	CLA	CAA-C2A-C3A	-3.16	108.74	116.10
34	T	614	LUT	C21-C26-C27	-3.15	108.71	112.70
33	5	317	CHL	CAC-C3C-C4C	3.15	128.90	124.81
33	P	609	CHL	C1-C2-C3	3.15	131.50	126.04
25	G	202	CLA	CHB-C1B-NB	3.15	127.59	124.26
25	A	808	CLA	C3B-C4B-NB	-3.15	107.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	851	BCR	C15-C14-C13	-3.15	122.81	127.31
28	A	849	BCR	C8-C9-C10	3.15	123.78	118.94
25	6	615	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
33	R	608	CHL	C1D-ND-C4D	3.15	108.57	106.33
25	A	839	CLA	C3B-C4B-NB	-3.15	107.59	110.52
25	H	205	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	A	819	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	B	814	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	3	314	CLA	C3B-C4B-NB	-3.15	107.60	110.52
28	A	846	BCR	C38-C26-C25	-3.15	121.00	124.53
25	S	303	CLA	C3B-C4B-NB	-3.15	107.60	110.52
33	7	305	CHL	C1D-CHD-C4C	-3.14	119.27	126.06
28	B	844	BCR	C20-C21-C22	-3.14	122.82	127.31
36	U	316	NEX	C17-C1-C6	-3.14	107.66	110.47
25	7	302	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	9	310	CLA	C3B-C4B-NB	-3.14	107.60	110.52
33	U	305	CHL	CHD-C4C-NC	3.14	129.15	124.20
34	5	318	LUT	C18-C5-C6	-3.14	121.00	124.53
25	B	809	CLA	C3B-C4B-NB	-3.14	107.60	110.52
34	a	314	LUT	C30-C31-C32	-3.14	113.42	123.22
25	3	310	CLA	C3B-C4B-NB	-3.14	107.60	110.52
36	U	316	NEX	C35-C15-C14	-3.14	117.04	123.47
27	A	844	LHG	C5-O7-C7	-3.14	110.06	117.79
25	A	832	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	B	824	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	8	304	CLA	C3B-C4B-NB	-3.14	107.60	110.52
25	A	812	CLA	CHB-C1B-NB	3.14	127.58	124.26
33	Q	607	CHL	C1D-ND-C4D	3.14	108.56	106.33
33	U	306	CHL	C1D-CHD-C4C	-3.14	119.29	126.06
25	B	831	CLA	C3B-C4B-NB	-3.14	107.61	110.52
25	a	302	CLA	C3B-C4B-NB	-3.14	107.61	110.52
33	4	314	CHL	CHB-C1B-NB	-3.14	120.94	124.26
25	A	814	CLA	C3B-C4B-NB	-3.13	107.61	110.52
25	O	201	CLA	C3B-C4B-NB	-3.13	107.61	110.52
25	a	307	CLA	C3B-C4B-NB	-3.13	107.61	110.52
33	S	302	CHL	C1-C2-C3	-3.13	120.62	126.04
25	B	807	CLA	O2D-CGD-CBD	3.13	116.83	111.27
34	P	615	LUT	C21-C26-C27	-3.13	108.74	112.70
25	A	817	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
28	B	843	BCR	C11-C10-C9	-3.13	122.84	127.31
25	1	609	CLA	C3C-C4C-NC	-3.13	107.06	110.57
33	R	601	CHL	CAC-C3C-C4C	3.13	128.87	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	307	CLA	C3B-C4B-NB	-3.13	107.61	110.52
33	5	317	CHL	C3B-C4B-NB	3.13	113.42	110.52
33	S	310	CHL	CHD-C4C-NC	3.13	129.14	124.20
25	a	303	CLA	C5-C3-C2	-3.13	114.78	121.12
33	R	607	CHL	C1D-ND-C4D	3.13	108.56	106.33
28	3	318	BCR	C28-C27-C26	-3.13	108.49	114.08
36	U	301	NEX	C31-C30-C29	-3.13	122.84	127.31
25	A	820	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
33	P	601	CHL	CAC-C3C-C4C	3.13	128.87	124.81
27	T	617	LHG	O7-C7-C8	3.13	118.24	111.50
34	T	614	LUT	C8-C7-C6	-3.13	118.42	127.20
25	a	312	CLA	C3B-C4B-NB	-3.13	107.61	110.52
25	2	313	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
34	a	316	LUT	C7-C8-C9	-3.12	121.51	126.23
25	L	206	CLA	C3B-C4B-NB	-3.12	107.62	110.52
28	A	845	BCR	C7-C8-C9	-3.12	121.52	126.23
33	S	308	CHL	C1D-ND-C4D	3.12	108.55	106.33
33	U	307	CHL	CAC-C3C-C4C	3.12	128.86	124.81
33	Q	607	CHL	CHB-C1B-NB	-3.12	120.95	124.26
25	a	303	CLA	C2D-C1D-ND	-3.12	107.81	110.10
33	4	305	CHL	C1-C2-C3	-3.12	121.71	126.75
34	Q	615	LUT	C21-C26-C27	-3.12	108.76	112.70
33	Q	608	CHL	C1-C2-C3	3.12	131.44	126.04
34	9	312	LUT	C15-C14-C13	-3.12	122.86	127.31
33	P	619	CHL	CHD-C4C-NC	3.12	129.12	124.20
28	6	621	BCR	C8-C9-C10	3.12	123.72	118.94
25	2	313	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	R	612	CLA	O2A-CGA-CBA	3.12	121.69	111.91
25	A	809	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
33	R	606	CHL	O2A-CGA-CBA	3.12	121.69	111.91
28	4	317	BCR	C33-C5-C6	-3.12	121.03	124.53
28	4	321	BCR	C34-C9-C10	-3.12	118.56	122.92
25	B	829	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
25	A	824	CLA	C3B-C4B-NB	-3.12	107.62	110.52
25	8	303	CLA	C3B-C4B-NB	-3.12	107.62	110.52
33	6	617	CHL	CHB-C1B-NB	-3.12	120.96	124.26
25	5	306	CLA	C3B-C4B-NB	-3.12	107.62	110.52
28	8	318	BCR	C15-C16-C17	-3.12	117.09	123.47
25	2	312	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
33	3	306	CHL	C1D-CHD-C4C	-3.11	119.34	126.06
33	a	305	CHL	CHD-C4C-NC	3.11	129.11	124.20
33	R	608	CHL	CHB-C1B-NB	-3.11	120.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	U	305	CHL	CHB-C4A-NA	3.11	128.81	124.51
25	5	313	CLA	C2D-C1D-ND	-3.11	107.81	110.10
33	S	309	CHL	CAC-C3C-C4C	3.11	128.85	124.81
33	R	609	CHL	C1-C2-C3	3.11	131.42	126.04
33	Q	601	CHL	CAC-C3C-C4C	3.11	128.84	124.81
33	P	607	CHL	CHD-C4C-NC	3.11	129.10	124.20
34	3	316	LUT	C11-C10-C9	-3.11	122.88	127.31
27	6	618	LHG	C5-O7-C7	-3.11	110.14	117.79
33	P	608	CHL	CHB-C1B-NB	-3.11	120.97	124.26
25	B	817	CLA	C3B-C4B-NB	-3.11	107.63	110.52
25	1	609	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
26	A	841	PQN	C14-C13-C15	3.10	120.49	115.27
33	S	321	CHL	C1D-CHD-C4C	-3.10	119.36	126.06
33	S	306	CHL	C1D-CHD-C4C	-3.10	119.37	126.06
28	L	204	BCR	C20-C21-C22	-3.10	122.88	127.31
25	7	303	CLA	CHB-C1B-NB	3.10	127.54	124.26
25	S	320	CLA	CHB-C4A-NA	3.10	128.80	124.51
25	T	609	CLA	C3B-C4B-NB	-3.10	107.64	110.52
25	4	301	CLA	C3B-C4B-NB	-3.10	107.64	110.52
25	4	303	CLA	C3B-C4B-NB	-3.10	107.64	110.52
33	4	305	CHL	CHD-C4C-NC	3.10	129.09	124.20
35	T	615	XAT	C7-C8-C9	-3.10	120.72	125.53
28	L	204	BCR	C38-C26-C27	3.10	119.57	113.62
25	A	839	CLA	C1-C2-C3	-3.10	120.68	126.04
25	A	829	CLA	C3B-C4B-NB	-3.10	107.64	110.52
28	8	318	BCR	C21-C20-C19	-3.10	113.55	123.22
28	4	321	BCR	C27-C26-C25	-3.10	118.23	122.73
28	F	801	BCR	C16-C15-C14	-3.10	117.13	123.47
25	P	612	CLA	O2A-CGA-CBA	3.10	121.62	111.91
34	2	315	LUT	C30-C31-C32	-3.10	113.56	123.22
25	U	303	CLA	CHB-C4A-NA	3.10	128.79	124.51
25	O	202	CLA	C3B-C4B-NB	-3.10	107.64	110.52
34	a	314	LUT	C35-C15-C14	-3.10	117.13	123.47
33	R	601	CHL	C1D-CHD-C4C	-3.10	119.38	126.06
28	B	840	BCR	C38-C26-C25	-3.10	121.05	124.53
25	B	811	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
25	A	802	CLA	C3B-C4B-NB	-3.09	107.64	110.52
33	R	605	CHL	CMB-C2B-C1B	3.09	130.08	125.37
33	T	605	CHL	C1D-CHD-C4C	-3.09	119.38	126.06
33	S	302	CHL	OBD-CAD-C3D	-3.09	121.08	128.52
25	9	308	CLA	C1-C2-C3	-3.09	121.75	126.75
25	5	324	CLA	O2D-CGD-O1D	-3.09	117.79	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	616	LUT	C16-C1-C6	-3.09	105.28	110.30
25	2	312	CLA	C3B-C4B-NB	-3.09	107.65	110.52
28	L	203	BCR	C33-C5-C4	3.09	119.55	113.62
34	5	318	LUT	C30-C31-C32	-3.09	113.58	123.22
33	P	601	CHL	C1D-CHD-C4C	-3.09	119.40	126.06
33	T	601	CHL	C1D-CHD-C4C	-3.09	119.40	126.06
25	1	608	CLA	C3B-C4B-NB	-3.09	107.65	110.52
33	S	310	CHL	C3B-C4B-NB	3.09	113.38	110.52
33	4	322	CHL	C3B-C4B-NB	3.09	113.38	110.52
33	R	606	CHL	CAC-C3C-C4C	3.08	128.81	124.81
33	T	605	CHL	CAC-C3C-C4C	3.08	128.81	124.81
25	A	816	CLA	C3B-C4B-NB	-3.08	107.66	110.52
33	R	607	CHL	CHD-C4C-NC	3.08	129.06	124.20
34	5	318	LUT	C35-C15-C14	-3.08	117.16	123.47
33	T	607	CHL	C1D-CHD-C4C	-3.08	119.41	126.06
25	R	610	CLA	C1-C2-C3	-3.08	120.71	126.04
25	5	306	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
25	B	803	CLA	CHB-C4A-NA	3.08	128.77	124.51
33	5	317	CHL	C1D-CHD-C4C	-3.08	119.41	126.06
33	R	606	CHL	CHD-C4C-NC	3.08	129.06	124.20
25	5	316	CLA	C3B-C4B-NB	-3.08	107.66	110.52
25	B	808	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
34	P	615	LUT	C19-C9-C8	3.08	122.93	118.08
33	U	307	CHL	C1D-ND-C4D	3.08	108.52	106.33
25	9	308	CLA	C3B-C4B-NB	-3.08	107.66	110.52
25	A	810	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
33	S	302	CHL	C4-C3-C5	3.08	120.44	115.27
33	S	321	CHL	C1D-ND-C4D	3.07	108.52	106.33
25	1	607	CLA	C3B-C4B-NB	-3.07	107.66	110.52
28	L	203	BCR	C24-C23-C22	-3.07	121.59	126.23
25	B	821	CLA	C3B-C4B-NB	-3.07	107.67	110.52
33	P	605	CHL	C3C-C4C-NC	3.07	114.01	110.57
25	1	614	CLA	C3B-C4B-NB	-3.07	107.67	110.52
28	O	204	BCR	C33-C5-C6	-3.07	121.08	124.53
33	Q	601	CHL	C1D-CHD-C4C	-3.07	119.44	126.06
33	P	622	CHL	C3B-C4B-NB	3.07	113.36	110.52
28	B	841	BCR	C33-C5-C4	3.07	119.50	113.62
25	3	320	CLA	CHB-C4A-NA	3.07	128.75	124.51
25	4	310	CLA	CHB-C1B-NB	3.07	127.50	124.26
32	6	602	LMG	O8-C28-C29	3.06	121.52	111.91
25	A	851	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
34	6	619	LUT	C35-C15-C14	-3.06	117.20	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	847	BCR	C33-C5-C6	-3.06	121.09	124.53
25	B	802	CLA	C3B-C4B-NB	-3.06	107.67	110.52
25	5	309	CLA	C3B-C4B-NB	-3.06	107.67	110.52
33	P	606	CHL	C3B-C4B-NB	3.06	113.35	110.52
28	B	841	BCR	C30-C25-C26	-3.06	118.31	122.61
25	L	209	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	2	312	CLA	C1-C2-C3	-3.06	120.75	126.04
28	4	317	BCR	C23-C24-C25	-3.06	118.61	127.20
25	B	824	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
33	T	605	CHL	O2A-CGA-CBA	3.06	121.50	111.91
25	T	609	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	1	603	CLA	C3B-C4B-NB	-3.06	107.68	110.52
33	U	305	CHL	CAC-C3C-C4C	3.06	128.78	124.81
25	9	303	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	O	202	CLA	C2D-C1D-ND	-3.05	107.85	110.10
34	7	314	LUT	C15-C14-C13	-3.05	122.95	127.31
25	7	312	CLA	C3B-C4B-NB	-3.05	107.68	110.52
25	1	613	CLA	C3B-C4B-NB	-3.05	107.68	110.52
34	9	313	LUT	C10-C11-C12	-3.05	113.69	123.22
33	6	608	CHL	CMB-C2B-C1B	3.05	130.02	125.37
25	a	311	CLA	CHB-C4A-NA	3.05	128.73	124.51
33	T	606	CHL	CMB-C2B-C1B	3.05	130.01	125.37
34	3	316	LUT	C7-C8-C9	-3.05	121.63	126.23
33	4	306	CHL	CMB-C2B-C1B	3.05	130.01	125.37
34	Q	615	LUT	C19-C9-C8	3.05	122.88	118.08
33	4	306	CHL	C3B-C4B-NB	3.04	113.34	110.52
28	A	849	BCR	C16-C17-C18	-3.04	122.97	127.31
28	4	317	BCR	C15-C16-C17	-3.04	117.25	123.47
28	K	206	BCR	C19-C18-C17	3.04	123.61	118.94
25	A	823	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
34	R	616	LUT	C10-C11-C12	-3.04	113.73	123.22
28	B	845	BCR	C29-C30-C25	3.04	115.16	110.48
28	4	317	BCR	C38-C26-C27	3.04	119.45	113.62
25	A	806	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
28	3	318	BCR	C3-C4-C5	-3.04	108.66	114.08
34	2	315	LUT	C35-C15-C14	-3.04	117.25	123.47
33	1	601	CHL	CAC-C3C-C4C	3.04	128.75	124.81
33	S	307	CHL	CHD-C4C-NC	3.04	128.99	124.20
34	P	615	LUT	C35-C34-C33	-3.04	122.98	127.31
33	P	605	CHL	CAC-C3C-C4C	3.03	128.75	124.81
25	K	205	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
25	3	303	CLA	O2D-CGD-O1D	-3.03	117.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Q	601	CHL	CMB-C2B-C1B	3.03	129.99	125.37
33	7	305	CHL	C3C-C4C-NC	3.03	113.97	110.57
33	6	608	CHL	C1-C2-C3	-3.03	121.84	126.75
33	Q	606	CHL	C1D-CHD-C4C	-3.03	119.52	126.06
27	7	317	LHG	C5-O7-C7	-3.03	110.33	117.79
28	5	320	BCR	C2-C1-C6	3.03	115.15	110.48
33	S	307	CHL	O1D-CGD-CBD	-3.03	118.28	124.48
32	J	104	LMG	C8-O7-C10	-3.03	110.33	117.79
28	5	320	BCR	C31-C1-C6	-3.03	105.38	110.30
28	6	621	BCR	C23-C24-C25	-3.03	118.69	127.20
25	8	308	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
34	P	615	LUT	C8-C7-C6	-3.03	118.69	127.20
33	U	309	CHL	C1D-CHD-C4C	-3.03	119.52	126.06
25	Q	613	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
33	R	605	CHL	CHD-C4C-NC	3.02	128.97	124.20
25	2	309	CLA	C3B-C4B-NB	-3.02	107.71	110.52
25	a	306	CLA	C1-C2-C3	-3.02	120.82	126.04
25	B	832	CLA	C3B-C4B-NB	-3.02	107.71	110.52
28	3	318	BCR	C34-C9-C10	-3.02	118.69	122.92
33	7	305	CHL	C3B-C4B-NB	3.02	113.32	110.52
33	Q	606	CHL	CMB-C2B-C1B	3.02	129.97	125.37
33	P	601	CHL	CMB-C2B-C1B	3.02	129.97	125.37
28	8	301	BCR	C16-C17-C18	-3.02	123.00	127.31
32	7	319	LMG	O8-C28-C29	3.02	121.37	111.91
33	T	604	CHL	C3C-C4C-NC	3.02	113.95	110.57
25	B	805	CLA	CHB-C4A-NA	3.02	128.68	124.51
33	4	322	CHL	CMD-C2D-C3D	-3.02	120.68	127.61
25	B	803	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	1	612	CLA	C3A-C2A-C1A	3.02	105.86	101.34
25	A	853	CLA	C3B-C4B-NB	-3.01	107.72	110.52
33	9	307	CHL	CHD-C4C-NC	3.01	128.95	124.20
28	F	801	BCR	C28-C27-C26	-3.01	108.69	114.08
25	K	203	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	F	802	CLA	C3B-C4B-NB	-3.01	107.72	110.52
34	2	316	LUT	C18-C5-C4	3.01	119.94	114.36
33	T	604	CHL	CMB-C2B-C1B	3.01	129.96	125.37
25	3	320	CLA	C3B-C4B-NB	-3.01	107.72	110.52
25	8	311	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	9	311	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
33	5	307	CHL	C3B-C4B-NB	3.01	113.31	110.52
25	U	313	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
33	S	307	CHL	C1D-CHD-C4C	-3.01	119.56	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	T	607	CHL	CMB-C2B-C1B	3.01	129.95	125.37
25	3	313	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
28	O	205	BCR	C8-C9-C10	3.01	123.56	118.94
25	R	604	CLA	C3B-C4B-NB	-3.01	107.72	110.52
33	U	305	CHL	CMB-C2B-C1B	3.01	129.95	125.37
25	B	823	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
28	B	851	BCR	C8-C7-C6	-3.01	118.76	127.20
33	9	306	CHL	C1D-ND-C4D	3.01	108.47	106.33
33	T	607	CHL	C1-C2-C3	-3.01	120.84	126.04
25	7	313	CLA	C3B-C4B-NB	-3.01	107.73	110.52
33	P	606	CHL	C1D-CHD-C4C	-3.01	119.57	126.06
28	B	844	BCR	C33-C5-C4	3.01	119.39	113.62
25	6	616	CLA	C3B-C4B-NB	-3.01	107.73	110.52
33	R	601	CHL	CMB-C2B-C1B	3.01	129.95	125.37
25	B	809	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
25	B	819	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
25	8	313	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
33	S	321	CHL	CAC-C3C-C4C	3.00	128.71	124.81
25	5	319	CLA	C3B-C4B-NB	-3.00	107.73	110.52
36	R	617	NEX	C11-C12-C13	-3.00	117.98	126.42
25	5	316	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
33	U	307	CHL	C1D-CHD-C4C	-3.00	119.58	126.06
28	6	621	BCR	C11-C12-C13	-3.00	117.98	126.42
34	R	615	LUT	C18-C5-C4	3.00	119.92	114.36
25	8	315	CLA	C3B-C4B-NB	-3.00	107.73	110.52
33	Q	606	CHL	CHD-C4C-NC	3.00	128.93	124.20
34	Q	615	LUT	C18-C5-C6	-3.00	121.16	124.53
36	T	616	NEX	C24-C23-C22	-3.00	104.98	110.77
25	B	808	CLA	C3B-C4B-NB	-3.00	107.73	110.52
28	4	317	BCR	C2-C1-C6	3.00	115.10	110.48
34	7	315	LUT	C15-C14-C13	-3.00	123.03	127.31
33	4	314	CHL	CHC-C1C-NC	3.00	128.75	124.20
33	9	306	CHL	C3B-C4B-NB	3.00	113.30	110.52
33	1	601	CHL	O2A-CGA-CBA	3.00	121.31	111.91
25	S	314	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
28	B	845	BCR	C16-C15-C14	-3.00	117.34	123.47
25	1	614	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
25	A	822	CLA	C3B-C4B-NB	-2.99	107.74	110.52
36	U	301	NEX	C35-C15-C14	-2.99	117.34	123.47
25	G	201	CLA	C3B-C4B-NB	-2.99	107.74	110.52
33	T	604	CHL	CAC-C3C-C4C	2.99	128.69	124.81
33	P	606	CHL	CAC-C3C-C4C	2.99	128.69	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	306	CLA	CAA-C2A-C3A	-2.99	109.12	116.10
25	B	810	CLA	CHB-C1B-NB	2.99	127.42	124.26
25	R	604	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
34	8	317	LUT	C35-C34-C33	-2.99	123.04	127.31
25	7	310	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	5	302	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	5	315	CLA	C3B-C4B-NB	-2.99	107.74	110.52
35	P	623	XAT	C8-C9-C10	-2.99	118.16	124.81
33	T	601	CHL	CAC-C3C-C4C	2.99	128.69	124.81
32	4	320	LMG	O8-C28-C29	2.99	121.28	111.91
25	L	205	CLA	O2D-CGD-CBD	2.99	116.58	111.27
25	A	828	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	B	805	CLA	C3B-C4B-NB	-2.99	107.74	110.52
25	R	610	CLA	C3B-C4B-NB	-2.99	107.74	110.52
34	8	316	LUT	C21-C26-C27	-2.99	108.93	112.70
33	5	308	CHL	C1D-CHD-C4C	-2.99	119.62	126.06
25	A	811	CLA	C3B-C4B-NB	-2.99	107.75	110.52
33	4	322	CHL	O2A-CGA-CBA	2.99	121.28	111.91
28	A	845	BCR	C20-C21-C22	-2.98	123.05	127.31
25	L	206	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
33	Q	606	CHL	C3C-C4C-NC	2.98	113.92	110.57
33	S	308	CHL	C3C-C4C-NC	2.98	113.92	110.57
33	1	601	CHL	CHC-C1C-NC	2.98	128.73	124.20
33	P	605	CHL	CMB-C2B-C1B	2.98	129.91	125.37
25	S	311	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	B	831	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
28	L	208	BCR	C28-C27-C26	-2.98	108.75	114.08
34	1	615	LUT	C8-C7-C6	-2.98	118.83	127.20
35	Q	616	XAT	C35-C15-C14	-2.98	117.37	123.47
25	1	607	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
34	a	315	LUT	C16-C1-C6	-2.98	105.47	110.30
28	O	204	BCR	C27-C26-C25	-2.98	118.41	122.73
28	B	851	BCR	C24-C23-C22	-2.98	121.74	126.23
34	S	316	LUT	C21-C26-C27	-2.98	108.94	112.70
28	3	318	BCR	C33-C5-C4	2.98	119.33	113.62
28	G	203	BCR	C3-C4-C5	-2.97	108.77	114.08
25	A	804	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
25	a	301	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
28	6	621	BCR	C16-C17-C18	-2.97	123.07	127.31
33	S	309	CHL	CMB-C2B-C1B	2.97	129.90	125.37
33	U	309	CHL	CHD-C4C-NC	2.97	128.89	124.20
25	A	838	CLA	C3B-C4B-NB	-2.97	107.76	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	606	CHL	C1D-CHD-C4C	-2.97	119.64	126.06
34	2	316	LUT	C35-C15-C14	-2.97	117.39	123.47
34	Q	614	LUT	C3-C4-C5	-2.97	105.93	111.85
25	A	828	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
25	B	819	CLA	C3B-C4B-NB	-2.97	107.76	110.52
25	7	310	CLA	CHB-C4A-NA	2.97	128.62	124.51
28	6	621	BCR	C8-C7-C6	-2.97	118.86	127.20
33	T	606	CHL	CHB-C1B-NB	-2.97	121.11	124.26
25	A	821	CLA	CHB-C4A-NA	2.97	128.62	124.51
33	S	309	CHL	C1D-ND-C4D	2.97	108.44	106.33
36	P	617	NEX	C24-C23-C22	-2.97	105.04	110.77
25	S	301	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
28	7	316	BCR	C21-C20-C19	-2.97	113.95	123.22
28	6	621	BCR	C34-C9-C10	-2.97	118.76	122.92
33	6	606	CHL	CHB-C1B-NB	-2.97	121.11	124.26
25	3	312	CLA	C3B-C4B-NB	-2.97	107.76	110.52
36	P	621	NEX	C2-C1-C6	2.97	112.09	109.21
25	A	816	CLA	CAA-CBA-CGA	-2.97	104.58	113.25
25	A	808	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
33	P	619	CHL	CMB-C2B-C1B	2.97	129.89	125.37
25	6	604	CLA	C3B-C4B-NB	-2.97	107.76	110.52
33	Q	608	CHL	O2A-CGA-CBA	2.97	121.22	111.91
33	4	304	CHL	C3C-C4C-NC	2.97	113.90	110.57
28	8	318	BCR	C38-C26-C27	2.97	119.31	113.62
25	B	836	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
28	K	206	BCR	C27-C26-C25	-2.96	118.43	122.73
34	Q	615	LUT	C16-C1-C6	-2.96	105.49	110.30
33	P	609	CHL	O2A-CGA-CBA	2.96	121.20	111.91
33	Q	605	CHL	C3C-C4C-NC	2.96	113.89	110.57
25	A	805	CLA	CHB-C4A-NA	2.96	128.61	124.51
33	R	609	CHL	O2A-CGA-CBA	2.96	121.19	111.91
33	S	310	CHL	CMB-C2B-C1B	2.96	129.88	125.37
34	Q	615	LUT	C15-C35-C34	-2.96	117.41	123.47
33	4	314	CHL	CMB-C2B-C1B	2.96	129.88	125.37
25	5	305	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	H	203	CLA	C3B-C4B-NB	-2.96	107.77	110.52
25	H	205	CLA	CHB-C4A-NA	2.96	128.60	124.51
25	4	313	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
33	U	309	CHL	O2D-CGD-O1D	-2.96	118.06	123.84
33	S	307	CHL	O2A-CGA-CBA	2.96	121.19	111.91
25	Q	604	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	B	830	CLA	C1-C2-C3	-2.96	120.93	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	607	CHL	CMB-C2B-C1B	2.95	129.87	125.37
25	2	308	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
25	B	836	CLA	C3B-C4B-NB	-2.95	107.78	110.52
25	9	311	CLA	C3B-C4B-NB	-2.95	107.78	110.52
34	3	316	LUT	C30-C31-C32	-2.95	114.00	123.22
33	S	310	CHL	C1D-CHD-C4C	-2.95	119.69	126.06
28	B	842	BCR	C21-C20-C19	-2.95	114.00	123.22
33	6	608	CHL	C1D-CHD-C4C	-2.95	119.69	126.06
25	S	315	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
33	P	607	CHL	CMB-C2B-C1B	2.95	129.86	125.37
33	R	605	CHL	C3B-C4B-NB	2.95	113.25	110.52
28	A	849	BCR	C16-C15-C14	-2.95	117.43	123.47
33	U	307	CHL	CMB-C2B-C1B	2.95	129.86	125.37
25	T	609	CLA	O1D-CGD-CBD	2.95	130.52	124.48
34	R	616	LUT	C18-C5-C4	2.95	119.82	114.36
28	L	204	BCR	C24-C23-C22	-2.95	121.78	126.23
34	6	619	LUT	C16-C1-C6	-2.95	105.52	110.30
33	S	306	CHL	C3C-C4C-NC	2.95	113.88	110.57
33	T	607	CHL	O2A-CGA-CBA	2.95	121.16	111.91
33	T	607	CHL	CAC-C3C-C4C	2.95	128.63	124.81
33	3	306	CHL	CAC-C3C-C4C	2.95	128.63	124.81
28	B	842	BCR	C37-C22-C21	-2.95	118.80	122.92
33	5	308	CHL	C3B-C4B-NB	2.95	113.25	110.52
28	B	843	BCR	C3-C4-C5	-2.95	108.82	114.08
28	4	317	BCR	C16-C17-C18	-2.95	123.11	127.31
33	Q	605	CHL	CHB-C4A-NA	2.95	128.59	124.51
28	A	847	BCR	C3-C4-C5	-2.94	108.82	114.08
25	8	314	CLA	C3B-C4B-NB	-2.94	107.78	110.52
34	8	316	LUT	C20-C13-C12	2.94	122.72	118.08
33	U	308	CHL	CHB-C1B-NB	-2.94	121.14	124.26
25	A	810	CLA	C3B-C4B-NB	-2.94	107.78	110.52
33	a	305	CHL	CAC-C3C-C4C	2.94	128.63	124.81
25	B	807	CLA	C3B-C4B-NB	-2.94	107.79	110.52
25	S	305	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	8	315	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	T	610	CLA	O2D-CGD-CBD	2.94	116.49	111.27
33	P	609	CHL	C3B-C4B-NB	-2.94	107.79	110.52
33	S	309	CHL	C1D-CHD-C4C	-2.94	119.72	126.06
25	U	313	CLA	C3B-C4B-NB	-2.94	107.79	110.52
33	6	606	CHL	CHC-C1C-NC	2.94	128.66	124.20
25	B	834	CLA	C3B-C4B-NB	-2.94	107.79	110.52
33	3	306	CHL	O2A-CGA-CBA	2.94	121.12	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	316	LUT	C2-C3-C4	2.94	114.32	110.30
28	L	208	BCR	C38-C26-C27	2.93	119.25	113.62
28	5	323	BCR	C8-C9-C10	2.93	123.44	118.94
25	B	835	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
28	8	318	BCR	C31-C1-C6	-2.93	105.55	110.30
28	A	848	BCR	C20-C21-C22	-2.93	123.13	127.31
33	3	306	CHL	C3C-C4C-NC	2.93	113.86	110.57
25	A	816	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	A	839	CLA	CHB-C4A-NA	2.93	128.56	124.51
25	A	817	CLA	C3B-C4B-NB	-2.93	107.80	110.52
33	U	305	CHL	CHC-C1C-NC	2.93	128.64	124.20
33	U	309	CHL	O2A-CGA-CBA	2.93	121.09	111.91
34	6	622	LUT	C15-C14-C13	-2.93	123.13	127.31
25	B	807	CLA	CHB-C4A-NA	2.92	128.56	124.51
33	Q	608	CHL	C3B-C4B-NB	-2.92	107.80	110.52
33	6	607	CHL	OMC-CMC-C2C	-2.92	119.08	125.69
26	B	839	PQN	C11-C3-C4	2.92	121.63	118.50
36	T	616	NEX	C35-C15-C14	-2.92	117.48	123.47
34	R	615	LUT	C31-C30-C29	-2.92	123.14	127.31
25	B	817	CLA	CHB-C1B-NB	2.92	127.35	124.26
28	L	208	BCR	C20-C21-C22	-2.92	123.14	127.31
25	9	304	CLA	CHB-C1B-NB	2.92	127.35	124.26
25	S	303	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
33	P	606	CHL	CHB-C1B-NB	-2.92	121.17	124.26
28	B	845	BCR	C37-C22-C21	-2.92	118.83	122.92
25	U	313	CLA	CHB-C4A-NA	2.92	128.55	124.51
33	6	606	CHL	C3C-C4C-NC	2.92	113.84	110.57
34	5	318	LUT	C21-C26-C27	-2.92	109.01	112.70
33	P	605	CHL	C1D-ND-C4D	2.92	108.41	106.33
33	T	606	CHL	CAC-C3C-C4C	2.92	128.60	124.81
28	B	841	BCR	C23-C24-C25	-2.92	119.01	127.20
34	2	315	LUT	C10-C11-C12	-2.92	114.12	123.22
25	8	314	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
36	P	621	NEX	C16-C1-C2	-2.92	95.96	109.05
33	T	604	CHL	O2A-CGA-CBA	2.91	121.06	111.91
28	L	208	BCR	C1-C6-C5	-2.91	118.51	122.61
25	K	203	CLA	C3B-C4B-NB	-2.91	107.81	110.52
33	R	605	CHL	CHC-C1C-NC	2.91	128.62	124.20
33	S	321	CHL	CHC-C1C-NC	2.91	128.62	124.20
33	P	622	CHL	C4A-NA-C1A	2.91	108.02	106.71
33	8	307	CHL	CHC-C1C-NC	2.91	128.62	124.20
33	S	308	CHL	C1D-CHD-C4C	-2.91	119.78	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	U	314	LUT	C20-C13-C14	-2.91	118.85	122.92
25	A	829	CLA	C1-C2-C3	-2.91	121.01	126.04
33	6	617	CHL	CHC-C1C-NC	2.91	128.61	124.20
33	6	617	CHL	CMB-C2B-C1B	2.91	129.80	125.37
25	5	302	CLA	CHC-C4B-NB	2.91	127.33	124.26
25	a	306	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
25	a	312	CLA	O1D-CGD-CBD	2.91	130.43	124.48
34	a	314	LUT	C10-C11-C12	-2.91	114.15	123.22
33	9	306	CHL	CHC-C1C-NC	2.91	128.61	124.20
33	6	606	CHL	CHD-C1D-ND	-2.91	121.78	124.45
34	1	617	LUT	C1-C2-C3	2.90	120.20	113.64
25	3	313	CLA	C3B-C4B-NB	-2.90	107.82	110.52
25	6	611	CLA	C3B-C4B-NB	-2.90	107.82	110.52
25	8	306	CLA	C3B-C4B-NB	-2.90	107.82	110.52
34	5	322	LUT	C18-C5-C4	2.90	119.73	114.36
25	3	302	CLA	C3B-C4B-NB	-2.90	107.82	110.52
28	L	204	BCR	C21-C20-C19	-2.90	114.17	123.22
34	9	313	LUT	C20-C13-C12	2.90	122.65	118.08
25	a	313	CLA	C3B-C4B-NB	-2.90	107.83	110.52
25	H	203	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
33	Q	605	CHL	CMB-C2B-C1B	2.90	129.78	125.37
33	U	307	CHL	CHC-C1C-NC	2.90	128.60	124.20
34	1	617	LUT	C4-C5-C6	-2.90	114.39	120.85
25	8	303	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	9	303	CLA	C3B-C4B-NB	-2.90	107.83	110.52
34	Q	615	LUT	C8-C7-C6	-2.90	119.06	127.20
28	J	106	BCR	C3-C4-C5	-2.90	108.90	114.08
28	L	208	BCR	C33-C5-C4	2.90	119.18	113.62
25	a	301	CLA	C3B-C4B-NB	-2.90	107.83	110.52
33	a	305	CHL	O2A-CGA-CBA	2.90	120.99	111.91
33	P	605	CHL	CHC-C1C-NC	2.89	128.59	124.20
28	B	845	BCR	C10-C11-C12	-2.89	114.18	123.22
33	5	317	CHL	CHB-C4A-NA	2.89	128.51	124.51
25	8	305	CLA	C3B-C4B-NB	-2.89	107.83	110.52
28	F	803	BCR	C34-C9-C10	-2.89	118.87	122.92
33	R	606	CHL	C3C-C4C-NC	2.89	113.82	110.57
33	P	606	CHL	C3C-C4C-NC	2.89	113.81	110.57
25	B	802	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	B	830	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
28	J	106	BCR	C38-C26-C27	2.89	119.17	113.62
25	8	311	CLA	C3B-C4B-NB	-2.89	107.83	110.52
25	6	613	CLA	CHB-C4A-NA	2.89	128.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	4	315	LUT	C8-C7-C6	-2.89	119.08	127.20
25	6	623	CLA	CHB-C4A-NA	2.89	128.51	124.51
28	3	317	BCR	C11-C10-C9	-2.89	123.18	127.31
34	5	318	LUT	C15-C14-C13	-2.89	123.18	127.31
25	B	833	CLA	C3B-C4B-NB	-2.89	107.83	110.52
28	B	851	BCR	C7-C8-C9	-2.89	121.87	126.23
25	2	312	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	Q	610	CLA	C3B-C4B-NB	-2.89	107.83	110.52
34	6	622	LUT	C21-C26-C27	-2.89	109.05	112.70
28	A	847	BCR	C10-C11-C12	-2.89	114.20	123.22
35	P	616	XAT	C7-C8-C9	-2.89	121.05	125.53
33	P	619	CHL	C1D-CHD-C4C	-2.89	119.83	126.06
25	2	306	CLA	C3B-C4B-NB	-2.89	107.83	110.52
28	B	851	BCR	C38-C26-C25	-2.89	121.29	124.53
33	U	306	CHL	CHB-C1B-NB	-2.89	121.20	124.26
25	A	812	CLA	C3B-C4B-NB	-2.89	107.84	110.52
34	a	315	LUT	C20-C13-C12	2.89	122.62	118.08
28	3	318	BCR	C8-C9-C10	2.89	123.37	118.94
34	5	318	LUT	C20-C13-C12	2.89	122.62	118.08
25	P	610	CLA	C3B-C4B-NB	-2.89	107.84	110.52
25	3	305	CLA	C3B-C4B-NB	-2.89	107.84	110.52
33	R	609	CHL	C3B-C4B-NB	-2.89	107.84	110.52
33	P	607	CHL	C1D-CHD-C4C	-2.88	119.83	126.06
33	6	617	CHL	C1D-CHD-C4C	-2.88	119.83	126.06
25	A	839	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	B	801	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	B	826	CLA	CHB-C1B-NB	2.88	127.31	124.26
25	T	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	a	303	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
33	4	322	CHL	CHC-C1C-NC	2.88	128.58	124.20
25	2	307	CLA	C3B-C4B-NB	-2.88	107.84	110.52
25	a	306	CLA	C3B-C4B-NB	-2.88	107.84	110.52
25	7	308	CLA	CHB-C4A-NA	2.88	128.50	124.51
33	Q	606	CHL	O2A-CGA-CBA	2.88	120.95	111.91
28	O	204	BCR	C29-C30-C25	2.88	114.91	110.48
25	6	612	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
33	4	306	CHL	C1D-CHD-C4C	-2.88	119.85	126.06
28	L	208	BCR	C30-C25-C26	-2.88	118.56	122.61
25	B	814	CLA	C3B-C4B-NB	-2.88	107.84	110.52
25	R	611	CLA	CHB-C4A-NA	2.88	128.49	124.51
33	U	305	CHL	C3C-C4C-NC	2.88	113.80	110.57
25	6	605	CLA	O2A-CGA-O1A	-2.88	116.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	322	CHL	O2D-CGD-O1D	-2.88	118.21	123.84
28	F	803	BCR	C12-C13-C14	2.88	123.36	118.94
33	S	302	CHL	CHC-C1C-NC	2.88	128.57	124.20
25	3	301	CLA	C3B-C4B-NB	-2.88	107.85	110.52
28	4	317	BCR	C34-C9-C10	-2.88	118.89	122.92
25	B	816	CLA	CHB-C4A-NA	2.88	128.49	124.51
28	I	201	BCR	C37-C22-C21	-2.88	118.89	122.92
25	B	833	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
33	Q	605	CHL	CHC-C1C-NC	2.87	128.56	124.20
33	T	606	CHL	CHC-C1C-NC	2.87	128.56	124.20
33	T	606	CHL	C1D-CHD-C4C	-2.87	119.86	126.06
34	a	314	LUT	C8-C7-C6	-2.87	119.13	127.20
34	S	316	LUT	C3-C4-C5	-2.87	106.13	111.85
35	S	318	XAT	C27-C28-C29	-2.87	121.07	125.53
33	S	309	CHL	C3C-C4C-NC	2.87	113.79	110.57
25	O	201	CLA	CHB-C4A-NA	2.87	128.48	124.51
25	L	202	CLA	C3B-C4B-NB	-2.87	107.85	110.52
25	A	822	CLA	CHB-C4A-NA	2.87	128.48	124.51
33	U	305	CHL	C1D-CHD-C4C	-2.87	119.87	126.06
28	J	106	BCR	C23-C24-C25	-2.87	119.14	127.20
34	R	615	LUT	C20-C13-C14	-2.87	118.91	122.92
25	6	605	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
33	4	314	CHL	C1D-CHD-C4C	-2.87	119.87	126.06
33	S	306	CHL	CMB-C2B-C1B	2.87	129.74	125.37
34	P	614	LUT	C31-C30-C29	-2.87	123.22	127.31
28	A	854	BCR	C30-C25-C26	-2.87	118.58	122.61
33	U	306	CHL	C3C-C4C-NC	2.87	113.79	110.57
25	2	309	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	J	105	CLA	C3B-C4B-NB	-2.87	107.86	110.52
25	R	603	CLA	CHB-C4A-NA	2.87	128.47	124.51
28	A	849	BCR	C28-C27-C26	-2.86	108.96	114.08
34	1	615	LUT	C30-C31-C32	-2.86	114.28	123.22
25	a	304	CLA	C3B-C4B-NB	-2.86	107.86	110.52
25	R	612	CLA	O2D-CGD-CBD	2.86	116.36	111.27
33	9	307	CHL	C3C-C4C-NC	2.86	113.78	110.57
33	R	607	CHL	C1D-CHD-C4C	-2.86	119.89	126.06
34	T	614	LUT	C18-C5-C6	-2.86	121.32	124.53
25	R	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
35	P	620	XAT	C7-C8-C9	-2.86	121.09	125.53
25	P	612	CLA	O2D-CGD-CBD	2.86	116.35	111.27
34	3	315	LUT	C20-C13-C12	2.86	122.58	118.08
33	Q	605	CHL	C1D-CHD-C4C	-2.86	119.89	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	308	CLA	C3B-C4B-NB	-2.86	107.86	110.52
33	T	601	CHL	CMB-C2B-C1B	2.86	129.72	125.37
25	K	201	CLA	C3B-C4B-NB	-2.86	107.86	110.52
34	S	316	LUT	C15-C14-C13	-2.86	123.23	127.31
36	P	621	NEX	C39-C29-C30	-2.86	118.92	122.92
25	7	306	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
25	3	311	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	8	308	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	R	602	CLA	C3B-C4B-NB	-2.85	107.87	110.52
35	Q	616	XAT	C20-C13-C12	2.85	122.57	118.08
33	T	605	CHL	C3C-C4C-NC	2.85	113.77	110.57
25	7	307	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
33	U	306	CHL	O2A-CGA-CBA	2.85	120.86	111.91
25	2	305	CLA	C3B-C4B-NB	-2.85	107.87	110.52
25	S	313	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
34	8	317	LUT	C16-C1-C6	-2.85	105.68	110.30
33	P	606	CHL	O2A-CGA-CBA	2.85	120.85	111.91
33	S	302	CHL	CHD-C1D-ND	-2.85	121.83	124.45
25	A	804	CLA	CHB-C1B-NB	2.85	127.27	124.26
25	6	615	CLA	CHB-C1B-NB	2.85	127.27	124.26
34	T	613	LUT	C31-C30-C29	-2.85	123.24	127.31
28	A	847	BCR	C38-C26-C27	2.85	119.09	113.62
34	a	314	LUT	C20-C13-C12	2.85	122.56	118.08
28	B	851	BCR	C28-C27-C26	-2.85	108.99	114.08
25	2	311	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	6	609	CLA	C3B-C4B-NB	-2.85	107.87	110.52
25	P	602	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	A	838	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
33	T	604	CHL	CHC-C1C-NC	2.84	128.52	124.20
34	P	615	LUT	C18-C5-C6	-2.84	121.34	124.53
25	7	312	CLA	O2D-CGD-CBD	2.84	116.32	111.27
27	B	847	LHG	C6-C5-C4	-2.84	105.07	111.79
28	A	845	BCR	C38-C26-C25	-2.84	121.34	124.53
28	L	208	BCR	C38-C26-C25	-2.84	121.34	124.53
25	A	815	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	B	802	CLA	C1-C2-C3	-2.84	121.13	126.04
25	B	832	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
34	S	316	LUT	C8-C7-C6	-2.84	119.23	127.20
25	J	105	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
28	8	301	BCR	C15-C14-C13	-2.84	123.26	127.31
25	B	804	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	2	310	CLA	C3B-C4B-NB	-2.84	107.88	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2	301	LMG	O8-C28-C29	2.84	120.81	111.91
33	6	608	CHL	CHC-C1C-NC	2.83	128.50	124.20
33	T	605	CHL	CHB-C1B-NB	-2.83	121.26	124.26
33	P	619	CHL	CHC-C1C-NC	2.83	128.50	124.20
34	U	315	LUT	C18-C5-C4	2.83	119.61	114.36
36	T	616	NEX	C39-C29-C30	-2.83	118.95	122.92
25	3	309	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
34	T	613	LUT	C18-C5-C4	2.83	119.60	114.36
33	5	317	CHL	O2D-CGD-O1D	-2.83	118.30	123.84
33	S	310	CHL	C3C-C4C-NC	2.83	113.75	110.57
28	B	841	BCR	C15-C16-C17	-2.83	117.67	123.47
25	A	823	CLA	C3B-C4B-NB	-2.83	107.89	110.52
25	4	313	CLA	C3B-C4B-NB	-2.83	107.89	110.52
25	3	303	CLA	C3B-C4B-NB	-2.83	107.89	110.52
25	U	303	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
33	1	601	CHL	CBA-CAA-C2A	-2.83	105.52	113.86
25	K	202	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	A	827	CLA	CHB-C1B-NB	2.83	127.25	124.26
25	5	319	CLA	CHB-C1B-NB	2.83	127.25	124.26
25	B	802	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	Q	610	CLA	CHB-C4A-NA	2.83	128.42	124.51
33	4	322	CHL	CMB-C2B-C1B	2.83	129.67	125.37
28	F	801	BCR	C7-C8-C9	-2.83	121.97	126.23
33	U	308	CHL	C1D-CHD-C4C	-2.82	119.96	126.06
25	R	611	CLA	O1D-CGD-CBD	2.82	130.26	124.48
34	6	619	LUT	C20-C13-C12	2.82	122.53	118.08
25	A	851	CLA	C1-C2-C3	-2.82	121.16	126.04
28	B	842	BCR	C34-C9-C10	-2.82	118.97	122.92
25	2	313	CLA	CAA-CBA-CGA	-2.82	105.01	113.25
25	T	612	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	8	302	CLA	C3B-C4B-NB	-2.82	107.90	110.52
33	7	305	CHL	CHC-C1C-NC	2.82	128.48	124.20
34	3	315	LUT	C30-C31-C32	-2.82	114.42	123.22
28	K	206	BCR	C38-C26-C27	2.82	119.03	113.62
28	A	854	BCR	C38-C26-C27	2.82	119.03	113.62
26	A	841	PQN	C11-C3-C4	2.82	121.52	118.50
25	A	842	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	L	201	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	R	614	CLA	C3B-C4B-NB	-2.82	107.90	110.52
25	S	304	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	A	803	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
25	B	823	CLA	C3B-C4B-NB	-2.82	107.90	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	605	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
33	9	306	CHL	CMB-C2B-C1B	2.82	129.66	125.37
25	S	301	CLA	CAA-CBA-CGA	-2.82	105.03	113.25
32	1	619	LMG	O8-C28-C29	2.82	120.74	111.91
25	A	826	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
25	9	305	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
25	B	828	CLA	C3B-C4B-NB	-2.81	107.90	110.52
25	S	311	CLA	C3B-C4B-NB	-2.81	107.90	110.52
33	6	607	CHL	C6-C5-C3	-2.81	110.02	114.62
34	4	315	LUT	C39-C29-C28	2.81	122.51	118.08
33	1	606	CHL	O2A-CGA-CBA	2.81	120.74	111.91
35	Q	616	XAT	C38-C25-C24	2.81	117.44	114.28
33	T	607	CHL	CHD-C4C-NC	2.81	128.63	124.20
25	3	308	CLA	C3B-C4B-NB	-2.81	107.91	110.52
34	S	317	LUT	C18-C5-C6	-2.81	121.37	124.53
31	B	850	SQD	O6-C1-C2	2.81	112.69	108.30
28	A	845	BCR	C11-C10-C9	-2.81	123.30	127.31
34	R	616	LUT	C15-C35-C34	-2.81	117.72	123.47
33	T	604	CHL	C1D-CHD-C4C	-2.81	120.00	126.06
33	P	622	CHL	CHC-C4B-NB	-2.81	121.28	124.26
33	P	607	CHL	CHC-C1C-NC	2.81	128.47	124.20
25	2	306	CLA	CMA-C3A-C2A	-2.81	109.54	116.10
25	B	815	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
25	B	824	CLA	CAC-C3C-C4C	2.81	128.45	124.81
33	1	606	CHL	CAC-C3C-C4C	2.81	128.45	124.81
28	B	843	BCR	C16-C17-C18	-2.81	123.30	127.31
33	6	606	CHL	O2A-CGA-CBA	2.81	120.72	111.91
30	B	848	DGD	O6D-C1D-C2D	2.81	116.29	110.35
25	Q	604	CLA	C1-C2-C3	-2.81	122.21	126.75
25	B	837	CLA	CHB-C4A-NA	2.81	128.39	124.51
28	K	206	BCR	C35-C13-C12	2.80	122.50	118.08
25	K	202	CLA	C3B-C4B-NB	-2.80	107.91	110.52
25	F	802	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	1	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	T	611	CLA	C3B-C4B-NB	-2.80	107.92	110.52
28	5	323	BCR	C36-C18-C17	-2.80	119.00	122.92
33	U	307	CHL	C3C-C4C-NC	2.80	113.71	110.57
33	R	608	CHL	C1D-CHD-C4C	-2.80	120.01	126.06
25	S	315	CLA	C3B-C4B-NB	-2.80	107.92	110.52
33	S	321	CHL	C1-C2-C3	-2.80	122.22	126.75
25	B	811	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	1	607	CLA	C1-C2-C3	-2.80	121.20	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	301	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	6	603	CLA	C1-C2-C3	-2.80	121.20	126.04
25	a	303	CLA	CHB-C4A-NA	2.80	128.38	124.51
34	3	315	LUT	C35-C34-C33	-2.80	123.32	127.31
25	B	818	CLA	C3B-C4B-NB	-2.80	107.92	110.52
25	A	825	CLA	CHB-C1B-NB	2.80	127.22	124.26
28	O	204	BCR	C38-C26-C27	2.80	118.99	113.62
35	P	620	XAT	C24-C23-C22	-2.80	105.37	110.77
33	8	307	CHL	C3B-C4B-NB	2.80	113.11	110.52
28	8	318	BCR	C33-C5-C4	2.80	118.99	113.62
25	A	825	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
28	A	847	BCR	C15-C16-C17	-2.79	117.75	123.47
25	8	314	CLA	CHB-C4A-NA	2.79	128.38	124.51
25	A	818	CLA	C3B-C4B-NB	-2.79	107.92	110.52
33	U	306	CHL	CHC-C1C-NC	2.79	128.44	124.20
25	7	303	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	5	303	CLA	CMC-C2C-C1C	2.79	129.29	125.04
33	5	307	CHL	CHB-C4A-NA	2.79	128.37	124.51
25	9	305	CLA	C3B-C4B-NB	-2.79	107.93	110.52
25	A	836	CLA	CHB-C1B-NB	2.79	127.21	124.26
25	2	302	CLA	CHB-C1B-NB	2.79	127.21	124.26
32	H	204	LMG	C9-C8-C7	-2.79	105.19	111.79
32	J	102	LMG	C8-O7-C10	-2.79	110.93	117.79
33	S	308	CHL	CHC-C1C-NC	2.79	128.43	124.20
33	R	605	CHL	OBD-CAD-C3D	-2.79	121.81	128.52
34	R	615	LUT	C3-C4-C5	-2.79	106.31	111.85
33	T	604	CHL	CHB-C4A-NA	2.79	128.36	124.51
33	U	306	CHL	CAC-C3C-C4C	2.79	128.42	124.81
25	U	310	CLA	C3B-C4B-NB	-2.79	107.93	110.52
25	G	202	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	P	611	CLA	C4A-NA-C1A	2.78	107.96	106.71
33	R	607	CHL	CHC-C1C-NC	2.78	128.42	124.20
33	P	608	CHL	C1D-CHD-C4C	-2.78	120.06	126.06
25	T	609	CLA	C2A-C1A-CHA	2.78	128.72	123.86
25	5	304	CLA	CHB-C4A-NA	2.78	128.36	124.51
27	1	618	LHG	O8-C23-C24	2.78	120.63	111.91
25	A	838	CLA	C1-C2-C3	-2.78	121.24	126.04
34	Q	615	LUT	C40-C33-C32	2.78	122.46	118.08
28	B	844	BCR	C21-C20-C19	-2.78	114.55	123.22
33	4	306	CHL	O2D-CGD-O1D	-2.78	118.41	123.84
25	9	305	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	A	835	CLA	CHB-C4A-NA	2.77	128.35	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	4	322	CHL	CHB-C4A-NA	2.77	128.35	124.51
28	G	203	BCR	C15-C14-C13	-2.77	123.35	127.31
25	8	309	CLA	CHB-C4A-NA	2.77	128.35	124.51
34	a	315	LUT	C3-C4-C5	-2.77	106.33	111.85
28	5	320	BCR	C33-C5-C4	2.77	118.94	113.62
33	R	601	CHL	O2A-CGA-CBA	2.77	120.61	111.91
28	J	101	BCR	C33-C5-C4	2.77	118.94	113.62
33	R	605	CHL	C2A-C3A-C4A	-2.77	97.39	101.87
32	H	204	LMG	C8-O7-C10	-2.77	110.97	117.79
25	4	309	CLA	C3B-C4B-NB	-2.77	107.94	110.52
32	7	318	LMG	O8-C28-C29	2.77	120.60	111.91
25	4	313	CLA	CAA-C2A-C3A	-2.77	109.63	116.10
36	R	617	NEX	C39-C29-C30	-2.77	119.04	122.92
33	R	607	CHL	C4-C3-C5	2.77	119.15	115.98
25	U	310	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
28	4	317	BCR	C2-C3-C4	-2.77	105.19	111.38
34	5	318	LUT	C10-C11-C12	-2.77	114.58	123.22
25	Q	618	CLA	CHB-C1B-NB	2.77	127.19	124.26
25	3	302	CLA	CHB-C1B-NB	2.77	127.19	124.26
33	T	601	CHL	O2A-CGA-CBA	2.77	120.59	111.91
33	5	317	CHL	C1D-ND-C4D	2.77	108.30	106.33
25	5	315	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
34	4	315	LUT	C30-C31-C32	-2.77	114.59	123.22
33	Q	601	CHL	O2A-CGA-CBA	2.76	120.58	111.91
25	S	303	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
33	S	306	CHL	CHB-C4A-NA	2.76	128.33	124.51
25	2	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
33	5	308	CHL	CAA-CBA-CGA	-2.76	105.18	113.25
25	A	827	CLA	O2D-CGD-CBD	2.76	116.17	111.27
33	Q	607	CHL	C1D-CHD-C4C	-2.76	120.10	126.06
25	A	830	CLA	C3B-C4B-NB	-2.76	107.95	110.52
36	P	621	NEX	C17-C1-C2	-2.76	96.65	109.05
33	P	606	CHL	CMB-C2B-C1B	2.76	129.57	125.37
33	3	306	CHL	CHC-C1C-NC	2.76	128.39	124.20
33	P	605	CHL	CHB-C4A-NA	2.76	128.33	124.51
25	B	826	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	J	103	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
28	4	321	BCR	C38-C26-C25	-2.76	121.43	124.53
28	3	317	BCR	C38-C26-C27	2.76	118.91	113.62
25	T	603	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	7	311	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
36	U	301	NEX	C39-C29-C30	-2.76	119.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	815	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	H	202	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
33	P	601	CHL	O2A-CGA-CBA	2.76	120.56	111.91
25	A	810	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	A	811	CLA	CHB-C4A-NA	2.76	128.32	124.51
28	J	101	BCR	C21-C20-C19	-2.75	114.62	123.22
25	B	805	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
33	P	607	CHL	C4-C3-C5	2.75	119.13	115.98
25	T	602	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
33	P	607	CHL	C3C-C4C-NC	2.75	113.66	110.57
25	B	818	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	P	604	CLA	CHB-C4A-NA	2.75	128.32	124.51
33	P	619	CHL	C4-C3-C5	2.75	119.13	115.98
28	4	317	BCR	C1-C6-C5	-2.75	118.74	122.61
25	R	603	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
33	4	306	CHL	O2A-CGA-CBA	2.75	120.54	111.91
25	9	301	CLA	CHB-C4A-NA	2.75	128.31	124.51
35	S	318	XAT	C10-C11-C12	-2.75	114.64	123.22
25	Q	610	CLA	O1D-CGD-CBD	2.75	130.11	124.48
32	J	102	LMG	O8-C28-C29	2.75	120.53	111.91
33	P	619	CHL	C3C-C4C-NC	2.75	113.65	110.57
28	J	101	BCR	C31-C1-C6	-2.75	105.84	110.30
33	S	308	CHL	CMB-C2B-C1B	2.75	129.55	125.37
34	U	314	LUT	C20-C13-C12	2.75	122.40	118.08
25	U	302	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
34	4	315	LUT	C31-C30-C29	-2.75	123.39	127.31
28	5	323	BCR	C37-C22-C21	2.75	126.77	122.92
28	O	204	BCR	C8-C7-C6	-2.74	119.49	127.20
25	5	313	CLA	CHD-C1D-C2D	2.74	131.24	125.48
33	U	307	CHL	C4A-NA-C1A	-2.74	105.47	106.71
25	B	814	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	5	319	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	3	314	CLA	CHB-C4A-NA	2.74	128.31	124.51
36	U	316	NEX	C39-C29-C30	-2.74	119.08	122.92
28	I	201	BCR	C4-C5-C6	-2.74	118.75	122.73
34	1	615	LUT	C20-C13-C12	2.74	122.40	118.08
25	A	806	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	P	611	CLA	C3B-C4B-NB	2.74	113.05	110.52
25	7	304	CLA	C3B-C4B-NB	-2.74	107.98	110.52
28	L	204	BCR	C3-C4-C5	-2.74	109.19	114.08
25	A	831	CLA	C3B-C4B-NB	-2.73	107.98	110.52
25	A	814	CLA	CHD-C1D-ND	-2.73	121.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	847	BCR	C23-C24-C25	-2.73	119.52	127.20
28	5	320	BCR	C28-C27-C26	-2.73	109.19	114.08
25	B	834	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	B	826	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	7	304	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
36	P	621	NEX	C4-C3-C2	-2.73	105.50	110.77
33	9	307	CHL	OMC-CMC-C2C	-2.73	119.51	125.69
25	A	831	CLA	CHB-C4A-NA	2.73	128.29	124.51
33	8	307	CHL	OMC-CMC-C2C	-2.73	119.51	125.69
25	A	809	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	J	105	CLA	CHB-C4A-NA	2.73	128.29	124.51
33	1	601	CHL	CHB-C4A-NA	2.73	128.29	124.51
25	7	306	CLA	C1-C2-C3	-2.73	122.33	126.75
33	S	302	CHL	OMC-CMC-C2C	-2.73	119.52	125.69
33	S	309	CHL	CHB-C1B-NB	-2.73	121.37	124.26
25	B	813	CLA	CHB-C4A-NA	2.73	128.28	124.51
31	B	850	SQD	O7-S-C6	2.73	110.18	106.94
28	L	208	BCR	C15-C16-C17	-2.73	117.89	123.47
28	B	840	BCR	C21-C20-C19	-2.73	114.71	123.22
25	8	303	CLA	CHB-C4A-NA	2.73	128.28	124.51
33	P	605	CHL	C1D-CHD-C4C	-2.73	120.18	126.06
25	1	612	CLA	C1-C2-C3	-2.73	121.33	126.04
34	P	614	LUT	C20-C13-C14	-2.72	119.11	122.92
25	A	819	CLA	CHB-C1B-NB	2.72	127.14	124.26
25	Q	604	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	K	204	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
33	S	321	CHL	C3C-C4C-NC	2.72	113.63	110.57
28	8	318	BCR	C11-C10-C9	-2.72	123.42	127.31
25	L	201	CLA	CHB-C4A-NA	2.72	128.28	124.51
34	1	616	LUT	C11-C10-C9	-2.72	123.42	127.31
25	T	608	CLA	C3B-C4B-NB	-2.72	107.99	110.52
28	A	845	BCR	C29-C30-C25	2.72	114.67	110.48
25	8	313	CLA	C3B-C4B-NB	-2.72	107.99	110.52
33	S	321	CHL	CMB-C2B-C1B	2.72	129.51	125.37
28	B	840	BCR	C33-C5-C6	-2.72	121.47	124.53
33	R	607	CHL	C3C-C4C-NC	2.72	113.62	110.57
25	B	826	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
25	6	614	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
33	R	605	CHL	CAC-C3C-C4C	2.72	128.34	124.81
33	T	605	CHL	CHC-C1C-NC	2.72	128.33	124.20
25	3	320	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
34	a	316	LUT	C11-C10-C9	-2.72	123.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	605	CHL	C1D-CHD-C4C	-2.72	120.19	126.06
34	9	312	LUT	C8-C7-C6	-2.72	119.56	127.20
25	3	301	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	7	307	CLA	CHB-C4A-NA	2.72	128.27	124.51
33	R	608	CHL	CHC-C1C-NC	2.72	128.33	124.20
33	R	605	CHL	C4A-NA-C1A	-2.72	105.48	106.71
36	P	621	NEX	C38-C25-C24	2.72	117.34	114.28
25	B	812	CLA	CHB-C4A-NA	2.72	128.27	124.51
34	P	614	LUT	C18-C5-C4	2.72	119.39	114.36
28	7	316	BCR	C11-C10-C9	-2.72	123.43	127.31
34	7	314	LUT	C16-C1-C6	-2.72	105.89	110.30
25	A	805	CLA	CHB-C1B-NB	2.72	127.13	124.26
33	9	307	CHL	CHC-C1C-NC	2.72	128.32	124.20
25	7	309	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
33	8	307	CHL	C3C-C4C-NC	2.72	113.62	110.57
25	8	305	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
34	1	616	LUT	C3-C4-C5	-2.71	106.45	111.85
25	1	611	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	6	601	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	P	603	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
34	S	316	LUT	C31-C30-C29	-2.71	123.44	127.31
36	P	621	NEX	C31-C30-C29	-2.71	123.44	127.31
25	A	833	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
25	Q	612	CLA	C3B-C4B-NB	-2.71	108.00	110.52
25	a	310	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
33	P	622	CHL	CHC-C1C-NC	2.71	128.32	124.20
25	A	823	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	U	312	CLA	CHB-C4A-NA	2.71	128.26	124.51
33	S	309	CHL	CHC-C1C-NC	2.71	128.31	124.20
36	P	621	NEX	C15-C35-C34	-2.71	117.92	123.47
25	7	306	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	H	205	CLA	CAA-C2A-C1A	-2.71	106.14	112.14
30	B	848	DGD	O1G-C1A-C2A	2.71	120.41	111.91
25	A	805	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	P	610	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	A	808	CLA	CHB-C4A-NA	2.71	128.26	124.51
28	A	845	BCR	C10-C11-C12	-2.71	114.77	123.22
27	A	843	LHG	C5-O7-C7	-2.71	111.12	117.79
25	B	835	CLA	C3B-C4B-NB	-2.71	108.00	110.52
26	A	841	PQN	C11-C12-C13	-2.71	122.28	126.79
31	B	850	SQD	O9-S-C6	2.71	110.16	106.94
25	R	613	CLA	O2D-CGD-O1D	-2.71	118.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	S	318	XAT	C35-C34-C33	-2.71	123.45	127.31
33	3	306	CHL	CHB-C1B-NB	-2.71	121.39	124.26
25	8	313	CLA	CHB-C1B-NB	2.71	127.12	124.26
34	S	316	LUT	C22-C23-C24	2.71	114.82	111.74
33	P	608	CHL	CHC-C1C-NC	2.70	128.31	124.20
28	F	803	BCR	C23-C24-C25	-2.70	119.61	127.20
25	9	309	CLA	CHB-C4A-NA	2.70	128.25	124.51
34	1	616	LUT	C4-C5-C6	-2.70	114.82	120.85
33	9	307	CHL	C3B-C4B-NB	2.70	113.02	110.52
34	9	312	LUT	C39-C29-C28	2.70	122.33	118.08
25	6	610	CLA	CHB-C4A-NA	2.70	128.25	124.51
32	J	104	LMG	O8-C28-C29	2.70	120.39	111.91
25	A	835	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	9	309	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	4	312	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	2	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	Q	613	CLA	C3B-C4B-NB	-2.70	108.01	110.52
25	3	304	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	5	321	LHG	O8-C23-C24	2.70	120.38	111.91
28	3	319	BCR	C16-C15-C14	-2.70	117.95	123.47
28	L	204	BCR	C30-C25-C24	2.70	123.41	115.78
25	B	804	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
33	S	321	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
25	B	818	CLA	C1-C2-C3	-2.70	121.38	126.04
28	A	854	BCR	C7-C8-C9	-2.70	122.16	126.23
27	A	844	LHG	O8-C23-C24	2.69	120.36	111.91
25	A	807	CLA	CHB-C1B-NB	2.69	127.11	124.26
25	A	816	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	5	315	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	R	610	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	A	801	CLA	CBA-CAA-C2A	-2.69	105.92	113.86
33	Q	607	CHL	CHC-C1C-NC	2.69	128.29	124.20
34	S	316	LUT	C35-C15-C14	-2.69	117.96	123.47
36	R	617	NEX	C24-C23-C22	-2.69	105.57	110.77
25	8	312	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	9	301	CLA	CMB-C2B-C3B	2.69	130.56	123.59
25	A	832	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	H	202	CLA	C3B-C4B-NB	-2.69	108.02	110.52
33	P	622	CHL	CHD-C4C-NC	2.69	128.44	124.20
33	R	606	CHL	CHC-C1C-NC	2.69	128.28	124.20
25	B	838	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
33	Q	605	CHL	C2A-C3A-C4A	-2.69	98.35	101.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	842	BCR	C8-C7-C6	-2.69	119.65	127.20
33	6	608	CHL	CHB-C4A-NA	2.69	128.23	124.51
25	B	806	CLA	C3B-C4B-NB	-2.69	108.02	110.52
25	a	313	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
25	B	815	CLA	CHC-C4B-NB	2.69	127.10	124.26
25	A	815	CLA	C3B-C4B-NB	-2.69	108.02	110.52
25	A	842	CLA	CMC-C2C-C1C	-2.69	120.95	125.04
33	5	307	CHL	C3C-C4C-NC	2.68	113.58	110.57
25	A	813	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	4	302	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
33	U	308	CHL	C3C-C4C-NC	2.68	113.58	110.57
32	J	107	LMG	C1-C2-C3	2.68	115.58	110.00
25	5	305	CLA	C3B-C4B-NB	-2.68	108.03	110.52
28	J	101	BCR	C38-C26-C27	2.68	118.77	113.62
28	L	208	BCR	C33-C5-C6	-2.68	121.52	124.53
36	U	316	NEX	C24-C23-C22	-2.68	105.59	110.77
25	P	604	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	5	316	CLA	CHB-C4A-NA	2.68	128.22	124.51
32	7	319	LMG	O1-C1-C2	2.68	112.49	108.30
28	L	207	BCR	C3-C4-C5	-2.68	109.29	114.08
28	B	840	BCR	C16-C15-C14	-2.68	117.98	123.47
28	J	106	BCR	C33-C5-C4	2.68	118.76	113.62
34	8	316	LUT	C30-C31-C32	-2.68	114.86	123.22
25	A	807	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	P	602	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	2	304	CLA	C3B-C4B-NB	-2.68	108.03	110.52
25	a	311	CLA	C1-C2-C3	-2.68	121.41	126.04
25	B	804	CLA	CHB-C1B-NB	2.68	127.09	124.26
34	4	316	LUT	C10-C11-C12	-2.68	114.87	123.22
25	H	201	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
34	9	312	LUT	C30-C31-C32	-2.67	114.87	123.22
25	R	611	CLA	C3B-C4B-NB	-2.67	108.03	110.52
28	B	845	BCR	C15-C14-C13	-2.67	123.50	127.31
25	U	302	CLA	C3B-C4B-NB	-2.67	108.04	110.52
25	2	303	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	A	822	CLA	O2D-CGD-CBD	2.67	116.02	111.27
25	A	834	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	2	302	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	8	306	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	O	202	CLA	CBD-CHA-C1A	2.67	131.65	128.50
25	7	308	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	6	615	CLA	CHB-C4A-NA	2.67	128.20	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	309	CLA	C1-C2-C3	-2.67	121.43	126.04
25	3	303	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
33	Q	608	CHL	CHD-C1D-ND	-2.67	122.00	124.45
25	9	310	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	2	307	CLA	CHB-C4A-NA	2.67	128.20	124.51
34	2	316	LUT	C30-C31-C32	-2.67	114.90	123.22
25	A	842	CLA	C1-C2-C3	-2.67	121.43	126.04
25	A	837	CLA	CHB-C4A-NA	2.66	128.20	124.51
25	6	614	CLA	CHB-C4A-NA	2.66	128.20	124.51
25	A	835	CLA	CHB-C1B-NB	2.66	127.08	124.26
25	P	612	CLA	C1-C2-C3	2.66	130.65	126.04
33	R	601	CHL	CHD-C4C-NC	2.66	128.40	124.20
25	6	612	CLA	CHB-C1B-NB	2.66	127.08	124.26
34	P	615	LUT	C3-C4-C5	-2.66	106.55	111.85
25	5	314	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
25	S	315	CLA	CHB-C4A-NA	2.66	128.19	124.51
34	a	314	LUT	C11-C10-C9	-2.66	123.51	127.31
33	U	309	CHL	CAC-C3C-C4C	2.66	128.26	124.81
25	Q	609	CLA	C3B-C4B-NB	-2.66	108.05	110.52
25	4	312	CLA	C3B-C4B-NB	-2.66	108.05	110.52
25	5	305	CLA	CHC-C4B-NB	2.66	127.07	124.26
33	P	622	CHL	O2A-CGA-CBA	2.66	120.25	111.91
28	4	317	BCR	C21-C20-C19	-2.66	114.92	123.22
25	B	807	CLA	O2A-CGA-O1A	-2.66	116.89	123.59
25	B	849	CLA	C3B-C4B-NB	-2.66	108.05	110.52
25	8	312	CLA	C3B-C4B-NB	-2.66	108.05	110.52
33	7	305	CHL	C4-C3-C5	2.66	119.74	115.27
25	8	308	CLA	C1-C2-C3	-2.66	122.45	126.75
33	P	619	CHL	O2D-CGD-O1D	-2.66	118.65	123.84
34	1	616	LUT	C20-C13-C12	2.66	122.26	118.08
25	3	303	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	a	312	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
26	A	841	PQN	C2M-C2-C3	-2.65	120.07	124.40
25	A	842	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	A	846	BCR	C33-C5-C4	2.65	118.71	113.62
28	J	106	BCR	C4-C5-C6	-2.65	118.88	122.73
25	A	827	CLA	C1-C2-C3	-2.65	121.45	126.04
33	R	606	CHL	CHB-C1B-NB	-2.65	121.45	124.26
33	5	317	CHL	CHB-C1B-NB	-2.65	121.45	124.26
33	6	607	CHL	C1-C2-C3	-2.65	121.46	126.04
25	U	304	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
35	P	616	XAT	C35-C15-C14	-2.65	118.04	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	311	CLA	O2D-CGD-CBD	2.65	115.98	111.27
25	6	603	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	1	614	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	Q	603	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
28	3	318	BCR	C1-C6-C7	2.65	123.27	115.78
36	U	301	NEX	C24-C23-C22	-2.65	105.66	110.77
34	3	316	LUT	C35-C34-C33	-2.65	123.53	127.31
28	3	318	BCR	C30-C25-C26	-2.65	118.88	122.61
25	2	311	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	7	303	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	J	103	CLA	C3B-C4B-NB	-2.65	108.06	110.52
25	2	304	CLA	CHB-C4A-NA	2.65	128.17	124.51
33	U	308	CHL	CHC-C1C-NC	2.65	128.22	124.20
25	P	611	CLA	CED-O2D-CGD	2.65	121.92	115.94
25	Q	612	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
25	G	201	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	8	308	CLA	C3B-C4B-NB	-2.65	108.06	110.52
28	G	203	BCR	C33-C5-C4	2.64	118.69	113.62
33	P	601	CHL	CHD-C4C-NC	2.64	128.37	124.20
25	B	831	CLA	CHB-C4A-NA	2.64	128.17	124.51
25	A	824	CLA	CHB-C1B-NB	2.64	127.06	124.26
34	4	316	LUT	C21-C26-C27	-2.64	109.36	112.70
34	U	314	LUT	C18-C5-C4	2.64	119.25	114.36
33	S	302	CHL	C3B-C4B-NB	2.64	112.97	110.52
28	J	101	BCR	C35-C13-C12	2.64	122.24	118.08
34	4	316	LUT	C3-C4-C5	-2.64	106.59	111.85
36	P	621	NEX	C17-C1-C6	-2.64	108.11	110.47
25	6	605	CLA	CHB-C1B-NB	2.64	127.05	124.26
33	1	601	CHL	O2D-CGD-O1D	-2.64	118.68	123.84
28	G	203	BCR	C28-C27-C26	-2.64	109.37	114.08
25	3	301	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	B	838	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	A	802	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
34	P	614	LUT	C20-C13-C12	2.64	122.23	118.08
33	T	604	CHL	CAA-CBA-CGA	-2.64	105.55	113.25
25	R	612	CLA	C1-C2-C3	2.64	130.60	126.04
28	4	321	BCR	C35-C13-C14	-2.64	119.23	122.92
25	a	303	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
36	P	621	NEX	C20-C13-C14	-2.64	119.23	122.92
25	8	304	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
25	A	814	CLA	CHB-C1B-NB	2.64	127.05	124.26
25	U	304	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1	615	LUT	C16-C1-C6	-2.64	106.03	110.30
25	5	303	CLA	CHB-C4A-NA	2.63	128.16	124.51
33	Q	601	CHL	CHD-C4C-NC	2.63	128.35	124.20
33	5	308	CHL	CHD-C1D-ND	-2.63	122.03	124.45
30	B	848	DGD	C6E-C5E-C4E	-2.63	106.84	113.00
33	P	607	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
25	6	613	CLA	C1-C2-C3	-2.63	121.49	126.04
25	Q	612	CLA	CHD-C1D-ND	-2.63	122.04	124.45
34	8	317	LUT	C10-C11-C12	-2.63	115.01	123.22
25	9	302	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	B	824	CLA	CHB-C1B-NB	2.63	127.04	124.26
25	R	613	CLA	C3B-C4B-NB	-2.63	108.08	110.52
33	P	609	CHL	CHD-C1D-ND	-2.63	122.04	124.45
25	3	304	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	9	308	CLA	CHB-C4A-NA	2.63	128.14	124.51
34	9	312	LUT	C18-C5-C6	-2.63	121.58	124.53
35	T	615	XAT	C15-C35-C34	-2.63	118.09	123.47
25	A	851	CLA	C3B-C4B-NB	-2.63	108.08	110.52
25	B	827	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
35	P	616	XAT	C24-C23-C22	-2.62	105.70	110.77
25	B	821	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
34	7	314	LUT	C8-C7-C6	-2.62	119.83	127.20
25	U	312	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
28	3	319	BCR	C34-C9-C10	-2.62	119.25	122.92
25	Q	613	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
25	G	201	CLA	C1-C2-C3	-2.62	122.51	126.75
25	K	201	CLA	CHB-C4A-NA	2.62	128.14	124.51
34	4	315	LUT	C18-C5-C4	2.62	119.21	114.36
25	H	202	CLA	CMA-C3A-C2A	-2.62	109.98	116.10
33	7	305	CHL	O2A-CGA-CBA	2.62	120.14	111.91
32	4	320	LMG	C3-C4-C5	2.62	114.92	110.24
25	3	301	CLA	CHC-C4B-NB	2.62	127.03	124.26
27	Q	617	LHG	O8-C23-C24	2.62	120.14	111.91
34	3	315	LUT	C39-C29-C28	2.62	122.21	118.08
25	A	834	CLA	C3B-C4B-NB	-2.62	108.08	110.52
25	9	304	CLA	CHB-C4A-NA	2.62	128.14	124.51
33	4	305	CHL	CHC-C4B-NB	-2.62	121.48	124.26
33	3	306	CHL	CHB-C4A-NA	2.62	128.14	124.51
25	Q	610	CLA	CED-O2D-CGD	2.62	121.86	115.94
33	5	317	CHL	CHC-C1C-NC	2.62	128.18	124.20
28	B	851	BCR	C38-C26-C27	2.62	118.65	113.62
34	a	315	LUT	C4-C5-C6	-2.62	115.01	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	204	BCR	C34-C9-C10	-2.62	119.26	122.92
34	T	614	LUT	C19-C9-C8	2.62	122.20	118.08
33	6	617	CHL	C3C-C4C-NC	2.62	113.51	110.57
33	R	609	CHL	CHD-C1D-ND	-2.62	122.05	124.45
28	A	846	BCR	C37-C22-C21	-2.62	119.26	122.92
25	A	824	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
28	3	317	BCR	C33-C5-C4	2.62	118.64	113.62
33	R	607	CHL	O2D-CGD-O1D	-2.61	118.73	123.84
28	O	205	BCR	C38-C26-C27	2.61	118.64	113.62
25	3	305	CLA	CHB-C4A-NA	2.61	128.12	124.51
28	B	842	BCR	C16-C15-C14	-2.61	118.12	123.47
27	4	318	LHG	C5-O7-C7	-2.61	111.36	117.79
25	2	304	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	R	614	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	S	313	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	T	609	CLA	C1-C2-C3	-2.61	121.53	126.04
25	A	833	CLA	C3B-C4B-NB	-2.61	108.09	110.52
25	U	312	CLA	C3B-C4B-NB	-2.61	108.09	110.52
25	a	312	CLA	CHB-C1B-NB	2.61	127.02	124.26
25	A	814	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	2	313	CLA	CHB-C1B-NB	2.61	127.02	124.26
28	J	101	BCR	C23-C24-C25	-2.61	119.88	127.20
34	3	316	LUT	C10-C11-C12	-2.61	115.08	123.22
25	7	301	CLA	C3B-C4B-NB	-2.61	108.10	110.52
35	S	318	XAT	C25-C24-C23	2.61	117.91	112.75
25	R	614	CLA	CHB-C1B-NB	2.61	127.02	124.26
25	6	601	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	H	201	CLA	CHC-C4B-NB	2.61	127.02	124.26
25	8	304	CLA	CHB-C1B-NB	2.61	127.02	124.26
30	B	848	DGD	O5D-C6D-C5D	2.61	113.87	109.05
25	Q	609	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	8	309	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	T	603	CLA	CHB-C4A-NA	2.60	128.11	124.51
34	5	322	LUT	C8-C7-C6	-2.60	119.89	127.20
28	L	203	BCR	C16-C17-C18	-2.60	123.59	127.31
25	P	613	CLA	C3B-C4B-NB	-2.60	108.10	110.52
25	A	832	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	5	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
28	5	320	BCR	C8-C7-C6	-2.60	119.89	127.20
34	9	313	LUT	C31-C30-C29	-2.60	123.59	127.31
25	1	610	CLA	CHB-C1B-NB	2.60	127.01	124.26
33	P	606	CHL	CHC-C1C-NC	2.60	128.15	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	608	CHL	C3C-C4C-NC	2.60	113.49	110.57
34	R	616	LUT	C19-C9-C8	2.60	122.17	118.08
33	6	607	CHL	CHB-C4A-NA	2.60	128.11	124.51
25	3	302	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	a	308	CLA	CHC-C1C-NC	2.60	128.14	124.20
30	B	848	DGD	O6E-C1E-C2E	2.60	115.85	110.35
34	U	314	LUT	C3-C4-C5	-2.60	106.68	111.85
33	4	304	CHL	CHC-C1C-NC	2.60	128.14	124.20
25	3	307	CLA	C1-C2-C3	-2.60	122.55	126.75
28	B	840	BCR	C20-C21-C22	-2.60	123.60	127.31
28	L	203	BCR	C10-C11-C12	-2.60	115.11	123.22
28	B	851	BCR	C36-C18-C17	-2.60	119.29	122.92
27	6	618	LHG	O8-C23-C24	2.60	120.06	111.91
25	2	313	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	a	306	CLA	CHB-C4A-NA	2.60	128.10	124.51
28	6	621	BCR	C1-C6-C7	2.60	123.12	115.78
25	Q	613	CLA	CHB-C1B-NB	2.60	127.00	124.26
25	L	205	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	S	305	CLA	C1-C2-C3	-2.60	122.55	126.75
25	A	821	CLA	CHB-C1B-NB	2.59	127.00	124.26
25	L	205	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	P	604	CLA	C1-C2-C3	-2.59	122.55	126.75
25	Q	618	CLA	C2A-C3A-C4A	-2.59	98.98	103.59
25	B	835	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
33	8	307	CHL	C4-C3-C5	2.59	119.63	115.27
34	a	316	LUT	C20-C13-C14	-2.59	119.29	122.92
34	4	315	LUT	C1-C2-C3	2.59	119.50	113.64
25	T	602	CLA	C3B-C4B-NB	-2.59	108.11	110.52
25	T	611	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	a	309	CLA	CHB-C1B-NB	2.59	127.00	124.26
25	O	203	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	6	601	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	K	205	CLA	C3B-C4B-NB	-2.59	108.11	110.52
27	4	319	LHG	O8-C23-C24	2.59	120.03	111.91
25	6	623	CLA	O2D-CGD-CBD	2.59	115.87	111.27
25	B	820	CLA	CHC-C4B-NB	2.59	127.00	124.26
32	4	320	LMG	C8-O7-C10	-2.59	111.42	117.79
25	B	810	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	6	609	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
28	3	319	BCR	C8-C9-C10	2.59	122.91	118.94
34	1	617	LUT	C3-C4-C5	-2.59	106.70	111.85
25	5	324	CLA	CHB-C1B-NB	2.59	127.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	312	CLA	C3B-C4B-NB	-2.59	108.11	110.52
34	U	315	LUT	C15-C35-C34	-2.59	118.17	123.47
25	L	202	CLA	CHB-C4A-NA	2.59	128.09	124.51
33	Q	606	CHL	CHC-C1C-NC	2.59	128.13	124.20
33	S	306	CHL	CHD-C4C-NC	2.59	128.28	124.20
25	9	310	CLA	CHB-C1B-NB	2.59	127.00	124.26
25	5	305	CLA	C1-C2-C3	-2.59	122.57	126.75
25	1	607	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	8	315	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	B	803	CLA	CHB-C1B-NB	2.58	126.99	124.26
25	3	307	CLA	CHB-C1B-NB	2.58	126.99	124.26
33	6	606	CHL	C1-C2-C3	-2.58	121.58	126.04
27	P	618	LHG	O8-C23-C24	2.58	120.01	111.91
25	3	309	CLA	C3B-C4B-NB	-2.58	108.12	110.52
25	A	819	CLA	CHB-C4A-NA	2.58	128.08	124.51
28	L	203	BCR	C11-C10-C9	-2.58	123.62	127.31
25	Q	611	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	O	204	BCR	C7-C8-C9	-2.58	122.34	126.23
34	7	314	LUT	C3-C4-C5	-2.58	106.72	111.85
28	3	318	BCR	C1-C6-C5	-2.58	118.98	122.61
33	P	622	CHL	C4-C3-C5	2.58	119.61	115.27
32	J	107	LMG	C1-O6-C5	2.58	118.75	113.69
25	A	818	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	B	811	CLA	CHB-C1B-NB	2.58	126.99	124.26
33	P	608	CHL	C3C-C4C-NC	2.58	113.46	110.57
25	6	613	CLA	C3B-C4B-NB	-2.58	108.12	110.52
28	L	204	BCR	C30-C25-C26	-2.58	118.98	122.61
25	P	611	CLA	CMA-C3A-C2A	-2.58	110.08	116.10
25	R	604	CLA	CHB-C4A-NA	2.58	128.08	124.51
33	4	306	CHL	C3C-C4C-NC	2.58	113.46	110.57
25	8	302	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
28	K	206	BCR	C34-C9-C10	-2.58	119.31	122.92
25	4	302	CLA	CHB-C1B-NB	2.58	126.98	124.26
25	1	613	CLA	CHB-C4A-NA	2.58	128.07	124.51
35	T	615	XAT	C24-C23-C22	-2.58	105.80	110.77
25	O	203	CLA	CAB-C3B-C2B	2.58	130.26	123.59
34	a	314	LUT	C15-C14-C13	-2.57	123.64	127.31
25	3	308	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
25	6	623	CLA	C3B-C4B-NB	-2.57	108.13	110.52
25	5	304	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
34	a	314	LUT	C39-C29-C28	2.57	122.13	118.08
25	L	202	CLA	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	830	CLA	CHB-C1B-NB	2.57	126.98	124.26
25	S	304	CLA	C3B-C4B-NB	-2.57	108.13	110.52
25	A	837	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
34	Q	614	LUT	C31-C30-C29	-2.57	123.64	127.31
32	J	107	LMG	O8-C28-C29	2.57	119.98	111.91
25	6	620	CLA	C3B-C4B-NB	-2.57	108.13	110.52
28	B	845	BCR	C38-C26-C25	-2.57	121.64	124.53
33	Q	607	CHL	C3C-C4C-NC	2.57	113.45	110.57
25	T	609	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
25	H	202	CLA	CHB-C1B-NB	2.57	126.98	124.26
25	U	303	CLA	C3B-C4B-NB	-2.57	108.13	110.52
25	A	820	CLA	CHB-C4A-NA	2.57	128.07	124.51
35	Q	616	XAT	C20-C13-C14	-2.57	119.32	122.92
34	U	315	LUT	C19-C9-C8	2.57	122.13	118.08
34	2	316	LUT	C35-C34-C33	-2.57	123.64	127.31
25	3	311	CLA	C3B-C4B-NB	-2.57	108.13	110.52
28	B	840	BCR	C23-C24-C25	-2.57	119.99	127.20
25	8	305	CLA	CHB-C1B-NB	2.57	126.98	124.26
25	U	313	CLA	O2A-CGA-O1A	-2.57	116.90	123.30
25	B	836	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	J	103	CLA	CHB-C4A-NA	2.57	128.06	124.51
33	6	608	CHL	CAA-C2A-C1A	-2.57	103.56	111.97
25	3	314	CLA	CHB-C1B-NB	2.57	126.97	124.26
28	I	201	BCR	C36-C18-C17	-2.57	119.33	122.92
34	R	616	LUT	C38-C25-C24	-2.57	118.07	123.56
33	9	306	CHL	OMC-CMC-C2C	-2.57	119.89	125.69
25	B	817	CLA	CHC-C4B-NB	2.57	126.97	124.26
25	a	310	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	B	820	CLA	CHB-C4A-NA	2.56	128.06	124.51
34	S	316	LUT	C20-C13-C12	2.56	122.12	118.08
25	A	807	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
28	A	848	BCR	C28-C27-C26	-2.56	109.50	114.08
27	B	847	LHG	O8-C23-C24	2.56	119.95	111.91
25	4	308	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	9	309	CLA	C3B-C4B-NB	-2.56	108.14	110.52
25	7	312	CLA	CHB-C1B-NB	2.56	126.97	124.26
34	1	617	LUT	C1-C6-C7	2.56	123.02	115.78
25	B	849	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	A	812	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	B	833	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
34	4	316	LUT	C18-C5-C4	2.56	119.10	114.36
33	6	608	CHL	CAA-CBA-CGA	-2.56	105.78	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	833	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	Q	611	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
25	U	311	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
35	S	318	XAT	C40-C33-C32	2.56	122.11	118.08
25	5	319	CLA	C2A-C1A-CHA	2.56	128.33	123.86
25	4	311	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	R	602	CLA	CHB-C1B-NB	2.56	126.96	124.26
34	9	313	LUT	C16-C1-C6	-2.56	106.15	110.30
26	A	841	PQN	C21-C22-C23	-2.56	107.66	115.92
25	J	103	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
25	a	303	CLA	CHB-C1B-NB	2.56	126.96	124.26
34	6	622	LUT	C8-C7-C6	-2.56	120.02	127.20
28	K	206	BCR	C33-C5-C4	2.56	118.53	113.62
25	1	609	CLA	C2B-C1B-NB	2.56	111.94	110.23
33	P	619	CHL	CHB-C1B-NB	-2.56	121.55	124.26
25	4	301	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
25	5	313	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
25	H	203	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	B	826	CLA	C1-C2-C3	-2.55	121.63	126.04
28	8	301	BCR	C33-C5-C4	2.55	118.52	113.62
25	a	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
28	G	203	BCR	C16-C15-C14	-2.55	118.24	123.47
25	2	303	CLA	C3B-C4B-NB	-2.55	108.15	110.52
34	1	615	LUT	C10-C11-C12	-2.55	115.25	123.22
25	U	302	CLA	CHB-C4A-NA	2.55	128.04	124.51
33	T	601	CHL	C3B-C4B-NB	2.55	112.88	110.52
28	A	846	BCR	C16-C15-C14	-2.55	118.25	123.47
36	U	301	NEX	C26-C27-C28	-2.55	120.60	125.99
28	A	846	BCR	C21-C20-C19	-2.55	115.26	123.22
25	5	303	CLA	CHC-C4B-NB	2.55	126.96	124.26
25	P	603	CLA	C3B-C4B-NB	-2.55	108.15	110.52
28	A	846	BCR	C28-C27-C26	-2.55	109.53	114.08
25	Q	602	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
33	4	306	CHL	C5-C3-C4	2.55	120.23	114.60
25	A	826	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	4	303	CLA	CHB-C4A-NA	2.55	128.03	124.51
33	T	601	CHL	CHD-C4C-NC	2.55	128.22	124.20
33	T	606	CHL	C3C-C4C-NC	2.55	113.43	110.57
25	1	612	CLA	C2A-C1A-CHA	2.55	128.31	123.86
25	B	813	CLA	C3B-C4B-NB	-2.54	108.15	110.52
25	B	811	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	A	816	CLA	CHB-C1B-NB	2.54	126.95	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	311	CLA	CHB-C1B-NB	2.54	126.95	124.26
25	H	201	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	5	314	CLA	C3B-C4B-NB	-2.54	108.16	110.52
25	O	201	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
35	P	623	XAT	O23-C23-C24	-2.54	104.75	109.80
25	a	309	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
25	P	610	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	a	301	CLA	O1D-CGD-CBD	2.54	129.68	124.48
33	P	607	CHL	CHB-C1B-NB	-2.54	121.57	124.26
34	a	315	LUT	C1-C6-C5	-2.54	119.04	122.61
25	B	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
27	S	319	LHG	O8-C23-C24	2.54	119.88	111.91
33	U	309	CHL	CHC-C4B-NB	-2.54	121.57	124.26
28	F	801	BCR	C20-C19-C18	-2.54	119.28	126.42
33	4	304	CHL	CHD-C1D-ND	-2.54	122.12	124.45
25	Q	602	CLA	CMB-C2B-C1B	-2.54	121.50	125.37
34	2	316	LUT	C16-C1-C6	-2.54	106.18	110.30
25	A	809	CLA	O2D-CGD-CBD	2.54	115.78	111.27
25	A	818	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
25	7	301	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
25	A	838	CLA	CHB-C1B-NB	2.54	126.94	124.26
25	L	206	CLA	CHB-C4A-NA	2.53	128.02	124.51
28	B	842	BCR	C10-C11-C12	-2.53	115.31	123.22
25	T	612	CLA	CHB-C4A-NA	2.53	128.02	124.51
28	F	801	BCR	C15-C14-C13	-2.53	123.70	127.31
25	Q	602	CLA	C3B-C4B-NB	-2.53	108.17	110.52
34	P	615	LUT	C15-C35-C34	-2.53	118.29	123.47
33	5	308	CHL	CHB-C1B-NB	-2.53	121.58	124.26
27	T	617	LHG	O8-C23-C24	2.53	119.85	111.91
33	T	605	CHL	CMB-C2B-C1B	2.53	129.22	125.37
25	a	301	CLA	CHB-C4A-NA	2.53	128.01	124.51
28	B	844	BCR	C28-C27-C26	-2.53	109.56	114.08
25	3	310	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
25	4	307	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	A	835	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
25	7	306	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
32	H	204	LMG	O8-C28-C29	2.53	119.84	111.91
28	B	843	BCR	C33-C5-C4	2.53	118.47	113.62
28	A	847	BCR	C21-C20-C19	-2.53	115.33	123.22
25	K	205	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	S	314	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	Q	609	CLA	CHD-C1D-ND	-2.53	122.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	314	CLA	CHB-C4A-NA	2.53	128.00	124.51
25	8	304	CLA	CHB-C4A-NA	2.53	128.00	124.51
28	A	846	BCR	C38-C26-C27	2.53	118.47	113.62
25	B	825	CLA	C3B-C4B-NB	-2.53	108.17	110.52
25	a	312	CLA	CHB-C4A-NA	2.53	128.00	124.51
33	U	307	CHL	O2A-CGA-CBA	2.52	119.83	111.91
34	S	316	LUT	C30-C31-C32	-2.52	115.34	123.22
25	S	320	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
33	R	605	CHL	CHB-C1B-NB	-2.52	121.58	124.26
34	1	616	LUT	C1-C6-C5	-2.52	119.06	122.61
25	Q	609	CLA	CHB-C1B-NB	2.52	126.93	124.26
33	S	308	CHL	CHB-C1B-NB	-2.52	121.59	124.26
33	4	306	CHL	CHC-C1C-NC	2.52	128.03	124.20
25	O	202	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
25	Q	603	CLA	C3B-C4B-NB	-2.52	108.18	110.52
25	1	602	CLA	C3B-C4B-NB	-2.52	108.18	110.52
25	6	610	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
25	K	201	CLA	O2D-CGD-CBD	2.52	115.74	111.27
34	T	613	LUT	C3-C4-C5	-2.52	106.84	111.85
25	K	203	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	4	312	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	H	201	CLA	C3B-C4B-NB	-2.52	108.18	110.52
28	B	843	BCR	C33-C5-C6	-2.52	121.70	124.53
33	R	607	CHL	CHB-C1B-NB	-2.52	121.59	124.26
25	8	303	CLA	CHC-C4B-NB	2.52	126.92	124.26
25	B	820	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
28	3	317	BCR	C36-C18-C19	2.52	122.04	118.08
28	I	201	BCR	C8-C7-C6	-2.52	120.14	127.20
34	7	315	LUT	C30-C31-C32	-2.52	115.37	123.22
25	B	830	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	6	615	CLA	CAA-CBA-CGA	-2.51	105.90	113.25
25	3	310	CLA	CHB-C4A-NA	2.51	127.99	124.51
25	a	308	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
25	A	828	CLA	CHC-C4B-NB	2.51	126.92	124.26
27	4	319	LHG	C5-O7-C7	-2.51	111.61	117.79
34	9	313	LUT	C18-C5-C6	-2.51	121.71	124.53
28	L	204	BCR	C10-C11-C12	-2.51	115.39	123.22
25	7	313	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	R	613	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	R	603	CLA	C3B-C4B-NB	-2.51	108.19	110.52
35	P	616	XAT	C15-C35-C34	-2.51	118.34	123.47
33	R	606	CHL	CHB-C4A-NA	2.51	127.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	312	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
25	T	611	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
33	U	306	CHL	CMB-C2B-C1B	2.51	129.19	125.37
25	1	609	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
33	4	305	CHL	O2A-CGA-CBA	2.50	119.77	111.91
34	a	314	LUT	C19-C9-C8	2.50	122.02	118.08
25	B	831	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
28	G	203	BCR	C10-C11-C12	-2.50	115.41	123.22
25	6	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	4	308	CLA	CAC-C3C-C4C	2.50	128.06	124.81
33	5	308	CHL	CMB-C2B-C1B	2.50	129.18	125.37
34	8	316	LUT	C20-C13-C14	-2.50	119.42	122.92
25	a	302	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	A	811	CLA	CHB-C1B-NB	2.50	126.91	124.26
32	J	107	LMG	O1-C1-C2	2.50	112.21	108.30
25	6	609	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	a	313	CLA	CHC-C4B-NB	2.50	126.90	124.26
25	F	802	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	A	830	CLA	O2D-CGD-CBD	2.50	115.71	111.27
28	J	101	BCR	C2-C1-C6	2.50	114.33	110.48
28	A	847	BCR	C7-C8-C9	-2.50	122.46	126.23
26	B	839	PQN	C14-C13-C15	2.50	119.47	115.27
33	6	607	CHL	C4-C3-C5	2.50	119.47	115.27
28	B	845	BCR	C11-C10-C9	-2.50	123.75	127.31
25	2	302	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	T	608	CLA	CHB-C4A-NA	2.50	127.96	124.51
25	4	302	CLA	CHB-C4A-NA	2.50	127.96	124.51
25	7	301	CLA	CHB-C4A-NA	2.50	127.96	124.51
34	7	314	LUT	C10-C11-C12	-2.50	115.43	123.22
25	B	825	CLA	C1-C2-C3	-2.50	121.73	126.04
33	R	601	CHL	C3B-C4B-NB	2.49	112.83	110.52
27	P	624	LHG	O8-C23-C24	2.49	119.73	111.91
28	O	204	BCR	C39-C30-C25	-2.49	106.25	110.30
30	B	846	DGD	O1G-C1A-C2A	2.49	119.73	111.91
25	A	815	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	5	309	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
25	O	203	CLA	CMB-C2B-C3B	2.49	130.05	123.59
34	1	615	LUT	C18-C5-C4	2.49	118.97	114.36
33	U	308	CHL	C4A-NA-C1A	-2.49	105.59	106.71
25	A	837	CLA	CAA-CBA-CGA	-2.49	105.97	113.25
33	9	306	CHL	CHB-C4A-NA	2.49	127.96	124.51
33	S	302	CHL	O2A-CGA-CBA	2.49	119.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	P	611	CLA	CGD-CBD-CAD	-2.49	102.67	110.73
34	3	316	LUT	C3-C4-C5	-2.49	106.89	111.85
34	6	622	LUT	C10-C11-C12	-2.49	115.45	123.22
27	A	852	LHG	O8-C23-C24	2.49	119.72	111.91
25	a	310	CLA	C3B-C4B-NB	-2.49	108.21	110.52
28	4	321	BCR	C16-C17-C18	-2.49	123.76	127.31
34	4	315	LUT	C21-C26-C27	-2.49	109.56	112.70
28	4	321	BCR	C7-C6-C5	-2.49	115.43	121.46
25	R	602	CLA	CHB-C4A-NA	2.49	127.95	124.51
34	7	314	LUT	C30-C31-C32	-2.49	115.45	123.22
33	R	605	CHL	C3C-C4C-NC	2.49	113.36	110.57
36	U	316	NEX	C26-C27-C28	-2.49	120.73	125.99
28	A	854	BCR	C27-C26-C25	-2.49	119.12	122.73
25	B	817	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
34	T	614	LUT	C15-C35-C34	-2.49	118.38	123.47
25	A	827	CLA	C11-C12-C13	-2.49	107.88	115.92
33	S	308	CHL	C4-C3-C5	2.49	118.83	115.98
25	B	829	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	R	618	LHG	O8-C23-C24	2.49	119.71	111.91
25	a	308	CLA	C2B-C1B-NB	2.49	111.90	110.23
33	4	314	CHL	C3C-C4C-NC	2.49	113.36	110.57
35	P	623	XAT	C15-C35-C34	-2.48	118.38	123.47
25	A	812	CLA	C2D-C1D-ND	-2.48	108.27	110.10
28	B	843	BCR	C15-C16-C17	-2.48	118.39	123.47
25	7	302	CLA	CHB-C4A-NA	2.48	127.95	124.51
25	A	842	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
25	1	605	CLA	CHB-C1B-NB	2.48	126.89	124.26
25	7	308	CLA	CHB-C1B-NB	2.48	126.89	124.26
25	B	802	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	B	832	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	6	618	LHG	O7-C7-O9	-2.48	117.71	123.70
34	3	316	LUT	C15-C14-C13	-2.48	123.77	127.31
25	B	819	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	5	312	CLA	CHB-C4A-NA	2.48	127.94	124.51
33	T	604	CHL	CHB-C1B-NB	-2.48	121.63	124.26
25	A	829	CLA	O2D-CGD-CBD	2.48	115.67	111.27
25	R	610	CLA	CHD-C1D-ND	-2.48	122.18	124.45
25	Q	604	CLA	C3B-C4B-NB	-2.48	108.22	110.52
28	B	851	BCR	C4-C5-C6	-2.48	119.14	122.73
34	4	315	LUT	C16-C1-C6	-2.48	106.28	110.30
25	A	837	CLA	C3B-C4B-NB	-2.47	108.22	110.52
33	T	607	CHL	C3B-C4B-NB	2.47	112.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	8	318	BCR	C2-C1-C6	2.47	114.29	110.48
25	P	611	CLA	CBB-CAB-C3B	-2.47	115.31	127.62
25	4	309	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
25	7	311	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	F	803	BCR	C38-C26-C27	2.47	118.37	113.62
25	Q	612	CLA	CHB-C4A-NA	2.47	127.93	124.51
34	a	314	LUT	C31-C30-C29	-2.47	123.78	127.31
25	7	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
33	4	304	CHL	CAA-C2A-C3A	-2.47	110.33	116.10
34	6	622	LUT	C31-C30-C29	-2.47	123.78	127.31
33	1	601	CHL	CHB-C1B-NB	-2.47	121.64	124.26
25	A	825	CLA	CAC-C3C-C4C	2.47	128.02	124.81
33	a	305	CHL	C3C-C4C-NC	2.47	113.34	110.57
33	P	605	CHL	CHB-C1B-NB	-2.47	121.64	124.26
25	A	842	CLA	CHC-C4B-NB	2.47	126.87	124.26
35	P	620	XAT	C15-C35-C34	-2.47	118.42	123.47
25	3	310	CLA	CHB-C1B-NB	2.47	126.87	124.26
34	3	316	LUT	C8-C7-C6	-2.47	120.27	127.20
25	A	830	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	A	838	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	T	612	CLA	CHB-C1B-NB	2.47	126.87	124.26
33	U	305	CHL	CHB-C1B-NB	-2.47	121.64	124.26
25	B	815	CLA	O2D-CGD-CBD	2.47	115.65	111.27
25	K	202	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	H	205	CLA	C3B-C4B-NB	-2.47	108.23	110.52
25	7	302	CLA	CHB-C1B-NB	2.47	126.87	124.26
25	5	310	CLA	C3B-C4B-NB	-2.47	108.23	110.52
34	5	318	LUT	C16-C1-C6	-2.47	106.30	110.30
25	B	806	CLA	O2D-CGD-CBD	2.47	115.65	111.27
25	1	613	CLA	CHB-C1B-NB	2.47	126.87	124.26
28	F	801	BCR	C37-C22-C21	-2.47	119.47	122.92
34	a	315	LUT	C30-C31-C32	-2.46	115.53	123.22
28	F	801	BCR	C8-C7-C6	-2.46	120.28	127.20
25	A	851	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
25	K	201	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
25	B	813	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
33	9	307	CHL	O2A-CGA-CBA	2.46	119.64	111.91
34	2	316	LUT	C10-C11-C12	-2.46	115.53	123.22
35	Q	616	XAT	C31-C32-C33	-2.46	119.50	126.42
31	B	850	SQD	O48-C23-C24	2.46	119.64	111.91
33	1	601	CHL	CMD-C2D-C3D	-2.46	121.95	127.61
25	B	822	CLA	O2D-CGD-CBD	2.46	115.64	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	O	204	BCR	C4-C5-C6	-2.46	119.16	122.73
28	A	854	BCR	C38-C26-C25	-2.46	121.76	124.53
25	A	804	CLA	CHB-C4A-NA	2.46	127.92	124.51
34	T	614	LUT	C18-C5-C4	2.46	118.91	114.36
34	8	317	LUT	C18-C5-C4	2.46	118.91	114.36
25	9	302	CLA	CHC-C4B-NB	2.46	126.86	124.26
34	7	315	LUT	C18-C5-C4	2.46	118.91	114.36
28	B	841	BCR	C38-C26-C27	2.46	118.34	113.62
25	P	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
33	3	306	CHL	C4-C3-C5	2.46	119.41	115.27
25	A	828	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
34	a	314	LUT	C16-C1-C6	-2.46	106.31	110.30
25	B	822	CLA	C1-C2-C3	-2.46	121.80	126.04
25	A	840	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	2	305	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	9	305	CLA	C1-C2-C3	-2.45	122.78	126.75
33	5	308	CHL	OBD-CAD-C3D	-2.45	122.61	128.52
25	2	302	CLA	CAA-CBA-CGA	-2.45	106.08	113.25
33	5	307	CHL	CHB-C1B-NB	-2.45	121.66	124.26
25	3	314	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
33	P	606	CHL	O2D-CGD-O1D	-2.45	119.04	123.84
34	4	315	LUT	C35-C15-C14	-2.45	118.45	123.47
25	S	312	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
32	J	104	LMG	C7-O1-C1	-2.45	108.95	113.74
28	3	318	BCR	C37-C22-C21	-2.45	119.49	122.92
27	8	319	LHG	C6-C5-C4	-2.45	106.00	111.79
25	2	308	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	8	306	CLA	CHB-C4A-NA	2.45	127.90	124.51
35	S	318	XAT	C7-C8-C9	-2.45	121.73	125.53
25	8	310	CLA	C1-C2-C3	-2.45	121.81	126.04
25	S	305	CLA	CHB-C4A-NA	2.45	127.90	124.51
34	a	316	LUT	C40-C33-C34	-2.45	119.50	122.92
25	3	313	CLA	CHB-C4A-NA	2.45	127.90	124.51
27	8	319	LHG	O8-C23-C24	2.45	119.59	111.91
34	1	615	LUT	C15-C14-C13	-2.45	123.82	127.31
25	2	310	CLA	CHB-C4A-NA	2.45	127.89	124.51
33	5	308	CHL	O2D-CGD-O1D	-2.45	119.06	123.84
33	P	601	CHL	C3B-C4B-NB	2.44	112.78	110.52
25	A	806	CLA	CHC-C4B-NB	2.44	126.84	124.26
33	Q	601	CHL	C3B-C4B-NB	2.44	112.78	110.52
32	6	602	LMG	C1-O6-C5	-2.44	108.89	113.69
35	P	623	XAT	C35-C15-C14	-2.44	118.47	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	849	BCR	C37-C22-C21	-2.44	119.50	122.92
25	6	604	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
25	1	610	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
28	F	801	BCR	C33-C5-C4	2.44	118.30	113.62
33	Q	608	CHL	C2A-C3A-C4A	2.44	105.81	101.87
33	6	607	CHL	O2A-CGA-CBA	2.44	119.56	111.91
25	A	853	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
25	B	834	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
25	7	312	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	7	311	CLA	C3B-C4B-NB	-2.44	108.25	110.52
25	B	823	CLA	CHB-C1B-NB	2.44	126.84	124.26
25	S	305	CLA	C3B-C4B-NB	-2.44	108.25	110.52
34	Q	615	LUT	C18-C5-C4	2.44	118.87	114.36
28	B	844	BCR	C8-C7-C6	-2.44	120.36	127.20
33	R	609	CHL	C2A-C3A-C4A	2.44	105.81	101.87
25	5	304	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
25	Q	603	CLA	CHD-C1D-ND	-2.44	122.22	124.45
25	A	839	CLA	CHB-C1B-NB	2.44	126.84	124.26
36	R	617	NEX	C40-C33-C34	-2.44	119.51	122.92
25	P	613	CLA	CHB-C4A-NA	2.43	127.88	124.51
34	1	617	LUT	C39-C29-C30	-2.43	119.51	122.92
28	L	203	BCR	C15-C14-C13	-2.43	123.84	127.31
28	4	317	BCR	C11-C12-C13	-2.43	119.58	126.42
25	B	837	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
33	P	609	CHL	C2A-C3A-C4A	2.43	105.80	101.87
25	5	313	CLA	C3B-C4B-NB	-2.43	108.26	110.52
32	2	301	LMG	C7-O1-C1	-2.43	108.99	113.74
33	S	309	CHL	OBD-CAD-C3D	-2.43	122.67	128.52
33	9	307	CHL	CED-O2D-CGD	2.43	121.44	115.94
34	4	315	LUT	C15-C35-C34	-2.43	118.50	123.47
25	3	312	CLA	CHB-C1B-NB	2.43	126.83	124.26
25	4	311	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
25	8	308	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
28	O	204	BCR	C11-C10-C9	-2.43	123.84	127.31
33	4	305	CHL	O1D-CGD-CBD	-2.43	119.51	124.48
25	G	202	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B	827	CLA	CHB-C1B-NB	2.43	126.83	124.26
33	4	306	CHL	CBC-CAC-C3C	-2.43	105.73	112.43
25	P	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	4	313	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B	833	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	a	309	CLA	CHB-C4A-NA	2.43	127.87	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	807	CLA	C1-C2-C3	-2.43	121.84	126.04
25	A	831	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
33	P	607	CHL	O2A-CGA-CBA	2.43	119.53	111.91
25	B	830	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
33	T	601	CHL	CHC-C4B-NB	-2.43	121.69	124.26
34	9	312	LUT	C10-C11-C12	-2.43	115.64	123.22
25	S	304	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	7	302	CLA	CAA-C2A-C1A	-2.43	104.03	111.97
25	B	817	CLA	CHB-C4A-NA	2.43	127.87	124.51
33	5	308	CHL	CHB-C4A-NA	2.43	127.87	124.51
33	6	608	CHL	C1D-ND-C4D	2.43	108.06	106.33
25	5	302	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
27	5	301	LHG	O8-C23-C24	2.43	119.52	111.91
25	O	203	CLA	O2D-CGD-O1D	-2.42	118.58	124.09
34	6	619	LUT	C3-C4-C5	-2.42	107.02	111.85
25	B	828	CLA	CHB-C4A-NA	2.42	127.86	124.51
28	8	301	BCR	C39-C30-C25	-2.42	106.37	110.30
25	Q	602	CLA	CHD-C1D-ND	-2.42	122.23	124.45
28	3	317	BCR	C29-C30-C25	2.42	114.21	110.48
25	B	804	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
34	U	314	LUT	C31-C30-C29	-2.42	123.86	127.31
25	a	304	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	A	802	CLA	O1D-CGD-CBD	2.42	129.44	124.48
25	A	804	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
33	P	619	CHL	O2A-CGA-CBA	2.42	119.50	111.91
25	1	610	CLA	C2D-C1D-ND	-2.42	108.32	110.10
33	R	607	CHL	O2A-CGA-CBA	2.42	119.50	111.91
34	a	315	LUT	C31-C30-C29	-2.42	123.86	127.31
25	3	302	CLA	CAA-CBA-CGA	-2.42	106.19	113.25
25	S	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	2	303	CLA	C2D-C1D-ND	-2.42	108.32	110.10
25	4	307	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	A	819	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
25	5	313	CLA	C3C-C4C-NC	-2.42	107.86	110.57
28	A	854	BCR	C10-C11-C12	-2.41	115.68	123.22
25	6	603	CLA	CHB-C1B-NB	2.41	126.81	124.26
25	4	313	CLA	CMA-C3A-C2A	-2.41	110.46	116.10
34	9	312	LUT	C35-C15-C14	-2.41	118.53	123.47
25	7	313	CLA	CHB-C4A-NA	2.41	127.85	124.51
33	9	307	CHL	C5-C3-C4	2.41	119.93	114.60
25	S	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
33	T	605	CHL	O2D-CGD-O1D	-2.41	119.12	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	316	LUT	C39-C29-C28	2.41	121.88	118.08
28	6	621	BCR	C21-C20-C19	-2.41	115.69	123.22
35	Q	616	XAT	C15-C35-C34	-2.41	118.53	123.47
33	Q	605	CHL	CHB-C1B-NB	-2.41	121.70	124.26
28	A	854	BCR	C20-C21-C22	-2.41	123.87	127.31
25	5	302	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	A	806	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
34	1	617	LUT	C20-C13-C14	-2.41	119.54	122.92
25	6	601	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
25	1	602	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	Q	609	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	A	814	CLA	C16-C15-C13	-2.41	108.13	115.92
25	A	804	CLA	C1-C2-C3	-2.41	121.87	126.04
28	J	101	BCR	C10-C11-C12	-2.41	115.69	123.22
25	2	310	CLA	CAA-C2A-C3A	-2.41	110.47	116.10
25	R	604	CLA	C1-C2-C3	-2.41	122.85	126.75
34	S	317	LUT	C16-C1-C6	-2.41	106.39	110.30
28	A	854	BCR	C15-C16-C17	-2.41	118.54	123.47
34	Q	614	LUT	C22-C23-C24	2.41	114.48	111.74
25	A	815	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
33	5	308	CHL	C5-C3-C4	2.41	119.92	114.60
25	A	812	CLA	CHB-C4A-NA	2.41	127.84	124.51
28	3	318	BCR	C16-C15-C14	-2.41	118.54	123.47
33	T	601	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
25	B	815	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
33	S	308	CHL	O2A-CGA-CBA	2.41	119.47	111.91
25	B	814	CLA	C1-C2-C3	-2.41	121.88	126.04
33	T	601	CHL	CHD-C1D-C2D	2.41	130.53	125.48
25	Q	611	CLA	C4D-CHA-C1A	2.41	124.18	121.25
28	J	106	BCR	C8-C7-C6	-2.41	120.44	127.20
25	9	309	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
25	A	826	CLA	C2D-C1D-ND	-2.41	108.33	110.10
25	B	830	CLA	O2D-CGD-CBD	2.41	115.54	111.27
34	3	316	LUT	C35-C15-C14	-2.40	118.55	123.47
33	S	309	CHL	O2A-CGA-CBA	2.40	119.45	111.91
25	1	603	CLA	C2D-C1D-ND	-2.40	108.33	110.10
25	a	307	CLA	CHB-C1B-NB	2.40	126.80	124.26
33	U	307	CHL	CHB-C1B-NB	-2.40	121.71	124.26
25	1	604	CLA	C3B-C4B-NB	-2.40	108.28	110.52
27	7	317	LHG	O8-C23-C24	2.40	119.45	111.91
33	R	601	CHL	CHD-C1D-C2D	2.40	130.52	125.48
25	3	308	CLA	CHB-C4A-NA	2.40	127.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	P	615	LUT	C38-C25-C24	-2.40	118.42	123.56
28	K	206	BCR	C2-C1-C6	2.40	114.18	110.48
25	B	828	CLA	CHB-C1B-NB	2.40	126.80	124.26
25	B	827	CLA	CHB-C4A-NA	2.40	127.83	124.51
34	5	322	LUT	C30-C31-C32	-2.40	115.73	123.22
28	A	845	BCR	C31-C1-C6	-2.40	106.41	110.30
25	2	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	Q	611	CLA	O1D-CGD-CBD	2.40	129.39	124.48
28	L	208	BCR	C4-C5-C6	-2.40	119.25	122.73
33	P	608	CHL	C4A-NA-C1A	-2.40	105.63	106.71
25	9	308	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
36	U	316	NEX	C38-C25-C24	2.40	116.98	114.28
25	7	313	CLA	CHB-C1B-NB	2.40	126.80	124.26
25	B	825	CLA	CHB-C4A-NA	2.40	127.83	124.51
33	P	601	CHL	CHD-C1D-C2D	2.40	130.51	125.48
25	S	312	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
33	U	307	CHL	C4-C3-C5	2.40	119.30	115.27
25	A	809	CLA	CHB-C1B-NB	2.40	126.79	124.26
33	P	601	CHL	OMC-CMC-C2C	-2.40	120.27	125.69
28	A	854	BCR	C21-C20-C19	-2.40	115.74	123.22
25	9	303	CLA	CHB-C4A-NA	2.40	127.82	124.51
33	Q	601	CHL	CHD-C1D-C2D	2.39	130.50	125.48
25	9	308	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
34	S	317	LUT	C10-C11-C12	-2.39	115.74	123.22
27	4	318	LHG	O8-C23-C24	2.39	119.42	111.91
34	8	316	LUT	C8-C7-C6	-2.39	120.48	127.20
28	L	203	BCR	C2-C1-C6	2.39	114.17	110.48
25	B	823	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
33	T	605	CHL	CHB-C4A-NA	2.39	127.82	124.51
25	A	826	CLA	CHB-C1B-NB	2.39	126.79	124.26
25	9	311	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	a	311	CLA	O1D-CGD-CBD	2.39	129.38	124.48
34	2	315	LUT	C28-C29-C30	-2.39	115.27	118.94
25	B	824	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	G	202	CLA	C3B-C4B-NB	-2.39	108.30	110.52
33	5	308	CHL	CHC-C1C-NC	2.39	127.83	124.20
33	6	608	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
25	B	812	CLA	CAC-C3C-C4C	2.39	127.91	124.81
34	a	315	LUT	C35-C15-C14	-2.39	118.58	123.47
25	2	308	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
25	B	829	CLA	CHB-C1B-NB	2.39	126.78	124.26
33	R	601	CHL	C4A-NA-C1A	2.39	107.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	617	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
25	S	314	CLA	CHC-C4B-NB	2.39	126.78	124.26
34	U	315	LUT	C38-C25-C24	-2.39	118.45	123.56
33	4	305	CHL	CHD-C1D-C2D	2.39	130.48	125.48
33	S	302	CHL	C6-C5-C3	-2.39	110.72	114.62
25	8	310	CLA	CHB-C4A-NA	2.38	127.81	124.51
33	R	601	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
28	7	316	BCR	C1-C6-C7	2.38	122.52	115.78
34	1	617	LUT	C2-C3-C4	2.38	113.57	110.30
25	a	307	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
33	Q	605	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
28	3	317	BCR	C1-C6-C7	2.38	122.52	115.78
25	3	305	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	7	306	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	a	308	CLA	C2D-C1D-ND	-2.38	108.35	110.10
34	6	619	LUT	C22-C23-C24	2.38	114.45	111.74
25	B	849	CLA	CHB-C1B-NB	2.38	126.78	124.26
25	6	620	CLA	CHB-C1B-NB	2.38	126.78	124.26
33	Q	601	CHL	C4A-NA-C1A	2.38	107.78	106.71
25	4	311	CLA	C3B-C4B-NB	-2.38	108.31	110.52
25	U	310	CLA	CHB-C4A-NA	2.38	127.81	124.51
33	R	606	CHL	O2A-CGA-O1A	-2.38	117.58	123.59
28	B	843	BCR	C8-C7-C6	-2.38	120.51	127.20
25	A	830	CLA	CHC-C4B-NB	2.38	126.78	124.26
25	B	813	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
25	B	814	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
34	3	316	LUT	C2-C3-C4	-2.38	107.05	110.30
25	a	302	CLA	CHB-C1B-NB	2.38	126.78	124.26
33	Q	601	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
25	S	320	CLA	C3B-C4B-NB	-2.38	108.31	110.52
34	3	316	LUT	C38-C25-C24	-2.38	118.47	123.56
33	U	305	CHL	C2A-C3A-C4A	-2.38	98.03	101.87
25	A	840	CLA	O2D-CGD-CBD	2.38	115.49	111.27
25	A	801	CLA	CHB-C1B-NB	2.38	126.77	124.26
25	A	812	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
33	5	307	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
33	1	601	CHL	O1D-CGD-CBD	-2.38	119.62	124.48
33	T	601	CHL	CHC-C1C-NC	2.38	127.81	124.20
33	S	308	CHL	CHB-C4A-NA	2.38	127.80	124.51
25	T	609	CLA	CHA-C1A-NA	-2.38	120.96	126.40
25	B	836	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
33	R	601	CHL	CHC-C4B-NB	-2.37	121.74	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	851	BCR	C11-C10-C9	-2.37	123.92	127.31
25	A	823	CLA	CHB-C1B-NB	2.37	126.77	124.26
33	S	309	CHL	CED-O2D-CGD	2.37	121.31	115.94
25	5	314	CLA	O2D-CGD-CBD	2.37	115.49	111.27
25	A	842	CLA	CMC-C2C-C3C	2.37	132.56	126.12
25	A	853	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	6	620	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	U	304	CLA	C1-C2-C3	-2.37	122.91	126.75
34	1	615	LUT	C7-C8-C9	-2.37	122.65	126.23
34	5	318	LUT	C7-C8-C9	-2.37	122.65	126.23
25	A	822	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
34	2	315	LUT	C40-C33-C34	-2.37	119.60	122.92
25	K	202	CLA	O2A-CGA-O1A	-2.37	117.39	123.30
25	4	309	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
30	B	848	DGD	O6D-C5D-C4D	-2.37	105.39	109.69
25	6	611	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	A	807	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	1	603	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	F	801	BCR	C11-C10-C9	-2.37	123.93	127.31
25	B	816	CLA	CHB-C1B-NB	2.37	126.77	124.26
25	9	302	CLA	CHB-C1B-NB	2.37	126.77	124.26
33	S	306	CHL	O2A-CGA-CBA	2.37	119.34	111.91
28	4	321	BCR	C15-C16-C17	-2.37	118.62	123.47
25	R	604	CLA	CHB-C1B-NB	2.37	126.77	124.26
34	3	315	LUT	C10-C11-C12	-2.37	115.82	123.22
25	6	604	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	B	842	BCR	C23-C22-C21	2.37	122.57	118.94
25	A	837	CLA	O2D-CGD-CBD	2.37	115.47	111.27
34	8	316	LUT	C3-C4-C5	-2.37	107.14	111.85
25	9	308	CLA	CHB-C1B-NB	2.37	126.76	124.26
25	5	304	CLA	C3B-C4B-NB	-2.37	108.32	110.52
28	B	851	BCR	C23-C24-C25	-2.37	120.55	127.20
34	7	315	LUT	C21-C26-C27	-2.37	109.71	112.70
34	7	315	LUT	C16-C1-C6	-2.37	106.46	110.30
25	a	307	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
33	Q	601	CHL	CHC-C4B-NB	-2.37	121.75	124.26
25	6	604	CLA	CHB-C1B-NB	2.37	126.76	124.26
34	8	317	LUT	C30-C31-C32	-2.37	115.84	123.22
25	R	612	CLA	C3A-C2A-C1A	2.36	104.88	101.34
25	1	605	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	6	616	CLA	CHB-C4A-NA	2.36	127.78	124.51
34	R	616	LUT	C8-C9-C10	-2.36	115.31	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5	307	CHL	C5-C3-C4	2.36	119.83	114.60
28	J	101	BCR	C15-C14-C13	-2.36	123.94	127.31
25	P	612	CLA	C3A-C2A-C1A	2.36	104.88	101.34
25	B	823	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	A	821	CLA	C2D-C1D-ND	-2.36	108.36	110.10
34	4	316	LUT	C20-C13-C12	2.36	121.80	118.08
25	3	308	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
33	S	309	CHL	CHB-C4A-NA	2.36	127.78	124.51
25	8	302	CLA	CAC-C3C-C4C	2.36	127.88	124.81
25	S	303	CLA	C1-C2-C3	-2.36	121.96	126.04
33	P	601	CHL	C4A-NA-C1A	2.36	107.77	106.71
27	a	317	LHG	O8-C23-C24	2.36	119.32	111.91
28	A	845	BCR	C34-C9-C10	-2.36	119.61	122.92
34	7	315	LUT	C10-C11-C12	-2.36	115.85	123.22
25	8	314	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
33	S	321	CHL	CHB-C4A-NA	2.36	127.78	124.51
28	B	840	BCR	C36-C18-C17	-2.36	119.62	122.92
35	P	620	XAT	C31-C32-C33	-2.36	119.78	126.42
25	7	311	CLA	C1-C2-C3	-2.36	121.96	126.04
28	F	801	BCR	C36-C18-C17	-2.36	119.62	122.92
25	B	822	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	Q	613	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	S	313	CLA	C3B-C4B-NB	-2.36	108.33	110.52
25	F	802	CLA	CHB-C1B-NB	2.36	126.75	124.26
25	6	603	CLA	CHC-C4B-NB	2.36	126.75	124.26
33	7	305	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
25	4	310	CLA	C3B-C4B-NB	-2.36	108.33	110.52
25	A	830	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	5	309	CLA	C1-C2-C3	-2.36	122.94	126.75
33	P	619	CHL	C4A-NA-C1A	-2.36	105.65	106.71
34	a	314	LUT	C18-C5-C4	2.36	118.72	114.36
25	A	839	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	9	301	CLA	CAB-C3B-C2B	2.36	129.70	123.59
25	P	604	CLA	C3B-C4B-NB	-2.36	108.33	110.52
34	P	615	LUT	C18-C5-C4	2.36	118.72	114.36
33	U	309	CHL	CHD-C1D-C2D	2.36	130.42	125.48
34	1	617	LUT	C40-C33-C34	-2.36	119.62	122.92
36	U	301	NEX	C19-C9-C10	-2.36	119.62	122.92
25	1	608	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
28	O	204	BCR	C10-C11-C12	-2.36	115.87	123.22
36	P	617	NEX	C40-C33-C34	-2.36	119.62	122.92
25	1	611	CLA	CHB-C4A-NA	2.35	127.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	R	607	CHL	CHB-C4A-NA	2.35	127.77	124.51
33	R	606	CHL	CMB-C2B-C1B	2.35	128.96	125.37
25	A	813	CLA	O2D-CGD-CBD	2.35	115.45	111.27
25	R	614	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
25	B	833	CLA	CHC-C4B-NB	2.35	126.75	124.26
25	K	204	CLA	C3B-C4B-NB	-2.35	108.33	110.52
25	1	612	CLA	CHC-C4B-NB	2.35	126.75	124.26
28	A	848	BCR	C21-C20-C19	-2.35	115.87	123.22
33	T	607	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
25	A	829	CLA	CHB-C4A-NA	2.35	127.77	124.51
25	1	613	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
25	B	835	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	8	302	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	B	825	CLA	CHC-C4B-NB	2.35	126.75	124.26
25	4	302	CLA	C3B-C4B-NB	-2.35	108.33	110.52
34	6	619	LUT	C20-C13-C14	-2.35	119.63	122.92
25	3	309	CLA	CHB-C4A-NA	2.35	127.76	124.51
33	P	601	CHL	CHC-C4B-NB	-2.35	121.77	124.26
25	B	826	CLA	O2D-CGD-CBD	2.35	115.44	111.27
28	B	844	BCR	C16-C17-C18	-2.35	123.96	127.31
35	P	623	XAT	C4-C3-C2	-2.35	106.24	110.77
25	A	821	CLA	O2D-CGD-CBD	2.35	115.44	111.27
25	3	311	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
25	B	808	CLA	C1-C2-C3	-2.35	121.98	126.04
28	A	845	BCR	C36-C18-C17	-2.35	119.63	122.92
25	B	822	CLA	C3B-C4B-NB	-2.35	108.34	110.52
25	5	305	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	B	835	CLA	CHB-C1B-NB	2.35	126.74	124.26
25	5	311	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	R	613	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
34	T	613	LUT	C22-C23-C24	2.35	114.41	111.74
25	S	304	CLA	CHD-C1D-ND	-2.34	122.30	124.45
25	T	603	CLA	C3B-C4B-NB	-2.34	108.34	110.52
33	Q	607	CHL	C4A-NA-C1A	-2.34	105.65	106.71
28	L	208	BCR	C16-C17-C18	-2.34	123.97	127.31
25	T	610	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
25	6	614	CLA	C3B-C4B-NB	-2.34	108.34	110.52
25	4	311	CLA	O2D-CGD-CBD	2.34	115.43	111.27
34	6	619	LUT	C8-C7-C6	-2.34	120.62	127.20
34	6	622	LUT	C18-C5-C4	2.34	118.70	114.36
25	L	205	CLA	CHC-C4B-NB	2.34	126.74	124.26
34	1	615	LUT	C39-C29-C28	2.34	121.77	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	613	CLA	C16-C15-C13	-2.34	108.35	115.92
25	1	604	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
25	A	802	CLA	CMB-C2B-C1B	-2.34	121.80	125.37
25	4	310	CLA	CHA-C1A-NA	-2.34	121.03	126.40
25	1	603	CLA	CHB-C1B-NB	2.34	126.74	124.26
34	7	315	LUT	C35-C15-C14	-2.34	118.68	123.47
25	5	302	CLA	C2D-C1D-ND	-2.34	108.38	110.10
25	B	811	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
25	5	309	CLA	CHB-C1B-NB	2.34	126.73	124.26
25	S	301	CLA	C2D-C1D-ND	-2.34	108.38	110.10
28	A	848	BCR	C34-C9-C10	-2.34	119.65	122.92
33	6	608	CHL	C3B-C4B-NB	2.34	112.69	110.52
35	P	623	XAT	C31-C32-C33	-2.34	119.84	126.42
25	4	308	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	A	825	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
25	B	849	CLA	CHB-C4A-NA	2.34	127.74	124.51
33	P	605	CHL	C2A-C3A-C4A	-2.34	98.09	101.87
25	B	807	CLA	CHC-C4B-NB	2.34	126.73	124.26
25	3	307	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
33	6	608	CHL	CHA-C1A-NA	2.34	131.75	126.40
25	B	819	CLA	CHB-C1B-NB	2.34	126.73	124.26
25	B	816	CLA	CAA-CBA-CGA	-2.34	106.43	113.25
34	1	616	LUT	C38-C25-C24	-2.34	118.56	123.56
33	P	619	CHL	CHB-C4A-NA	2.34	127.74	124.51
34	4	316	LUT	C8-C7-C6	-2.34	120.64	127.20
34	8	316	LUT	C10-C11-C12	-2.33	115.93	123.22
25	A	824	CLA	CHB-C4A-NA	2.33	127.74	124.51
34	6	619	LUT	C7-C8-C9	-2.33	122.71	126.23
25	4	307	CLA	CHB-C1B-NB	2.33	126.73	124.26
33	P	622	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
33	R	608	CHL	C4A-NA-C1A	-2.33	105.66	106.71
25	B	834	CLA	CHB-C1B-NB	2.33	126.73	124.26
33	P	607	CHL	CHB-C4A-NA	2.33	127.74	124.51
25	1	612	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
28	4	321	BCR	C21-C20-C19	-2.33	115.94	123.22
34	1	616	LUT	C19-C9-C10	-2.33	119.66	122.92
25	T	602	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	T	603	CLA	C1-C2-C3	-2.33	122.98	126.75
34	7	315	LUT	C20-C13-C12	2.33	121.75	118.08
25	S	301	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
33	S	306	CHL	CHB-C1B-NB	-2.33	121.79	124.26
25	T	602	CLA	CHB-C1B-NB	2.33	126.72	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	610	CLA	CHB-C4A-NA	2.33	127.73	124.51
28	K	206	BCR	C29-C30-C25	2.33	114.07	110.48
34	7	314	LUT	C1-C2-C3	2.33	118.90	113.64
28	J	101	BCR	C11-C10-C9	-2.33	123.99	127.31
25	G	202	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
33	S	310	CHL	CHC-C1C-NC	2.33	127.73	124.20
25	Q	602	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	S	301	CLA	CHC-C4B-NB	2.33	126.72	124.26
25	5	316	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	U	311	CLA	CHA-C1A-NA	-2.33	121.07	126.40
25	T	608	CLA	CHB-C1B-NB	2.33	126.72	124.26
25	U	302	CLA	CMB-C2B-C1B	-2.33	121.83	125.37
28	A	846	BCR	C10-C11-C12	-2.32	115.96	123.22
34	4	316	LUT	C15-C14-C13	-2.32	123.99	127.31
25	A	814	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
28	A	845	BCR	C38-C26-C27	2.32	118.08	113.62
25	R	602	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
25	6	610	CLA	CHB-C1B-NB	2.32	126.72	124.26
34	1	616	LUT	C21-C26-C27	-2.32	109.77	112.70
33	U	305	CHL	C4A-NA-C1A	-2.32	105.66	106.71
25	H	202	CLA	CHB-C4A-NA	2.32	127.72	124.51
25	R	610	CLA	CHB-C1B-NB	2.32	126.72	124.26
26	B	839	PQN	C2M-C2-C3	-2.32	120.61	124.40
34	1	616	LUT	C30-C31-C32	-2.32	115.97	123.22
34	1	616	LUT	C31-C30-C29	-2.32	124.00	127.31
33	Q	606	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
35	S	318	XAT	C18-C5-C4	2.32	116.89	114.28
35	P	616	XAT	C10-C11-C12	-2.32	115.98	123.22
25	5	304	CLA	CHB-C1B-NB	2.32	126.71	124.26
28	5	323	BCR	C36-C18-C19	-2.32	114.42	118.08
25	B	819	CLA	O2D-CGD-CBD	2.32	115.39	111.27
25	2	309	CLA	C7-C6-C5	-2.32	107.06	113.36
34	U	315	LUT	C39-C29-C30	-2.32	119.67	122.92
33	T	606	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
25	R	604	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
34	2	316	LUT	C3-C4-C5	-2.32	107.24	111.85
28	B	841	BCR	C21-C20-C19	-2.32	115.98	123.22
34	5	322	LUT	C11-C10-C9	-2.32	124.00	127.31
34	1	616	LUT	C35-C15-C14	-2.32	118.73	123.47
25	2	306	CLA	CHB-C4A-NA	2.32	127.72	124.51
25	U	310	CLA	CHB-C1B-NB	2.32	126.71	124.26
33	S	307	CHL	C3C-C4C-NC	2.32	113.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	304	CLA	C3B-C4B-NB	-2.32	108.37	110.52
25	B	827	CLA	O1D-CGD-CBD	2.32	129.22	124.48
28	B	840	BCR	C34-C9-C10	-2.32	119.68	122.92
25	A	825	CLA	O1D-CGD-CBD	2.32	129.22	124.48
28	O	205	BCR	C37-C22-C21	-2.32	119.68	122.92
25	2	310	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
28	O	204	BCR	C20-C19-C18	-2.31	119.91	126.42
33	1	606	CHL	CHC-C1C-NC	2.31	127.72	124.20
25	5	310	CLA	O1D-CGD-CBD	2.31	129.22	124.48
28	K	206	BCR	C15-C16-C17	2.31	128.22	123.47
25	K	203	CLA	CHB-C1B-NB	2.31	126.71	124.26
33	R	609	CHL	OMC-CMC-C2C	-2.31	120.45	125.69
33	S	309	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
34	5	322	LUT	C10-C11-C12	-2.31	116.00	123.22
25	A	842	CLA	CBC-CAC-C3C	2.31	118.81	112.43
33	S	321	CHL	O1D-CGD-CBD	-2.31	119.75	124.48
33	4	305	CHL	C5-C3-C4	2.31	119.71	114.60
25	R	612	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
25	2	311	CLA	C2A-C1A-CHA	2.31	127.90	123.86
25	A	809	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
25	A	802	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
33	R	606	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
25	A	836	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
25	U	310	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	B	806	CLA	CHB-C4A-NA	2.31	127.70	124.51
28	B	842	BCR	C15-C16-C17	-2.31	118.75	123.47
28	3	317	BCR	C37-C22-C21	-2.31	119.69	122.92
30	B	846	DGD	O6D-C5D-C6D	2.31	111.32	106.67
33	U	307	CHL	CHB-C4A-NA	2.31	127.70	124.51
25	3	302	CLA	C2D-C1D-ND	-2.31	108.40	110.10
25	A	820	CLA	C3B-C4B-NB	-2.31	108.38	110.52
25	B	829	CLA	CHC-C4B-NB	2.31	126.70	124.26
28	A	846	BCR	C31-C1-C6	-2.31	106.56	110.30
33	Q	608	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
28	A	847	BCR	C8-C7-C6	-2.31	120.73	127.20
34	3	316	LUT	C16-C1-C6	-2.31	106.56	110.30
25	H	203	CLA	CHB-C1B-NB	2.31	126.70	124.26
25	A	810	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
36	U	316	NEX	C40-C33-C34	-2.31	119.69	122.92
25	Q	602	CLA	CHB-C4A-NA	2.30	127.70	124.51
34	R	616	LUT	C16-C1-C6	-2.30	106.56	110.30
25	P	604	CLA	O2A-CGA-O1A	-2.30	117.78	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	P	601	CHL	CHC-C1C-NC	2.30	127.70	124.20
25	R	611	CLA	C2A-C1A-CHA	2.30	127.89	123.86
25	1	602	CLA	CHB-C4A-NA	2.30	127.70	124.51
25	A	806	CLA	CHB-C1B-NB	2.30	126.70	124.26
25	5	303	CLA	CHB-C1B-NB	2.30	126.70	124.26
33	S	321	CHL	O2A-CGA-CBA	2.30	119.14	111.91
25	G	202	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
25	A	803	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
25	A	840	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
33	U	307	CHL	C6-C5-C3	-2.30	110.85	114.62
25	B	801	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	3	313	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	P	612	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
28	F	803	BCR	C37-C22-C23	2.30	121.70	118.08
25	6	603	CLA	CHB-C4A-NA	2.30	127.70	124.51
25	6	605	CLA	CHB-C4A-NA	2.30	127.70	124.51
33	6	606	CHL	C4-C3-C5	2.30	119.14	115.27
25	B	821	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	F	802	CLA	O2A-CGA-O1A	-2.30	117.56	123.30
25	a	306	CLA	CHD-C1D-ND	-2.30	122.34	124.45
27	5	301	LHG	C6-C5-C4	-2.30	106.34	111.79
25	R	610	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	R	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	1	609	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
25	R	604	CLA	CMC-C2C-C1C	-2.30	121.53	125.04
25	9	308	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
28	I	201	BCR	C15-C14-C13	-2.30	124.03	127.31
25	8	310	CLA	CHB-C1B-NB	2.30	126.69	124.26
34	1	617	LUT	C11-C10-C9	-2.30	124.03	127.31
34	Q	615	LUT	C40-C33-C34	-2.30	119.70	122.92
28	B	842	BCR	C4-C5-C6	-2.30	119.39	122.73
28	L	208	BCR	C27-C26-C25	-2.30	119.39	122.73
28	O	205	BCR	C4-C5-C6	-2.30	119.39	122.73
25	8	303	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	a	311	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
25	A	802	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	3	304	CLA	CHB-C4A-NA	2.30	127.69	124.51
36	P	621	NEX	C19-C9-C10	-2.30	119.71	122.92
25	B	838	CLA	CHB-C1B-NB	2.30	126.69	124.26
25	O	202	CLA	CHB-C4A-NA	2.29	127.69	124.51
25	B	825	CLA	O2D-CGD-CBD	2.29	115.34	111.27
25	A	828	CLA	CHB-C4A-NA	2.29	127.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	9	306	CHL	OBD-CAD-C3D	-2.29	123.00	128.52
25	7	309	CLA	CHB-C1B-NB	2.29	126.69	124.26
33	P	607	CHL	C4A-NA-C1A	-2.29	105.67	106.71
25	5	309	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	S	314	CLA	C3B-C4B-NB	-2.29	108.39	110.52
28	4	321	BCR	C8-C9-C10	2.29	122.46	118.94
34	U	314	LUT	C22-C23-C24	2.29	114.35	111.74
33	P	609	CHL	OMC-CMC-C2C	-2.29	120.50	125.69
28	5	323	BCR	C33-C5-C4	2.29	118.02	113.62
25	L	206	CLA	CHB-C1B-NB	2.29	126.68	124.26
34	3	315	LUT	C7-C8-C9	-2.29	122.78	126.23
33	S	306	CHL	CHB-C1B-C2B	-2.29	120.77	127.24
27	7	317	LHG	O7-C7-O9	-2.29	118.17	123.70
25	A	832	CLA	C1-C2-C3	-2.29	122.08	126.04
25	4	309	CLA	CHB-C1B-NB	2.29	126.68	124.26
25	T	608	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	A	825	CLA	CHB-C4A-NA	2.29	127.68	124.51
28	7	316	BCR	C23-C24-C25	-2.29	120.78	127.20
33	3	306	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
25	9	311	CLA	O2D-CGD-CBD	2.29	115.33	111.27
33	R	607	CHL	C4A-NA-C1A	-2.29	105.68	106.71
25	B	808	CLA	CBA-CAA-C2A	-2.29	107.11	113.86
25	B	820	CLA	C3B-C4B-NB	-2.29	108.39	110.52
25	U	302	CLA	CHD-C1D-ND	-2.29	122.35	124.45
33	T	607	CHL	CED-O2D-CGD	2.29	121.11	115.94
25	5	306	CLA	CHB-C4A-NA	2.29	127.67	124.51
36	T	616	NEX	C40-C33-C34	-2.29	119.72	122.92
25	9	301	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
33	S	306	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
33	Q	601	CHL	CHC-C1C-NC	2.29	127.67	124.20
25	B	827	CLA	O2A-CGA-O1A	-2.29	117.83	123.59
33	a	305	CHL	CHC-C1C-NC	2.28	127.67	124.20
25	1	607	CLA	CHD-C1D-ND	-2.28	122.36	124.45
28	L	204	BCR	C36-C18-C17	-2.28	119.72	122.92
25	2	306	CLA	CHD-C1D-ND	-2.28	122.36	124.45
34	P	615	LUT	C16-C1-C6	-2.28	106.60	110.30
28	A	845	BCR	C2-C1-C6	2.28	113.99	110.48
25	Q	618	CLA	O1D-CGD-CBD	2.28	129.15	124.48
25	1	602	CLA	O1D-CGD-CBD	2.28	129.15	124.48
34	a	315	LUT	C1-C2-C3	2.28	118.79	113.64
34	Q	614	LUT	C20-C13-C12	2.28	121.67	118.08
25	5	305	CLA	O2D-CGD-CBD	2.28	115.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	829	CLA	CHB-C1B-NB	2.28	126.67	124.26
25	6	603	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
34	Q	615	LUT	C39-C29-C30	-2.28	119.73	122.92
28	B	843	BCR	C23-C24-C25	-2.28	120.80	127.20
33	7	305	CHL	CHB-C4A-NA	2.28	127.66	124.51
34	3	316	LUT	C20-C13-C12	2.28	121.67	118.08
33	9	307	CHL	C1-C2-C3	-2.28	123.06	126.75
25	B	837	CLA	CHB-C1B-NB	2.28	126.67	124.26
33	U	305	CHL	CED-O2D-CGD	2.28	121.09	115.94
25	5	319	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
25	A	833	CLA	C2D-C1D-ND	-2.28	108.43	110.10
25	6	623	CLA	C3A-C2A-C1A	2.28	104.75	101.34
32	6	602	LMG	C8-O7-C10	-2.28	112.19	117.79
33	8	307	CHL	O2A-CGA-CBA	2.28	119.05	111.91
36	P	617	NEX	C26-C27-C28	-2.28	121.18	125.99
28	A	846	BCR	C34-C9-C10	-2.28	119.74	122.92
33	6	606	CHL	C6-C5-C3	-2.27	110.90	114.62
25	3	309	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	B	816	CLA	C3B-C4B-NB	-2.27	108.41	110.52
36	P	621	NEX	C40-C33-C34	-2.27	119.74	122.92
36	R	617	NEX	C19-C9-C10	-2.27	119.74	122.92
25	B	808	CLA	CHC-C4B-NB	2.27	126.66	124.26
25	B	832	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	6	613	CLA	CHD-C1D-ND	-2.27	122.37	124.45
34	2	315	LUT	C39-C29-C28	2.27	121.66	118.08
25	B	822	CLA	CHC-C4B-NB	2.27	126.66	124.26
25	Q	618	CLA	CED-O2D-CGD	2.27	121.07	115.94
28	4	317	BCR	C37-C22-C23	2.27	121.65	118.08
25	9	302	CLA	C3B-C4B-NB	-2.27	108.41	110.52
25	A	808	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	S	311	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	S	315	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
28	B	844	BCR	C10-C11-C12	-2.27	116.14	123.22
25	Q	610	CLA	CHB-C1B-NB	2.27	126.66	124.26
28	A	849	BCR	C36-C18-C17	-2.27	119.75	122.92
33	4	305	CHL	C3B-C4B-NB	2.27	112.62	110.52
25	T	602	CLA	CHD-C1D-ND	-2.27	122.37	124.45
33	P	605	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
25	J	103	CLA	CHB-C1B-NB	2.27	126.66	124.26
25	B	808	CLA	CHB-C1B-NB	2.27	126.66	124.26
33	R	601	CHL	CHC-C1C-NC	2.27	127.64	124.20
28	B	841	BCR	C27-C26-C25	-2.27	119.44	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	R	615	LUT	C38-C25-C24	-2.27	118.71	123.56
25	3	312	CLA	CHB-C4A-NA	2.26	127.64	124.51
25	9	311	CLA	CHD-C1D-ND	-2.26	122.37	124.45
25	U	311	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	8	305	CLA	CHB-C4A-NA	2.26	127.64	124.51
25	3	312	CLA	O2D-CGD-CBD	2.26	115.29	111.27
34	4	315	LUT	C10-C11-C12	-2.26	116.16	123.22
33	P	622	CHL	CHD-C1D-C2D	2.26	130.22	125.48
36	T	616	NEX	C26-C27-C28	-2.26	121.21	125.99
33	S	306	CHL	CAA-C2A-C3A	-2.26	106.59	112.78
25	S	314	CLA	CGD-CBD-CAD	-2.26	103.41	110.73
33	R	606	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
27	B	847	LHG	C5-O7-C7	-2.26	112.23	117.79
25	Q	609	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
34	R	616	LUT	C3-C4-C5	-2.26	107.36	111.85
25	G	201	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
25	B	836	CLA	CHB-C1B-NB	2.26	126.65	124.26
33	T	601	CHL	OMC-CMC-C2C	-2.26	120.58	125.69
32	J	102	LMG	C7-O1-C1	-2.26	109.33	113.74
33	4	322	CHL	CHB-C1B-C2B	-2.26	120.86	127.24
25	B	809	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	A	820	CLA	O2D-CGD-CBD	2.26	115.28	111.27
27	A	843	LHG	O8-C23-C24	2.26	118.99	111.91
28	A	854	BCR	C36-C18-C17	-2.26	119.76	122.92
25	A	820	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
32	7	319	LMG	C8-O7-C10	-2.26	112.24	117.79
25	5	310	CLA	CHB-C4A-NA	2.26	127.63	124.51
28	J	106	BCR	C10-C11-C12	-2.25	116.18	123.22
34	7	314	LUT	C21-C26-C27	-2.25	109.85	112.70
28	G	203	BCR	C20-C19-C18	-2.25	120.08	126.42
33	1	606	CHL	C3C-C4C-NC	2.25	113.10	110.57
25	2	314	CLA	O2D-CGD-CBD	2.25	115.27	111.27
33	T	606	CHL	C2A-C3A-C4A	-2.25	98.23	101.87
25	A	824	CLA	O2D-CGD-CBD	2.25	115.27	111.27
25	B	824	CLA	C1-C2-C3	-2.25	122.15	126.04
25	S	301	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	3	301	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	3	311	CLA	CHB-C1B-NB	2.25	126.64	124.26
25	6	616	CLA	O2D-CGD-CBD	2.25	115.27	111.27
34	T	614	LUT	C38-C25-C24	-2.25	118.74	123.56
25	A	818	CLA	O2D-CGD-CBD	2.25	115.27	111.27
25	P	603	CLA	O2A-CGA-O1A	-2.25	117.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	302	CLA	O1D-CGD-CBD	2.25	129.09	124.48
34	S	316	LUT	C39-C29-C28	2.25	121.62	118.08
28	K	206	BCR	C10-C11-C12	-2.25	116.20	123.22
25	A	810	CLA	CHC-C4B-NB	2.25	126.64	124.26
25	1	611	CLA	CHB-C1B-NB	2.25	126.64	124.26
33	P	622	CHL	C4B-CHC-C1C	-2.25	121.00	126.34
33	1	606	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
34	P	614	LUT	C3-C4-C5	-2.25	107.38	111.85
34	4	316	LUT	C35-C34-C33	-2.25	124.10	127.31
25	S	305	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
34	P	614	LUT	C40-C33-C34	-2.25	119.78	122.92
25	Q	611	CLA	CHA-C1A-NA	-2.25	121.25	126.40
34	T	614	LUT	C40-C33-C32	2.25	121.62	118.08
25	A	816	CLA	C1-C2-C3	-2.24	122.16	126.04
25	S	301	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
28	8	301	BCR	C29-C30-C25	2.24	113.94	110.48
25	4	313	CLA	CHD-C1D-ND	-2.24	122.39	124.45
25	B	818	CLA	CHB-C1B-NB	2.24	126.63	124.26
28	B	842	BCR	C1-C6-C5	-2.24	119.45	122.61
25	6	609	CLA	O1D-CGD-CBD	2.24	129.07	124.48
25	A	835	CLA	CHA-C1A-NA	-2.24	121.26	126.40
33	T	606	CHL	C4A-NA-C1A	-2.24	105.70	106.71
25	a	304	CLA	CHB-C1B-NB	2.24	126.63	124.26
27	A	852	LHG	C6-C5-C4	-2.24	106.49	111.79
25	B	803	CLA	O2A-CGA-O1A	-2.24	117.72	123.30
34	8	317	LUT	C3-C4-C5	-2.24	107.39	111.85
28	B	843	BCR	C16-C15-C14	-2.24	118.89	123.47
34	8	316	LUT	C18-C5-C4	2.24	118.50	114.36
25	7	306	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	A	853	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
34	5	322	LUT	C20-C13-C12	2.24	121.60	118.08
35	S	318	XAT	C30-C31-C32	-2.24	116.23	123.22
35	Q	616	XAT	C17-C1-C16	2.24	110.67	107.37
28	B	845	BCR	C35-C13-C12	2.24	121.60	118.08
25	L	209	CLA	CHC-C4B-NB	2.24	126.62	124.26
25	7	304	CLA	CHC-C4B-NB	2.24	126.62	124.26
25	A	806	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
25	A	831	CLA	CHB-C1B-NB	2.24	126.62	124.26
25	a	303	CLA	CHC-C4B-NB	2.24	126.62	124.26
36	R	617	NEX	C2-C1-C6	2.24	111.38	109.21
25	8	314	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
30	B	848	DGD	C4D-C3D-C2D	2.24	114.73	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	301	CLA	C1-C2-C3	-2.24	122.18	126.04
25	A	853	CLA	CHB-C1B-NB	2.23	126.62	124.26
25	1	614	CLA	CHC-C4B-NB	2.23	126.62	124.26
28	B	844	BCR	C39-C30-C25	-2.23	106.67	110.30
25	1	610	CLA	CHB-C4A-NA	2.23	127.60	124.51
28	I	201	BCR	C10-C11-C12	-2.23	116.24	123.22
33	S	306	CHL	C1C-C2C-C3C	-2.23	105.34	107.11
25	B	816	CLA	C2D-C1D-ND	-2.23	108.46	110.10
25	2	309	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
36	U	301	NEX	C38-C25-C24	2.23	116.79	114.28
25	A	820	CLA	C2D-C1D-ND	-2.23	108.46	110.10
34	Q	615	LUT	C38-C25-C24	-2.23	118.79	123.56
36	P	621	NEX	C11-C12-C13	-2.23	120.15	126.42
33	P	622	CHL	C3C-C4C-NC	2.23	113.07	110.57
33	U	305	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
34	S	317	LUT	C32-C33-C34	2.23	122.36	118.94
25	B	811	CLA	CHC-C4B-NB	2.23	126.62	124.26
34	R	616	LUT	C39-C29-C30	-2.23	119.80	122.92
25	7	311	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
25	P	603	CLA	CHD-C1D-ND	-2.23	122.41	124.45
25	a	304	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	A	808	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
34	R	615	LUT	C20-C13-C12	2.23	121.59	118.08
25	2	314	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	Q	618	CLA	CHA-C1A-NA	-2.23	121.41	126.41
25	B	814	CLA	CHC-C4B-NB	2.23	126.61	124.26
25	5	305	CLA	CHB-C1B-NB	2.23	126.61	124.26
25	Q	618	CLA	C4D-CHA-C1A	2.23	123.96	121.25
25	1	607	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
28	5	320	BCR	C20-C19-C18	-2.22	120.17	126.42
34	7	315	LUT	C35-C34-C33	-2.22	124.14	127.31
25	B	816	CLA	O2D-CGD-CBD	2.22	115.22	111.27
33	U	307	CHL	C1-C2-C3	-2.22	122.20	126.04
35	Q	616	XAT	O4-C5-C6	-2.22	57.12	58.96
34	1	615	LUT	C31-C30-C29	-2.22	124.14	127.31
31	B	850	SQD	O8-S-C6	2.22	109.28	105.74
25	A	802	CLA	C16-C15-C13	-2.22	108.73	115.92
27	1	618	LHG	C25-C24-C23	-2.22	105.53	113.62
28	I	201	BCR	C1-C6-C5	-2.22	119.48	122.61
25	2	306	CLA	C3C-C4C-NC	-2.22	108.08	110.57
33	U	307	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
25	A	823	CLA	O2A-CGA-O1A	-2.22	117.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	604	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
25	1	611	CLA	C2D-C1D-ND	-2.22	108.47	110.10
25	5	314	CLA	O2A-CGA-O1A	-2.22	117.76	123.30
34	a	315	LUT	C38-C25-C24	-2.22	118.80	123.56
25	2	313	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
33	P	606	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
33	6	617	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
34	1	616	LUT	C1-C2-C3	2.22	118.66	113.64
25	P	613	CLA	CHD-C1D-ND	-2.22	122.41	124.45
25	B	829	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	R	604	CLA	O1D-CGD-CBD	2.22	129.03	124.48
25	1	609	CLA	C3B-C4B-NB	-2.22	108.45	110.52
28	B	851	BCR	C1-C6-C5	-2.22	119.49	122.61
25	2	303	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	2	313	CLA	CHD-C1D-ND	-2.22	122.41	124.45
25	2	305	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
28	L	204	BCR	C33-C5-C4	2.22	117.88	113.62
25	A	810	CLA	CAA-CBA-CGA	-2.22	106.77	113.25
34	7	315	LUT	C7-C8-C9	-2.22	122.88	126.23
33	S	310	CHL	O2A-CGA-CBA	2.22	118.87	111.91
25	B	809	CLA	CAA-CBA-CGA	-2.22	106.77	113.25
25	9	311	CLA	O2A-CGA-O1A	-2.22	117.77	123.30
25	8	310	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
28	B	845	BCR	C8-C7-C6	-2.22	120.97	127.20
25	P	602	CLA	CHB-C1B-NB	2.22	126.61	124.26
25	P	611	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
33	a	305	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
25	2	307	CLA	CHC-C4B-NB	2.22	126.60	124.26
25	1	605	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
34	P	614	LUT	C22-C23-C24	2.22	114.26	111.74
25	6	616	CLA	CHD-C1D-ND	-2.22	122.42	124.45
28	L	207	BCR	C38-C26-C27	2.22	117.87	113.62
28	L	204	BCR	C23-C24-C25	-2.22	120.98	127.20
25	a	311	CLA	C3B-C4B-NB	-2.22	108.46	110.52
25	4	303	CLA	CHB-C1B-NB	2.22	126.60	124.26
25	4	312	CLA	O2A-CGA-O1A	-2.22	117.78	123.30
25	B	805	CLA	CHD-C1D-ND	-2.22	122.42	124.45
25	B	815	CLA	CHD-C1D-ND	-2.22	122.42	124.45
25	4	312	CLA	O1A-CGA-CBA	2.22	130.20	123.08
33	S	321	CHL	CHB-C1B-NB	-2.22	121.91	124.26
28	5	323	BCR	C28-C27-C26	-2.21	110.12	114.08
34	1	616	LUT	C15-C14-C13	-2.21	124.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	106	BCR	C34-C9-C8	2.21	121.57	118.08
34	5	318	LUT	C8-C7-C6	-2.21	120.98	127.20
28	K	206	BCR	C20-C19-C18	-2.21	120.20	126.42
33	4	322	CHL	O1D-CGD-CBD	-2.21	119.95	124.48
25	4	309	CLA	C2D-C1D-ND	-2.21	108.47	110.10
25	6	601	CLA	CHB-C1B-NB	2.21	126.60	124.26
25	7	302	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
25	U	304	CLA	CMC-C2C-C1C	-2.21	121.67	125.04
25	A	817	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	P	613	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
25	B	815	CLA	C2D-C1D-ND	-2.21	108.47	110.10
33	5	307	CHL	O1D-CGD-CBD	-2.21	119.96	124.48
28	B	840	BCR	C37-C22-C23	2.21	121.56	118.08
25	1	612	CLA	O2D-CGD-CBD	2.21	115.19	111.27
25	1	604	CLA	CHB-C1B-NB	2.21	126.60	124.26
25	3	308	CLA	CHB-C1B-NB	2.21	126.60	124.26
34	R	616	LUT	C40-C33-C32	2.21	121.56	118.08
25	3	302	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
28	F	801	BCR	C38-C26-C25	-2.21	122.05	124.53
25	B	824	CLA	C2D-C1D-ND	-2.21	108.48	110.10
25	2	313	CLA	O2D-CGD-CBD	2.21	115.19	111.27
28	I	201	BCR	C34-C9-C10	-2.21	119.83	122.92
25	B	831	CLA	CHB-C1B-NB	2.21	126.59	124.26
33	6	606	CHL	CHB-C4A-NA	2.21	127.56	124.51
25	A	831	CLA	C2D-C1D-ND	-2.21	108.48	110.10
35	T	615	XAT	C35-C15-C14	-2.21	118.96	123.47
25	B	814	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	G	202	CLA	CHD-C1D-ND	-2.20	122.43	124.45
25	A	827	CLA	CHB-C4A-NA	2.20	127.56	124.51
34	9	312	LUT	C16-C1-C6	-2.20	106.72	110.30
35	P	620	XAT	C10-C11-C12	-2.20	116.34	123.22
33	U	308	CHL	C2A-C3A-C4A	-2.20	98.31	101.87
25	S	303	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
25	A	801	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
25	J	105	CLA	C2D-C1D-ND	-2.20	108.48	110.10
35	T	615	XAT	C10-C11-C12	-2.20	116.35	123.22
25	U	302	CLA	CHB-C1B-NB	2.20	126.59	124.26
25	H	205	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
33	S	306	CHL	CHC-C1C-NC	2.20	127.54	124.20
28	L	207	BCR	C21-C20-C19	-2.20	116.35	123.22
25	2	304	CLA	CHC-C4B-NB	2.20	126.58	124.26
34	P	615	LUT	C8-C9-C10	-2.20	115.57	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	320	BCR	C16-C15-C14	-2.20	118.97	123.47
25	5	310	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
28	A	845	BCR	C33-C5-C4	2.20	117.84	113.62
25	7	308	CLA	C1-C2-C3	-2.20	122.24	126.04
33	4	322	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
25	a	306	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
25	A	840	CLA	C1-C2-C3	-2.20	122.25	126.04
28	O	205	BCR	C11-C12-C13	-2.20	120.25	126.42
25	3	301	CLA	CHB-C1B-NB	2.20	126.58	124.26
28	A	848	BCR	C24-C23-C22	-2.19	122.92	126.23
25	K	204	CLA	CHA-C1A-NA	-2.19	121.37	126.40
33	6	617	CHL	CHB-C4A-NA	2.19	127.55	124.51
25	2	307	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	3	305	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
25	2	312	CLA	CHB-C1B-NB	2.19	126.58	124.26
33	4	304	CHL	OBD-CAD-C3D	-2.19	123.24	128.52
34	3	315	LUT	C16-C1-C6	-2.19	106.74	110.30
34	T	613	LUT	C20-C13-C12	2.19	121.53	118.08
25	4	310	CLA	C3A-C2A-C1A	2.19	104.62	101.34
33	P	601	CHL	C5-C3-C4	2.19	119.44	114.60
25	A	813	CLA	C2D-C1D-ND	-2.19	108.49	110.10
25	S	312	CLA	CHB-C1B-NB	2.19	126.58	124.26
25	1	608	CLA	CHB-C1B-NB	2.19	126.58	124.26
25	2	309	CLA	CHB-C1B-NB	2.19	126.58	124.26
25	5	315	CLA	CHB-C1B-NB	2.19	126.58	124.26
33	Q	601	CHL	C5-C3-C4	2.19	119.44	114.60
25	A	838	CLA	C11-C12-C13	-2.19	108.84	115.92
25	K	205	CLA	CHB-C1B-NB	2.19	126.58	124.26
25	O	202	CLA	CHB-C1B-NB	2.19	126.58	124.26
33	R	601	CHL	C5-C3-C4	2.19	119.44	114.60
34	9	313	LUT	C7-C8-C9	-2.19	122.93	126.23
25	2	304	CLA	CHB-C1B-NB	2.19	126.58	124.26
25	L	205	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
25	S	313	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
25	a	307	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	a	303	CLA	O2A-CGA-CBA	2.19	118.77	111.91
25	T	611	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
28	B	843	BCR	C10-C11-C12	-2.19	116.39	123.22
33	P	609	CHL	C2C-C3C-C4C	2.19	108.05	106.49
25	A	823	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
34	9	312	LUT	C7-C8-C9	-2.19	122.93	126.23
33	6	606	CHL	CED-O2D-CGD	2.19	120.88	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	303	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
28	J	101	BCR	C30-C25-C24	2.19	121.96	115.78
25	B	834	CLA	O2D-CGD-CBD	2.18	115.15	111.27
33	T	607	CHL	C3C-C4C-NC	2.18	113.02	110.57
36	U	301	NEX	C16-C1-C6	-2.18	108.52	110.47
25	1	612	CLA	CGD-CBD-CAD	2.18	117.81	110.73
33	9	306	CHL	CMA-C3A-C2A	-2.18	111.00	116.10
25	P	604	CLA	CMC-C2C-C1C	-2.18	121.71	125.04
25	7	301	CLA	CHB-C1B-NB	2.18	126.57	124.26
33	P	605	CHL	CHA-C1A-NA	2.18	131.40	126.40
25	P	602	CLA	CHD-C1D-ND	-2.18	122.45	124.45
32	J	107	LMG	O6-C1-O1	-2.18	104.81	109.97
25	3	312	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
28	8	318	BCR	C37-C22-C23	2.18	121.52	118.08
25	3	303	CLA	O2D-CGD-CBD	2.18	115.14	111.27
25	a	303	CLA	C3B-C4B-NB	-2.18	108.49	110.52
25	S	303	CLA	O1D-CGD-CBD	2.18	128.95	124.48
33	6	617	CHL	OBD-CAD-C3D	-2.18	123.27	128.52
28	O	204	BCR	C2-C1-C6	2.18	113.84	110.48
25	B	806	CLA	CHC-C4B-NB	2.18	126.57	124.26
25	O	202	CLA	CHC-C4B-NB	2.18	126.57	124.26
25	1	603	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	a	301	CLA	CAC-C3C-C4C	2.18	127.64	124.81
25	8	310	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	9	304	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	R	614	CLA	CAA-CBA-CGA	-2.18	106.88	113.25
25	7	310	CLA	CHC-C4B-NB	2.18	126.56	124.26
25	T	602	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	9	301	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	B	849	CLA	CHC-C4B-NB	2.18	126.56	124.26
25	5	312	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
28	A	848	BCR	C31-C1-C6	-2.18	106.77	110.30
25	2	308	CLA	CHD-C1D-ND	-2.18	122.45	124.45
36	P	617	NEX	C2-C1-C6	2.18	111.33	109.21
25	a	303	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
25	U	312	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
25	T	603	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	2	311	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
34	9	313	LUT	C15-C35-C34	-2.18	119.02	123.47
25	H	203	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
33	P	622	CHL	CMB-C2B-C1B	2.18	128.68	125.37
25	L	202	CLA	CHC-C4B-NB	2.18	126.56	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	838	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
33	P	605	CHL	CHB-C1B-C2B	-2.18	121.09	127.24
25	G	201	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	S	311	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
28	O	205	BCR	C33-C5-C4	2.17	117.79	113.62
33	a	305	CHL	C3B-C4B-NB	2.17	112.53	110.52
33	P	606	CHL	CHB-C4A-NA	2.17	127.52	124.51
25	S	303	CLA	CHB-C1B-NB	2.17	126.56	124.26
25	6	611	CLA	CHB-C4A-NA	2.17	127.52	124.51
33	T	604	CHL	C2A-C3A-C4A	-2.17	98.36	101.87
33	P	619	CHL	C2A-C3A-C4A	-2.17	98.36	101.87
25	5	310	CLA	CHB-C1B-NB	2.17	126.56	124.26
28	4	321	BCR	C12-C13-C14	2.17	122.27	118.94
25	6	616	CLA	CHB-C1B-NB	2.17	126.56	124.26
25	P	611	CLA	C2C-C1C-NC	2.17	112.00	109.97
25	5	302	CLA	O2D-CGD-CBD	2.17	115.12	111.27
25	2	311	CLA	CHC-C4B-NB	2.17	126.55	124.26
28	3	319	BCR	C38-C26-C27	2.17	117.78	113.62
25	2	306	CLA	O2D-CGD-CBD	2.17	115.12	111.27
25	7	308	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
33	S	308	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
25	R	611	CLA	CHA-C1A-NA	-2.17	121.43	126.40
25	B	817	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	B	849	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
28	B	840	BCR	C3-C4-C5	-2.17	110.20	114.08
25	1	610	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
33	P	622	CHL	CED-O2D-CGD	2.17	120.84	115.94
33	S	302	CHL	CED-O2D-CGD	2.17	120.84	115.94
25	T	609	CLA	CED-O2D-CGD	2.17	120.84	115.94
35	P	620	XAT	C30-C31-C32	-2.17	116.46	123.22
33	U	306	CHL	CHB-C4A-NA	2.17	127.51	124.51
33	P	601	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
25	Q	612	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
33	Q	605	CHL	CHB-C1B-C2B	-2.17	121.12	127.24
25	J	103	CLA	C1-C2-C3	-2.17	122.30	126.04
25	H	205	CLA	CHB-C1B-NB	2.16	126.55	124.26
28	L	204	BCR	C37-C22-C21	-2.16	119.89	122.92
25	K	203	CLA	C2D-C1D-ND	-2.16	108.51	110.10
25	4	310	CLA	CHB-C1B-C2B	-2.16	121.13	127.24
25	B	803	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
25	4	301	CLA	CHB-C1B-NB	2.16	126.55	124.26
33	8	307	CHL	CED-O2D-CGD	2.16	120.83	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Q	607	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
28	7	316	BCR	C1-C6-C5	-2.16	119.57	122.61
33	R	601	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
25	8	314	CLA	O2D-CGD-CBD	2.16	115.11	111.27
25	A	801	CLA	CHC-C4B-NB	2.16	126.54	124.26
34	S	316	LUT	C10-C11-C12	-2.16	116.48	123.22
25	2	303	CLA	CHB-C1B-NB	2.16	126.54	124.26
25	A	802	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
25	8	306	CLA	O1D-CGD-CBD	2.16	128.90	124.48
25	U	302	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
34	2	316	LUT	C21-C26-C27	-2.16	109.97	112.70
25	A	804	CLA	C11-C10-C8	-2.16	108.94	115.92
34	6	619	LUT	C39-C29-C28	2.16	121.48	118.08
33	R	609	CHL	C2C-C3C-C4C	2.16	108.03	106.49
33	4	305	CHL	CED-O2D-CGD	2.16	120.82	115.94
25	P	610	CLA	CHB-C1B-NB	2.16	126.54	124.26
25	a	306	CLA	CHB-C1B-NB	2.16	126.54	124.26
34	7	315	LUT	C8-C7-C6	-2.16	121.14	127.20
25	U	303	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	T	614	LUT	C8-C9-C10	-2.16	115.63	118.94
25	R	603	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	2	312	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	a	312	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
25	L	205	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
33	5	308	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
34	8	316	LUT	C39-C29-C28	2.15	121.47	118.08
25	A	821	CLA	O1D-CGD-CBD	2.15	128.89	124.48
28	J	106	BCR	C35-C13-C14	-2.15	119.91	122.92
25	6	620	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
25	A	851	CLA	CHB-C4A-NA	2.15	127.49	124.51
25	A	827	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
28	8	301	BCR	C37-C22-C21	-2.15	119.91	122.92
25	B	820	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
27	8	319	LHG	C5-O7-C7	-2.15	112.49	117.79
25	3	313	CLA	CHC-C4B-NB	2.15	126.54	124.26
25	A	801	CLA	C11-C10-C8	-2.15	108.96	115.92
28	G	203	BCR	C34-C9-C10	-2.15	119.91	122.92
33	Q	601	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
28	A	847	BCR	C11-C10-C9	-2.15	124.24	127.31
34	a	316	LUT	C15-C35-C34	-2.15	119.07	123.47
25	7	310	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
33	T	604	CHL	O2D-CGD-O1D	-2.15	119.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	8	311	CLA	CHB-C4A-NA	2.15	127.48	124.51
28	L	204	BCR	C8-C7-C6	-2.15	121.16	127.20
31	B	850	SQD	C44-O6-C1	-2.15	109.54	113.74
33	P	608	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
25	A	812	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
36	T	616	NEX	C4-C3-C2	-2.15	106.62	110.77
25	B	808	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
25	B	810	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
35	P	620	XAT	C18-C5-C4	2.15	116.70	114.28
25	6	614	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	A	807	CLA	C7-C6-C5	-2.15	107.53	113.36
33	Q	607	CHL	C2A-C3A-C4A	-2.15	98.40	101.87
36	P	621	NEX	C12-C13-C14	2.15	122.24	118.94
25	U	313	CLA	CHB-C1B-NB	2.15	126.53	124.26
33	T	606	CHL	CHB-C4A-NA	2.15	127.48	124.51
25	A	826	CLA	O2D-CGD-CBD	2.15	115.08	111.27
28	B	845	BCR	C39-C30-C25	-2.15	106.82	110.30
25	A	825	CLA	C2D-C1D-ND	-2.15	108.52	110.10
33	R	608	CHL	O2D-CGD-O1D	-2.15	119.64	123.84
33	R	605	CHL	CHB-C1B-C2B	-2.15	121.17	127.24
25	P	611	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
25	3	320	CLA	O1D-CGD-CBD	2.15	128.88	124.48
28	I	201	BCR	C35-C13-C12	2.15	121.46	118.08
25	O	201	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	A	819	CLA	O2D-CGD-CBD	2.15	115.08	111.27
25	T	602	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
25	L	209	CLA	C2A-C1A-CHA	2.15	127.60	123.85
25	A	801	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
25	B	819	CLA	CGD-CBD-CAD	-2.15	103.79	110.73
28	A	848	BCR	C2-C1-C6	2.14	113.78	110.48
25	6	613	CLA	O2D-CGD-CBD	2.14	115.08	111.27
25	A	819	CLA	CHC-C4B-NB	2.14	126.53	124.26
25	3	307	CLA	CHB-C4A-NA	2.14	127.48	124.51
25	B	811	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	P	611	CLA	CHD-C1D-ND	-2.14	122.48	124.45
34	U	315	LUT	C8-C9-C10	-2.14	115.65	118.94
25	5	306	CLA	CHB-C1B-NB	2.14	126.53	124.26
34	1	615	LUT	C1-C2-C3	2.14	118.48	113.64
25	A	840	CLA	C11-C12-C13	-2.14	108.99	115.92
25	8	311	CLA	CHB-C1B-NB	2.14	126.53	124.26
25	B	833	CLA	CHA-C1A-NA	-2.14	121.49	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	2	315	LUT	C20-C13-C12	2.14	121.45	118.08
25	6	614	CLA	CAC-C3C-C4C	2.14	127.59	124.81
25	6	615	CLA	CHD-C1D-ND	-2.14	122.49	124.45
25	A	823	CLA	O2D-CGD-CBD	2.14	115.07	111.27
33	U	306	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
25	a	309	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	4	303	CLA	C1-C2-C3	-2.14	123.29	126.75
25	5	313	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
33	U	305	CHL	CHB-C1B-C2B	-2.14	121.20	127.24
33	P	605	CHL	CAA-C2A-C3A	-2.14	106.92	112.78
28	8	318	BCR	C8-C7-C6	-2.14	121.20	127.20
28	L	207	BCR	C35-C13-C14	-2.14	119.93	122.92
33	6	608	CHL	CHB-C1B-C2B	-2.14	121.20	127.24
25	5	303	CLA	O2D-CGD-CBD	2.14	115.06	111.27
25	A	809	CLA	CHC-C4B-NB	2.14	126.52	124.26
25	5	312	CLA	CHB-C1B-NB	2.14	126.52	124.26
25	S	320	CLA	CHD-C1D-ND	-2.14	122.49	124.45
28	B	845	BCR	C38-C26-C27	2.14	117.72	113.62
28	A	848	BCR	C28-C29-C30	-2.14	106.97	114.60
34	9	313	LUT	C19-C9-C8	2.14	121.44	118.08
25	B	820	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
25	5	311	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	1	609	CLA	C2D-C1D-ND	-2.13	108.53	110.10
33	4	314	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
25	1	605	CLA	C6-C5-C3	-2.13	111.13	114.62
25	A	830	CLA	C2D-C1D-ND	-2.13	108.53	110.10
25	A	811	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	1	608	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
33	P	607	CHL	C2A-C3A-C4A	-2.13	98.42	101.87
28	A	847	BCR	C34-C9-C8	2.13	121.44	118.08
27	A	852	LHG	O8-C23-O10	-2.13	118.21	123.59
25	5	306	CLA	CHC-C4B-NB	2.13	126.51	124.26
25	B	813	CLA	C2D-C1D-ND	-2.13	108.53	110.10
33	5	308	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
33	T	607	CHL	CHD-C1D-C2D	2.13	129.95	125.48
33	a	305	CHL	CHD-C1D-C2D	2.13	129.95	125.48
33	U	305	CHL	O2A-CGA-O1A	-2.13	117.99	123.30
25	B	810	CLA	O2D-CGD-CBD	2.13	115.05	111.27
25	B	825	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	A	802	CLA	CHB-C1B-NB	2.13	126.51	124.26
25	9	310	CLA	CHD-C1D-ND	-2.13	122.50	124.45
34	1	616	LUT	C10-C11-C12	-2.13	116.58	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	3	315	LUT	C21-C26-C27	-2.13	110.01	112.70
34	9	312	LUT	C38-C25-C24	-2.13	119.01	123.56
25	7	304	CLA	CHB-C4A-NA	2.13	127.45	124.51
28	A	848	BCR	C11-C12-C13	-2.13	120.44	126.42
33	P	608	CHL	C2A-C3A-C4A	-2.13	98.43	101.87
36	R	617	NEX	C1-C2-C3	-2.13	108.84	113.64
28	A	845	BCR	C8-C7-C6	-2.13	121.23	127.20
25	9	303	CLA	C2D-C1D-ND	-2.13	108.54	110.10
30	B	848	DGD	C1E-O6E-C5E	2.13	117.86	113.69
33	R	607	CHL	C2A-C3A-C4A	-2.13	98.44	101.87
28	F	803	BCR	C4-C5-C6	-2.13	119.64	122.73
25	A	840	CLA	CHB-C1B-NB	2.13	126.51	124.26
34	8	317	LUT	C35-C15-C14	-2.12	119.12	123.47
25	3	311	CLA	CHD-C1D-ND	-2.12	122.50	124.45
25	A	814	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
25	U	304	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
34	9	313	LUT	C21-C26-C25	-2.12	107.61	111.42
33	4	322	CHL	CHB-C1B-NB	-2.12	122.01	124.26
25	L	206	CLA	CHC-C4B-NB	2.12	126.50	124.26
25	R	612	CLA	CED-O2D-CGD	2.12	120.74	115.94
25	A	836	CLA	CHC-C4B-NB	2.12	126.50	124.26
25	1	613	CLA	C2D-C1D-ND	-2.12	108.54	110.10
25	8	312	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
33	R	608	CHL	C2A-C3A-C4A	-2.12	98.44	101.87
25	A	822	CLA	CHC-C4B-NB	2.12	126.50	124.26
25	A	808	CLA	CHD-C1D-ND	-2.12	122.50	124.45
25	K	204	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
25	3	320	CLA	CHB-C1B-NB	2.12	126.50	124.26
28	A	845	BCR	C16-C15-C14	-2.12	119.13	123.47
28	L	207	BCR	C16-C15-C14	-2.12	119.13	123.47
34	P	615	LUT	C20-C13-C12	2.12	121.42	118.08
25	4	309	CLA	CHB-C4A-NA	2.12	127.44	124.51
28	F	803	BCR	C36-C18-C19	2.12	121.42	118.08
34	2	316	LUT	C20-C13-C12	2.12	121.42	118.08
33	4	305	CHL	CHC-C1C-NC	2.12	127.42	124.20
33	T	604	CHL	C4A-NA-C1A	-2.12	105.75	106.71
33	T	607	CHL	CHC-C4B-NB	-2.12	122.01	124.26
28	7	316	BCR	C39-C30-C25	-2.12	106.86	110.30
34	5	322	LUT	C15-C14-C13	-2.12	124.28	127.31
33	S	302	CHL	CHB-C4A-NA	2.12	127.44	124.51
28	6	621	BCR	C2-C1-C6	-2.12	107.22	110.48
25	P	602	CLA	CMB-C2B-C1B	-2.12	122.14	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	T	607	CHL	O2A-CGA-O1A	-2.12	118.25	123.59
25	H	203	CLA	CHC-C4B-NB	2.12	126.50	124.26
25	3	312	CLA	CHC-C4B-NB	2.12	126.50	124.26
34	4	316	LUT	C7-C8-C9	-2.12	123.03	126.23
34	6	619	LUT	C10-C11-C12	-2.12	116.61	123.22
25	P	602	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
27	5	321	LHG	O8-C23-O10	-2.12	118.25	123.59
25	A	837	CLA	CHB-C1B-NB	2.12	126.50	124.26
25	P	610	CLA	C1-C2-C3	-2.12	122.38	126.04
27	S	319	LHG	C5-O7-C7	-2.12	112.58	117.79
25	B	817	CLA	O2D-CGD-CBD	2.12	115.03	111.27
34	U	314	LUT	C8-C7-C6	-2.12	121.26	127.20
33	5	307	CHL	C2A-C3A-C4A	-2.12	98.45	101.87
28	A	846	BCR	C8-C7-C6	-2.12	121.26	127.20
33	S	306	CHL	CMB-C2B-C3B	2.11	131.71	126.59
33	6	606	CHL	O1D-CGD-CBD	-2.11	120.16	124.48
33	T	604	CHL	CHB-C1B-C2B	-2.11	121.27	127.24
33	6	606	CHL	OMC-CMC-C2C	-2.11	120.91	125.69
35	P	620	XAT	C35-C15-C14	-2.11	119.14	123.47
25	8	313	CLA	CHC-C4B-NB	2.11	126.49	124.26
34	R	615	LUT	C22-C23-C24	2.11	114.15	111.74
25	U	310	CLA	C1-C2-C3	-2.11	122.39	126.04
25	P	611	CLA	C2A-C1A-CHA	-2.11	120.17	123.85
36	R	617	NEX	C26-C27-C28	-2.11	121.53	125.99
25	H	205	CLA	CHC-C4B-NB	2.11	126.49	124.26
25	B	811	CLA	C16-C15-C13	-2.11	109.09	115.92
25	5	313	CLA	CHA-C4D-ND	2.11	136.92	132.50
28	A	845	BCR	C23-C24-C25	-2.11	121.27	127.20
25	8	313	CLA	C1-C2-C3	-2.11	122.39	126.04
25	A	808	CLA	O2D-CGD-CBD	2.11	115.02	111.27
25	A	835	CLA	C2A-C1A-CHA	2.11	127.55	123.86
36	P	617	NEX	C38-C25-C24	2.11	116.65	114.28
34	a	314	LUT	C1-C2-C3	2.11	118.41	113.64
36	U	316	NEX	C5-C6-C1	2.11	121.79	119.70
34	U	315	LUT	C16-C1-C6	-2.11	106.88	110.30
33	5	307	CHL	O2A-CGA-O1A	-2.11	118.27	123.59
28	6	621	BCR	C37-C22-C23	2.11	121.40	118.08
25	F	802	CLA	CHC-C4B-NB	2.11	126.49	124.26
25	P	612	CLA	CED-O2D-CGD	2.11	120.70	115.94
35	T	615	XAT	C31-C32-C33	-2.11	120.50	126.42
25	P	611	CLA	C3C-C4C-NC	-2.11	108.21	110.57
25	A	817	CLA	CHC-C4B-NB	2.11	126.49	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	849	BCR	C38-C26-C27	2.11	117.66	113.62
34	6	622	LUT	C22-C23-C24	-2.11	109.34	111.74
25	T	612	CLA	CAA-CBA-CGA	-2.11	107.10	113.25
25	U	310	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
30	B	846	DGD	O3G-C3G-C2G	-2.11	105.82	110.90
33	R	607	CHL	OMC-CMC-C2C	-2.11	120.93	125.69
34	9	312	LUT	C21-C26-C27	-2.11	110.04	112.70
28	4	321	BCR	C1-C6-C5	-2.10	119.65	122.61
33	R	607	CHL	C1-C2-C3	-2.10	122.40	126.04
34	1	615	LUT	C11-C10-C9	-2.10	124.31	127.31
28	8	318	BCR	C10-C11-C12	-2.10	116.65	123.22
33	S	321	CHL	C2A-C3A-C4A	-2.10	98.47	101.87
33	P	608	CHL	CHB-C4A-NA	2.10	127.42	124.51
34	2	315	LUT	C38-C25-C24	-2.10	119.06	123.56
34	5	322	LUT	C40-C33-C34	-2.10	119.98	122.92
33	T	601	CHL	C4A-NA-C1A	2.10	107.65	106.71
25	P	603	CLA	CMA-C3A-C4A	-2.10	106.12	111.77
33	Q	607	CHL	CHB-C4A-NA	2.10	127.42	124.51
25	Q	609	CLA	C1-C2-C3	-2.10	122.41	126.04
25	3	309	CLA	CAC-C3C-C4C	2.10	127.54	124.81
28	O	205	BCR	C1-C6-C5	-2.10	119.66	122.61
32	J	102	LMG	O8-C28-O10	-2.10	118.29	123.59
25	7	301	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	a	303	CLA	CMB-C2B-C3B	2.10	131.67	126.59
33	1	601	CHL	C4-C3-C5	2.10	118.80	115.27
25	S	313	CLA	CHB-C1B-NB	2.10	126.48	124.26
25	4	309	CLA	CHC-C4B-NB	2.10	126.48	124.26
28	L	207	BCR	C34-C9-C10	-2.10	119.98	122.92
25	5	310	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
28	B	845	BCR	C33-C5-C4	2.10	117.65	113.62
25	A	802	CLA	CHC-C4B-NB	2.10	126.48	124.26
35	P	616	XAT	C31-C32-C33	-2.10	120.52	126.42
33	P	619	CHL	OMC-CMC-C2C	-2.10	120.94	125.69
33	P	607	CHL	OMC-CMC-C2C	-2.10	120.94	125.69
25	9	301	CLA	O2D-CGD-CBD	2.10	114.99	111.27
25	A	840	CLA	CHC-C4B-NB	2.10	126.48	124.26
25	a	312	CLA	CHD-C1D-ND	-2.10	122.53	124.45
33	1	601	CHL	CHB-C1B-C2B	-2.10	121.32	127.24
25	U	311	CLA	C3B-C4B-NB	-2.10	108.57	110.52
25	3	305	CLA	CHD-C1D-ND	-2.09	122.53	124.45
25	B	807	CLA	C11-C12-C13	-2.09	109.15	115.92
25	9	308	CLA	C3A-C2A-C1A	2.09	104.48	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Q	606	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
25	S	315	CLA	C2D-C1D-ND	-2.09	108.56	110.10
28	L	204	BCR	C11-C10-C9	-2.09	124.32	127.31
25	R	603	CLA	CHD-C1D-ND	-2.09	122.53	124.45
26	A	841	PQN	C2M-C2-C1	2.09	119.74	116.27
33	P	619	CHL	C1-C2-C3	-2.09	122.42	126.04
33	P	607	CHL	C1-C2-C3	-2.09	122.42	126.04
25	5	309	CLA	C2D-C1D-ND	-2.09	108.56	110.10
25	O	201	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	Q	611	CLA	CHB-C1B-NB	2.09	126.47	124.26
25	2	311	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	P	615	LUT	C40-C33-C32	2.09	121.37	118.08
27	2	317	LHG	O8-C23-C24	2.09	118.47	111.91
25	3	314	CLA	CHC-C4B-NB	2.09	126.47	124.26
25	5	314	CLA	CHB-C1B-NB	2.09	126.47	124.26
34	U	315	LUT	C40-C33-C32	2.09	121.37	118.08
28	B	841	BCR	C10-C11-C12	-2.09	116.69	123.22
33	4	314	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
34	a	316	LUT	C31-C32-C33	-2.09	120.54	126.42
25	B	801	CLA	C16-C15-C13	-2.09	109.17	115.92
25	L	201	CLA	CHB-C1B-NB	2.09	126.47	124.26
35	T	615	XAT	C4-C3-C2	-2.09	106.74	110.77
25	U	313	CLA	CMB-C2B-C3B	2.09	131.65	126.59
25	S	311	CLA	CHD-C1D-ND	-2.09	122.53	124.45
34	6	622	LUT	C38-C25-C24	-2.09	119.09	123.56
34	5	318	LUT	C18-C5-C4	2.09	118.22	114.36
25	1	604	CLA	CHB-C4A-NA	2.09	127.40	124.51
25	L	201	CLA	CHC-C4B-NB	2.09	126.47	124.26
28	A	849	BCR	C33-C5-C6	-2.09	122.18	124.53
34	P	615	LUT	C39-C29-C30	-2.09	120.00	122.92
25	A	813	CLA	CHB-C1B-NB	2.09	126.47	124.26
33	U	309	CHL	C3C-C4C-NC	2.09	112.91	110.57
25	8	306	CLA	CAA-C2A-C3A	-2.09	109.05	114.26
25	6	615	CLA	O2A-CGA-O1A	-2.09	116.60	123.14
25	B	819	CLA	CHD-C1D-ND	-2.09	122.54	124.45
25	5	316	CLA	CHD-C1D-ND	-2.09	122.54	124.45
33	S	310	CHL	O1D-CGD-CBD	-2.09	120.22	124.48
25	A	830	CLA	C16-C15-C13	-2.09	109.18	115.92
25	B	827	CLA	C2D-C1D-ND	-2.09	108.57	110.10
33	S	308	CHL	CED-O2D-CGD	2.09	120.65	115.94
27	4	319	LHG	O7-C7-O9	-2.09	118.66	123.70
25	4	307	CLA	O2A-CGA-O1A	-2.08	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F	801	BCR	C38-C26-C27	2.08	117.62	113.62
28	B	841	BCR	C38-C26-C25	-2.08	122.19	124.53
35	P	623	XAT	C30-C31-C32	-2.08	116.71	123.22
25	H	205	CLA	O2D-CGD-CBD	2.08	114.97	111.27
25	1	608	CLA	CHB-C4A-NA	2.08	127.39	124.51
34	3	315	LUT	C38-C25-C24	-2.08	119.10	123.56
25	4	310	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
25	7	304	CLA	CAA-C2A-C3A	-2.08	109.05	114.26
33	S	307	CHL	CHC-C1C-NC	2.08	127.36	124.20
25	3	302	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
28	J	101	BCR	C16-C17-C18	-2.08	124.34	127.31
25	Q	611	CLA	CHB-C4A-NA	2.08	127.39	124.51
33	R	608	CHL	CHB-C4A-NA	2.08	127.39	124.51
25	S	320	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
33	S	306	CHL	CED-O2D-CGD	2.08	120.65	115.94
28	G	203	BCR	C31-C1-C6	-2.08	106.92	110.30
25	A	842	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	B	836	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	A	825	CLA	C1-C2-C3	-2.08	122.44	126.04
33	4	314	CHL	CED-O2D-CGD	2.08	120.64	115.94
33	S	307	CHL	C3B-C4B-NB	2.08	112.45	110.52
25	B	804	CLA	C11-C12-C13	-2.08	109.19	115.92
25	B	803	CLA	CHC-C4B-NB	2.08	126.46	124.26
25	K	201	CLA	CHB-C1B-NB	2.08	126.46	124.26
33	4	304	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
36	R	617	NEX	C4-C3-C2	-2.08	106.76	110.77
33	5	317	CHL	OBD-CAD-C3D	-2.08	123.52	128.52
25	J	105	CLA	CHC-C4B-NB	2.08	126.46	124.26
25	8	302	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
33	S	307	CHL	CHD-C1D-C2D	2.08	129.84	125.48
33	S	307	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
25	A	810	CLA	C2D-C1D-ND	-2.08	108.57	110.10
33	5	308	CHL	C4A-NA-C1A	-2.08	105.77	106.71
34	4	315	LUT	C40-C33-C32	2.08	121.35	118.08
25	9	305	CLA	O1D-CGD-CBD	2.08	128.73	124.48
28	B	843	BCR	C39-C30-C25	-2.08	106.93	110.30
28	5	320	BCR	C35-C13-C14	-2.08	120.01	122.92
25	2	303	CLA	CAC-C3C-C4C	2.08	127.50	124.81
25	5	319	CLA	C2D-C1D-ND	-2.08	108.57	110.10
25	7	309	CLA	CMA-C3A-C2A	-2.08	111.25	116.10
34	8	317	LUT	C20-C13-C14	-2.08	120.02	122.92
25	6	610	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	5	320	BCR	C20-C21-C22	-2.08	124.35	127.31
25	A	814	CLA	C1-C2-C3	-2.07	122.45	126.04
28	8	318	BCR	C35-C13-C14	-2.07	120.02	122.92
25	3	303	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	A	836	CLA	O1D-CGD-CBD	2.07	128.73	124.48
25	A	803	CLA	CHB-C4A-NA	2.07	127.38	124.51
33	9	307	CHL	CAA-CBA-CGA	-2.07	107.19	113.25
28	A	848	BCR	C23-C24-C25	-2.07	121.38	127.20
33	1	606	CHL	C3B-C4B-NB	2.07	112.44	110.52
25	A	825	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	A	812	CLA	C3C-C4C-NC	-2.07	108.25	110.57
34	a	316	LUT	C1-C6-C7	2.07	121.64	115.78
34	5	318	LUT	C38-C25-C24	-2.07	119.13	123.56
25	A	829	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
34	4	316	LUT	C19-C9-C8	2.07	121.34	118.08
25	9	303	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	1	603	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	B	842	BCR	C36-C18-C17	-2.07	120.02	122.92
28	8	301	BCR	C38-C26-C27	2.07	117.59	113.62
25	Q	610	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	6	609	CLA	CHC-C4B-NB	2.07	126.45	124.26
25	8	306	CLA	CHB-C1B-NB	2.07	126.45	124.26
33	6	608	CHL	C3D-C4D-CHA	-2.07	107.99	112.72
33	Q	608	CHL	C2C-C3C-C4C	2.07	107.96	106.49
25	a	301	CLA	CHB-C1B-NB	2.07	126.45	124.26
33	S	321	CHL	CHB-C1B-C2B	-2.07	121.40	127.24
28	5	320	BCR	C11-C12-C13	-2.07	120.61	126.42
25	B	823	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
25	B	830	CLA	C2D-C1D-ND	-2.07	108.58	110.10
33	P	622	CHL	OBD-CAD-C3D	-2.07	123.55	128.52
25	a	301	CLA	CHC-C4B-NB	2.07	126.44	124.26
32	4	320	LMG	C6-C5-C4	-2.07	108.17	113.00
33	9	306	CHL	CHB-C1B-NB	-2.06	122.07	124.26
25	6	609	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	4	308	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
33	6	608	CHL	C4A-NA-C1A	-2.06	105.78	106.71
35	P	623	XAT	C18-C5-C4	2.06	116.60	114.28
34	a	315	LUT	C10-C11-C12	-2.06	116.78	123.22
25	2	313	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
34	Q	614	LUT	C8-C7-C6	-2.06	121.41	127.20
33	6	608	CHL	C2A-C3A-C4A	-2.06	98.54	101.87
25	6	604	CLA	CAA-CBA-CGA	-2.06	107.23	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	P	619	CHL	C3D-C4D-CHA	-2.06	108.00	112.72
25	5	311	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
34	3	316	LUT	C15-C35-C34	-2.06	119.25	123.47
34	5	322	LUT	C38-C25-C24	-2.06	119.15	123.56
25	8	308	CLA	CHC-C4B-NB	2.06	126.44	124.26
36	P	617	NEX	C4-C3-C2	-2.06	106.79	110.77
25	B	802	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	5	312	CLA	CBA-CAA-C2A	-2.06	107.78	113.86
25	Q	602	CLA	CMB-C2B-C3B	2.06	131.58	126.59
25	B	826	CLA	C2D-C1D-ND	-2.06	108.59	110.10
25	a	309	CLA	C2D-C1D-ND	-2.06	108.59	110.10
25	A	806	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
33	1	601	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
25	B	832	CLA	CHC-C4B-NB	2.06	126.44	124.26
33	R	607	CHL	C3D-C4D-CHA	-2.06	108.01	112.72
35	Q	616	XAT	C4-C3-C2	-2.06	106.80	110.77
25	K	201	CLA	C2D-C1D-ND	-2.06	108.59	110.10
25	3	310	CLA	C2D-C1D-ND	-2.06	108.59	110.10
33	R	609	CHL	C2B-C1B-NB	-2.06	108.85	110.23
25	a	308	CLA	C4D-CHA-C1A	-2.06	118.74	121.25
25	B	833	CLA	CHB-C1B-NB	2.06	126.44	124.26
25	2	309	CLA	CHC-C4B-NB	2.06	126.44	124.26
25	8	302	CLA	C2D-C1D-ND	-2.06	108.59	110.10
28	I	201	BCR	C32-C1-C6	-2.06	106.96	110.30
25	A	842	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	a	306	CLA	O1D-CGD-CBD	2.06	128.69	124.48
28	A	847	BCR	C33-C5-C4	2.06	117.56	113.62
25	J	105	CLA	CHB-C1B-NB	2.06	126.43	124.26
25	4	313	CLA	CHB-C1B-NB	2.06	126.43	124.26
25	L	202	CLA	C16-C15-C13	-2.05	109.28	115.92
25	8	302	CLA	CHC-C4B-NB	2.05	126.43	124.26
33	U	308	CHL	CHB-C4A-NA	2.05	127.35	124.51
25	B	824	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
33	4	306	CHL	OBD-CAD-C3D	-2.05	123.58	128.52
33	6	608	CHL	C5-C3-C4	2.05	119.14	114.60
25	B	828	CLA	CHC-C4B-NB	2.05	126.43	124.26
28	F	803	BCR	C24-C23-C22	-2.05	123.13	126.23
25	R	612	CLA	C3B-C4B-NB	-2.05	108.61	110.52
33	S	310	CHL	CED-O2D-CGD	2.05	120.58	115.94
25	B	822	CLA	C2D-C1D-ND	-2.05	108.59	110.10
27	5	321	LHG	O7-C7-O9	-2.05	118.74	123.70
33	9	306	CHL	CHB-C1B-C2B	-2.05	121.44	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	841	BCR	C34-C9-C10	-2.05	120.05	122.92
25	B	801	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
33	S	310	CHL	O2D-CGD-O1D	-2.05	119.83	123.84
25	B	818	CLA	C2D-C1D-ND	-2.05	108.59	110.10
34	a	316	LUT	C39-C29-C30	-2.05	120.05	122.92
25	A	820	CLA	CHB-C1B-NB	2.05	126.43	124.26
25	1	604	CLA	CHC-C4B-NB	2.05	126.43	124.26
34	2	316	LUT	C15-C14-C13	-2.05	124.38	127.31
33	R	606	CHL	O2D-CGD-O1D	-2.05	119.83	123.84
25	R	602	CLA	CAC-C3C-C4C	2.05	127.47	124.81
33	P	607	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
25	a	302	CLA	C2D-C1D-ND	-2.05	108.59	110.10
33	T	607	CHL	CHC-C1C-NC	2.05	127.31	124.20
28	L	204	BCR	C8-C9-C10	2.05	122.09	118.94
25	P	611	CLA	CMC-C2C-C1C	2.05	128.16	125.04
28	7	316	BCR	C37-C22-C23	2.05	121.31	118.08
34	6	622	LUT	C39-C29-C28	2.05	121.31	118.08
25	5	314	CLA	CHC-C4B-NB	2.05	126.43	124.26
25	a	311	CLA	CHC-C4B-NB	2.05	126.43	124.26
34	U	315	LUT	C20-C13-C12	2.05	121.31	118.08
28	J	101	BCR	C1-C6-C7	2.05	121.57	115.78
25	Q	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
34	T	613	LUT	C8-C7-C6	-2.05	121.45	127.20
33	P	609	CHL	C2A-C1A-CHA	2.05	127.44	123.86
33	U	306	CHL	OBD-CAD-C3D	-2.05	123.59	128.52
25	R	612	CLA	C2B-C1B-NB	-2.05	108.86	110.23
33	S	306	CHL	C4A-NA-C1A	-2.05	105.79	106.71
25	1	609	CLA	C4D-CHA-C1A	-2.05	118.76	121.25
28	A	854	BCR	C35-C13-C14	-2.05	120.06	122.92
34	8	317	LUT	C38-C25-C24	-2.05	119.18	123.56
25	2	314	CLA	C3B-C4B-NB	-2.05	108.62	110.52
25	L	205	CLA	CHB-C1B-NB	2.05	126.42	124.26
25	3	310	CLA	CHC-C4B-NB	2.05	126.42	124.26
25	3	307	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	7	310	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
25	T	608	CLA	C1-C2-C3	-2.04	122.51	126.04
25	A	821	CLA	CHC-C4B-NB	2.04	126.42	124.26
33	T	606	CHL	OBD-CAD-C3D	-2.04	123.60	128.52
28	8	318	BCR	C29-C30-C25	2.04	113.63	110.48
25	5	304	CLA	CMB-C2B-C3B	2.04	131.54	126.59
34	9	313	LUT	C8-C7-C6	-2.04	121.47	127.20
25	A	819	CLA	O2A-CGA-O1A	-2.04	118.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	2	310	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	A	821	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
25	1	612	CLA	O1D-CGD-CBD	2.04	128.66	124.48
25	a	308	CLA	O1D-CGD-CBD	2.04	128.66	124.48
34	9	313	LUT	C39-C29-C28	2.04	121.29	118.08
25	4	303	CLA	O1D-CGD-CBD	2.04	128.66	124.48
25	3	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	B	822	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	6	614	CLA	O1A-CGA-CBA	2.04	129.64	123.08
33	8	307	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
25	A	815	CLA	C1-C2-C3	-2.04	122.51	126.04
25	5	324	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	2	308	CLA	C2D-C1D-ND	-2.04	108.60	110.10
25	B	809	CLA	CHB-C1B-NB	2.04	126.42	124.26
25	9	301	CLA	CHD-C1D-ND	-2.04	122.58	124.45
34	1	617	LUT	C15-C35-C34	-2.04	119.30	123.47
25	7	308	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
33	Q	608	CHL	C2B-C1B-NB	-2.04	108.86	110.23
34	1	617	LUT	C31-C32-C33	-2.04	120.69	126.42
25	U	302	CLA	CMB-C2B-C3B	2.04	131.53	126.59
34	P	614	LUT	C16-C1-C6	-2.04	106.99	110.30
34	6	622	LUT	C20-C13-C12	2.04	121.29	118.08
25	B	809	CLA	CHC-C4B-NB	2.04	126.41	124.26
28	L	208	BCR	C8-C7-C6	-2.04	121.48	127.20
34	P	615	LUT	C30-C31-C32	-2.04	116.86	123.22
25	2	304	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	R	604	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
25	3	303	CLA	CHC-C4B-NB	2.04	126.41	124.26
25	T	602	CLA	C2D-C1D-ND	-2.04	108.60	110.10
28	B	840	BCR	C1-C6-C5	-2.04	119.75	122.61
34	R	616	LUT	C30-C31-C32	-2.04	116.87	123.22
25	S	314	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	B	804	CLA	O1D-CGD-CBD	2.03	128.65	124.48
34	S	317	LUT	C39-C29-C30	-2.03	120.07	122.92
32	4	320	LMG	O6-C1-C2	-2.03	106.04	110.35
25	G	201	CLA	CHB-C1B-NB	2.03	126.41	124.26
25	1	612	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
28	7	316	BCR	C36-C18-C17	-2.03	120.08	122.92
33	S	308	CHL	C4A-NA-C1A	-2.03	105.79	106.71
33	S	308	CHL	CHB-C1B-C2B	-2.03	121.50	127.24
33	6	607	CHL	CED-O2D-CGD	2.03	120.53	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	611	CLA	CHB-C1B-NB	2.03	126.41	124.26
25	6	623	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	S	312	CLA	CHC-C4B-NB	2.03	126.41	124.26
25	5	311	CLA	CHC-C4B-NB	2.03	126.41	124.26
25	6	623	CLA	CHB-C1B-NB	2.03	126.41	124.26
28	6	621	BCR	C35-C13-C14	-2.03	120.08	122.92
25	U	302	CLA	C2D-C1D-ND	-2.03	108.61	110.10
34	U	315	LUT	C30-C31-C32	-2.03	116.88	123.22
25	B	808	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	9	309	CLA	CHD-C1D-ND	-2.03	122.59	124.45
33	S	308	CHL	C1-C2-C3	-2.03	122.53	126.04
25	2	307	CLA	C2D-C1D-ND	-2.03	108.61	110.10
28	O	204	BCR	C16-C15-C14	-2.03	119.32	123.47
25	7	309	CLA	O2D-CGD-CBD	2.03	114.87	111.27
33	P	622	CHL	C1-O2A-CGA	2.03	121.77	116.44
25	S	315	CLA	CHB-C1B-NB	2.03	126.41	124.26
25	8	304	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
34	7	314	LUT	C20-C13-C12	2.03	121.27	118.08
25	7	302	CLA	O2D-CGD-CBD	2.03	114.87	111.27
27	A	852	LHG	O7-C7-O9	-2.03	118.80	123.70
25	A	811	CLA	C16-C15-C13	-2.03	109.36	115.92
28	L	203	BCR	C23-C24-C25	-2.03	121.51	127.20
28	F	801	BCR	C10-C11-C12	-2.03	116.89	123.22
25	A	830	CLA	CHB-C1B-NB	2.03	126.40	124.26
25	2	305	CLA	CHB-C1B-NB	2.03	126.40	124.26
25	7	313	CLA	CHC-C4B-NB	2.03	126.40	124.26
32	7	319	LMG	O8-C28-O10	-2.03	118.48	123.59
25	B	824	CLA	O2D-CGD-CBD	2.03	114.87	111.27
25	6	610	CLA	CHC-C4B-NB	2.03	126.40	124.26
33	R	609	CHL	C2A-C1A-CHA	2.03	127.40	123.86
32	2	301	LMG	C9-C8-C7	-2.03	107.00	111.79
25	B	821	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
34	Q	615	LUT	C3-C4-C5	-2.02	107.82	111.85
25	P	612	CLA	C2B-C1B-NB	-2.02	108.88	110.23
25	Q	613	CLA	CHD-C1D-ND	-2.02	122.59	124.45
25	3	301	CLA	C7-C6-C5	-2.02	107.86	113.36
25	B	827	CLA	CHC-C4B-NB	2.02	126.40	124.26
25	T	610	CLA	CHB-C1B-NB	2.02	126.40	124.26
25	P	612	CLA	C3B-C4B-NB	-2.02	108.64	110.52
25	A	803	CLA	CHC-C4B-NB	2.02	126.40	124.26
25	B	819	CLA	CHC-C4B-NB	2.02	126.40	124.26
25	3	305	CLA	CHC-C4B-NB	2.02	126.40	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	302	CLA	CHB-C1B-NB	2.02	126.40	124.26
25	9	309	CLA	CHC-C4B-NB	2.02	126.40	124.26
27	a	317	LHG	O7-C7-O9	-2.02	118.81	123.70
28	L	203	BCR	C28-C29-C30	-2.02	107.37	114.60
33	U	305	CHL	CAA-C2A-C3A	-2.02	107.24	112.78
35	P	620	XAT	C38-C25-C24	2.02	116.55	114.28
25	L	209	CLA	CHA-C1A-NA	-2.02	121.77	126.40
33	P	609	CHL	C2B-C1B-NB	-2.02	108.88	110.23
25	K	201	CLA	CAC-C3C-C4C	2.02	127.43	124.81
25	1	605	CLA	O2D-CGD-CBD	2.02	114.86	111.27
25	A	802	CLA	C1-C2-C3	-2.02	122.55	126.04
25	Q	604	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
25	9	311	CLA	CHB-C1B-NB	2.02	126.39	124.26
28	A	848	BCR	C16-C15-C14	-2.02	119.34	123.47
33	1	606	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
25	B	806	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
35	P	616	XAT	O4-C5-C6	-2.02	57.29	58.96
33	T	605	CHL	OMC-CMC-C2C	-2.02	121.12	125.69
25	1	611	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	R	602	CLA	C2D-C1D-ND	-2.02	108.62	110.10
25	A	831	CLA	C1-C2-C3	-2.02	123.49	126.75
25	B	802	CLA	O1D-CGD-CBD	2.02	128.61	124.48
35	P	620	XAT	C4-C3-C2	-2.02	106.88	110.77
34	3	315	LUT	C20-C13-C14	-2.02	120.10	122.92
25	8	305	CLA	CHD-C1D-ND	-2.02	122.60	124.45
35	T	615	XAT	C38-C25-C24	2.02	116.55	114.28
25	S	314	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	T	609	CLA	CHB-C1B-NB	2.02	126.39	124.26
25	Q	611	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	A	822	CLA	CHB-C1B-NB	2.01	126.39	124.26
36	U	316	NEX	C31-C32-C33	-2.01	120.76	126.42
33	5	317	CHL	CHB-C1B-C2B	-2.01	121.55	127.24
35	S	318	XAT	C4-C3-C2	-2.01	106.88	110.77
33	3	306	CHL	OBD-CAD-C3D	-2.01	123.67	128.52
33	T	601	CHL	C4B-CHC-C1C	-2.01	121.56	126.34
25	A	835	CLA	CHC-C4B-NB	2.01	126.39	124.26
33	U	306	CHL	OMC-CMC-C2C	-2.01	121.13	125.69
28	A	846	BCR	C23-C24-C25	-2.01	121.55	127.20
25	R	602	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
27	B	847	LHG	O8-C23-O10	-2.01	118.51	123.59
32	H	204	LMG	O7-C10-O9	-2.01	118.84	123.70
33	Q	608	CHL	C2A-C1A-CHA	2.01	127.38	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	S	302	CHL	CAA-CBA-CGA	-2.01	107.38	113.25
34	7	314	LUT	C35-C15-C14	-2.01	119.36	123.47
25	2	312	CLA	C3C-C4C-NC	-2.01	108.32	110.57
34	1	617	LUT	C19-C9-C8	2.01	121.25	118.08
34	a	316	LUT	C16-C1-C6	-2.01	107.04	110.30
33	P	606	CHL	OBD-CAD-C3D	-2.01	123.68	128.52
25	1	612	CLA	C3B-C4B-NB	-2.01	108.65	110.52
33	P	609	CHL	C4D-CHA-C1A	2.01	123.69	121.25
32	J	104	LMG	O8-C28-O10	-2.01	118.52	123.59
25	7	303	CLA	C2D-C1D-ND	-2.01	108.62	110.10
25	S	303	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
33	4	304	CHL	CMA-C3A-C2A	-2.01	111.41	116.10
25	7	312	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
25	8	314	CLA	C2A-C3A-C4A	2.01	105.11	101.87
28	L	204	BCR	C3-C2-C1	-2.01	107.42	114.60
25	1	614	CLA	CHB-C1B-NB	2.01	126.38	124.26
25	U	311	CLA	CHB-C4A-NA	2.01	127.29	124.51
25	a	308	CLA	CMC-C2C-C1C	-2.01	121.98	125.04
34	S	316	LUT	C11-C10-C9	-2.01	124.44	127.31
25	R	613	CLA	CHB-C1B-NB	2.01	126.38	124.26
34	R	616	LUT	C7-C8-C9	-2.01	123.20	126.23
34	3	315	LUT	C19-C9-C8	2.01	121.24	118.08
28	B	843	BCR	C4-C5-C6	-2.01	119.82	122.73
25	A	807	CLA	CHC-C4B-NB	2.01	126.38	124.26
25	7	301	CLA	CHC-C4B-NB	2.01	126.38	124.26
25	G	201	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
25	8	313	CLA	CHB-C4A-NA	2.01	127.29	124.51
25	8	314	CLA	CMA-C3A-C2A	-2.01	105.74	113.83
34	T	614	LUT	C3-C4-C5	-2.01	107.86	111.85
25	R	610	CLA	C3A-C2A-C1A	2.01	104.34	101.34
28	O	204	BCR	C37-C22-C21	-2.01	120.11	122.92
25	Q	613	CLA	CHC-C4B-NB	2.00	126.38	124.26
25	S	313	CLA	CHC-C4B-NB	2.00	126.38	124.26
25	R	613	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	Q	612	CLA	C3A-C2A-C1A	2.00	104.34	101.34
25	B	849	CLA	C2D-C1D-ND	-2.00	108.63	110.10
25	Q	612	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	P	613	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	G	202	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
25	3	309	CLA	C2D-C1D-ND	-2.00	108.63	110.10
25	B	812	CLA	CHB-C1B-NB	2.00	126.38	124.26
28	I	201	BCR	C27-C26-C25	-2.00	119.82	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	9	313	LUT	C21-C26-C27	-2.00	110.17	112.70
25	S	303	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
33	P	601	CHL	C4B-CHC-C1C	-2.00	121.59	126.34
34	Q	614	LUT	C20-C13-C14	-2.00	120.12	122.92
34	9	312	LUT	C40-C33-C34	-2.00	120.12	122.92
25	B	825	CLA	CHB-C1B-NB	2.00	126.38	124.26
25	6	620	CLA	CHC-C4B-NB	2.00	126.38	124.26
25	7	301	CLA	C2D-C1D-ND	-2.00	108.63	110.10
25	U	304	CLA	CMC-C2C-C3C	2.00	131.55	126.12
36	P	621	NEX	O24-C25-C26	-2.00	57.30	58.96
25	Q	603	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
34	S	316	LUT	C7-C8-C9	-2.00	123.21	126.23
25	Q	612	CLA	CAC-C3C-C4C	2.00	127.41	124.81
25	7	311	CLA	CHB-C1B-NB	2.00	126.38	124.26

There are no chirality outliers.

All (4042) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CBD-CGD-O2D-CED
25	A	804	CLA	C2B-C3B-CAB-CBB
25	A	804	CLA	C4B-C3B-CAB-CBB
25	A	804	CLA	CAD-CBD-CGD-O1D
25	A	804	CLA	CAD-CBD-CGD-O2D
25	A	806	CLA	CHA-CBD-CGD-O1D
25	A	806	CLA	CHA-CBD-CGD-O2D
25	A	808	CLA	C2-C3-C5-C6
25	A	808	CLA	C4-C3-C5-C6
25	A	809	CLA	C3A-C2A-CAA-CBA
25	A	809	CLA	C2B-C3B-CAB-CBB
25	A	809	CLA	C4B-C3B-CAB-CBB
25	A	809	CLA	CHA-CBD-CGD-O2D
25	A	810	CLA	C2B-C3B-CAB-CBB
25	A	810	CLA	C4B-C3B-CAB-CBB
25	A	810	CLA	CBD-CGD-O2D-CED
25	A	813	CLA	C2B-C3B-CAB-CBB
25	A	813	CLA	C4B-C3B-CAB-CBB
25	A	815	CLA	CHA-CBD-CGD-O1D
25	A	815	CLA	CHA-CBD-CGD-O2D
25	A	815	CLA	CAD-CBD-CGD-O1D
25	A	815	CLA	CAD-CBD-CGD-O2D
25	A	816	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	816	CLA	C4B-C3B-CAB-CBB
25	A	816	CLA	CHA-CBD-CGD-O1D
25	A	816	CLA	CHA-CBD-CGD-O2D
25	A	817	CLA	C2B-C3B-CAB-CBB
25	A	817	CLA	C4B-C3B-CAB-CBB
25	A	818	CLA	CHA-CBD-CGD-O1D
25	A	818	CLA	CHA-CBD-CGD-O2D
25	A	819	CLA	C1A-C2A-CAA-CBA
25	A	819	CLA	C3A-C2A-CAA-CBA
25	A	819	CLA	C4B-C3B-CAB-CBB
25	A	820	CLA	C1A-C2A-CAA-CBA
25	A	820	CLA	C3A-C2A-CAA-CBA
25	A	823	CLA	C3A-C2A-CAA-CBA
25	A	823	CLA	CHA-CBD-CGD-O1D
25	A	823	CLA	CHA-CBD-CGD-O2D
25	A	824	CLA	C2B-C3B-CAB-CBB
25	A	824	CLA	C4B-C3B-CAB-CBB
25	A	824	CLA	CHA-CBD-CGD-O1D
25	A	824	CLA	CHA-CBD-CGD-O2D
25	A	825	CLA	C4B-C3B-CAB-CBB
25	A	825	CLA	CHA-CBD-CGD-O1D
25	A	825	CLA	CHA-CBD-CGD-O2D
25	A	828	CLA	C1A-C2A-CAA-CBA
25	A	828	CLA	C3A-C2A-CAA-CBA
25	A	828	CLA	CHA-CBD-CGD-O1D
25	A	828	CLA	CHA-CBD-CGD-O2D
25	A	828	CLA	CBD-CGD-O2D-CED
25	A	829	CLA	C2B-C3B-CAB-CBB
25	A	829	CLA	C4B-C3B-CAB-CBB
25	A	831	CLA	C1A-C2A-CAA-CBA
25	A	831	CLA	C3A-C2A-CAA-CBA
25	A	831	CLA	CHA-CBD-CGD-O1D
25	A	831	CLA	CHA-CBD-CGD-O2D
25	A	831	CLA	CAD-CBD-CGD-O1D
25	A	834	CLA	C1A-C2A-CAA-CBA
25	A	834	CLA	C4B-C3B-CAB-CBB
25	A	834	CLA	CAD-CBD-CGD-O2D
25	A	835	CLA	C2B-C3B-CAB-CBB
25	A	835	CLA	C4B-C3B-CAB-CBB
25	A	836	CLA	C2B-C3B-CAB-CBB
25	A	836	CLA	C4B-C3B-CAB-CBB
25	A	836	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	836	CLA	C4-C3-C5-C6
25	A	837	CLA	C4B-C3B-CAB-CBB
25	A	838	CLA	C2B-C3B-CAB-CBB
25	A	838	CLA	C4B-C3B-CAB-CBB
25	A	838	CLA	CHA-CBD-CGD-O1D
25	A	838	CLA	CHA-CBD-CGD-O2D
25	A	839	CLA	C2-C3-C5-C6
25	A	839	CLA	C4-C3-C5-C6
25	A	840	CLA	C4B-C3B-CAB-CBB
25	A	853	CLA	C4B-C3B-CAB-CBB
25	A	853	CLA	CHA-CBD-CGD-O1D
25	A	853	CLA	CHA-CBD-CGD-O2D
25	B	801	CLA	C2B-C3B-CAB-CBB
25	B	801	CLA	C4B-C3B-CAB-CBB
25	B	801	CLA	CHA-CBD-CGD-O1D
25	B	801	CLA	CHA-CBD-CGD-O2D
25	B	801	CLA	CBD-CGD-O2D-CED
25	B	802	CLA	CBD-CGD-O2D-CED
25	B	803	CLA	CHA-CBD-CGD-O1D
25	B	803	CLA	CHA-CBD-CGD-O2D
25	B	804	CLA	C3A-C2A-CAA-CBA
25	B	806	CLA	C2B-C3B-CAB-CBB
25	B	806	CLA	C4B-C3B-CAB-CBB
25	B	807	CLA	C2B-C3B-CAB-CBB
25	B	807	CLA	C4B-C3B-CAB-CBB
25	B	807	CLA	CHA-CBD-CGD-O1D
25	B	807	CLA	CHA-CBD-CGD-O2D
25	B	808	CLA	C2B-C3B-CAB-CBB
25	B	808	CLA	C4B-C3B-CAB-CBB
25	B	809	CLA	CAD-CBD-CGD-O1D
25	B	809	CLA	C11-C12-C13-C14
25	B	812	CLA	C2B-C3B-CAB-CBB
25	B	812	CLA	C4B-C3B-CAB-CBB
25	B	815	CLA	C2B-C3B-CAB-CBB
25	B	815	CLA	C4B-C3B-CAB-CBB
25	B	816	CLA	C1A-C2A-CAA-CBA
25	B	816	CLA	C3A-C2A-CAA-CBA
25	B	817	CLA	CHA-CBD-CGD-O1D
25	B	817	CLA	CHA-CBD-CGD-O2D
25	B	818	CLA	CHA-CBD-CGD-O1D
25	B	818	CLA	CHA-CBD-CGD-O2D
25	B	818	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	819	CLA	C2B-C3B-CAB-CBB
25	B	819	CLA	C4B-C3B-CAB-CBB
25	B	821	CLA	CBD-CGD-O2D-CED
25	B	824	CLA	C2B-C3B-CAB-CBB
25	B	824	CLA	C4B-C3B-CAB-CBB
25	B	825	CLA	C1A-C2A-CAA-CBA
25	B	825	CLA	C3A-C2A-CAA-CBA
25	B	826	CLA	C1A-C2A-CAA-CBA
25	B	826	CLA	C3A-C2A-CAA-CBA
25	B	826	CLA	CHA-CBD-CGD-O1D
25	B	826	CLA	CHA-CBD-CGD-O2D
25	B	828	CLA	C1A-C2A-CAA-CBA
25	B	828	CLA	C3A-C2A-CAA-CBA
25	B	831	CLA	C2B-C3B-CAB-CBB
25	B	831	CLA	C4B-C3B-CAB-CBB
25	B	832	CLA	C1A-C2A-CAA-CBA
25	B	832	CLA	C3A-C2A-CAA-CBA
25	B	832	CLA	C2B-C3B-CAB-CBB
25	B	832	CLA	C4B-C3B-CAB-CBB
25	B	832	CLA	CBD-CGD-O2D-CED
25	B	833	CLA	CHA-CBD-CGD-O1D
25	B	833	CLA	CHA-CBD-CGD-O2D
25	B	833	CLA	CAD-CBD-CGD-O1D
25	B	833	CLA	CAD-CBD-CGD-O2D
25	B	834	CLA	C4B-C3B-CAB-CBB
25	B	834	CLA	CHA-CBD-CGD-O1D
25	B	834	CLA	CHA-CBD-CGD-O2D
25	B	834	CLA	CAD-CBD-CGD-O1D
25	B	836	CLA	C2B-C3B-CAB-CBB
25	B	836	CLA	C4B-C3B-CAB-CBB
25	B	837	CLA	C2A-CAA-CBA-CGA
25	B	849	CLA	C1A-C2A-CAA-CBA
25	B	849	CLA	C4B-C3B-CAB-CBB
25	F	802	CLA	C2B-C3B-CAB-CBB
25	F	802	CLA	C4B-C3B-CAB-CBB
25	F	802	CLA	CBD-CGD-O2D-CED
25	G	201	CLA	C2B-C3B-CAB-CBB
25	G	201	CLA	C4B-C3B-CAB-CBB
25	G	201	CLA	CHA-CBD-CGD-O1D
25	G	201	CLA	CHA-CBD-CGD-O2D
25	G	202	CLA	C2B-C3B-CAB-CBB
25	G	202	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	H	201	CLA	C1A-C2A-CAA-CBA
25	H	201	CLA	C3A-C2A-CAA-CBA
25	H	202	CLA	C2B-C3B-CAB-CBB
25	H	202	CLA	C4B-C3B-CAB-CBB
25	H	202	CLA	CBD-CGD-O2D-CED
25	H	202	CLA	O1D-CGD-O2D-CED
25	H	203	CLA	C1A-C2A-CAA-CBA
25	H	203	CLA	C2B-C3B-CAB-CBB
25	H	203	CLA	C4B-C3B-CAB-CBB
25	J	103	CLA	C3A-C2A-CAA-CBA
25	J	103	CLA	C4B-C3B-CAB-CBB
25	J	105	CLA	C2B-C3B-CAB-CBB
25	J	105	CLA	C4B-C3B-CAB-CBB
25	J	105	CLA	CHA-CBD-CGD-O1D
25	J	105	CLA	CHA-CBD-CGD-O2D
25	J	105	CLA	CAD-CBD-CGD-O1D
25	K	203	CLA	C2B-C3B-CAB-CBB
25	K	203	CLA	C4B-C3B-CAB-CBB
25	K	204	CLA	C4B-C3B-CAB-CBB
25	K	204	CLA	CBD-CGD-O2D-CED
25	K	205	CLA	C2A-CAA-CBA-CGA
25	L	202	CLA	C2B-C3B-CAB-CBB
25	L	202	CLA	C4B-C3B-CAB-CBB
25	L	202	CLA	CHA-CBD-CGD-O1D
25	L	202	CLA	CHA-CBD-CGD-O2D
25	L	202	CLA	C4-C3-C5-C6
25	L	206	CLA	C1A-C2A-CAA-CBA
25	L	206	CLA	C3A-C2A-CAA-CBA
25	O	201	CLA	CHA-CBD-CGD-O1D
25	O	201	CLA	CHA-CBD-CGD-O2D
25	O	201	CLA	CAD-CBD-CGD-O1D
25	O	201	CLA	CBD-CGD-O2D-CED
25	P	603	CLA	C4B-C3B-CAB-CBB
25	P	610	CLA	CBD-CGD-O2D-CED
25	P	611	CLA	CBD-CGD-O2D-CED
25	P	611	CLA	O1D-CGD-O2D-CED
25	Q	603	CLA	C4B-C3B-CAB-CBB
25	Q	610	CLA	C2B-C3B-CAB-CBB
25	Q	610	CLA	C4B-C3B-CAB-CBB
25	Q	613	CLA	C2B-C3B-CAB-CBB
25	Q	613	CLA	C4B-C3B-CAB-CBB
25	Q	613	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	Q	613	CLA	CAD-CBD-CGD-O2D
25	Q	618	CLA	C2B-C3B-CAB-CBB
25	Q	618	CLA	C4B-C3B-CAB-CBB
25	R	610	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	C2B-C3B-CAB-CBB
25	R	611	CLA	C4B-C3B-CAB-CBB
25	R	614	CLA	C2B-C3B-CAB-CBB
25	R	614	CLA	C4B-C3B-CAB-CBB
25	R	614	CLA	CAD-CBD-CGD-O1D
25	R	614	CLA	CAD-CBD-CGD-O2D
25	S	301	CLA	C2B-C3B-CAB-CBB
25	S	301	CLA	C4B-C3B-CAB-CBB
25	S	301	CLA	CAD-CBD-CGD-O1D
25	S	301	CLA	CAD-CBD-CGD-O2D
25	S	305	CLA	C1A-C2A-CAA-CBA
25	S	305	CLA	C3A-C2A-CAA-CBA
25	S	313	CLA	C2B-C3B-CAB-CBB
25	S	313	CLA	C4B-C3B-CAB-CBB
25	S	313	CLA	CBD-CGD-O2D-CED
25	S	315	CLA	CAD-CBD-CGD-O1D
25	S	315	CLA	CAD-CBD-CGD-O2D
25	S	320	CLA	C4B-C3B-CAB-CBB
25	T	608	CLA	CBD-CGD-O2D-CED
25	T	609	CLA	C1A-C2A-CAA-CBA
25	T	609	CLA	C3A-C2A-CAA-CBA
25	T	609	CLA	C2B-C3B-CAB-CBB
25	T	609	CLA	C4B-C3B-CAB-CBB
25	T	612	CLA	C2B-C3B-CAB-CBB
25	T	612	CLA	C4B-C3B-CAB-CBB
25	T	612	CLA	CAD-CBD-CGD-O1D
25	T	612	CLA	CAD-CBD-CGD-O2D
25	U	303	CLA	C4B-C3B-CAB-CBB
25	U	313	CLA	C2B-C3B-CAB-CBB
25	U	313	CLA	C4B-C3B-CAB-CBB
25	U	313	CLA	CAD-CBD-CGD-O1D
25	U	313	CLA	CAD-CBD-CGD-O2D
25	1	602	CLA	C2B-C3B-CAB-CBB
25	1	602	CLA	C4B-C3B-CAB-CBB
25	1	602	CLA	CBD-CGD-O2D-CED
25	1	603	CLA	C2B-C3B-CAB-CBB
25	1	603	CLA	C4B-C3B-CAB-CBB
25	1	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	1	603	CLA	C4-C3-C5-C6
25	1	605	CLA	C3-C5-C6-C7
25	1	608	CLA	C3A-C2A-CAA-CBA
25	1	610	CLA	CBD-CGD-O2D-CED
25	1	612	CLA	CBD-CGD-O2D-CED
25	1	613	CLA	C2B-C3B-CAB-CBB
25	1	613	CLA	C4B-C3B-CAB-CBB
25	1	614	CLA	CHA-CBD-CGD-O1D
25	1	614	CLA	CHA-CBD-CGD-O2D
25	2	302	CLA	C3A-C2A-CAA-CBA
25	2	302	CLA	CHA-CBD-CGD-O1D
25	2	302	CLA	CHA-CBD-CGD-O2D
25	2	302	CLA	CAD-CBD-CGD-O1D
25	2	302	CLA	CAD-CBD-CGD-O2D
25	2	303	CLA	C2B-C3B-CAB-CBB
25	2	303	CLA	C4B-C3B-CAB-CBB
25	2	304	CLA	C2B-C3B-CAB-CBB
25	2	304	CLA	C4B-C3B-CAB-CBB
25	2	307	CLA	C1A-C2A-CAA-CBA
25	2	307	CLA	C3A-C2A-CAA-CBA
25	2	308	CLA	C2B-C3B-CAB-CBB
25	2	308	CLA	C4B-C3B-CAB-CBB
25	2	308	CLA	CBD-CGD-O2D-CED
25	2	309	CLA	C2-C3-C5-C6
25	2	309	CLA	C4-C3-C5-C6
25	2	310	CLA	C2B-C3B-CAB-CBB
25	2	310	CLA	C4B-C3B-CAB-CBB
25	2	310	CLA	CBD-CGD-O2D-CED
25	2	312	CLA	C2B-C3B-CAB-CBB
25	2	312	CLA	C4B-C3B-CAB-CBB
25	2	313	CLA	C1A-C2A-CAA-CBA
25	3	302	CLA	CBD-CGD-O2D-CED
25	3	303	CLA	C1A-C2A-CAA-CBA
25	3	303	CLA	C3A-C2A-CAA-CBA
25	3	304	CLA	C2B-C3B-CAB-CBB
25	3	304	CLA	C4B-C3B-CAB-CBB
25	3	305	CLA	C2B-C3B-CAB-CBB
25	3	305	CLA	C4B-C3B-CAB-CBB
25	3	305	CLA	C11-C10-C8-C9
25	3	308	CLA	C2B-C3B-CAB-CBB
25	3	308	CLA	C4B-C3B-CAB-CBB
25	3	309	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	3	309	CLA	C4B-C3B-CAB-CBB
25	3	309	CLA	CHA-CBD-CGD-O1D
25	3	309	CLA	CHA-CBD-CGD-O2D
25	3	310	CLA	C2B-C3B-CAB-CBB
25	3	310	CLA	C4B-C3B-CAB-CBB
25	3	312	CLA	C2B-C3B-CAB-CBB
25	3	312	CLA	C4B-C3B-CAB-CBB
25	3	314	CLA	C4B-C3B-CAB-CBB
25	3	320	CLA	C4B-C3B-CAB-CBB
25	3	320	CLA	C2-C3-C5-C6
25	3	320	CLA	C4-C3-C5-C6
25	4	301	CLA	C2B-C3B-CAB-CBB
25	4	301	CLA	C4B-C3B-CAB-CBB
25	4	307	CLA	C1A-C2A-CAA-CBA
25	4	309	CLA	CBD-CGD-O2D-CED
25	4	309	CLA	C2-C3-C5-C6
25	4	309	CLA	C4-C3-C5-C6
25	4	311	CLA	C1A-C2A-CAA-CBA
25	4	311	CLA	C3A-C2A-CAA-CBA
25	4	311	CLA	C2B-C3B-CAB-CBB
25	4	311	CLA	C4B-C3B-CAB-CBB
25	4	311	CLA	CHA-CBD-CGD-O1D
25	4	311	CLA	CHA-CBD-CGD-O2D
25	4	312	CLA	C2B-C3B-CAB-CBB
25	4	312	CLA	C4B-C3B-CAB-CBB
25	5	302	CLA	C2A-CAA-CBA-CGA
25	5	302	CLA	C2B-C3B-CAB-CBB
25	5	302	CLA	C4B-C3B-CAB-CBB
25	5	309	CLA	C1A-C2A-CAA-CBA
25	5	309	CLA	C3A-C2A-CAA-CBA
25	5	309	CLA	C2B-C3B-CAB-CBB
25	5	309	CLA	C4B-C3B-CAB-CBB
25	5	311	CLA	C2B-C3B-CAB-CBB
25	5	311	CLA	C4B-C3B-CAB-CBB
25	5	312	CLA	C4B-C3B-CAB-CBB
25	5	312	CLA	C3-C5-C6-C7
25	5	313	CLA	C4B-C3B-CAB-CBB
25	5	315	CLA	CBD-CGD-O2D-CED
25	5	316	CLA	C2B-C3B-CAB-CBB
25	5	316	CLA	C4B-C3B-CAB-CBB
25	5	316	CLA	CHA-CBD-CGD-O1D
25	5	316	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	5	319	CLA	C2A-CAA-CBA-CGA
25	5	319	CLA	CHA-CBD-CGD-O1D
25	5	319	CLA	CHA-CBD-CGD-O2D
25	5	324	CLA	C4B-C3B-CAB-CBB
25	5	324	CLA	CHA-CBD-CGD-O1D
25	5	324	CLA	CHA-CBD-CGD-O2D
25	5	324	CLA	CAD-CBD-CGD-O1D
25	5	324	CLA	CAD-CBD-CGD-O2D
25	6	601	CLA	CHA-CBD-CGD-O1D
25	6	601	CLA	CHA-CBD-CGD-O2D
25	6	601	CLA	CAD-CBD-CGD-O1D
25	6	603	CLA	C2B-C3B-CAB-CBB
25	6	603	CLA	C4B-C3B-CAB-CBB
25	6	603	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	C4B-C3B-CAB-CBB
25	6	609	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	C2-C3-C5-C6
25	6	610	CLA	C4-C3-C5-C6
25	6	611	CLA	C2B-C3B-CAB-CBB
25	6	611	CLA	C4B-C3B-CAB-CBB
25	6	611	CLA	C2-C3-C5-C6
25	6	611	CLA	C4-C3-C5-C6
25	6	612	CLA	C4B-C3B-CAB-CBB
25	6	612	CLA	C3-C5-C6-C7
25	6	615	CLA	C1A-C2A-CAA-CBA
25	6	615	CLA	C3A-C2A-CAA-CBA
25	6	615	CLA	C2B-C3B-CAB-CBB
25	6	615	CLA	C4B-C3B-CAB-CBB
25	6	616	CLA	C2B-C3B-CAB-CBB
25	6	616	CLA	C4B-C3B-CAB-CBB
25	6	616	CLA	CHA-CBD-CGD-O1D
25	6	616	CLA	CHA-CBD-CGD-O2D
25	6	620	CLA	C1A-C2A-CAA-CBA
25	6	620	CLA	C3A-C2A-CAA-CBA
25	6	620	CLA	C2B-C3B-CAB-CBB
25	6	620	CLA	C4B-C3B-CAB-CBB
25	6	620	CLA	CHA-CBD-CGD-O1D
25	6	620	CLA	CHA-CBD-CGD-O2D
25	6	620	CLA	CAD-CBD-CGD-O1D
25	6	620	CLA	CAD-CBD-CGD-O2D
25	6	623	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	6	623	CLA	C4B-C3B-CAB-CBB
25	6	623	CLA	CHA-CBD-CGD-O1D
25	6	623	CLA	CHA-CBD-CGD-O2D
25	7	301	CLA	C2B-C3B-CAB-CBB
25	7	301	CLA	C4B-C3B-CAB-CBB
25	7	304	CLA	C4B-C3B-CAB-CBB
25	7	304	CLA	CHA-CBD-CGD-O1D
25	7	304	CLA	CHA-CBD-CGD-O2D
25	7	304	CLA	CAD-CBD-CGD-O1D
25	7	307	CLA	C1A-C2A-CAA-CBA
25	7	310	CLA	C2B-C3B-CAB-CBB
25	7	310	CLA	C4B-C3B-CAB-CBB
25	7	310	CLA	C3-C5-C6-C7
25	7	311	CLA	CHA-CBD-CGD-O1D
25	7	311	CLA	CHA-CBD-CGD-O2D
25	7	313	CLA	C2B-C3B-CAB-CBB
25	7	313	CLA	C4B-C3B-CAB-CBB
25	8	302	CLA	CHA-CBD-CGD-O1D
25	8	302	CLA	CHA-CBD-CGD-O2D
25	8	302	CLA	CAD-CBD-CGD-O1D
25	8	302	CLA	CAD-CBD-CGD-O2D
25	8	306	CLA	C2B-C3B-CAB-CBB
25	8	306	CLA	C4B-C3B-CAB-CBB
25	8	308	CLA	C1A-C2A-CAA-CBA
25	8	309	CLA	C1A-C2A-CAA-CBA
25	8	309	CLA	C3A-C2A-CAA-CBA
25	8	310	CLA	C2B-C3B-CAB-CBB
25	8	310	CLA	C4B-C3B-CAB-CBB
25	8	311	CLA	C4B-C3B-CAB-CBB
25	8	313	CLA	C4B-C3B-CAB-CBB
25	8	315	CLA	C4B-C3B-CAB-CBB
25	8	315	CLA	CHA-CBD-CGD-O1D
25	8	315	CLA	CHA-CBD-CGD-O2D
25	9	302	CLA	C2B-C3B-CAB-CBB
25	9	302	CLA	C4B-C3B-CAB-CBB
25	9	302	CLA	CHA-CBD-CGD-O1D
25	9	302	CLA	CHA-CBD-CGD-O2D
25	9	302	CLA	CAD-CBD-CGD-O1D
25	9	302	CLA	CBD-CGD-O2D-CED
25	9	303	CLA	C2-C3-C5-C6
25	9	303	CLA	C4-C3-C5-C6
25	9	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	9	305	CLA	C4B-C3B-CAB-CBB
25	9	308	CLA	C1A-C2A-CAA-CBA
25	9	308	CLA	C3A-C2A-CAA-CBA
25	9	308	CLA	C4B-C3B-CAB-CBB
25	9	310	CLA	C4B-C3B-CAB-CBB
25	a	301	CLA	C2B-C3B-CAB-CBB
25	a	301	CLA	C4B-C3B-CAB-CBB
25	a	301	CLA	CBD-CGD-O2D-CED
25	a	302	CLA	C2B-C3B-CAB-CBB
25	a	302	CLA	C4B-C3B-CAB-CBB
25	a	302	CLA	C2-C3-C5-C6
25	a	302	CLA	C4-C3-C5-C6
25	a	303	CLA	O1A-CGA-O2A-C1
25	a	303	CLA	O2A-C1-C2-C3
25	a	304	CLA	C3-C5-C6-C7
25	a	306	CLA	CBD-CGD-O2D-CED
25	a	307	CLA	C3A-C2A-CAA-CBA
25	a	309	CLA	CBD-CGD-O2D-CED
25	a	311	CLA	CBD-CGD-O2D-CED
25	a	312	CLA	C2B-C3B-CAB-CBB
25	a	312	CLA	C4B-C3B-CAB-CBB
25	a	313	CLA	CHA-CBD-CGD-O1D
25	a	313	CLA	CHA-CBD-CGD-O2D
27	A	843	LHG	C3-O3-P-O5
27	A	843	LHG	C4-O6-P-O4
27	A	844	LHG	C3-O3-P-O5
27	A	844	LHG	C3-O3-P-O6
27	A	844	LHG	C4-O6-P-O3
27	A	844	LHG	C4-O6-P-O4
27	A	844	LHG	C4-O6-P-O5
27	A	852	LHG	C3-O3-P-O4
27	A	852	LHG	C3-O3-P-O5
27	A	852	LHG	C3-O3-P-O6
27	A	852	LHG	C4-O6-P-O4
27	A	852	LHG	O9-C7-O7-C5
27	A	852	LHG	C8-C7-O7-C5
27	B	847	LHG	O1-C1-C2-C3
27	B	847	LHG	C4-O6-P-O4
27	B	847	LHG	O7-C5-C6-O8
27	B	847	LHG	C8-C7-O7-C5
27	P	618	LHG	C4-O6-P-O5
27	P	624	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
27	Q	617	LHG	C4-O6-P-O5
27	R	618	LHG	C4-O6-P-O5
27	T	617	LHG	C4-O6-P-O5
27	1	618	LHG	C24-C23-O8-C6
27	2	317	LHG	C4-O6-P-O5
27	4	318	LHG	C1-C2-C3-O3
27	4	318	LHG	O2-C2-C3-O3
27	4	319	LHG	C4-O6-P-O5
27	5	301	LHG	C3-O3-P-O4
27	5	301	LHG	C3-O3-P-O5
27	5	301	LHG	C3-O3-P-O6
27	5	321	LHG	C3-O3-P-O5
27	5	321	LHG	C4-O6-P-O3
27	5	321	LHG	C4-O6-P-O4
27	6	618	LHG	C4-O6-P-O3
27	7	317	LHG	C4-O6-P-O3
27	7	317	LHG	C4-O6-P-O4
27	7	317	LHG	C4-O6-P-O5
27	8	319	LHG	C3-O3-P-O6
27	a	317	LHG	C24-C23-O8-C6
28	A	845	BCR	C1-C6-C7-C8
28	A	848	BCR	C7-C8-C9-C10
28	A	848	BCR	C7-C8-C9-C34
28	A	848	BCR	C37-C22-C23-C24
28	A	849	BCR	C7-C8-C9-C10
28	A	849	BCR	C7-C8-C9-C34
28	A	854	BCR	C21-C22-C23-C24
28	A	854	BCR	C37-C22-C23-C24
28	B	840	BCR	C7-C8-C9-C34
28	B	841	BCR	C7-C8-C9-C10
28	B	841	BCR	C7-C8-C9-C34
28	B	843	BCR	C1-C6-C7-C8
28	B	844	BCR	C21-C22-C23-C24
28	B	844	BCR	C37-C22-C23-C24
28	B	845	BCR	C21-C22-C23-C24
28	B	845	BCR	C37-C22-C23-C24
28	F	801	BCR	C17-C18-C19-C20
28	F	801	BCR	C36-C18-C19-C20
28	I	201	BCR	C17-C18-C19-C20
28	I	201	BCR	C36-C18-C19-C20
28	I	201	BCR	C21-C22-C23-C24
28	I	201	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
28	J	101	BCR	C23-C24-C25-C26
28	J	101	BCR	C23-C24-C25-C30
28	J	106	BCR	C7-C8-C9-C10
28	J	106	BCR	C7-C8-C9-C34
28	J	106	BCR	C17-C18-C19-C20
28	J	106	BCR	C36-C18-C19-C20
28	K	206	BCR	C19-C20-C21-C22
28	L	203	BCR	C9-C10-C11-C12
28	L	204	BCR	C36-C18-C19-C20
28	L	207	BCR	C36-C18-C19-C20
28	L	207	BCR	C21-C22-C23-C24
28	L	207	BCR	C37-C22-C23-C24
28	L	207	BCR	C23-C24-C25-C26
28	L	207	BCR	C23-C24-C25-C30
28	O	205	BCR	C23-C24-C25-C26
28	3	317	BCR	C21-C22-C23-C24
28	3	317	BCR	C37-C22-C23-C24
28	3	318	BCR	C5-C6-C7-C8
28	3	318	BCR	C21-C22-C23-C24
28	3	318	BCR	C37-C22-C23-C24
28	4	317	BCR	C11-C12-C13-C14
28	4	317	BCR	C11-C12-C13-C35
28	4	321	BCR	C1-C6-C7-C8
28	4	321	BCR	C5-C6-C7-C8
28	4	321	BCR	C11-C12-C13-C14
28	4	321	BCR	C11-C12-C13-C35
28	5	320	BCR	C1-C6-C7-C8
28	5	320	BCR	C23-C24-C25-C30
28	5	323	BCR	C11-C12-C13-C14
28	5	323	BCR	C11-C12-C13-C35
28	5	323	BCR	C17-C18-C19-C20
28	5	323	BCR	C36-C18-C19-C20
28	5	323	BCR	C21-C22-C23-C24
28	5	323	BCR	C37-C22-C23-C24
28	6	621	BCR	C5-C6-C7-C8
28	7	316	BCR	C23-C24-C25-C30
28	8	318	BCR	C36-C18-C19-C20
30	B	846	DGD	C2B-C1B-O2G-C2G
30	B	846	DGD	O6D-C1D-O3G-C3G
31	B	850	SQD	C2-C1-O6-C44
31	B	850	SQD	O5-C1-O6-C44
32	J	102	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
32	J	104	LMG	C11-C10-O7-C8
32	1	619	LMG	C11-C10-O7-C8
32	6	602	LMG	C11-C10-O7-C8
32	7	318	LMG	C11-C10-O7-C8
32	7	319	LMG	O6-C1-O1-C7
33	P	601	CHL	C3C-C2C-CMC-OMC
33	P	606	CHL	C3C-C2C-CMC-OMC
33	P	607	CHL	C3C-C2C-CMC-OMC
33	P	608	CHL	C1A-C2A-CAA-CBA
33	P	609	CHL	C1A-C2A-CAA-CBA
33	P	609	CHL	C3A-C2A-CAA-CBA
33	P	609	CHL	C11-C10-C8-C9
33	P	619	CHL	C3C-C2C-CMC-OMC
33	P	622	CHL	C1C-C2C-CMC-OMC
33	P	622	CHL	C3C-C2C-CMC-OMC
33	Q	601	CHL	C3C-C2C-CMC-OMC
33	Q	606	CHL	C3C-C2C-CMC-OMC
33	Q	607	CHL	C1A-C2A-CAA-CBA
33	Q	608	CHL	C1A-C2A-CAA-CBA
33	Q	608	CHL	C3A-C2A-CAA-CBA
33	Q	608	CHL	C11-C10-C8-C9
33	R	601	CHL	C3C-C2C-CMC-OMC
33	R	606	CHL	C3C-C2C-CMC-OMC
33	R	607	CHL	C3C-C2C-CMC-OMC
33	R	608	CHL	C1A-C2A-CAA-CBA
33	R	609	CHL	C1A-C2A-CAA-CBA
33	R	609	CHL	C3A-C2A-CAA-CBA
33	R	609	CHL	C11-C10-C8-C9
33	S	302	CHL	C3A-C2A-CAA-CBA
33	S	302	CHL	C2A-CAA-CBA-CGA
33	S	302	CHL	C1C-C2C-CMC-OMC
33	S	302	CHL	C3C-C2C-CMC-OMC
33	S	302	CHL	C4-C3-C5-C6
33	S	306	CHL	C2B-C3B-CAB-CBB
33	S	306	CHL	C3C-C2C-CMC-OMC
33	S	307	CHL	C2B-C3B-CAB-CBB
33	S	307	CHL	C4B-C3B-CAB-CBB
33	S	307	CHL	C1C-C2C-CMC-OMC
33	S	307	CHL	C3C-C2C-CMC-OMC
33	S	308	CHL	C2A-CAA-CBA-CGA
33	S	308	CHL	CHA-CBD-CGD-O1D
33	S	308	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
33	S	310	CHL	C3C-C2C-CMC-OMC
33	S	321	CHL	C3C-C2C-CMC-OMC
33	T	601	CHL	C3C-C2C-CMC-OMC
33	T	605	CHL	C3C-C2C-CMC-OMC
33	T	606	CHL	C1A-C2A-CAA-CBA
33	U	305	CHL	C1A-C2A-CAA-CBA
33	U	305	CHL	C3A-C2A-CAA-CBA
33	U	306	CHL	C3C-C2C-CMC-OMC
33	U	307	CHL	C3C-C2C-CMC-OMC
33	U	307	CHL	C3-C5-C6-C7
33	U	308	CHL	C1A-C2A-CAA-CBA
33	1	606	CHL	C2B-C3B-CAB-CBB
33	1	606	CHL	C4B-C3B-CAB-CBB
33	1	606	CHL	C3C-C2C-CMC-OMC
33	1	606	CHL	CBD-CGD-O2D-CED
33	3	306	CHL	CBD-CGD-O2D-CED
33	4	314	CHL	C3C-C2C-CMC-OMC
33	5	307	CHL	C1C-C2C-CMC-OMC
33	5	307	CHL	C3C-C2C-CMC-OMC
33	5	308	CHL	C1A-C2A-CAA-CBA
33	5	308	CHL	C3A-C2A-CAA-CBA
33	6	607	CHL	C1C-C2C-CMC-OMC
33	6	607	CHL	C3C-C2C-CMC-OMC
33	6	607	CHL	CBD-CGD-O2D-CED
33	6	608	CHL	C1C-C2C-CMC-OMC
33	6	608	CHL	C3C-C2C-CMC-OMC
33	6	608	CHL	CBD-CGD-O2D-CED
33	6	617	CHL	C3C-C2C-CMC-OMC
33	7	305	CHL	C1C-C2C-CMC-OMC
33	7	305	CHL	C3C-C2C-CMC-OMC
33	8	307	CHL	C1C-C2C-CMC-OMC
33	8	307	CHL	C3C-C2C-CMC-OMC
33	9	306	CHL	C3C-C2C-CMC-OMC
33	9	306	CHL	CBD-CGD-O2D-CED
33	9	307	CHL	C3C-C2C-CMC-OMC
33	a	305	CHL	C2B-C3B-CAB-CBB
33	a	305	CHL	C4B-C3B-CAB-CBB
33	a	305	CHL	C3C-C2C-CMC-OMC
33	a	305	CHL	CBD-CGD-O2D-CED
34	P	615	LUT	C1-C6-C7-C8
34	R	616	LUT	C1-C6-C7-C8
34	S	317	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
34	S	317	LUT	C31-C32-C33-C40
34	U	315	LUT	C1-C6-C7-C8
34	1	616	LUT	C1-C6-C7-C8
34	1	616	LUT	C7-C8-C9-C10
34	1	616	LUT	C7-C8-C9-C19
34	1	617	LUT	C7-C8-C9-C10
34	1	617	LUT	C7-C8-C9-C19
34	1	617	LUT	C27-C28-C29-C30
34	1	617	LUT	C27-C28-C29-C39
34	2	315	LUT	C7-C8-C9-C10
34	2	315	LUT	C7-C8-C9-C19
34	2	315	LUT	C31-C32-C33-C34
34	2	315	LUT	C31-C32-C33-C40
34	4	316	LUT	C1-C6-C7-C8
34	a	315	LUT	C1-C6-C7-C8
34	a	315	LUT	C7-C8-C9-C10
34	a	315	LUT	C7-C8-C9-C19
34	a	316	LUT	C1-C6-C7-C8
34	a	316	LUT	C5-C6-C7-C8
34	a	316	LUT	C7-C8-C9-C10
34	a	316	LUT	C7-C8-C9-C19
34	a	316	LUT	C27-C28-C29-C30
34	a	316	LUT	C27-C28-C29-C39
35	P	616	XAT	C7-C8-C9-C19
35	P	620	XAT	C7-C8-C9-C19
35	S	318	XAT	C7-C8-C9-C19
35	S	318	XAT	C31-C32-C33-C34
35	S	318	XAT	C31-C32-C33-C40
36	P	621	NEX	C7-C8-C9-C19
36	P	621	NEX	C11-C12-C13-C14
36	P	621	NEX	C11-C12-C13-C20
36	P	621	NEX	O24-C26-C27-C28
36	P	621	NEX	C33-C34-C35-C15
25	A	801	CLA	O1D-CGD-O2D-CED
25	B	802	CLA	O1D-CGD-O2D-CED
25	P	610	CLA	O1D-CGD-O2D-CED
25	Q	609	CLA	O1D-CGD-O2D-CED
25	R	610	CLA	O1D-CGD-O2D-CED
25	T	608	CLA	O1D-CGD-O2D-CED
25	U	310	CLA	O1D-CGD-O2D-CED
25	2	303	CLA	O1D-CGD-O2D-CED
25	5	315	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	7	303	CLA	O1D-CGD-O2D-CED
25	8	306	CLA	O1D-CGD-O2D-CED
33	P	608	CHL	O1D-CGD-O2D-CED
33	Q	607	CHL	O1D-CGD-O2D-CED
33	R	608	CHL	O1D-CGD-O2D-CED
33	T	606	CHL	O1D-CGD-O2D-CED
33	U	308	CHL	O1D-CGD-O2D-CED
33	4	306	CHL	O1D-CGD-O2D-CED
25	P	612	CLA	C8-C10-C11-C12
25	R	612	CLA	C8-C10-C11-C12
33	P	609	CHL	C15-C16-C17-C18
33	Q	608	CHL	C15-C16-C17-C18
33	R	609	CHL	C15-C16-C17-C18
25	A	828	CLA	O1D-CGD-O2D-CED
25	A	853	CLA	O1D-CGD-O2D-CED
25	B	809	CLA	O1D-CGD-O2D-CED
25	F	802	CLA	O1D-CGD-O2D-CED
25	2	308	CLA	O1D-CGD-O2D-CED
25	2	309	CLA	O1D-CGD-O2D-CED
33	1	606	CHL	O1D-CGD-O2D-CED
33	a	305	CHL	O1D-CGD-O2D-CED
25	A	811	CLA	CBD-CGD-O2D-CED
25	A	834	CLA	CBD-CGD-O2D-CED
25	A	842	CLA	CBD-CGD-O2D-CED
25	A	853	CLA	CBD-CGD-O2D-CED
25	B	809	CLA	CBD-CGD-O2D-CED
25	B	812	CLA	CBD-CGD-O2D-CED
25	H	205	CLA	CBD-CGD-O2D-CED
25	J	103	CLA	CBD-CGD-O2D-CED
25	J	105	CLA	CBD-CGD-O2D-CED
25	K	201	CLA	CBD-CGD-O2D-CED
25	Q	609	CLA	CBD-CGD-O2D-CED
25	R	602	CLA	CBD-CGD-O2D-CED
25	S	303	CLA	CBD-CGD-O2D-CED
25	S	304	CLA	CBD-CGD-O2D-CED
25	S	311	CLA	CBD-CGD-O2D-CED
25	S	312	CLA	CBD-CGD-O2D-CED
25	S	315	CLA	CBD-CGD-O2D-CED
25	U	310	CLA	CBD-CGD-O2D-CED
25	1	607	CLA	CBD-CGD-O2D-CED
25	2	302	CLA	CBD-CGD-O2D-CED
25	2	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	306	CLA	CBD-CGD-O2D-CED
25	2	309	CLA	CBD-CGD-O2D-CED
25	2	311	CLA	CBD-CGD-O2D-CED
25	2	313	CLA	CBD-CGD-O2D-CED
25	4	301	CLA	CBD-CGD-O2D-CED
25	4	307	CLA	CBD-CGD-O2D-CED
25	5	306	CLA	CBD-CGD-O2D-CED
25	6	614	CLA	CBD-CGD-O2D-CED
25	7	303	CLA	CBD-CGD-O2D-CED
25	7	304	CLA	CBD-CGD-O2D-CED
25	7	306	CLA	CBD-CGD-O2D-CED
25	8	306	CLA	CBD-CGD-O2D-CED
25	8	308	CLA	CBD-CGD-O2D-CED
25	8	311	CLA	CBD-CGD-O2D-CED
25	9	304	CLA	CBD-CGD-O2D-CED
25	9	305	CLA	CBD-CGD-O2D-CED
25	a	303	CLA	CBD-CGD-O2D-CED
33	P	608	CHL	CBD-CGD-O2D-CED
33	Q	607	CHL	CBD-CGD-O2D-CED
33	R	608	CHL	CBD-CGD-O2D-CED
33	S	302	CHL	CBD-CGD-O2D-CED
33	T	606	CHL	CBD-CGD-O2D-CED
33	U	308	CHL	CBD-CGD-O2D-CED
33	4	306	CHL	CBD-CGD-O2D-CED
33	5	307	CHL	CBD-CGD-O2D-CED
33	5	308	CHL	CBD-CGD-O2D-CED
25	A	839	CLA	O1A-CGA-O2A-C1
25	Q	613	CLA	O1A-CGA-O2A-C1
27	1	618	LHG	O10-C23-O8-C6
27	a	317	LHG	O10-C23-O8-C6
32	1	619	LMG	O10-C28-O8-C9
32	4	320	LMG	O10-C28-O8-C9
32	7	319	LMG	O10-C28-O8-C9
33	P	605	CHL	O1A-CGA-O2A-C1
25	A	842	CLA	C2C-C3C-CAC-CBC
25	A	834	CLA	O1D-CGD-O2D-CED
25	K	204	CLA	O1D-CGD-O2D-CED
25	2	302	CLA	O1D-CGD-O2D-CED
25	2	311	CLA	O1D-CGD-O2D-CED
25	5	306	CLA	O1D-CGD-O2D-CED
25	7	306	CLA	O1D-CGD-O2D-CED
33	6	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	H	201	CLA	CBA-CGA-O2A-C1
25	B	832	CLA	O1D-CGD-O2D-CED
25	S	303	CLA	O1D-CGD-O2D-CED
25	S	313	CLA	O1D-CGD-O2D-CED
25	1	602	CLA	O1D-CGD-O2D-CED
25	1	610	CLA	O1D-CGD-O2D-CED
25	1	612	CLA	O1D-CGD-O2D-CED
25	2	310	CLA	O1D-CGD-O2D-CED
25	9	302	CLA	O1D-CGD-O2D-CED
25	a	301	CLA	O1D-CGD-O2D-CED
25	a	306	CLA	O1D-CGD-O2D-CED
25	a	311	CLA	O1D-CGD-O2D-CED
33	3	306	CHL	O1D-CGD-O2D-CED
25	A	839	CLA	CBA-CGA-O2A-C1
25	Q	613	CLA	CBA-CGA-O2A-C1
25	6	623	CLA	CBA-CGA-O2A-C1
32	1	619	LMG	C29-C28-O8-C9
32	4	320	LMG	C29-C28-O8-C9
32	7	319	LMG	C29-C28-O8-C9
25	A	812	CLA	CBD-CGD-O2D-CED
25	A	835	CLA	CBD-CGD-O2D-CED
25	B	826	CLA	CBD-CGD-O2D-CED
25	B	827	CLA	CBD-CGD-O2D-CED
25	B	838	CLA	CBD-CGD-O2D-CED
25	H	203	CLA	CBD-CGD-O2D-CED
25	L	209	CLA	CBD-CGD-O2D-CED
25	P	602	CLA	CBD-CGD-O2D-CED
25	Q	602	CLA	CBD-CGD-O2D-CED
25	T	602	CLA	CBD-CGD-O2D-CED
25	U	302	CLA	CBD-CGD-O2D-CED
25	1	604	CLA	CBD-CGD-O2D-CED
25	1	608	CLA	CBD-CGD-O2D-CED
25	1	611	CLA	CBD-CGD-O2D-CED
25	1	613	CLA	CBD-CGD-O2D-CED
25	5	314	CLA	CBD-CGD-O2D-CED
25	6	609	CLA	CBD-CGD-O2D-CED
25	7	310	CLA	CBD-CGD-O2D-CED
25	8	305	CLA	CBD-CGD-O2D-CED
25	8	312	CLA	CBD-CGD-O2D-CED
25	a	307	CLA	CBD-CGD-O2D-CED
25	a	310	CLA	CBD-CGD-O2D-CED
25	a	312	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	7	305	CHL	CBD-CGD-O2D-CED
25	A	842	CLA	C4C-C3C-CAC-CBC
25	A	806	CLA	O1A-CGA-O2A-C1
25	A	816	CLA	O1A-CGA-O2A-C1
25	B	809	CLA	O1A-CGA-O2A-C1
25	B	816	CLA	O1A-CGA-O2A-C1
25	B	820	CLA	O1A-CGA-O2A-C1
25	B	831	CLA	O1A-CGA-O2A-C1
25	P	603	CLA	O1A-CGA-O2A-C1
25	Q	603	CLA	O1A-CGA-O2A-C1
25	R	603	CLA	O1A-CGA-O2A-C1
25	R	614	CLA	O1A-CGA-O2A-C1
25	S	312	CLA	O1A-CGA-O2A-C1
25	S	320	CLA	O1A-CGA-O2A-C1
25	T	609	CLA	O1A-CGA-O2A-C1
25	U	303	CLA	O1A-CGA-O2A-C1
25	1	610	CLA	O1A-CGA-O2A-C1
25	a	309	CLA	O1A-CGA-O2A-C1
25	A	810	CLA	O1D-CGD-O2D-CED
25	B	801	CLA	O1D-CGD-O2D-CED
25	B	821	CLA	O1D-CGD-O2D-CED
25	O	201	CLA	O1D-CGD-O2D-CED
25	6	610	CLA	O1D-CGD-O2D-CED
25	a	309	CLA	O1D-CGD-O2D-CED
33	9	306	CHL	O1D-CGD-O2D-CED
25	4	309	CLA	O1D-CGD-O2D-CED
33	6	607	CHL	O1D-CGD-O2D-CED
25	A	829	CLA	CBD-CGD-O2D-CED
25	K	202	CLA	CBD-CGD-O2D-CED
25	Q	612	CLA	CBD-CGD-O2D-CED
25	6	623	CLA	CBD-CGD-O2D-CED
25	9	310	CLA	CBD-CGD-O2D-CED
25	Q	603	CLA	C5-C6-C7-C8
25	3	302	CLA	O1D-CGD-O2D-CED
25	6	603	CLA	O1D-CGD-O2D-CED
33	5	308	CHL	O1D-CGD-O2D-CED
27	B	847	LHG	O9-C7-O7-C5
30	B	846	DGD	O1B-C1B-O2G-C2G
32	1	619	LMG	O9-C10-O7-C8
32	6	602	LMG	O9-C10-O7-C8
32	7	318	LMG	O9-C10-O7-C8
25	A	812	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	A	830	CLA	C3-C5-C6-C7
25	A	832	CLA	C3-C5-C6-C7
25	A	840	CLA	C3-C5-C6-C7
25	A	851	CLA	C3-C5-C6-C7
25	B	805	CLA	C3-C5-C6-C7
25	B	806	CLA	C3-C5-C6-C7
25	B	807	CLA	C3-C5-C6-C7
25	B	808	CLA	C3-C5-C6-C7
25	B	813	CLA	C3-C5-C6-C7
25	B	816	CLA	C3-C5-C6-C7
25	B	820	CLA	C3-C5-C6-C7
25	B	838	CLA	C3-C5-C6-C7
25	L	201	CLA	C3-C5-C6-C7
25	Q	612	CLA	C3-C5-C6-C7
25	S	313	CLA	C3-C5-C6-C7
25	S	314	CLA	C3-C5-C6-C7
25	3	305	CLA	C3-C5-C6-C7
25	3	314	CLA	C3-C5-C6-C7
25	7	311	CLA	C3-C5-C6-C7
25	8	314	CLA	C3-C5-C6-C7
25	9	303	CLA	C3-C5-C6-C7
25	A	812	CLA	CBA-CGA-O2A-C1
25	A	820	CLA	CBA-CGA-O2A-C1
25	K	201	CLA	CBA-CGA-O2A-C1
25	P	603	CLA	CBA-CGA-O2A-C1
25	Q	603	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
25	R	614	CLA	CBA-CGA-O2A-C1
25	S	312	CLA	CBA-CGA-O2A-C1
25	S	320	CLA	CBA-CGA-O2A-C1
25	U	303	CLA	CBA-CGA-O2A-C1
25	2	312	CLA	CBA-CGA-O2A-C1
25	a	303	CLA	CBA-CGA-O2A-C1
25	1	607	CLA	O1D-CGD-O2D-CED
25	9	305	CLA	O1D-CGD-O2D-CED
33	S	302	CHL	O1D-CGD-O2D-CED
25	3	320	CLA	CBD-CGD-O2D-CED
25	5	303	CLA	CBD-CGD-O2D-CED
25	6	613	CLA	CBD-CGD-O2D-CED
25	7	301	CLA	CBD-CGD-O2D-CED
25	7	307	CLA	CBD-CGD-O2D-CED
33	4	305	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	H	201	CLA	O1A-CGA-O2A-C1
25	8	305	CLA	CBA-CGA-O2A-C1
33	3	306	CHL	C3-C5-C6-C7
33	6	607	CHL	C3-C5-C6-C7
33	8	307	CHL	C3-C5-C6-C7
25	6	609	CLA	C2C-C3C-CAC-CBC
25	A	802	CLA	C4-C3-C5-C6
25	A	814	CLA	C4-C3-C5-C6
25	B	816	CLA	C4-C3-C5-C6
25	B	837	CLA	C4-C3-C5-C6
25	A	802	CLA	C2-C3-C5-C6
25	L	202	CLA	C2-C3-C5-C6
33	S	302	CHL	C2-C3-C5-C6
25	A	823	CLA	CBD-CGD-O2D-CED
25	K	205	CLA	CBD-CGD-O2D-CED
25	Q	604	CLA	CBD-CGD-O2D-CED
25	T	603	CLA	CBD-CGD-O2D-CED
25	T	611	CLA	CBD-CGD-O2D-CED
25	U	312	CLA	CBD-CGD-O2D-CED
25	3	313	CLA	CBD-CGD-O2D-CED
25	4	311	CLA	CBD-CGD-O2D-CED
25	9	309	CLA	CBD-CGD-O2D-CED
25	A	809	CLA	C2A-CAA-CBA-CGA
25	A	834	CLA	C2A-CAA-CBA-CGA
25	A	851	CLA	C2A-CAA-CBA-CGA
25	B	809	CLA	C2A-CAA-CBA-CGA
25	B	822	CLA	C2A-CAA-CBA-CGA
25	B	825	CLA	C2A-CAA-CBA-CGA
25	B	832	CLA	C2A-CAA-CBA-CGA
25	F	802	CLA	C2A-CAA-CBA-CGA
25	3	305	CLA	C2A-CAA-CBA-CGA
25	5	314	CLA	C2A-CAA-CBA-CGA
33	P	605	CHL	C2A-CAA-CBA-CGA
33	R	605	CHL	C2A-CAA-CBA-CGA
33	S	306	CHL	C2A-CAA-CBA-CGA
33	U	305	CHL	C2A-CAA-CBA-CGA
33	3	306	CHL	C2A-CAA-CBA-CGA
33	8	307	CHL	C2A-CAA-CBA-CGA
25	A	828	CLA	O1A-CGA-O2A-C1
33	5	307	CHL	O1D-CGD-O2D-CED
25	A	801	CLA	C3-C5-C6-C7
25	A	853	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	P	613	CLA	C3-C5-C6-C7
25	R	613	CLA	C3-C5-C6-C7
25	T	611	CLA	C3-C5-C6-C7
25	U	312	CLA	C3-C5-C6-C7
25	8	302	CLA	C3-C5-C6-C7
25	9	301	CLA	C3-C5-C6-C7
25	9	309	CLA	C3-C5-C6-C7
25	A	806	CLA	CBA-CGA-O2A-C1
25	A	809	CLA	CBA-CGA-O2A-C1
25	A	816	CLA	CBA-CGA-O2A-C1
25	A	818	CLA	CBA-CGA-O2A-C1
25	A	836	CLA	CBA-CGA-O2A-C1
25	B	809	CLA	CBA-CGA-O2A-C1
25	B	816	CLA	CBA-CGA-O2A-C1
25	B	820	CLA	CBA-CGA-O2A-C1
25	B	829	CLA	CBA-CGA-O2A-C1
25	B	831	CLA	CBA-CGA-O2A-C1
25	J	103	CLA	CBA-CGA-O2A-C1
25	T	609	CLA	CBA-CGA-O2A-C1
25	T	612	CLA	CBA-CGA-O2A-C1
25	1	610	CLA	CBA-CGA-O2A-C1
25	4	309	CLA	CBA-CGA-O2A-C1
25	a	309	CLA	CBA-CGA-O2A-C1
32	H	204	LMG	C29-C28-O8-C9
33	P	605	CHL	CBA-CGA-O2A-C1
33	P	622	CHL	CBA-CGA-O2A-C1
33	7	305	CHL	CBA-CGA-O2A-C1
25	6	609	CLA	C4C-C3C-CAC-CBC
25	A	811	CLA	O1D-CGD-O2D-CED
25	2	306	CLA	O1D-CGD-O2D-CED
30	B	848	DGD	C4D-C5D-C6D-O5D
25	R	613	CLA	CBD-CGD-O2D-CED
25	R	614	CLA	CBD-CGD-O2D-CED
33	9	307	CHL	CBD-CGD-O2D-CED
25	K	201	CLA	O1D-CGD-O2D-CED
25	S	312	CLA	O1D-CGD-O2D-CED
25	2	313	CLA	O1D-CGD-O2D-CED
25	4	301	CLA	O1D-CGD-O2D-CED
32	J	104	LMG	O9-C10-O7-C8
32	4	320	LMG	O9-C10-O7-C8
25	A	812	CLA	O1A-CGA-O2A-C1
25	A	818	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	836	CLA	O1A-CGA-O2A-C1
25	B	829	CLA	O1A-CGA-O2A-C1
25	J	103	CLA	O1A-CGA-O2A-C1
25	K	201	CLA	O1A-CGA-O2A-C1
25	4	309	CLA	O1A-CGA-O2A-C1
25	8	305	CLA	O1A-CGA-O2A-C1
25	H	205	CLA	O1D-CGD-O2D-CED
25	J	105	CLA	O1D-CGD-O2D-CED
25	S	315	CLA	O1D-CGD-O2D-CED
28	L	203	BCR	C13-C14-C15-C16
28	O	205	BCR	C9-C10-C11-C12
28	5	320	BCR	C19-C20-C21-C22
25	A	830	CLA	CBD-CGD-O2D-CED
25	A	840	CLA	CBD-CGD-O2D-CED
25	B	805	CLA	CBD-CGD-O2D-CED
25	B	819	CLA	CBD-CGD-O2D-CED
25	P	604	CLA	CBD-CGD-O2D-CED
25	P	613	CLA	CBD-CGD-O2D-CED
25	Q	613	CLA	CBD-CGD-O2D-CED
25	S	301	CLA	CBD-CGD-O2D-CED
25	S	314	CLA	CBD-CGD-O2D-CED
25	T	612	CLA	CBD-CGD-O2D-CED
25	U	304	CLA	CBD-CGD-O2D-CED
25	U	313	CLA	CBD-CGD-O2D-CED
25	4	308	CLA	CBD-CGD-O2D-CED
25	5	304	CLA	CBD-CGD-O2D-CED
25	7	308	CLA	CBD-CGD-O2D-CED
25	9	303	CLA	CBD-CGD-O2D-CED
33	4	314	CHL	CBD-CGD-O2D-CED
33	6	606	CHL	CBD-CGD-O2D-CED
25	A	842	CLA	O1D-CGD-O2D-CED
25	J	103	CLA	O1D-CGD-O2D-CED
25	S	304	CLA	O1D-CGD-O2D-CED
25	8	308	CLA	O1D-CGD-O2D-CED
27	1	618	LHG	O2-C2-C3-O3
27	2	317	LHG	O2-C2-C3-O3
27	a	317	LHG	O2-C2-C3-O3
25	A	804	CLA	C3-C5-C6-C7
25	A	806	CLA	C3-C5-C6-C7
25	A	807	CLA	C3-C5-C6-C7
25	A	818	CLA	C3-C5-C6-C7
25	A	837	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	830	CLA	C3-C5-C6-C7
25	L	202	CLA	C3-C5-C6-C7
25	3	303	CLA	C3-C5-C6-C7
25	6	611	CLA	C3-C5-C6-C7
25	6	623	CLA	C3-C5-C6-C7
25	A	828	CLA	CBA-CGA-O2A-C1
33	P	601	CHL	CBA-CGA-O2A-C1
33	Q	601	CHL	CBA-CGA-O2A-C1
33	R	601	CHL	CBA-CGA-O2A-C1
33	S	302	CHL	CBA-CGA-O2A-C1
33	T	601	CHL	CBA-CGA-O2A-C1
25	A	820	CLA	O1A-CGA-O2A-C1
25	2	312	CLA	O1A-CGA-O2A-C1
33	P	622	CHL	O1A-CGA-O2A-C1
25	7	304	CLA	O1D-CGD-O2D-CED
25	9	304	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	C5-C6-C7-C8
25	S	320	CLA	C5-C6-C7-C8
25	U	303	CLA	C5-C6-C7-C8
32	4	320	LMG	C11-C10-O7-C8
25	2	302	CLA	CBA-CGA-O2A-C1
25	2	314	CLA	CBA-CGA-O2A-C1
25	7	313	CLA	CBA-CGA-O2A-C1
25	A	816	CLA	CBD-CGD-O2D-CED
25	A	836	CLA	CBD-CGD-O2D-CED
25	B	808	CLA	CBD-CGD-O2D-CED
25	4	303	CLA	CBD-CGD-O2D-CED
25	5	312	CLA	CBD-CGD-O2D-CED
33	P	601	CHL	CBD-CGD-O2D-CED
33	P	622	CHL	CBD-CGD-O2D-CED
33	Q	601	CHL	CBD-CGD-O2D-CED
33	R	601	CHL	CBD-CGD-O2D-CED
33	S	306	CHL	CBD-CGD-O2D-CED
33	S	310	CHL	CBD-CGD-O2D-CED
33	T	601	CHL	CBD-CGD-O2D-CED
25	P	603	CLA	C5-C6-C7-C8
25	a	303	CLA	O1D-CGD-O2D-CED
25	B	837	CLA	C2C-C3C-CAC-CBC
25	R	602	CLA	O1D-CGD-O2D-CED
25	3	312	CLA	CBD-CGD-O2D-CED
33	6	617	CHL	CBD-CGD-O2D-CED
25	A	802	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	A	814	CLA	C3-C5-C6-C7
25	T	612	CLA	O1A-CGA-O2A-C1
32	H	204	LMG	O10-C28-O8-C9
33	P	601	CHL	O1A-CGA-O2A-C1
33	Q	601	CHL	O1A-CGA-O2A-C1
33	R	601	CHL	O1A-CGA-O2A-C1
33	S	302	CHL	O1A-CGA-O2A-C1
33	T	601	CHL	O1A-CGA-O2A-C1
33	7	305	CHL	O1A-CGA-O2A-C1
25	A	818	CLA	C4-C3-C5-C6
25	A	830	CLA	C4-C3-C5-C6
25	L	201	CLA	C4-C3-C5-C6
25	1	602	CLA	C4-C3-C5-C6
25	2	305	CLA	C4-C3-C5-C6
25	a	301	CLA	C4-C3-C5-C6
33	6	607	CHL	C4-C3-C5-C6
25	A	818	CLA	C2-C3-C5-C6
25	A	830	CLA	C2-C3-C5-C6
25	B	816	CLA	C2-C3-C5-C6
25	L	201	CLA	C2-C3-C5-C6
25	1	602	CLA	C2-C3-C5-C6
25	2	305	CLA	C2-C3-C5-C6
25	a	301	CLA	C2-C3-C5-C6
33	6	607	CHL	C2-C3-C5-C6
25	A	814	CLA	CBD-CGD-O2D-CED
25	A	823	CLA	C2A-CAA-CBA-CGA
25	A	839	CLA	C2A-CAA-CBA-CGA
25	3	320	CLA	C2A-CAA-CBA-CGA
33	4	305	CHL	C2A-CAA-CBA-CGA
33	4	306	CHL	C2A-CAA-CBA-CGA
25	4	307	CLA	O1D-CGD-O2D-CED
25	8	311	CLA	O1D-CGD-O2D-CED
25	A	809	CLA	O1A-CGA-O2A-C1
25	6	611	CLA	CBA-CGA-O2A-C1
25	L	202	CLA	CBD-CGD-O2D-CED
25	B	812	CLA	O1D-CGD-O2D-CED
25	6	614	CLA	O1D-CGD-O2D-CED
25	B	819	CLA	CBA-CGA-O2A-C1
25	3	310	CLA	CBA-CGA-O2A-C1
25	A	835	CLA	O1D-CGD-O2D-CED
25	Q	602	CLA	O1D-CGD-O2D-CED
25	S	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	604	CLA	O1D-CGD-O2D-CED
25	1	608	CLA	O1D-CGD-O2D-CED
33	7	305	CHL	O1D-CGD-O2D-CED
25	P	602	CLA	O1D-CGD-O2D-CED
25	T	602	CLA	O1D-CGD-O2D-CED
25	1	613	CLA	O1D-CGD-O2D-CED
25	5	314	CLA	O1D-CGD-O2D-CED
25	a	307	CLA	O1D-CGD-O2D-CED
25	a	312	CLA	O1D-CGD-O2D-CED
25	A	822	CLA	CBD-CGD-O2D-CED
25	2	314	CLA	CBD-CGD-O2D-CED
25	6	611	CLA	O1A-CGA-O2A-C1
25	9	310	CLA	O1A-CGA-O2A-C1
25	B	810	CLA	C3-C5-C6-C7
25	B	827	CLA	O1D-CGD-O2D-CED
25	H	203	CLA	O1D-CGD-O2D-CED
25	6	609	CLA	O1D-CGD-O2D-CED
25	A	805	CLA	CBA-CGA-O2A-C1
25	A	807	CLA	CBA-CGA-O2A-C1
25	A	815	CLA	CBA-CGA-O2A-C1
25	A	835	CLA	CBA-CGA-O2A-C1
25	A	840	CLA	CBA-CGA-O2A-C1
25	Q	611	CLA	CBA-CGA-O2A-C1
25	S	304	CLA	CBA-CGA-O2A-C1
25	S	313	CLA	CBA-CGA-O2A-C1
25	T	610	CLA	CBA-CGA-O2A-C1
25	U	311	CLA	CBA-CGA-O2A-C1
25	1	603	CLA	CBA-CGA-O2A-C1
25	2	304	CLA	CBA-CGA-O2A-C1
25	2	307	CLA	CBA-CGA-O2A-C1
25	2	311	CLA	CBA-CGA-O2A-C1
25	3	305	CLA	CBA-CGA-O2A-C1
25	4	310	CLA	CBA-CGA-O2A-C1
25	5	311	CLA	CBA-CGA-O2A-C1
25	6	612	CLA	CBA-CGA-O2A-C1
25	8	313	CLA	CBA-CGA-O2A-C1
25	9	301	CLA	CBA-CGA-O2A-C1
25	9	310	CLA	CBA-CGA-O2A-C1
25	a	302	CLA	CBA-CGA-O2A-C1
33	S	306	CHL	CBA-CGA-O2A-C1
33	8	307	CHL	CBA-CGA-O2A-C1
25	B	802	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	2	314	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	C10-C11-C12-C13
25	A	836	CLA	C13-C15-C16-C17
25	R	611	CLA	C5-C6-C7-C8
25	3	311	CLA	C5-C6-C7-C8
25	A	805	CLA	O1A-CGA-O2A-C1
25	2	302	CLA	O1A-CGA-O2A-C1
25	B	837	CLA	C4C-C3C-CAC-CBC
25	A	812	CLA	C10-C11-C12-C13
25	A	820	CLA	C13-C15-C16-C17
25	A	832	CLA	C5-C6-C7-C8
25	A	838	CLA	C15-C16-C17-C18
25	5	324	CLA	C5-C6-C7-C8
26	B	839	PQN	C20-C21-C22-C23
27	8	319	LHG	O2-C2-C3-O3
25	2	305	CLA	C3-C5-C6-C7
25	4	310	CLA	C3-C5-C6-C7
27	4	318	LHG	O7-C5-C6-O8
27	6	618	LHG	O7-C5-C6-O8
33	S	306	CHL	O1A-CGA-O2A-C1
25	A	832	CLA	C4-C3-C5-C6
25	A	814	CLA	C2-C3-C5-C6
25	B	837	CLA	C2-C3-C5-C6
25	A	806	CLA	C11-C10-C8-C9
25	A	815	CLA	C11-C10-C8-C9
25	A	825	CLA	C6-C7-C8-C9
25	A	826	CLA	C6-C7-C8-C9
25	A	836	CLA	C14-C13-C15-C16
25	A	851	CLA	C11-C12-C13-C14
25	B	810	CLA	C11-C12-C13-C14
25	P	612	CLA	C11-C10-C8-C9
25	R	612	CLA	C11-C10-C8-C9
25	S	304	CLA	C6-C7-C8-C9
25	1	609	CLA	C6-C7-C8-C9
25	2	304	CLA	C14-C13-C15-C16
25	3	308	CLA	C14-C13-C15-C16
25	3	320	CLA	C11-C12-C13-C14
25	5	303	CLA	C11-C12-C13-C14
25	7	308	CLA	C11-C10-C8-C9
25	a	308	CLA	C6-C7-C8-C9
26	A	841	PQN	C24-C23-C25-C26
25	A	812	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	838	CLA	O1D-CGD-O2D-CED
25	U	302	CLA	O1D-CGD-O2D-CED
25	A	807	CLA	C15-C16-C17-C18
25	6	603	CLA	C15-C16-C17-C18
25	A	840	CLA	C2A-CAA-CBA-CGA
25	2	307	CLA	C2A-CAA-CBA-CGA
25	2	314	CLA	C2A-CAA-CBA-CGA
33	a	305	CHL	C2A-CAA-CBA-CGA
28	A	848	BCR	C11-C12-C13-C35
28	J	106	BCR	C37-C22-C23-C24
28	K	206	BCR	C36-C18-C19-C20
28	K	206	BCR	C37-C22-C23-C24
28	L	203	BCR	C11-C12-C13-C35
28	O	204	BCR	C37-C22-C23-C24
28	4	317	BCR	C36-C18-C19-C20
28	5	320	BCR	C11-C12-C13-C35
28	5	320	BCR	C37-C22-C23-C24
34	S	316	LUT	C11-C12-C13-C20
34	7	314	LUT	C7-C8-C9-C19
35	Q	616	XAT	C7-C8-C9-C19
35	T	615	XAT	C7-C8-C9-C19
36	U	316	NEX	C11-C12-C13-C20
28	B	840	BCR	C7-C8-C9-C10
28	J	106	BCR	C21-C22-C23-C24
28	K	206	BCR	C17-C18-C19-C20
28	K	206	BCR	C21-C22-C23-C24
28	L	203	BCR	C11-C12-C13-C14
32	2	301	LMG	O6-C5-C6-O5
27	S	319	LHG	C7-C8-C9-C10
25	A	840	CLA	O1A-CGA-O2A-C1
25	2	304	CLA	O1A-CGA-O2A-C1
25	2	311	CLA	O1A-CGA-O2A-C1
25	6	612	CLA	O1A-CGA-O2A-C1
25	S	314	CLA	C8-C10-C11-C12
26	B	839	PQN	C15-C16-C17-C18
25	8	312	CLA	O1D-CGD-O2D-CED
25	A	825	CLA	CBD-CGD-O2D-CED
25	2	305	CLA	CBA-CGA-O2A-C1
25	A	802	CLA	C15-C16-C17-C18
25	A	803	CLA	C13-C15-C16-C17
25	A	807	CLA	C8-C10-C11-C12
25	A	840	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	804	CLA	C15-C16-C17-C18
25	B	815	CLA	C5-C6-C7-C8
25	B	827	CLA	C5-C6-C7-C8
25	B	834	CLA	C13-C15-C16-C17
25	B	834	CLA	C15-C16-C17-C18
25	S	303	CLA	C8-C10-C11-C12
25	3	302	CLA	C10-C11-C12-C13
25	3	308	CLA	C13-C15-C16-C17
30	B	848	DGD	O6D-C5D-C6D-O5D
25	A	827	CLA	C8-C10-C11-C12
25	A	830	CLA	C10-C11-C12-C13
25	A	830	CLA	C13-C15-C16-C17
25	B	802	CLA	C13-C15-C16-C17
25	B	804	CLA	C13-C15-C16-C17
25	B	808	CLA	C15-C16-C17-C18
25	B	849	CLA	C5-C6-C7-C8
25	Q	611	CLA	C5-C6-C7-C8
25	T	609	CLA	C8-C10-C11-C12
25	T	610	CLA	C5-C6-C7-C8
25	U	311	CLA	C5-C6-C7-C8
25	2	304	CLA	C13-C15-C16-C17
25	3	308	CLA	C10-C11-C12-C13
25	5	302	CLA	C13-C15-C16-C17
25	6	605	CLA	C15-C16-C17-C18
25	7	308	CLA	C5-C6-C7-C8
25	9	303	CLA	C5-C6-C7-C8
25	a	311	CLA	C10-C11-C12-C13
25	B	826	CLA	O1D-CGD-O2D-CED
27	B	847	LHG	O1-C1-C2-O2
27	A	843	LHG	C7-C8-C9-C10
27	6	618	LHG	C7-C8-C9-C10
27	7	317	LHG	C23-C24-C25-C26
32	6	602	LMG	C10-C11-C12-C13
25	A	819	CLA	CBD-CGD-O2D-CED
25	7	313	CLA	CBD-CGD-O2D-CED
25	B	810	CLA	C15-C16-C17-C18
25	B	830	CLA	C10-C11-C12-C13
25	5	302	CLA	C8-C10-C11-C12
25	7	301	CLA	C13-C15-C16-C17
25	B	825	CLA	C3-C5-C6-C7
25	A	801	CLA	CBA-CGA-O2A-C1
25	A	811	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	A	815	CLA	C5-C6-C7-C8
25	A	830	CLA	C8-C10-C11-C12
25	A	839	CLA	C5-C6-C7-C8
25	A	851	CLA	C13-C15-C16-C17
25	B	801	CLA	C13-C15-C16-C17
25	B	831	CLA	C5-C6-C7-C8
25	1	612	CLA	C10-C11-C12-C13
25	7	311	CLA	C5-C6-C7-C8
25	8	310	CLA	C5-C6-C7-C8
25	8	313	CLA	C15-C16-C17-C18
27	1	618	LHG	C7-C8-C9-C10
27	a	317	LHG	C7-C8-C9-C10
25	K	203	CLA	CBD-CGD-O2D-CED
25	4	310	CLA	CBD-CGD-O2D-CED
25	6	615	CLA	CBD-CGD-O2D-CED
25	A	817	CLA	C8-C10-C11-C12
25	B	813	CLA	C8-C10-C11-C12
30	B	848	DGD	C4E-C5E-C6E-O5E
25	7	313	CLA	O1A-CGA-O2A-C1
25	A	810	CLA	C4-C3-C5-C6
25	A	808	CLA	C11-C12-C13-C15
25	A	812	CLA	C6-C7-C8-C10
25	A	825	CLA	C6-C7-C8-C10
25	A	839	CLA	C6-C7-C8-C10
25	B	805	CLA	C11-C10-C8-C7
25	B	836	CLA	C6-C7-C8-C10
25	R	613	CLA	C11-C12-C13-C15
25	U	312	CLA	C11-C12-C13-C15
25	3	320	CLA	C12-C13-C15-C16
25	5	313	CLA	C6-C7-C8-C10
33	P	609	CHL	C12-C13-C15-C16
33	Q	608	CHL	C12-C13-C15-C16
33	R	609	CHL	C12-C13-C15-C16
25	A	807	CLA	O1A-CGA-O2A-C1
25	A	815	CLA	O1A-CGA-O2A-C1
25	A	835	CLA	O1A-CGA-O2A-C1
25	Q	611	CLA	O1A-CGA-O2A-C1
25	S	304	CLA	O1A-CGA-O2A-C1
25	S	313	CLA	O1A-CGA-O2A-C1
25	U	311	CLA	O1A-CGA-O2A-C1
25	4	310	CLA	O1A-CGA-O2A-C1
25	5	311	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	8	313	CLA	O1A-CGA-O2A-C1
25	9	301	CLA	O1A-CGA-O2A-C1
33	8	307	CHL	O1A-CGA-O2A-C1
28	O	205	BCR	C13-C14-C15-C16
28	4	321	BCR	C13-C14-C15-C16
34	S	317	LUT	C33-C34-C35-C15
25	B	826	CLA	CBA-CGA-O2A-C1
25	A	814	CLA	C2A-CAA-CBA-CGA
25	A	824	CLA	C2A-CAA-CBA-CGA
25	B	829	CLA	C2A-CAA-CBA-CGA
25	B	836	CLA	C2A-CAA-CBA-CGA
25	S	314	CLA	C2A-CAA-CBA-CGA
25	6	623	CLA	C2A-CAA-CBA-CGA
25	9	305	CLA	C2A-CAA-CBA-CGA
33	P	607	CHL	C2A-CAA-CBA-CGA
33	P	619	CHL	C2A-CAA-CBA-CGA
33	R	607	CHL	C2A-CAA-CBA-CGA
33	S	321	CHL	C2A-CAA-CBA-CGA
33	1	606	CHL	C2A-CAA-CBA-CGA
25	K	202	CLA	O1D-CGD-O2D-CED
25	Q	612	CLA	O1D-CGD-O2D-CED
25	1	611	CLA	O1D-CGD-O2D-CED
25	7	310	CLA	O1D-CGD-O2D-CED
25	8	305	CLA	O1D-CGD-O2D-CED
25	a	310	CLA	O1D-CGD-O2D-CED
25	B	805	CLA	C10-C11-C12-C13
25	B	811	CLA	C10-C11-C12-C13
25	B	831	CLA	C10-C11-C12-C13
25	B	836	CLA	C15-C16-C17-C18
25	T	610	CLA	O1A-CGA-O2A-C1
25	1	603	CLA	O1A-CGA-O2A-C1
25	B	849	CLA	CBD-CGD-O2D-CED
32	2	301	LMG	O6-C1-O1-C7
25	B	816	CLA	C8-C10-C11-C12
25	P	612	CLA	C10-C11-C12-C13
25	R	612	CLA	C10-C11-C12-C13
25	L	209	CLA	O1D-CGD-O2D-CED
32	J	104	LMG	C28-C29-C30-C31
25	A	822	CLA	C3-C5-C6-C7
25	B	824	CLA	C3-C5-C6-C7
25	4	311	CLA	C3-C5-C6-C7
25	A	840	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	809	CLA	C13-C15-C16-C17
25	4	308	CLA	C8-C10-C11-C12
25	7	308	CLA	C10-C11-C12-C13
25	a	306	CLA	C13-C15-C16-C17
25	2	307	CLA	O1A-CGA-O2A-C1
25	3	305	CLA	O1A-CGA-O2A-C1
25	a	302	CLA	O1A-CGA-O2A-C1
25	8	309	CLA	CBA-CGA-O2A-C1
25	A	836	CLA	C15-C16-C17-C18
25	S	304	CLA	C5-C6-C7-C8
25	S	304	CLA	C15-C16-C17-C18
25	S	312	CLA	C5-C6-C7-C8
25	2	313	CLA	C5-C6-C7-C8
25	5	302	CLA	C15-C16-C17-C18
25	5	324	CLA	C8-C10-C11-C12
25	6	601	CLA	C8-C10-C11-C12
25	6	601	CLA	C10-C11-C12-C13
25	A	829	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	O1D-CGD-O2D-CED
25	7	301	CLA	O1D-CGD-O2D-CED
25	9	310	CLA	O1D-CGD-O2D-CED
25	R	604	CLA	CBD-CGD-O2D-CED
32	J	107	LMG	C11-C10-O7-C8
25	9	309	CLA	O1D-CGD-O2D-CED
25	A	810	CLA	C5-C6-C7-C8
25	A	816	CLA	C13-C15-C16-C17
25	A	827	CLA	C15-C16-C17-C18
25	A	838	CLA	C8-C10-C11-C12
25	B	825	CLA	C8-C10-C11-C12
25	L	201	CLA	C8-C10-C11-C12
25	S	313	CLA	C5-C6-C7-C8
25	S	313	CLA	C10-C11-C12-C13
25	1	607	CLA	C13-C15-C16-C17
25	3	320	CLA	C8-C10-C11-C12
25	4	308	CLA	C5-C6-C7-C8
25	5	302	CLA	C10-C11-C12-C13
25	5	303	CLA	C8-C10-C11-C12
25	8	302	CLA	C8-C10-C11-C12
27	A	843	LHG	C4-O6-P-O3
27	B	847	LHG	C4-O6-P-O3
27	P	618	LHG	C4-O6-P-O3
27	P	624	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
27	Q	617	LHG	C4-O6-P-O3
27	R	618	LHG	C4-O6-P-O3
27	T	617	LHG	C4-O6-P-O3
27	2	317	LHG	C4-O6-P-O3
27	6	618	LHG	C3-O3-P-O6
27	7	317	LHG	C3-O3-P-O6
25	A	820	CLA	C3-C5-C6-C7
25	B	815	CLA	C3-C5-C6-C7
25	J	103	CLA	C3-C5-C6-C7
25	L	205	CLA	CBA-CGA-O2A-C1
25	3	314	CLA	CBA-CGA-O2A-C1
32	6	602	LMG	C29-C28-O8-C9
33	5	307	CHL	CBA-CGA-O2A-C1
25	K	205	CLA	O1D-CGD-O2D-CED
25	3	313	CLA	O1D-CGD-O2D-CED
25	5	303	CLA	O1D-CGD-O2D-CED
33	4	305	CHL	O1D-CGD-O2D-CED
25	8	314	CLA	CBD-CGD-O2D-CED
25	3	308	CLA	C8-C10-C11-C12
33	6	606	CHL	C3-C5-C6-C7
31	B	850	SQD	C24-C25-C26-C27
25	8	303	CLA	C13-C15-C16-C17
27	1	618	LHG	C1-C2-C3-O3
27	2	317	LHG	C1-C2-C3-O3
27	a	317	LHG	C1-C2-C3-O3
32	J	107	LMG	O9-C10-O7-C8
25	B	821	CLA	C4-C3-C5-C6
25	3	305	CLA	C4-C3-C5-C6
25	3	311	CLA	C4-C3-C5-C6
25	B	812	CLA	C8-C10-C11-C12
25	R	613	CLA	C8-C10-C11-C12
25	U	312	CLA	C8-C10-C11-C12
25	T	610	CLA	CBD-CGD-O2D-CED
25	A	818	CLA	C2A-CAA-CBA-CGA
25	K	204	CLA	C2A-CAA-CBA-CGA
25	S	303	CLA	C2A-CAA-CBA-CGA
25	1	609	CLA	C2A-CAA-CBA-CGA
25	5	303	CLA	C2A-CAA-CBA-CGA
25	8	303	CLA	C2A-CAA-CBA-CGA
25	a	303	CLA	C2A-CAA-CBA-CGA
25	a	308	CLA	C2A-CAA-CBA-CGA
25	A	811	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	822	CLA	CBA-CGA-O2A-C1
25	5	303	CLA	CBA-CGA-O2A-C1
25	7	310	CLA	CBA-CGA-O2A-C1
25	P	611	CLA	C2C-C3C-CAC-CBC
25	S	314	CLA	O1D-CGD-O2D-CED
32	J	107	LMG	C14-C15-C16-C17
25	R	614	CLA	O1D-CGD-O2D-CED
25	T	611	CLA	O1D-CGD-O2D-CED
25	U	312	CLA	O1D-CGD-O2D-CED
25	7	307	CLA	O1D-CGD-O2D-CED
25	A	827	CLA	C3-C5-C6-C7
25	B	831	CLA	C3-C5-C6-C7
25	5	311	CLA	C3-C5-C6-C7
27	A	852	LHG	C14-C15-C16-C17
27	4	318	LHG	C27-C28-C29-C30
32	H	204	LMG	C17-C18-C19-C20
32	1	619	LMG	C16-C17-C18-C19
25	A	801	CLA	O1A-CGA-O2A-C1
25	Q	613	CLA	O1D-CGD-O2D-CED
25	R	613	CLA	O1D-CGD-O2D-CED
25	6	623	CLA	O1D-CGD-O2D-CED
33	9	307	CHL	O1D-CGD-O2D-CED
25	B	814	CLA	C6-C7-C8-C10
25	P	610	CLA	C11-C12-C13-C14
25	R	613	CLA	C16-C17-C18-C19
25	2	309	CLA	C11-C12-C13-C15
25	3	303	CLA	CBA-CGA-O2A-C1
27	8	319	LHG	C16-C17-C18-C19
27	8	319	LHG	C32-C33-C34-C35
32	4	320	LMG	C16-C17-C18-C19
25	T	603	CLA	O1D-CGD-O2D-CED
25	T	612	CLA	O1D-CGD-O2D-CED
25	3	320	CLA	O1D-CGD-O2D-CED
25	1	610	CLA	C5-C6-C7-C8
25	6	623	CLA	C5-C6-C7-C8
25	6	623	CLA	C10-C11-C12-C13
25	a	309	CLA	C5-C6-C7-C8
27	B	847	LHG	C24-C25-C26-C27
27	R	618	LHG	C32-C33-C34-C35
27	2	317	LHG	C25-C26-C27-C28
27	4	318	LHG	C25-C26-C27-C28
25	Q	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	6	618	LHG	C16-C17-C18-C19
30	B	848	DGD	C5A-C6A-C7A-C8A
25	A	822	CLA	C15-C16-C17-C18
25	K	203	CLA	CBA-CGA-O2A-C1
27	A	844	LHG	O2-C2-C3-O3
27	A	843	LHG	C14-C15-C16-C17
25	P	613	CLA	O1D-CGD-O2D-CED
25	S	301	CLA	O1D-CGD-O2D-CED
25	U	313	CLA	O1D-CGD-O2D-CED
33	4	314	CHL	O1D-CGD-O2D-CED
33	6	606	CHL	O1D-CGD-O2D-CED
32	2	301	LMG	C2-C1-O1-C7
32	7	318	LMG	C2-C1-O1-C7
27	P	618	LHG	C32-C33-C34-C35
27	Q	617	LHG	C32-C33-C34-C35
32	J	107	LMG	C13-C14-C15-C16
25	1	604	CLA	C5-C6-C7-C8
25	2	305	CLA	O1A-CGA-O2A-C1
25	2	309	CLA	C11-C12-C13-C14
25	U	304	CLA	O1D-CGD-O2D-CED
25	4	311	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	C4-C3-C5-C6
33	P	609	CHL	C4-C3-C5-C6
33	Q	608	CHL	C4-C3-C5-C6
33	R	609	CHL	C4-C3-C5-C6
27	P	624	LHG	C32-C33-C34-C35
27	T	617	LHG	C32-C33-C34-C35
27	5	301	LHG	C15-C16-C17-C18
25	3	305	CLA	C2-C3-C5-C6
25	3	311	CLA	C2-C3-C5-C6
25	A	814	CLA	C11-C10-C8-C9
25	A	825	CLA	C14-C13-C15-C16
25	A	839	CLA	C6-C7-C8-C9
25	B	805	CLA	C11-C10-C8-C9
25	B	822	CLA	C11-C10-C8-C9
25	B	836	CLA	C6-C7-C8-C9
25	T	608	CLA	C14-C13-C15-C16
25	1	609	CLA	C11-C10-C8-C9
25	2	309	CLA	C11-C10-C8-C9
25	a	308	CLA	C11-C10-C8-C9
25	A	823	CLA	O1D-CGD-O2D-CED
25	P	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	J	104	LMG	C10-C11-C12-C13
27	8	319	LHG	C10-C11-C12-C13
25	B	807	CLA	C13-C15-C16-C17
25	Q	612	CLA	C8-C10-C11-C12
25	T	611	CLA	C8-C10-C11-C12
25	2	303	CLA	C5-C6-C7-C8
25	3	305	CLA	C10-C11-C12-C13
25	A	842	CLA	C2A-CAA-CBA-CGA
25	3	311	CLA	C2A-CAA-CBA-CGA
25	4	303	CLA	C2A-CAA-CBA-CGA
25	5	324	CLA	C2A-CAA-CBA-CGA
33	U	307	CHL	C2A-CAA-CBA-CGA
25	B	826	CLA	O1A-CGA-O2A-C1
32	6	602	LMG	O10-C28-O8-C9
28	B	842	BCR	C7-C8-C9-C34
28	B	851	BCR	C36-C18-C19-C20
28	F	801	BCR	C37-C22-C23-C24
28	L	207	BCR	C7-C8-C9-C34
28	6	621	BCR	C7-C8-C9-C34
27	5	321	LHG	C9-C10-C11-C12
32	H	204	LMG	C29-C30-C31-C32
27	4	318	LHG	O1-C1-C2-C3
27	5	301	LHG	O1-C1-C2-C3
27	6	618	LHG	O1-C1-C2-C3
28	B	851	BCR	C17-C18-C19-C20
28	F	801	BCR	C21-C22-C23-C24
28	L	207	BCR	C7-C8-C9-C10
28	O	204	BCR	C21-C22-C23-C24
28	4	317	BCR	C7-C8-C9-C10
28	5	320	BCR	C21-C22-C23-C24
28	6	621	BCR	C7-C8-C9-C10
34	S	317	LUT	C7-C8-C9-C10
25	L	202	CLA	C5-C6-C7-C8
25	P	613	CLA	C8-C10-C11-C12
27	A	843	LHG	C28-C29-C30-C31
27	2	317	LHG	C27-C28-C29-C30
31	B	850	SQD	C13-C14-C15-C16
27	4	318	LHG	C7-C8-C9-C10
27	2	317	LHG	C16-C17-C18-C19
25	L	205	CLA	O1A-CGA-O2A-C1
25	B	819	CLA	O1A-CGA-O2A-C1
25	A	807	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	A	808	CLA	C4B-C3B-CAB-CBB
25	A	821	CLA	C4B-C3B-CAB-CBB
25	A	823	CLA	C4B-C3B-CAB-CBB
25	A	832	CLA	C4B-C3B-CAB-CBB
25	A	839	CLA	C4B-C3B-CAB-CBB
25	B	817	CLA	C4B-C3B-CAB-CBB
25	B	822	CLA	C4B-C3B-CAB-CBB
25	B	828	CLA	C4B-C3B-CAB-CBB
25	B	835	CLA	C4B-C3B-CAB-CBB
25	B	837	CLA	C4B-C3B-CAB-CBB
25	B	838	CLA	C4B-C3B-CAB-CBB
25	K	201	CLA	C4B-C3B-CAB-CBB
25	K	205	CLA	C4B-C3B-CAB-CBB
25	L	206	CLA	C4B-C3B-CAB-CBB
25	L	209	CLA	C4B-C3B-CAB-CBB
25	O	201	CLA	C4B-C3B-CAB-CBB
25	R	603	CLA	C4B-C3B-CAB-CBB
25	S	312	CLA	C4B-C3B-CAB-CBB
25	S	314	CLA	C4B-C3B-CAB-CBB
25	S	315	CLA	C4B-C3B-CAB-CBB
25	1	604	CLA	C4B-C3B-CAB-CBB
25	1	607	CLA	C4B-C3B-CAB-CBB
25	1	611	CLA	C4B-C3B-CAB-CBB
25	1	614	CLA	C4B-C3B-CAB-CBB
25	2	314	CLA	C4B-C3B-CAB-CBB
25	3	307	CLA	C4B-C3B-CAB-CBB
25	3	311	CLA	C4B-C3B-CAB-CBB
25	4	303	CLA	C4B-C3B-CAB-CBB
25	4	313	CLA	C4B-C3B-CAB-CBB
25	5	306	CLA	C4B-C3B-CAB-CBB
25	5	314	CLA	C4B-C3B-CAB-CBB
25	6	601	CLA	C4B-C3B-CAB-CBB
25	6	609	CLA	C4B-C3B-CAB-CBB
25	6	610	CLA	C4B-C3B-CAB-CBB
25	6	613	CLA	C4B-C3B-CAB-CBB
25	7	306	CLA	C4B-C3B-CAB-CBB
25	7	309	CLA	C4B-C3B-CAB-CBB
25	7	311	CLA	C4B-C3B-CAB-CBB
25	8	302	CLA	C4B-C3B-CAB-CBB
25	8	308	CLA	C4B-C3B-CAB-CBB
25	8	314	CLA	C4B-C3B-CAB-CBB
25	9	309	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	9	311	CLA	C4B-C3B-CAB-CBB
25	a	303	CLA	C4B-C3B-CAB-CBB
25	a	306	CLA	C4B-C3B-CAB-CBB
25	a	310	CLA	C4B-C3B-CAB-CBB
25	a	313	CLA	C4B-C3B-CAB-CBB
33	S	306	CHL	C4B-C3B-CAB-CBB
33	4	306	CHL	C4B-C3B-CAB-CBB
25	A	801	CLA	C16-C17-C18-C19
25	P	610	CLA	C11-C12-C13-C15
25	P	612	CLA	C11-C12-C13-C15
25	R	612	CLA	C11-C12-C13-C15
25	3	311	CLA	C6-C7-C8-C9
25	B	818	CLA	C5-C6-C7-C8
25	9	301	CLA	C5-C6-C7-C8
25	a	303	CLA	C5-C6-C7-C8
27	A	852	LHG	C25-C26-C27-C28
27	4	318	LHG	C13-C14-C15-C16
32	6	602	LMG	C14-C15-C16-C17
25	A	807	CLA	CBD-CGD-O2D-CED
25	A	840	CLA	O1D-CGD-O2D-CED
25	4	308	CLA	O1D-CGD-O2D-CED
25	5	304	CLA	O1D-CGD-O2D-CED
27	5	301	LHG	C28-C29-C30-C31
32	J	102	LMG	C12-C13-C14-C15
27	B	847	LHG	C23-C24-C25-C26
30	B	848	DGD	C1A-C2A-C3A-C4A
25	A	810	CLA	C15-C16-C17-C18
25	B	815	CLA	C8-C10-C11-C12
25	R	610	CLA	C10-C11-C12-C13
25	7	301	CLA	C15-C16-C17-C18
25	3	314	CLA	O1A-CGA-O2A-C1
30	B	848	DGD	C7B-C8B-C9B-CAB
32	J	107	LMG	C16-C17-C18-C19
25	7	303	CLA	C3-C5-C6-C7
25	R	611	CLA	CBA-CGA-O2A-C1
25	8	303	CLA	CBA-CGA-O2A-C1
27	A	843	LHG	C27-C28-C29-C30
32	J	107	LMG	C34-C35-C36-C37
25	A	830	CLA	O1D-CGD-O2D-CED
25	A	803	CLA	C3A-C2A-CAA-CBA
25	A	804	CLA	C3A-C2A-CAA-CBA
25	A	807	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	832	CLA	C3A-C2A-CAA-CBA
25	B	811	CLA	C3A-C2A-CAA-CBA
25	B	822	CLA	C3A-C2A-CAA-CBA
25	K	204	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	1	611	CLA	C3A-C2A-CAA-CBA
25	3	313	CLA	C3A-C2A-CAA-CBA
25	4	307	CLA	C3A-C2A-CAA-CBA
25	5	302	CLA	C3A-C2A-CAA-CBA
25	6	609	CLA	C3A-C2A-CAA-CBA
25	8	308	CLA	C3A-C2A-CAA-CBA
25	a	310	CLA	C3A-C2A-CAA-CBA
33	P	605	CHL	C3A-C2A-CAA-CBA
33	P	607	CHL	C3A-C2A-CAA-CBA
33	P	619	CHL	C3A-C2A-CAA-CBA
33	R	607	CHL	C3A-C2A-CAA-CBA
33	S	321	CHL	C3A-C2A-CAA-CBA
33	U	307	CHL	C3A-C2A-CAA-CBA
33	5	307	CHL	C3A-C2A-CAA-CBA
25	P	610	CLA	C10-C11-C12-C13
25	R	610	CLA	C15-C16-C17-C18
32	6	602	LMG	C11-C12-C13-C14
25	B	805	CLA	O1D-CGD-O2D-CED
33	5	307	CHL	O1A-CGA-O2A-C1
25	3	310	CLA	O1A-CGA-O2A-C1
25	A	815	CLA	C11-C12-C13-C15
25	R	613	CLA	C16-C17-C18-C20
25	A	838	CLA	C2C-C3C-CAC-CBC
27	A	843	LHG	C9-C10-C11-C12
27	A	844	LHG	C11-C10-C9-C8
32	1	619	LMG	C7-C8-C9-O8
25	A	839	CLA	CBD-CGD-O2D-CED
32	H	204	LMG	C15-C16-C17-C18
25	B	808	CLA	O1D-CGD-O2D-CED
25	5	303	CLA	O1A-CGA-O2A-C1
25	7	301	CLA	C8-C10-C11-C12
25	7	311	CLA	C8-C10-C11-C12
25	A	825	CLA	C4-C3-C5-C6
25	B	825	CLA	C4-C3-C5-C6
25	P	612	CLA	C4-C3-C5-C6
25	Q	611	CLA	C4-C3-C5-C6
25	R	612	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	T	610	CLA	C4-C3-C5-C6
25	U	311	CLA	C4-C3-C5-C6
25	3	302	CLA	C4-C3-C5-C6
25	4	311	CLA	C4-C3-C5-C6
33	4	322	CHL	C4-C3-C5-C6
25	A	825	CLA	C2-C3-C5-C6
25	A	832	CLA	C2-C3-C5-C6
25	A	838	CLA	C2-C3-C5-C6
25	B	807	CLA	C2-C3-C5-C6
25	Q	611	CLA	C2-C3-C5-C6
25	U	311	CLA	C2-C3-C5-C6
25	4	311	CLA	C2-C3-C5-C6
25	6	613	CLA	C2-C3-C5-C6
33	1	601	CHL	C2-C3-C5-C6
33	4	322	CHL	C2-C3-C5-C6
25	P	612	CLA	O1A-CGA-O2A-C1
25	R	612	CLA	O1A-CGA-O2A-C1
25	7	310	CLA	O1A-CGA-O2A-C1
25	2	312	CLA	C16-C17-C18-C19
25	K	203	CLA	C2C-C3C-CAC-CBC
25	A	808	CLA	C2B-C3B-CAB-CBB
25	A	819	CLA	C2B-C3B-CAB-CBB
25	A	821	CLA	C2B-C3B-CAB-CBB
25	A	823	CLA	C2B-C3B-CAB-CBB
25	A	825	CLA	C2B-C3B-CAB-CBB
25	A	832	CLA	C2B-C3B-CAB-CBB
25	A	834	CLA	C2B-C3B-CAB-CBB
25	A	837	CLA	C2B-C3B-CAB-CBB
25	A	840	CLA	C2B-C3B-CAB-CBB
25	A	842	CLA	C2B-C3B-CAB-CBB
25	A	853	CLA	C2B-C3B-CAB-CBB
25	B	814	CLA	C2B-C3B-CAB-CBB
25	B	817	CLA	C2B-C3B-CAB-CBB
25	B	822	CLA	C2B-C3B-CAB-CBB
25	B	828	CLA	C2B-C3B-CAB-CBB
25	B	834	CLA	C2B-C3B-CAB-CBB
25	B	837	CLA	C2B-C3B-CAB-CBB
25	B	838	CLA	C2B-C3B-CAB-CBB
25	B	849	CLA	C2B-C3B-CAB-CBB
25	J	103	CLA	C2B-C3B-CAB-CBB
25	K	201	CLA	C2B-C3B-CAB-CBB
25	K	204	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	K	205	CLA	C2B-C3B-CAB-CBB
25	L	206	CLA	C2B-C3B-CAB-CBB
25	L	209	CLA	C2B-C3B-CAB-CBB
25	O	201	CLA	C2B-C3B-CAB-CBB
25	P	603	CLA	C2B-C3B-CAB-CBB
25	Q	603	CLA	C2B-C3B-CAB-CBB
25	R	603	CLA	C2B-C3B-CAB-CBB
25	S	312	CLA	C2B-C3B-CAB-CBB
25	S	314	CLA	C2B-C3B-CAB-CBB
25	S	315	CLA	C2B-C3B-CAB-CBB
25	S	320	CLA	C2B-C3B-CAB-CBB
25	U	303	CLA	C2B-C3B-CAB-CBB
25	1	604	CLA	C2B-C3B-CAB-CBB
25	1	607	CLA	C2B-C3B-CAB-CBB
25	1	611	CLA	C2B-C3B-CAB-CBB
25	1	614	CLA	C2B-C3B-CAB-CBB
25	2	307	CLA	C2B-C3B-CAB-CBB
25	2	314	CLA	C2B-C3B-CAB-CBB
25	3	307	CLA	C2B-C3B-CAB-CBB
25	3	311	CLA	C2B-C3B-CAB-CBB
25	3	314	CLA	C2B-C3B-CAB-CBB
25	3	320	CLA	C2B-C3B-CAB-CBB
25	4	303	CLA	C2B-C3B-CAB-CBB
25	4	313	CLA	C2B-C3B-CAB-CBB
25	5	306	CLA	C2B-C3B-CAB-CBB
25	5	312	CLA	C2B-C3B-CAB-CBB
25	5	313	CLA	C2B-C3B-CAB-CBB
25	5	314	CLA	C2B-C3B-CAB-CBB
25	5	315	CLA	C2B-C3B-CAB-CBB
25	5	324	CLA	C2B-C3B-CAB-CBB
25	6	601	CLA	C2B-C3B-CAB-CBB
25	6	604	CLA	C2B-C3B-CAB-CBB
25	6	609	CLA	C2B-C3B-CAB-CBB
25	6	610	CLA	C2B-C3B-CAB-CBB
25	6	612	CLA	C2B-C3B-CAB-CBB
25	6	613	CLA	C2B-C3B-CAB-CBB
25	6	623	CLA	C2B-C3B-CAB-CBB
25	7	302	CLA	C2B-C3B-CAB-CBB
25	7	304	CLA	C2B-C3B-CAB-CBB
25	7	306	CLA	C2B-C3B-CAB-CBB
25	7	309	CLA	C2B-C3B-CAB-CBB
25	7	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	8	302	CLA	C2B-C3B-CAB-CBB
25	8	308	CLA	C2B-C3B-CAB-CBB
25	8	311	CLA	C2B-C3B-CAB-CBB
25	8	313	CLA	C2B-C3B-CAB-CBB
25	8	314	CLA	C2B-C3B-CAB-CBB
25	8	315	CLA	C2B-C3B-CAB-CBB
25	9	308	CLA	C2B-C3B-CAB-CBB
25	9	309	CLA	C2B-C3B-CAB-CBB
25	9	310	CLA	C2B-C3B-CAB-CBB
25	9	311	CLA	C2B-C3B-CAB-CBB
25	a	303	CLA	C2B-C3B-CAB-CBB
25	a	306	CLA	C2B-C3B-CAB-CBB
25	a	310	CLA	C2B-C3B-CAB-CBB
25	a	313	CLA	C2B-C3B-CAB-CBB
27	A	843	LHG	O2-C2-C3-O3
33	4	306	CHL	C2B-C3B-CAB-CBB
25	R	603	CLA	C15-C16-C17-C18
25	A	809	CLA	C3-C5-C6-C7
25	B	818	CLA	C3-C5-C6-C7
25	A	811	CLA	O1A-CGA-O2A-C1
25	A	822	CLA	O1A-CGA-O2A-C1
25	A	826	CLA	CBD-CGD-O2D-CED
27	6	618	LHG	C1-C2-C3-O3
25	A	806	CLA	C2-C1-O2A-CGA
25	A	828	CLA	C2-C1-O2A-CGA
25	B	831	CLA	C2-C1-O2A-CGA
27	5	301	LHG	C29-C30-C31-C32
30	B	846	DGD	C3B-C4B-C5B-C6B
25	A	808	CLA	C13-C15-C16-C17
25	A	825	CLA	C10-C11-C12-C13
25	B	805	CLA	C15-C16-C17-C18
25	L	205	CLA	C8-C10-C11-C12
25	S	303	CLA	C10-C11-C12-C13
25	S	320	CLA	C15-C16-C17-C18
25	T	608	CLA	C10-C11-C12-C13
25	R	611	CLA	O1A-CGA-O2A-C1
25	3	303	CLA	O1A-CGA-O2A-C1
25	8	303	CLA	O1A-CGA-O2A-C1
25	A	836	CLA	C3-C5-C6-C7
25	P	612	CLA	C3-C5-C6-C7
25	R	612	CLA	C3-C5-C6-C7
28	A	845	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	A	847	BCR	C1-C6-C7-C8
28	A	847	BCR	C5-C6-C7-C8
28	B	841	BCR	C5-C6-C7-C8
28	J	101	BCR	C1-C6-C7-C8
28	J	101	BCR	C5-C6-C7-C8
28	L	204	BCR	C1-C6-C7-C8
28	L	204	BCR	C5-C6-C7-C8
28	O	205	BCR	C23-C24-C25-C30
28	3	317	BCR	C23-C24-C25-C26
28	3	317	BCR	C23-C24-C25-C30
28	3	318	BCR	C1-C6-C7-C8
28	5	320	BCR	C5-C6-C7-C8
28	5	320	BCR	C23-C24-C25-C26
28	5	323	BCR	C23-C24-C25-C26
28	5	323	BCR	C23-C24-C25-C30
28	6	621	BCR	C1-C6-C7-C8
28	6	621	BCR	C23-C24-C25-C26
28	6	621	BCR	C23-C24-C25-C30
28	7	316	BCR	C23-C24-C25-C26
28	8	301	BCR	C1-C6-C7-C8
28	8	301	BCR	C5-C6-C7-C8
28	8	318	BCR	C1-C6-C7-C8
28	8	318	BCR	C5-C6-C7-C8
34	Q	615	LUT	C1-C6-C7-C8
34	T	614	LUT	C1-C6-C7-C8
34	1	616	LUT	C5-C6-C7-C8
34	1	617	LUT	C1-C6-C7-C8
34	1	617	LUT	C5-C6-C7-C8
34	4	316	LUT	C5-C6-C7-C8
34	7	315	LUT	C1-C6-C7-C8
34	7	315	LUT	C5-C6-C7-C8
34	a	314	LUT	C1-C6-C7-C8
34	a	315	LUT	C5-C6-C7-C8
32	J	102	LMG	O6-C5-C6-O5
25	B	819	CLA	O1D-CGD-O2D-CED
25	3	311	CLA	CBA-CGA-O2A-C1
25	A	812	CLA	C8-C10-C11-C12
25	B	806	CLA	C13-C15-C16-C17
25	B	807	CLA	C15-C16-C17-C18
25	U	310	CLA	C10-C11-C12-C13
25	2	304	CLA	C5-C6-C7-C8
27	6	618	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	8	319	LHG	C31-C32-C33-C34
25	H	201	CLA	CBD-CGD-O2D-CED
27	Q	617	LHG	C7-C8-C9-C10
25	A	812	CLA	C13-C15-C16-C17
25	7	308	CLA	O1D-CGD-O2D-CED
25	A	838	CLA	C4-C3-C5-C6
25	B	801	CLA	C4-C3-C5-C6
25	B	807	CLA	C4-C3-C5-C6
25	1	607	CLA	C4-C3-C5-C6
25	1	613	CLA	C4-C3-C5-C6
25	a	312	CLA	C4-C3-C5-C6
33	1	601	CHL	C4-C3-C5-C6
25	L	202	CLA	O1D-CGD-O2D-CED
33	S	310	CHL	O1D-CGD-O2D-CED
25	A	808	CLA	C12-C13-C15-C16
25	A	809	CLA	C6-C7-C8-C10
25	A	818	CLA	C11-C12-C13-C15
25	A	819	CLA	C12-C13-C15-C16
25	A	820	CLA	C11-C12-C13-C15
25	A	825	CLA	C11-C10-C8-C7
25	A	826	CLA	C6-C7-C8-C10
25	B	801	CLA	C2-C3-C5-C6
25	B	810	CLA	C11-C12-C13-C15
25	B	822	CLA	C11-C10-C8-C7
25	B	822	CLA	C11-C12-C13-C15
25	B	822	CLA	C12-C13-C15-C16
25	B	825	CLA	C2-C3-C5-C6
25	B	830	CLA	C6-C7-C8-C10
25	B	830	CLA	C11-C12-C13-C15
25	B	836	CLA	C11-C12-C13-C15
25	B	838	CLA	C6-C7-C8-C10
25	P	612	CLA	C2-C3-C5-C6
25	R	612	CLA	C2-C3-C5-C6
25	S	313	CLA	C2-C3-C5-C6
25	S	314	CLA	C11-C10-C8-C7
25	T	610	CLA	C2-C3-C5-C6
25	1	607	CLA	C2-C3-C5-C6
25	1	609	CLA	C11-C10-C8-C7
25	1	613	CLA	C2-C3-C5-C6
25	2	309	CLA	C11-C10-C8-C7
25	3	302	CLA	C2-C3-C5-C6
25	7	303	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	8	313	CLA	C6-C7-C8-C10
25	a	306	CLA	C2-C3-C5-C6
25	a	308	CLA	C11-C10-C8-C7
25	a	312	CLA	C2-C3-C5-C6
26	A	841	PQN	C22-C23-C25-C26
33	P	609	CHL	C2-C3-C5-C6
33	Q	608	CHL	C2-C3-C5-C6
33	R	609	CHL	C2-C3-C5-C6
27	8	319	LHG	C30-C31-C32-C33
32	J	104	LMG	C12-C13-C14-C15
32	J	107	LMG	C22-C23-C24-C25
25	P	603	CLA	C15-C16-C17-C18
25	8	310	CLA	C8-C10-C11-C12
36	P	621	NEX	C29-C30-C31-C32
36	R	617	NEX	C13-C14-C15-C35
36	U	316	NEX	C29-C30-C31-C32
27	P	618	LHG	C7-C8-C9-C10
27	P	624	LHG	C7-C8-C9-C10
25	A	825	CLA	CBA-CGA-O2A-C1
25	A	842	CLA	CBA-CGA-O2A-C1
25	B	813	CLA	CBA-CGA-O2A-C1
25	B	823	CLA	CBA-CGA-O2A-C1
25	S	303	CLA	CBA-CGA-O2A-C1
25	1	604	CLA	CBA-CGA-O2A-C1
25	1	613	CLA	CBA-CGA-O2A-C1
25	5	324	CLA	CBA-CGA-O2A-C1
25	6	609	CLA	CBA-CGA-O2A-C1
25	a	311	CLA	CBA-CGA-O2A-C1
25	a	312	CLA	CBA-CGA-O2A-C1
27	B	847	LHG	C24-C23-O8-C6
27	5	301	LHG	C24-C23-O8-C6
33	6	607	CHL	CBA-CGA-O2A-C1
27	5	301	LHG	C12-C13-C14-C15
32	2	301	LMG	C16-C17-C18-C19
32	7	319	LMG	C13-C14-C15-C16
25	A	803	CLA	C2A-CAA-CBA-CGA
25	A	819	CLA	C2A-CAA-CBA-CGA
25	A	836	CLA	C2A-CAA-CBA-CGA
25	B	826	CLA	C2A-CAA-CBA-CGA
25	2	311	CLA	C2A-CAA-CBA-CGA
25	2	312	CLA	C2A-CAA-CBA-CGA
25	4	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	6	604	CLA	C2A-CAA-CBA-CGA
25	9	310	CLA	C2A-CAA-CBA-CGA
25	9	303	CLA	O1D-CGD-O2D-CED
25	J	103	CLA	C5-C6-C7-C8
25	2	304	CLA	C10-C11-C12-C13
25	2	312	CLA	C8-C10-C11-C12
25	8	302	CLA	C13-C15-C16-C17
25	2	308	CLA	C2A-CAA-CBA-CGA
33	P	601	CHL	O1D-CGD-O2D-CED
33	Q	601	CHL	O1D-CGD-O2D-CED
33	R	601	CHL	O1D-CGD-O2D-CED
33	S	306	CHL	O1D-CGD-O2D-CED
25	6	601	CLA	C12-C13-C15-C16
27	A	844	LHG	C7-C8-C9-C10
30	B	848	DGD	C1B-C2B-C3B-C4B
31	B	850	SQD	C7-C8-C9-C10
25	4	303	CLA	O1D-CGD-O2D-CED
25	5	312	CLA	O1D-CGD-O2D-CED
25	B	827	CLA	C10-C11-C12-C13
25	U	302	CLA	C8-C10-C11-C12
27	S	319	LHG	C32-C33-C34-C35
33	T	601	CHL	O1D-CGD-O2D-CED
25	A	838	CLA	C4C-C3C-CAC-CBC
27	B	847	LHG	C11-C10-C9-C8
27	B	847	LHG	C25-C26-C27-C28
27	5	321	LHG	C26-C27-C28-C29
27	5	321	LHG	C27-C28-C29-C30
33	S	309	CHL	CBD-CGD-O2D-CED
33	8	307	CHL	CBD-CGD-O2D-CED
25	A	853	CLA	C16-C17-C18-C20
32	7	318	LMG	O6-C1-O1-C7
25	P	602	CLA	C8-C10-C11-C12
25	R	602	CLA	C8-C10-C11-C12
25	T	602	CLA	C8-C10-C11-C12
25	2	314	CLA	O1D-CGD-O2D-CED
25	3	312	CLA	O1D-CGD-O2D-CED
33	P	622	CHL	O1D-CGD-O2D-CED
33	6	617	CHL	O1D-CGD-O2D-CED
25	B	812	CLA	C2C-C3C-CAC-CBC
27	Q	617	LHG	C11-C12-C13-C14
30	B	846	DGD	C2B-C3B-C4B-C5B
32	7	319	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	B	846	DGD	C3A-C4A-C5A-C6A
32	1	619	LMG	C13-C14-C15-C16
25	8	313	CLA	C3-C5-C6-C7
25	a	309	CLA	C3-C5-C6-C7
27	T	617	LHG	C7-C8-C9-C10
31	B	850	SQD	C28-C29-C30-C31
27	2	317	LHG	O7-C5-C6-O8
30	B	848	DGD	O1G-C1G-C2G-O2G
32	1	619	LMG	O7-C8-C9-O8
32	7	319	LMG	O7-C8-C9-O8
25	A	820	CLA	CBD-CGD-O2D-CED
25	3	303	CLA	CBD-CGD-O2D-CED
25	A	824	CLA	C6-C7-C8-C10
25	A	840	CLA	C16-C17-C18-C19
25	B	814	CLA	C6-C7-C8-C9
25	3	311	CLA	C6-C7-C8-C10
25	8	314	CLA	C6-C7-C8-C10
27	5	301	LHG	C11-C10-C9-C8
25	B	824	CLA	C5-C6-C7-C8
25	L	201	CLA	C10-C11-C12-C13
25	2	312	CLA	C5-C6-C7-C8
25	S	313	CLA	C4-C3-C5-C6
25	a	306	CLA	C4-C3-C5-C6
27	a	317	LHG	C23-C24-C25-C26
25	A	810	CLA	C2-C3-C5-C6
25	B	821	CLA	C2-C3-C5-C6
25	S	314	CLA	C2-C3-C5-C6
25	A	807	CLA	C14-C13-C15-C16
25	A	808	CLA	C11-C12-C13-C14
25	A	808	CLA	C14-C13-C15-C16
25	A	812	CLA	C6-C7-C8-C9
25	A	818	CLA	C11-C12-C13-C14
25	A	819	CLA	C14-C13-C15-C16
25	A	820	CLA	C11-C12-C13-C14
25	A	822	CLA	C6-C7-C8-C9
25	A	828	CLA	C6-C7-C8-C9
25	A	838	CLA	C11-C10-C8-C9
25	B	816	CLA	C6-C7-C8-C9
25	B	822	CLA	C11-C12-C13-C14
25	R	610	CLA	C11-C12-C13-C14
25	R	613	CLA	C14-C13-C15-C16
25	S	314	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	1	610	CLA	C11-C12-C13-C14
25	2	303	CLA	C14-C13-C15-C16
25	2	312	CLA	C14-C13-C15-C16
25	4	301	CLA	C11-C10-C8-C9
25	7	303	CLA	C6-C7-C8-C9
25	7	311	CLA	C14-C13-C15-C16
25	9	303	CLA	C6-C7-C8-C9
25	a	309	CLA	C11-C12-C13-C14
25	A	836	CLA	O1D-CGD-O2D-CED
25	U	303	CLA	C15-C16-C17-C18
25	A	838	CLA	C2A-CAA-CBA-CGA
25	3	314	CLA	C2A-CAA-CBA-CGA
25	5	313	CLA	C2A-CAA-CBA-CGA
25	9	309	CLA	C2A-CAA-CBA-CGA
33	6	606	CHL	C2A-CAA-CBA-CGA
32	H	204	LMG	C30-C31-C32-C33
27	1	618	LHG	C23-C24-C25-C26
28	A	846	BCR	C7-C8-C9-C34
28	I	201	BCR	C7-C8-C9-C34
28	O	204	BCR	C7-C8-C9-C34
28	4	317	BCR	C7-C8-C9-C34
25	A	816	CLA	O1D-CGD-O2D-CED
25	B	806	CLA	C15-C16-C17-C18
25	Q	603	CLA	C15-C16-C17-C18
27	Q	617	LHG	C24-C25-C26-C27
27	R	618	LHG	C24-C25-C26-C27
25	S	303	CLA	O1A-CGA-O2A-C1
25	3	311	CLA	O1A-CGA-O2A-C1
25	6	609	CLA	O1A-CGA-O2A-C1
33	6	607	CHL	O1A-CGA-O2A-C1
25	A	803	CLA	C1A-C2A-CAA-CBA
25	A	804	CLA	C1A-C2A-CAA-CBA
25	A	807	CLA	C1A-C2A-CAA-CBA
25	A	809	CLA	C1A-C2A-CAA-CBA
25	A	823	CLA	C1A-C2A-CAA-CBA
25	A	832	CLA	C1A-C2A-CAA-CBA
25	B	804	CLA	C1A-C2A-CAA-CBA
25	B	818	CLA	C1A-C2A-CAA-CBA
25	B	822	CLA	C1A-C2A-CAA-CBA
25	J	103	CLA	C1A-C2A-CAA-CBA
25	K	201	CLA	C1A-C2A-CAA-CBA
25	K	202	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	K	204	CLA	C1A-C2A-CAA-CBA
25	P	610	CLA	C1A-C2A-CAA-CBA
25	Q	604	CLA	C1A-C2A-CAA-CBA
25	Q	609	CLA	C1A-C2A-CAA-CBA
25	Q	613	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C1A-C2A-CAA-CBA
25	R	614	CLA	C1A-C2A-CAA-CBA
25	S	301	CLA	C1A-C2A-CAA-CBA
25	S	303	CLA	C1A-C2A-CAA-CBA
25	T	608	CLA	C1A-C2A-CAA-CBA
25	T	612	CLA	C1A-C2A-CAA-CBA
25	U	304	CLA	C1A-C2A-CAA-CBA
25	U	310	CLA	C1A-C2A-CAA-CBA
25	U	313	CLA	C1A-C2A-CAA-CBA
25	1	608	CLA	C1A-C2A-CAA-CBA
25	1	609	CLA	C1A-C2A-CAA-CBA
25	1	611	CLA	C1A-C2A-CAA-CBA
25	2	302	CLA	C1A-C2A-CAA-CBA
25	2	305	CLA	C1A-C2A-CAA-CBA
25	3	313	CLA	C1A-C2A-CAA-CBA
25	4	308	CLA	C1A-C2A-CAA-CBA
25	5	302	CLA	C1A-C2A-CAA-CBA
25	5	315	CLA	C1A-C2A-CAA-CBA
25	6	605	CLA	C1A-C2A-CAA-CBA
25	7	308	CLA	C1A-C2A-CAA-CBA
25	8	310	CLA	C1A-C2A-CAA-CBA
25	8	314	CLA	C1A-C2A-CAA-CBA
25	9	301	CLA	C1A-C2A-CAA-CBA
25	a	307	CLA	C1A-C2A-CAA-CBA
25	a	308	CLA	C1A-C2A-CAA-CBA
25	a	310	CLA	C1A-C2A-CAA-CBA
33	P	605	CHL	C1A-C2A-CAA-CBA
33	P	607	CHL	C1A-C2A-CAA-CBA
33	P	619	CHL	C1A-C2A-CAA-CBA
33	R	607	CHL	C1A-C2A-CAA-CBA
33	S	302	CHL	C1A-C2A-CAA-CBA
33	S	309	CHL	C1A-C2A-CAA-CBA
33	S	321	CHL	C1A-C2A-CAA-CBA
33	T	604	CHL	C1A-C2A-CAA-CBA
33	U	307	CHL	C1A-C2A-CAA-CBA
33	5	307	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	8	307	CHL	C1A-C2A-CAA-CBA
25	A	816	CLA	C16-C17-C18-C20
25	A	853	CLA	C16-C17-C18-C19
25	3	320	CLA	C16-C17-C18-C19
25	8	314	CLA	C6-C7-C8-C9
27	6	618	LHG	O9-C7-O7-C5
32	7	319	LMG	C11-C10-O7-C8
27	P	618	LHG	C11-C12-C13-C14
27	R	618	LHG	C11-C12-C13-C14
27	2	317	LHG	C17-C18-C19-C20
30	B	846	DGD	C4B-C5B-C6B-C7B
28	I	201	BCR	C19-C20-C21-C22
36	P	617	NEX	C29-C30-C31-C32
36	R	617	NEX	C29-C30-C31-C32
36	T	616	NEX	C29-C30-C31-C32
36	U	301	NEX	C29-C30-C31-C32
25	A	814	CLA	O1D-CGD-O2D-CED
25	A	815	CLA	C10-C11-C12-C13
25	B	824	CLA	C8-C10-C11-C12
25	Q	609	CLA	C10-C11-C12-C13
25	1	613	CLA	C15-C16-C17-C18
27	A	852	LHG	C4-O6-P-O3
25	A	837	CLA	CBD-CGD-O2D-CED
25	B	817	CLA	C3-C5-C6-C7
25	A	825	CLA	O1A-CGA-O2A-C1
25	A	801	CLA	C15-C16-C17-C18
25	A	825	CLA	C13-C15-C16-C17
25	A	827	CLA	C10-C11-C12-C13
25	Q	602	CLA	C8-C10-C11-C12
25	2	309	CLA	C10-C11-C12-C13
25	4	301	CLA	C10-C11-C12-C13
27	5	301	LHG	O6-C4-C5-C6
27	P	624	LHG	C24-C25-C26-C27
27	2	317	LHG	C23-C24-C25-C26
32	7	319	LMG	C28-C29-C30-C31
26	A	841	PQN	C23-C25-C26-C27
27	T	617	LHG	C24-C25-C26-C27
27	P	618	LHG	C24-C25-C26-C27
25	3	320	CLA	C5-C6-C7-C8
27	T	617	LHG	C11-C12-C13-C14
25	A	824	CLA	CBA-CGA-O2A-C1
25	1	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	a	310	CLA	CBA-CGA-O2A-C1
25	1	604	CLA	O1A-CGA-O2A-C1
32	J	104	LMG	O6-C5-C6-O5
25	B	834	CLA	C4-C3-C5-C6
25	2	304	CLA	C4-C3-C5-C6
25	7	304	CLA	C3A-C2A-CAA-CBA
25	A	806	CLA	C10-C11-C12-C13
25	B	825	CLA	C10-C11-C12-C13
25	B	837	CLA	C15-C16-C17-C18
27	5	301	LHG	C11-C12-C13-C14
25	B	813	CLA	O1A-CGA-O2A-C1
25	5	324	CLA	O1A-CGA-O2A-C1
27	B	847	LHG	O10-C23-O8-C6
27	P	624	LHG	C11-C12-C13-C14
32	J	107	LMG	C15-C16-C17-C18
25	6	603	CLA	C8-C10-C11-C12
25	2	312	CLA	C16-C17-C18-C20
25	9	303	CLA	C11-C12-C13-C15
32	1	619	LMG	O6-C5-C6-O5
25	K	203	CLA	C4C-C3C-CAC-CBC
27	A	844	LHG	C4-C5-C6-O8
31	B	850	SQD	O6-C44-C45-C46
32	J	104	LMG	O1-C7-C8-C9
32	J	107	LMG	O1-C7-C8-C9
25	8	310	CLA	C10-C11-C12-C13
32	J	104	LMG	C31-C32-C33-C34
31	B	850	SQD	C45-C44-O6-C1
27	2	317	LHG	C32-C33-C34-C35
25	B	815	CLA	CBD-CGD-O2D-CED
25	B	837	CLA	CBD-CGD-O2D-CED
25	A	827	CLA	C13-C15-C16-C17
25	B	824	CLA	C13-C15-C16-C17
25	T	609	CLA	C5-C6-C7-C8
25	a	312	CLA	C15-C16-C17-C18
27	5	321	LHG	C11-C10-C9-C8
27	R	618	LHG	C7-C8-C9-C10
25	A	842	CLA	O1A-CGA-O2A-C1
25	a	311	CLA	O1A-CGA-O2A-C1
25	a	312	CLA	O1A-CGA-O2A-C1
27	1	618	LHG	C25-C26-C27-C28
25	1	610	CLA	C3-C5-C6-C7
27	A	843	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	B	850	SQD	C27-C28-C29-C30
25	B	801	CLA	C8-C10-C11-C12
25	L	205	CLA	C5-C6-C7-C8
25	3	320	CLA	C13-C15-C16-C17
25	B	823	CLA	O1A-CGA-O2A-C1
25	1	613	CLA	O1A-CGA-O2A-C1
32	7	318	LMG	C28-C29-C30-C31
30	B	846	DGD	O6E-C5E-C6E-O5E
25	A	822	CLA	C4-C3-C5-C6
25	B	812	CLA	C4-C3-C5-C6
25	B	830	CLA	C4-C3-C5-C6
25	S	314	CLA	C4-C3-C5-C6
25	8	313	CLA	C4-C3-C5-C6
25	B	812	CLA	C2-C3-C5-C6
25	8	313	CLA	C2-C3-C5-C6
25	1	611	CLA	CBA-CGA-O2A-C1
32	2	301	LMG	C29-C28-O8-C9
25	B	810	CLA	CBD-CGD-O2D-CED
25	A	815	CLA	C8-C10-C11-C12
25	B	801	CLA	C10-C11-C12-C13
25	B	834	CLA	C8-C10-C11-C12
25	B	836	CLA	C13-C15-C16-C17
27	A	843	LHG	C19-C20-C21-C22
25	8	309	CLA	O1A-CGA-O2A-C1
25	K	203	CLA	O1D-CGD-O2D-CED
25	A	810	CLA	C2A-CAA-CBA-CGA
25	T	608	CLA	C2A-CAA-CBA-CGA
33	5	308	CHL	C2A-CAA-CBA-CGA
25	A	832	CLA	C13-C15-C16-C17
25	B	834	CLA	C5-C6-C7-C8
25	B	849	CLA	C15-C16-C17-C18
25	S	311	CLA	C10-C11-C12-C13
25	3	305	CLA	C8-C10-C11-C12
25	2	307	CLA	C2-C1-O2A-CGA
25	a	303	CLA	C2-C1-O2A-CGA
33	1	601	CHL	C2-C1-O2A-CGA
33	5	308	CHL	C2-C1-O2A-CGA
25	4	310	CLA	O1D-CGD-O2D-CED
25	7	313	CLA	O1D-CGD-O2D-CED
25	a	311	CLA	C3-C5-C6-C7
31	B	850	SQD	C31-C32-C33-C34
25	A	822	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	A	852	LHG	C24-C25-C26-C27
25	B	834	CLA	CBA-CGA-O2A-C1
25	3	320	CLA	CBA-CGA-O2A-C1
25	5	309	CLA	CBA-CGA-O2A-C1
33	P	609	CHL	CBA-CGA-O2A-C1
33	Q	608	CHL	CBA-CGA-O2A-C1
33	R	609	CHL	CBA-CGA-O2A-C1
27	4	318	LHG	O6-C4-C5-O7
27	5	321	LHG	O6-C4-C5-O7
25	A	824	CLA	C6-C7-C8-C9
25	7	301	CLA	C16-C17-C18-C19
25	9	303	CLA	C11-C12-C13-C14
27	5	301	LHG	O10-C23-O8-C6
25	A	839	CLA	C13-C15-C16-C17
25	S	304	CLA	C8-C10-C11-C12
33	P	609	CHL	C10-C11-C12-C13
33	Q	608	CHL	C10-C11-C12-C13
30	B	848	DGD	C2D-C1D-O3G-C3G
32	7	319	LMG	C2-C1-O1-C7
27	6	618	LHG	C9-C10-C11-C12
27	A	843	LHG	C24-C23-O8-C6
27	2	317	LHG	C24-C25-C26-C27
25	A	853	CLA	C15-C16-C17-C18
33	R	609	CHL	C10-C11-C12-C13
25	5	304	CLA	CBA-CGA-O2A-C1
25	A	825	CLA	O1D-CGD-O2D-CED
27	a	317	LHG	C25-C26-C27-C28
25	8	303	CLA	C8-C10-C11-C12
25	A	801	CLA	C6-C7-C8-C10
25	A	807	CLA	C11-C12-C13-C15
25	A	807	CLA	C12-C13-C15-C16
25	A	819	CLA	C11-C12-C13-C15
25	A	822	CLA	C6-C7-C8-C10
25	A	828	CLA	C6-C7-C8-C10
25	A	830	CLA	C11-C10-C8-C7
25	A	836	CLA	C12-C13-C15-C16
25	A	838	CLA	C11-C10-C8-C7
25	B	805	CLA	C11-C12-C13-C15
25	B	805	CLA	C12-C13-C15-C16
25	B	808	CLA	C11-C12-C13-C15
25	B	809	CLA	C11-C10-C8-C7
25	B	809	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	B	811	CLA	C11-C10-C8-C7
25	B	817	CLA	C12-C13-C15-C16
25	B	824	CLA	C11-C10-C8-C7
25	B	836	CLA	C12-C13-C15-C16
25	B	837	CLA	C12-C13-C15-C16
25	B	849	CLA	C11-C10-C8-C7
25	P	613	CLA	C11-C10-C8-C7
25	Q	609	CLA	C11-C12-C13-C15
25	Q	612	CLA	C11-C10-C8-C7
25	R	610	CLA	C11-C12-C13-C15
25	R	613	CLA	C11-C10-C8-C7
25	R	613	CLA	C12-C13-C15-C16
25	S	314	CLA	C12-C13-C15-C16
25	T	608	CLA	C11-C12-C13-C15
25	T	611	CLA	C11-C10-C8-C7
25	U	310	CLA	C11-C12-C13-C15
25	1	608	CLA	C11-C10-C8-C7
25	1	609	CLA	C6-C7-C8-C10
25	1	610	CLA	C11-C12-C13-C15
25	2	303	CLA	C12-C13-C15-C16
25	2	309	CLA	C6-C7-C8-C10
25	2	312	CLA	C11-C10-C8-C7
25	2	312	CLA	C12-C13-C15-C16
25	4	301	CLA	C11-C10-C8-C7
25	4	311	CLA	C6-C7-C8-C10
25	5	303	CLA	C11-C12-C13-C15
25	6	613	CLA	C6-C7-C8-C10
25	6	623	CLA	C6-C7-C8-C10
25	7	311	CLA	C12-C13-C15-C16
25	a	307	CLA	C11-C10-C8-C7
25	a	308	CLA	C6-C7-C8-C10
25	a	309	CLA	C11-C12-C13-C15
25	B	822	CLA	C3-C5-C6-C7
32	2	301	LMG	C14-C15-C16-C17
25	A	802	CLA	C11-C10-C8-C9
25	A	807	CLA	C11-C12-C13-C14
25	A	812	CLA	C14-C13-C15-C16
25	A	819	CLA	C11-C12-C13-C14
25	A	825	CLA	C11-C10-C8-C9
25	A	830	CLA	C11-C10-C8-C9
25	B	805	CLA	C11-C12-C13-C14
25	B	805	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	808	CLA	C11-C12-C13-C14
25	B	809	CLA	C11-C10-C8-C9
25	B	811	CLA	C11-C10-C8-C9
25	B	817	CLA	C14-C13-C15-C16
25	B	824	CLA	C11-C10-C8-C9
25	B	825	CLA	C6-C7-C8-C9
25	B	831	CLA	C11-C10-C8-C9
25	B	836	CLA	C14-C13-C15-C16
25	B	838	CLA	C6-C7-C8-C9
25	L	205	CLA	C11-C12-C13-C14
25	P	613	CLA	C11-C10-C8-C9
25	Q	609	CLA	C11-C12-C13-C14
25	Q	612	CLA	C11-C10-C8-C9
25	R	613	CLA	C11-C10-C8-C9
25	S	314	CLA	C14-C13-C15-C16
25	T	608	CLA	C11-C12-C13-C14
25	T	609	CLA	C11-C10-C8-C9
25	T	611	CLA	C11-C10-C8-C9
25	U	310	CLA	C11-C12-C13-C14
25	U	312	CLA	C11-C10-C8-C9
25	2	304	CLA	C11-C12-C13-C14
25	2	312	CLA	C11-C10-C8-C9
25	5	303	CLA	C14-C13-C15-C16
25	5	313	CLA	C6-C7-C8-C9
25	6	613	CLA	C6-C7-C8-C9
25	6	623	CLA	C6-C7-C8-C9
25	8	302	CLA	C11-C12-C13-C14
25	8	313	CLA	C6-C7-C8-C9
26	A	841	PQN	C19-C18-C20-C21
27	7	317	LHG	C27-C28-C29-C30
25	A	813	CLA	C2A-CAA-CBA-CGA
25	R	610	CLA	C2A-CAA-CBA-CGA
25	U	310	CLA	C2A-CAA-CBA-CGA
25	4	301	CLA	C2A-CAA-CBA-CGA
25	6	603	CLA	C2A-CAA-CBA-CGA
25	8	313	CLA	C2A-CAA-CBA-CGA
25	9	302	CLA	C2A-CAA-CBA-CGA
33	S	309	CHL	O1D-CGD-O2D-CED
25	a	310	CLA	O1A-CGA-O2A-C1
28	B	840	BCR	C37-C22-C23-C24
28	J	101	BCR	C37-C22-C23-C24
34	4	316	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
36	P	617	NEX	C11-C12-C13-C20
25	U	312	CLA	C16-C17-C18-C20
32	J	107	LMG	C10-C11-C12-C13
28	5	320	BCR	C11-C12-C13-C14
35	P	616	XAT	C7-C8-C9-C10
35	S	318	XAT	C7-C8-C9-C10
36	U	316	NEX	C11-C12-C13-C14
32	7	319	LMG	O9-C10-O7-C8
25	B	805	CLA	C8-C10-C11-C12
25	2	309	CLA	C8-C10-C11-C12
32	H	204	LMG	C18-C19-C20-C21
25	A	814	CLA	CBA-CGA-O2A-C1
25	B	804	CLA	CBA-CGA-O2A-C1
27	A	852	LHG	C24-C23-O8-C6
33	S	310	CHL	CBA-CGA-O2A-C1
25	1	602	CLA	C5-C6-C7-C8
25	K	203	CLA	O1A-CGA-O2A-C1
25	8	309	CLA	CBD-CGD-O2D-CED
25	A	801	CLA	C4B-C3B-CAB-CBB
25	A	805	CLA	C4B-C3B-CAB-CBB
25	A	812	CLA	C4B-C3B-CAB-CBB
25	A	815	CLA	C4B-C3B-CAB-CBB
25	A	818	CLA	C4B-C3B-CAB-CBB
25	A	828	CLA	C4B-C3B-CAB-CBB
25	A	842	CLA	C4B-C3B-CAB-CBB
25	A	851	CLA	C4B-C3B-CAB-CBB
25	B	814	CLA	C4B-C3B-CAB-CBB
25	B	821	CLA	C4B-C3B-CAB-CBB
25	B	825	CLA	C4B-C3B-CAB-CBB
25	B	827	CLA	C4B-C3B-CAB-CBB
25	B	829	CLA	C4B-C3B-CAB-CBB
25	O	202	CLA	C4B-C3B-CAB-CBB
25	P	611	CLA	C4B-C3B-CAB-CBB
25	2	305	CLA	C4B-C3B-CAB-CBB
25	2	307	CLA	C4B-C3B-CAB-CBB
25	2	311	CLA	C4B-C3B-CAB-CBB
25	4	308	CLA	C4B-C3B-CAB-CBB
25	4	309	CLA	C4B-C3B-CAB-CBB
25	4	310	CLA	C4B-C3B-CAB-CBB
25	5	315	CLA	C4B-C3B-CAB-CBB
25	5	319	CLA	C4B-C3B-CAB-CBB
25	7	302	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	7	312	CLA	C4B-C3B-CAB-CBB
25	8	303	CLA	C4B-C3B-CAB-CBB
25	8	304	CLA	C4B-C3B-CAB-CBB
25	8	305	CLA	C4B-C3B-CAB-CBB
25	8	312	CLA	C4B-C3B-CAB-CBB
33	S	302	CHL	C4B-C3B-CAB-CBB
25	U	312	CLA	C16-C17-C18-C19
25	3	320	CLA	C10-C11-C12-C13
25	a	301	CLA	C5-C6-C7-C8
27	4	318	LHG	O6-C4-C5-C6
27	1	618	LHG	C28-C29-C30-C31
25	8	304	CLA	CBD-CGD-O2D-CED
25	A	818	CLA	C10-C11-C12-C13
25	T	608	CLA	C15-C16-C17-C18
25	3	303	CLA	C4-C3-C5-C6
25	4	308	CLA	C4-C3-C5-C6
33	P	622	CHL	C4-C3-C5-C6
25	5	324	CLA	C10-C11-C12-C13
27	A	852	LHG	C11-C10-C9-C8
27	2	317	LHG	C9-C10-C11-C12
25	B	849	CLA	C3-C5-C6-C7
25	7	301	CLA	C16-C17-C18-C20
27	4	319	LHG	C11-C12-C13-C14
25	B	824	CLA	C10-C11-C12-C13
25	B	814	CLA	CBA-CGA-O2A-C1
27	2	317	LHG	C7-C8-C9-C10
27	S	319	LHG	C31-C32-C33-C34
25	R	604	CLA	O1D-CGD-O2D-CED
25	A	824	CLA	O1A-CGA-O2A-C1
25	A	834	CLA	C3A-C2A-CAA-CBA
25	B	837	CLA	C3A-C2A-CAA-CBA
25	H	203	CLA	C3A-C2A-CAA-CBA
25	K	201	CLA	C3A-C2A-CAA-CBA
25	P	604	CLA	C3A-C2A-CAA-CBA
25	Q	604	CLA	C3A-C2A-CAA-CBA
25	T	603	CLA	C3A-C2A-CAA-CBA
25	U	304	CLA	C3A-C2A-CAA-CBA
25	2	305	CLA	C3A-C2A-CAA-CBA
25	2	313	CLA	C3A-C2A-CAA-CBA
25	3	307	CLA	C3A-C2A-CAA-CBA
25	6	613	CLA	C3A-C2A-CAA-CBA
25	7	307	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
33	T	604	CHL	C3A-C2A-CAA-CBA
28	K	206	BCR	C15-C16-C17-C18
36	P	617	NEX	C13-C14-C15-C35
36	T	616	NEX	C13-C14-C15-C35
36	U	301	NEX	C13-C14-C15-C35
25	P	612	CLA	C11-C12-C13-C14
25	R	612	CLA	C11-C12-C13-C14
25	4	309	CLA	C6-C7-C8-C9
25	6	615	CLA	O1D-CGD-O2D-CED
25	B	812	CLA	CBA-CGA-O2A-C1
25	P	612	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBA-CGA-O2A-C1
33	3	306	CHL	CBA-CGA-O2A-C1
25	7	308	CLA	C8-C10-C11-C12
27	A	852	LHG	C4-C5-C6-O8
27	B	847	LHG	C4-C5-C6-O8
27	2	317	LHG	C4-C5-C6-O8
27	4	318	LHG	C4-C5-C6-O8
27	6	618	LHG	C4-C5-C6-O8
32	J	102	LMG	C7-C8-C9-O8
32	2	301	LMG	O1-C7-C8-C9
32	6	602	LMG	C7-C8-C9-O8
32	7	318	LMG	O1-C7-C8-C9
32	7	319	LMG	C7-C8-C9-O8
25	9	308	CLA	CBD-CGD-O2D-CED
25	1	611	CLA	O1A-CGA-O2A-C1
25	1	612	CLA	O1A-CGA-O2A-C1
25	8	314	CLA	O1D-CGD-O2D-CED
25	5	311	CLA	C4-C3-C5-C6
25	A	840	CLA	C16-C17-C18-C20
25	3	320	CLA	C16-C17-C18-C20
25	3	303	CLA	C2-C3-C5-C6
25	T	610	CLA	O1D-CGD-O2D-CED
25	3	309	CLA	CBD-CGD-O2D-CED
33	4	304	CHL	CBD-CGD-O2D-CED
32	H	204	LMG	C16-C17-C18-C19
33	P	608	CHL	C3C-C2C-CMC-OMC
33	Q	607	CHL	C3C-C2C-CMC-OMC
33	R	605	CHL	C3C-C2C-CMC-OMC
33	R	608	CHL	C3C-C2C-CMC-OMC
33	S	308	CHL	C3C-C2C-CMC-OMC
33	T	606	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
33	U	305	CHL	C3C-C2C-CMC-OMC
33	5	317	CHL	C3C-C2C-CMC-OMC
25	3	320	CLA	O1A-CGA-O2A-C1
25	A	819	CLA	O1D-CGD-O2D-CED
25	A	820	CLA	O1D-CGD-O2D-CED
25	B	849	CLA	O1D-CGD-O2D-CED
25	B	804	CLA	C3-C5-C6-C7
25	A	829	CLA	C2A-CAA-CBA-CGA
25	Q	609	CLA	C2A-CAA-CBA-CGA
27	7	317	LHG	O1-C1-C2-O2
27	A	843	LHG	C13-C14-C15-C16
27	4	318	LHG	C15-C16-C17-C18
32	J	104	LMG	C11-C12-C13-C14
25	A	817	CLA	CBA-CGA-O2A-C1
25	B	834	CLA	O1A-CGA-O2A-C1
32	2	301	LMG	O10-C28-O8-C9
25	A	815	CLA	C11-C12-C13-C14
25	A	816	CLA	C16-C17-C18-C19
25	A	851	CLA	C10-C11-C12-C13
25	A	805	CLA	C2B-C3B-CAB-CBB
25	A	807	CLA	C2B-C3B-CAB-CBB
25	A	818	CLA	C2B-C3B-CAB-CBB
25	A	828	CLA	C2B-C3B-CAB-CBB
25	A	839	CLA	C2B-C3B-CAB-CBB
25	A	851	CLA	C2B-C3B-CAB-CBB
25	B	821	CLA	C2B-C3B-CAB-CBB
25	B	827	CLA	C2B-C3B-CAB-CBB
25	B	829	CLA	C2B-C3B-CAB-CBB
25	B	835	CLA	C2B-C3B-CAB-CBB
25	P	611	CLA	C2B-C3B-CAB-CBB
25	2	305	CLA	C2B-C3B-CAB-CBB
25	4	308	CLA	C2B-C3B-CAB-CBB
25	4	309	CLA	C2B-C3B-CAB-CBB
25	5	319	CLA	C2B-C3B-CAB-CBB
25	8	304	CLA	C2B-C3B-CAB-CBB
25	8	305	CLA	C2B-C3B-CAB-CBB
27	S	319	LHG	O2-C2-C3-O3
33	S	302	CHL	C2B-C3B-CAB-CBB
33	6	608	CHL	C2B-C3B-CAB-CBB
32	2	301	LMG	C15-C16-C17-C18
25	A	853	CLA	C8-C10-C11-C12
25	5	309	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	A	852	LHG	C15-C16-C17-C18
27	A	844	LHG	O7-C5-C6-O8
25	R	611	CLA	CAA-CBA-CGA-O2A
30	B	848	DGD	C9B-CAB-CBB-CCB
27	S	319	LHG	C26-C27-C28-C29
27	a	317	LHG	C24-C25-C26-C27
32	H	204	LMG	C31-C32-C33-C34
25	A	807	CLA	C4-C3-C5-C6
25	A	828	CLA	C4-C3-C5-C6
25	A	818	CLA	C2-C1-O2A-CGA
25	A	853	CLA	C2-C1-O2A-CGA
25	3	314	CLA	C2-C1-O2A-CGA
25	6	605	CLA	C2-C1-O2A-CGA
25	7	310	CLA	C2-C1-O2A-CGA
33	3	306	CHL	C2-C1-O2A-CGA
33	4	305	CHL	C2-C1-O2A-CGA
33	8	307	CHL	C2-C1-O2A-CGA
25	A	825	CLA	C11-C12-C13-C14
25	A	830	CLA	C6-C7-C8-C9
25	B	813	CLA	C6-C7-C8-C9
25	B	823	CLA	C6-C7-C8-C9
25	B	830	CLA	C6-C7-C8-C9
25	B	836	CLA	C11-C12-C13-C14
25	B	849	CLA	C6-C7-C8-C9
25	U	312	CLA	C14-C13-C15-C16
25	2	309	CLA	C6-C7-C8-C9
25	3	308	CLA	C6-C7-C8-C9
25	7	301	CLA	C11-C10-C8-C9
25	7	301	CLA	C11-C12-C13-C14
25	7	311	CLA	C6-C7-C8-C9
25	A	814	CLA	C8-C10-C11-C12
25	B	810	CLA	C10-C11-C12-C13
25	B	806	CLA	C2A-CAA-CBA-CGA
25	B	814	CLA	C2A-CAA-CBA-CGA
25	P	610	CLA	C2A-CAA-CBA-CGA
25	P	613	CLA	C2A-CAA-CBA-CGA
25	S	305	CLA	C2A-CAA-CBA-CGA
25	7	311	CLA	C2A-CAA-CBA-CGA
25	A	829	CLA	C16-C17-C18-C20
28	B	841	BCR	C1-C6-C7-C8
28	B	843	BCR	C5-C6-C7-C8
28	B	843	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
28	B	845	BCR	C1-C6-C7-C8
28	B	845	BCR	C5-C6-C7-C8
28	K	206	BCR	C1-C6-C7-C8
28	K	206	BCR	C5-C6-C7-C8
28	K	206	BCR	C23-C24-C25-C26
28	K	206	BCR	C23-C24-C25-C30
28	L	208	BCR	C23-C24-C25-C26
28	L	208	BCR	C23-C24-C25-C30
28	3	317	BCR	C5-C6-C7-C8
34	Q	615	LUT	C5-C6-C7-C8
34	T	614	LUT	C5-C6-C7-C8
34	1	615	LUT	C1-C6-C7-C8
34	1	615	LUT	C5-C6-C7-C8
34	2	315	LUT	C5-C6-C7-C8
34	9	313	LUT	C1-C6-C7-C8
34	a	314	LUT	C5-C6-C7-C8
27	4	318	LHG	C26-C27-C28-C29
31	B	850	SQD	C35-C36-C37-C38
32	6	602	LMG	C33-C34-C35-C36
28	A	848	BCR	C11-C12-C13-C14
28	A	848	BCR	C21-C22-C23-C24
28	L	207	BCR	C17-C18-C19-C20
28	8	318	BCR	C17-C18-C19-C20
34	S	316	LUT	C11-C12-C13-C14
34	S	317	LUT	C31-C32-C33-C34
34	7	314	LUT	C7-C8-C9-C10
35	P	620	XAT	C7-C8-C9-C10
36	P	617	NEX	C11-C12-C13-C14
36	T	616	NEX	C11-C12-C13-C14
25	2	303	CLA	C15-C16-C17-C18
25	6	605	CLA	C8-C10-C11-C12
27	1	618	LHG	C24-C25-C26-C27
32	1	619	LMG	C14-C15-C16-C17
25	S	315	CLA	O2A-C1-C2-C3
25	A	801	CLA	C16-C17-C18-C20
25	Q	609	CLA	C16-C17-C18-C20
27	A	844	LHG	C15-C16-C17-C18
27	5	321	LHG	C24-C25-C26-C27
25	A	807	CLA	O1D-CGD-O2D-CED
25	H	201	CLA	O1D-CGD-O2D-CED
27	4	318	LHG	C14-C15-C16-C17
32	1	619	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	B	811	CLA	CBD-CGD-O2D-CED
25	A	808	CLA	C5-C6-C7-C8
27	5	301	LHG	O2-C2-C3-O3
25	A	802	CLA	C11-C10-C8-C7
25	A	807	CLA	C2-C3-C5-C6
25	A	815	CLA	C11-C10-C8-C7
25	A	840	CLA	C6-C7-C8-C10
25	B	806	CLA	C12-C13-C15-C16
25	B	813	CLA	C6-C7-C8-C10
25	B	823	CLA	C6-C7-C8-C10
25	B	825	CLA	C6-C7-C8-C10
25	B	830	CLA	C2-C3-C5-C6
25	B	831	CLA	C11-C10-C8-C7
25	B	831	CLA	C11-C12-C13-C15
25	B	834	CLA	C11-C10-C8-C7
25	B	849	CLA	C6-C7-C8-C10
25	L	202	CLA	C11-C12-C13-C15
25	L	205	CLA	C11-C12-C13-C15
25	S	304	CLA	C6-C7-C8-C10
25	U	312	CLA	C11-C10-C8-C7
25	U	312	CLA	C12-C13-C15-C16
25	2	304	CLA	C11-C12-C13-C15
25	3	305	CLA	C11-C10-C8-C7
25	3	308	CLA	C6-C7-C8-C10
25	3	308	CLA	C12-C13-C15-C16
25	5	303	CLA	C11-C10-C8-C7
25	5	303	CLA	C12-C13-C15-C16
25	6	601	CLA	C11-C10-C8-C7
25	7	301	CLA	C11-C10-C8-C7
25	8	302	CLA	C11-C12-C13-C15
26	A	841	PQN	C17-C18-C20-C21
25	B	812	CLA	O1A-CGA-O2A-C1
28	B	851	BCR	C19-C20-C21-C22
36	U	316	NEX	C13-C14-C15-C35
25	A	829	CLA	C16-C17-C18-C19
25	Q	612	CLA	C11-C12-C13-C15
25	T	611	CLA	C11-C12-C13-C15
25	4	309	CLA	C6-C7-C8-C10
27	8	319	LHG	C33-C34-C35-C36
25	6	603	CLA	CBA-CGA-O2A-C1
27	a	317	LHG	C28-C29-C30-C31
32	J	107	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
33	S	310	CHL	O1A-CGA-O2A-C1
25	6	601	CLA	C2A-CAA-CBA-CGA
25	5	313	CLA	CBD-CGD-O2D-CED
25	B	804	CLA	C10-C11-C12-C13
25	B	821	CLA	C10-C11-C12-C13
25	8	312	CLA	CBA-CGA-O2A-C1
27	2	317	LHG	C31-C32-C33-C34
27	6	618	LHG	C11-C10-C9-C8
27	7	317	LHG	C11-C10-C9-C8
25	A	806	CLA	C8-C10-C11-C12
25	A	814	CLA	O1A-CGA-O2A-C1
25	B	804	CLA	O1A-CGA-O2A-C1
27	2	317	LHG	C33-C34-C35-C36
25	A	805	CLA	CAD-CBD-CGD-O2D
25	B	809	CLA	CAD-CBD-CGD-O2D
25	B	810	CLA	CAD-CBD-CGD-O2D
25	H	203	CLA	CAD-CBD-CGD-O2D
25	J	105	CLA	CAD-CBD-CGD-O2D
25	O	201	CLA	CAD-CBD-CGD-O2D
25	P	604	CLA	CAD-CBD-CGD-O2D
25	P	612	CLA	CAD-CBD-CGD-O2D
25	Q	604	CLA	CAD-CBD-CGD-O2D
25	R	612	CLA	CAD-CBD-CGD-O2D
25	S	311	CLA	CAD-CBD-CGD-O2D
25	S	312	CLA	CAD-CBD-CGD-O2D
25	T	603	CLA	CAD-CBD-CGD-O2D
25	T	610	CLA	CAD-CBD-CGD-O2D
25	U	304	CLA	CAD-CBD-CGD-O2D
25	3	302	CLA	CAD-CBD-CGD-O2D
25	3	307	CLA	CAD-CBD-CGD-O2D
25	3	308	CLA	CAD-CBD-CGD-O2D
25	3	311	CLA	CAD-CBD-CGD-O2D
25	4	301	CLA	CAD-CBD-CGD-O2D
25	4	310	CLA	CAD-CBD-CGD-O2D
25	5	304	CLA	CAD-CBD-CGD-O2D
25	5	309	CLA	CAD-CBD-CGD-O2D
25	6	601	CLA	CAD-CBD-CGD-O2D
25	6	604	CLA	CAD-CBD-CGD-O2D
25	6	610	CLA	CAD-CBD-CGD-O2D
25	8	314	CLA	CAD-CBD-CGD-O2D
32	J	107	LMG	C9-C8-O7-C10
32	J	102	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	A	829	CLA	C5-C6-C7-C8
25	A	853	CLA	C5-C6-C7-C8
25	B	811	CLA	C8-C10-C11-C12
25	5	305	CLA	CBD-CGD-O2D-CED
27	6	618	LHG	C24-C23-O8-C6
25	A	837	CLA	O1D-CGD-O2D-CED
25	A	839	CLA	O1D-CGD-O2D-CED
25	B	822	CLA	C4-C3-C5-C6
25	a	311	CLA	C4-C3-C5-C6
33	7	305	CHL	C4-C3-C5-C6
25	3	308	CLA	C16-C17-C18-C19
25	B	814	CLA	C5-C6-C7-C8
25	A	828	CLA	C2-C3-C5-C6
25	B	822	CLA	C2-C3-C5-C6
33	7	305	CHL	C2-C3-C5-C6
27	A	852	LHG	C2-C3-O3-P
27	2	317	LHG	C2-C3-O3-P
30	B	848	DGD	O1G-C1G-C2G-C3G
32	J	107	LMG	C7-C8-C9-O8
25	B	836	CLA	CBD-CGD-O2D-CED
27	5	301	LHG	O6-C4-C5-O7
25	A	802	CLA	C8-C10-C11-C12
25	S	314	CLA	CBA-CGA-O2A-C1
25	1	604	CLA	C2A-CAA-CBA-CGA
25	6	613	CLA	C2A-CAA-CBA-CGA
25	B	814	CLA	O1A-CGA-O2A-C1
25	6	605	CLA	C16-C17-C18-C19
25	A	809	CLA	CHA-CBD-CGD-O1D
25	A	814	CLA	CHA-CBD-CGD-O1D
25	A	814	CLA	CHA-CBD-CGD-O2D
25	A	822	CLA	CHA-CBD-CGD-O1D
25	A	822	CLA	CHA-CBD-CGD-O2D
25	A	830	CLA	CHA-CBD-CGD-O1D
25	A	830	CLA	CHA-CBD-CGD-O2D
25	A	842	CLA	CHA-CBD-CGD-O1D
25	A	842	CLA	CHA-CBD-CGD-O2D
25	B	804	CLA	CHA-CBD-CGD-O1D
25	B	804	CLA	CHA-CBD-CGD-O2D
25	B	811	CLA	CHA-CBD-CGD-O1D
25	B	811	CLA	CHA-CBD-CGD-O2D
25	B	824	CLA	CHA-CBD-CGD-O1D
25	B	824	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	B	849	CLA	CHA-CBD-CGD-O1D
25	B	849	CLA	CHA-CBD-CGD-O2D
25	G	202	CLA	CHA-CBD-CGD-O1D
25	L	209	CLA	CHA-CBD-CGD-O1D
25	L	209	CLA	CHA-CBD-CGD-O2D
25	P	603	CLA	CHA-CBD-CGD-O1D
25	P	603	CLA	CHA-CBD-CGD-O2D
25	Q	603	CLA	CHA-CBD-CGD-O1D
25	Q	603	CLA	CHA-CBD-CGD-O2D
25	R	603	CLA	CHA-CBD-CGD-O1D
25	R	603	CLA	CHA-CBD-CGD-O2D
25	S	303	CLA	CHA-CBD-CGD-O1D
25	S	320	CLA	CHA-CBD-CGD-O1D
25	S	320	CLA	CHA-CBD-CGD-O2D
25	U	303	CLA	CHA-CBD-CGD-O1D
25	U	303	CLA	CHA-CBD-CGD-O2D
25	2	303	CLA	CHA-CBD-CGD-O1D
25	2	303	CLA	CHA-CBD-CGD-O2D
25	2	304	CLA	CHA-CBD-CGD-O1D
25	7	302	CLA	CHA-CBD-CGD-O1D
25	7	302	CLA	CHA-CBD-CGD-O2D
25	7	309	CLA	CHA-CBD-CGD-O1D
25	7	309	CLA	CHA-CBD-CGD-O2D
25	8	303	CLA	CHA-CBD-CGD-O1D
25	8	303	CLA	CHA-CBD-CGD-O2D
25	8	311	CLA	CHA-CBD-CGD-O1D
25	8	311	CLA	CHA-CBD-CGD-O2D
33	1	601	CHL	CHA-CBD-CGD-O1D
33	1	601	CHL	CHA-CBD-CGD-O2D
33	4	322	CHL	CHA-CBD-CGD-O1D
33	4	322	CHL	CHA-CBD-CGD-O2D
25	8	312	CLA	O1A-CGA-O2A-C1
27	A	843	LHG	O10-C23-O8-C6
27	A	852	LHG	O10-C23-O8-C6
33	3	306	CHL	O1A-CGA-O2A-C1
32	J	107	LMG	C17-C18-C19-C20
27	A	852	LHG	O7-C5-C6-O8
32	J	104	LMG	O1-C7-C8-O7
32	6	602	LMG	O7-C8-C9-O8
32	7	319	LMG	O1-C7-C8-O7
25	A	832	CLA	CBA-CGA-O2A-C1
25	B	806	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	B	815	CLA	C11-C12-C13-C14
27	6	618	LHG	C25-C26-C27-C28
25	5	305	CLA	O1D-CGD-O2D-CED
25	Q	611	CLA	C2C-C3C-CAC-CBC
27	S	319	LHG	C30-C31-C32-C33
25	8	303	CLA	C3-C5-C6-C7
25	A	853	CLA	C4-C3-C5-C6
25	A	817	CLA	O1A-CGA-O2A-C1
25	6	603	CLA	O1A-CGA-O2A-C1
32	H	204	LMG	C10-C11-C12-C13
25	A	822	CLA	C2-C3-C5-C6
27	5	301	LHG	O9-C7-O7-C5
25	B	815	CLA	C11-C10-C8-C9
25	5	303	CLA	C11-C10-C8-C9
25	5	310	CLA	C11-C10-C8-C9
25	8	309	CLA	O1D-CGD-O2D-CED
33	7	305	CHL	C5-C6-C7-C8
25	B	838	CLA	C15-C16-C17-C18
25	B	816	CLA	C2A-CAA-CBA-CGA
25	P	604	CLA	C2A-CAA-CBA-CGA
25	5	309	CLA	C2A-CAA-CBA-CGA
25	6	601	CLA	C14-C13-C15-C16
25	B	830	CLA	CAA-CBA-CGA-O2A
25	4	307	CLA	CBA-CGA-O2A-C1
25	A	842	CLA	C3-C5-C6-C7
25	T	608	CLA	C8-C10-C11-C12
30	B	846	DGD	C2A-C3A-C4A-C5A
25	3	303	CLA	O1D-CGD-O2D-CED
25	A	824	CLA	C1A-C2A-CAA-CBA
25	B	811	CLA	C1A-C2A-CAA-CBA
25	B	824	CLA	C1A-C2A-CAA-CBA
25	B	835	CLA	C1A-C2A-CAA-CBA
25	P	604	CLA	C1A-C2A-CAA-CBA
25	T	603	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C1A-C2A-CAA-CBA
25	3	307	CLA	C1A-C2A-CAA-CBA
25	4	301	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	C1A-C2A-CAA-CBA
33	S	306	CHL	C1A-C2A-CAA-CBA
32	7	318	LMG	C10-C11-C12-C13
27	5	301	LHG	C8-C7-O7-C5
25	A	851	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	5	321	LHG	C3-O3-P-O6
27	2	317	LHG	C28-C29-C30-C31
27	6	618	LHG	C33-C34-C35-C36
27	6	618	LHG	O2-C2-C3-O3
25	8	304	CLA	O1D-CGD-O2D-CED
25	1	608	CLA	C4-C3-C5-C6
25	1	612	CLA	C4-C3-C5-C6
25	B	837	CLA	O1D-CGD-O2D-CED
25	B	804	CLA	C4B-C3B-CAB-CBB
25	B	818	CLA	C4B-C3B-CAB-CBB
25	B	826	CLA	C4B-C3B-CAB-CBB
25	Q	611	CLA	C4B-C3B-CAB-CBB
25	S	304	CLA	C4B-C3B-CAB-CBB
25	T	610	CLA	C4B-C3B-CAB-CBB
25	U	311	CLA	C4B-C3B-CAB-CBB
25	1	608	CLA	C4B-C3B-CAB-CBB
25	2	302	CLA	C4B-C3B-CAB-CBB
25	4	302	CLA	C4B-C3B-CAB-CBB
25	6	605	CLA	C4B-C3B-CAB-CBB
25	7	308	CLA	C4B-C3B-CAB-CBB
25	a	307	CLA	C4B-C3B-CAB-CBB
27	A	852	LHG	C4-O6-P-O5
27	P	618	LHG	C4-O6-P-O4
27	P	624	LHG	C4-O6-P-O4
27	Q	617	LHG	C4-O6-P-O4
27	R	618	LHG	C4-O6-P-O4
27	T	617	LHG	C4-O6-P-O4
27	5	321	LHG	C4-O6-P-O5
27	6	618	LHG	C3-O3-P-O4
27	7	317	LHG	C3-O3-P-O5
27	8	319	LHG	C3-O3-P-O4
33	P	608	CHL	C4B-C3B-CAB-CBB
33	Q	607	CHL	C4B-C3B-CAB-CBB
33	R	608	CHL	C4B-C3B-CAB-CBB
33	T	606	CHL	C4B-C3B-CAB-CBB
33	U	308	CHL	C4B-C3B-CAB-CBB
33	4	314	CHL	C4B-C3B-CAB-CBB
33	5	307	CHL	C4B-C3B-CAB-CBB
33	5	317	CHL	C4B-C3B-CAB-CBB
33	6	608	CHL	C4B-C3B-CAB-CBB
33	6	617	CHL	C4B-C3B-CAB-CBB
25	A	819	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	R	611	CLA	C11-C12-C13-C15
25	A	805	CLA	CBD-CGD-O2D-CED
27	5	321	LHG	O6-C4-C5-C6
25	7	301	CLA	C5-C6-C7-C8
25	1	613	CLA	C3-C5-C6-C7
25	6	610	CLA	C3-C5-C6-C7
33	Q	608	CHL	O1A-CGA-O2A-C1
33	R	609	CHL	O1A-CGA-O2A-C1
25	a	311	CLA	C16-C17-C18-C19
25	A	806	CLA	CAD-CBD-CGD-O1D
25	A	814	CLA	CAD-CBD-CGD-O1D
25	A	816	CLA	CAD-CBD-CGD-O1D
25	A	825	CLA	CAD-CBD-CGD-O1D
25	A	836	CLA	CAD-CBD-CGD-O1D
25	A	842	CLA	CAD-CBD-CGD-O1D
25	B	804	CLA	CAD-CBD-CGD-O1D
25	B	811	CLA	CAD-CBD-CGD-O1D
25	B	812	CLA	CAD-CBD-CGD-O1D
25	B	824	CLA	CAD-CBD-CGD-O1D
25	G	202	CLA	CAD-CBD-CGD-O1D
25	S	303	CLA	CAD-CBD-CGD-O1D
25	2	303	CLA	CAD-CBD-CGD-O1D
25	2	304	CLA	CAD-CBD-CGD-O1D
25	6	623	CLA	CAD-CBD-CGD-O1D
36	P	621	NEX	C7-C8-C9-C10
25	5	319	CLA	CBD-CGD-O2D-CED
32	H	204	LMG	C28-C29-C30-C31
33	4	305	CHL	CAA-CBA-CGA-O2A
25	A	832	CLA	O1A-CGA-O2A-C1
33	P	609	CHL	O1A-CGA-O2A-C1
32	1	619	LMG	C10-C11-C12-C13
30	B	848	DGD	C3B-C4B-C5B-C6B
25	a	307	CLA	CBA-CGA-O2A-C1
25	4	307	CLA	O1A-CGA-O2A-C1
25	B	810	CLA	O1D-CGD-O2D-CED
25	B	811	CLA	C13-C15-C16-C17
25	A	814	CLA	C16-C17-C18-C19
25	A	806	CLA	C11-C10-C8-C7
25	A	851	CLA	C11-C12-C13-C15
25	A	851	CLA	C12-C13-C15-C16
25	B	801	CLA	C6-C7-C8-C10
25	B	806	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	B	813	CLA	C11-C10-C8-C7
25	B	815	CLA	C11-C10-C8-C7
25	B	824	CLA	C3A-C2A-CAA-CBA
25	L	202	CLA	C6-C7-C8-C10
25	P	612	CLA	C11-C10-C8-C7
25	R	612	CLA	C11-C10-C8-C7
25	1	612	CLA	C6-C7-C8-C10
25	3	320	CLA	C11-C12-C13-C15
25	5	310	CLA	C11-C10-C8-C7
25	5	324	CLA	C6-C7-C8-C10
25	6	603	CLA	C11-C10-C8-C7
25	6	605	CLA	C11-C10-C8-C7
25	6	605	CLA	C12-C13-C15-C16
25	a	311	CLA	C6-C7-C8-C10
33	P	609	CHL	C11-C10-C8-C7
33	Q	608	CHL	C11-C10-C8-C7
33	R	609	CHL	C11-C10-C8-C7
32	1	619	LMG	C29-C30-C31-C32
25	S	314	CLA	O1A-CGA-O2A-C1
25	B	825	CLA	CAA-CBA-CGA-O2A
25	8	302	CLA	C2C-C3C-CAC-CBC
30	B	846	DGD	C1B-C2B-C3B-C4B
27	B	847	LHG	C26-C27-C28-C29
27	4	318	LHG	C9-C10-C11-C12
32	2	301	LMG	C12-C13-C14-C15
33	U	309	CHL	C2C-C3C-CAC-CBC
27	7	317	LHG	C10-C11-C12-C13
25	8	315	CLA	CBD-CGD-O2D-CED
25	Q	604	CLA	C2A-CAA-CBA-CGA
25	U	304	CLA	C2A-CAA-CBA-CGA
25	1	602	CLA	C2A-CAA-CBA-CGA
25	S	314	CLA	C16-C17-C18-C20
25	a	312	CLA	C3-C5-C6-C7
27	8	319	LHG	C4-C5-C6-O8
32	7	319	LMG	O1-C7-C8-C9
33	P	601	CHL	C1C-C2C-CMC-OMC
33	P	606	CHL	C1C-C2C-CMC-OMC
33	P	607	CHL	C1C-C2C-CMC-OMC
33	P	608	CHL	C1C-C2C-CMC-OMC
33	P	619	CHL	C1C-C2C-CMC-OMC
33	Q	601	CHL	C1C-C2C-CMC-OMC
33	Q	606	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
33	Q	607	CHL	C1C-C2C-CMC-OMC
33	R	601	CHL	C1C-C2C-CMC-OMC
33	R	606	CHL	C1C-C2C-CMC-OMC
33	R	607	CHL	C1C-C2C-CMC-OMC
33	R	608	CHL	C1C-C2C-CMC-OMC
33	S	306	CHL	C1C-C2C-CMC-OMC
33	S	308	CHL	C1C-C2C-CMC-OMC
33	S	310	CHL	C1C-C2C-CMC-OMC
33	S	321	CHL	C1C-C2C-CMC-OMC
33	T	601	CHL	C1C-C2C-CMC-OMC
33	T	605	CHL	C1C-C2C-CMC-OMC
33	T	606	CHL	C1C-C2C-CMC-OMC
33	U	305	CHL	C1C-C2C-CMC-OMC
33	U	306	CHL	C1C-C2C-CMC-OMC
33	U	307	CHL	C1C-C2C-CMC-OMC
33	1	606	CHL	C1C-C2C-CMC-OMC
33	4	314	CHL	C1C-C2C-CMC-OMC
33	5	317	CHL	C1C-C2C-CMC-OMC
33	6	617	CHL	C1C-C2C-CMC-OMC
33	9	306	CHL	C1C-C2C-CMC-OMC
33	9	307	CHL	C1C-C2C-CMC-OMC
33	a	305	CHL	C1C-C2C-CMC-OMC
31	B	850	SQD	O6-C44-C45-O47
32	J	107	LMG	O7-C8-C9-O8
32	7	318	LMG	O1-C7-C8-O7
25	P	611	CLA	C4C-C3C-CAC-CBC
25	P	610	CLA	C8-C10-C11-C12
32	H	204	LMG	C35-C36-C37-C38
25	A	819	CLA	C16-C17-C18-C19
25	1	612	CLA	C16-C17-C18-C19
25	A	825	CLA	C3-C5-C6-C7
25	A	837	CLA	C4-C3-C5-C6
25	6	601	CLA	C4-C3-C5-C6
25	B	834	CLA	C2-C3-C5-C6
25	A	803	CLA	C11-C12-C13-C14
25	A	840	CLA	C6-C7-C8-C9
25	B	825	CLA	C14-C13-C15-C16
25	B	831	CLA	C11-C12-C13-C14
25	B	834	CLA	C11-C10-C8-C9
25	L	201	CLA	C11-C12-C13-C14
25	L	202	CLA	C6-C7-C8-C9
25	L	202	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	R	602	CLA	C6-C7-C8-C9
25	1	608	CLA	C11-C10-C8-C9
25	2	312	CLA	C6-C7-C8-C9
25	8	310	CLA	C11-C10-C8-C9
25	8	313	CLA	C11-C12-C13-C14
25	a	311	CLA	C6-C7-C8-C9
33	P	609	CHL	C14-C13-C15-C16
33	Q	608	CHL	C14-C13-C15-C16
33	R	609	CHL	C14-C13-C15-C16
25	A	826	CLA	O1D-CGD-O2D-CED
25	5	313	CLA	O1D-CGD-O2D-CED
33	4	304	CHL	O1D-CGD-O2D-CED
30	B	848	DGD	O6E-C5E-C6E-O5E
31	B	850	SQD	C26-C27-C28-C29
25	Q	609	CLA	C8-C10-C11-C12
36	T	616	NEX	C11-C12-C13-C20
25	U	310	CLA	C8-C10-C11-C12
25	A	812	CLA	C16-C17-C18-C19
28	L	204	BCR	C17-C18-C19-C20
27	a	317	LHG	C10-C11-C12-C13
25	A	801	CLA	C2B-C3B-CAB-CBB
25	A	812	CLA	C2B-C3B-CAB-CBB
25	A	815	CLA	C2B-C3B-CAB-CBB
25	A	831	CLA	C2B-C3B-CAB-CBB
25	B	802	CLA	C2B-C3B-CAB-CBB
25	B	825	CLA	C2B-C3B-CAB-CBB
25	L	201	CLA	C2B-C3B-CAB-CBB
25	O	202	CLA	C2B-C3B-CAB-CBB
25	S	311	CLA	C2B-C3B-CAB-CBB
25	T	603	CLA	C2B-C3B-CAB-CBB
25	U	304	CLA	C2B-C3B-CAB-CBB
25	1	612	CLA	C2B-C3B-CAB-CBB
25	2	302	CLA	C2B-C3B-CAB-CBB
25	2	311	CLA	C2B-C3B-CAB-CBB
25	4	310	CLA	C2B-C3B-CAB-CBB
25	5	305	CLA	C2B-C3B-CAB-CBB
25	5	310	CLA	C2B-C3B-CAB-CBB
25	6	614	CLA	C2B-C3B-CAB-CBB
25	7	308	CLA	C2B-C3B-CAB-CBB
25	7	312	CLA	C2B-C3B-CAB-CBB
25	8	303	CLA	C2B-C3B-CAB-CBB
25	8	312	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	a	311	CLA	C2B-C3B-CAB-CBB
33	P	608	CHL	C2B-C3B-CAB-CBB
33	Q	607	CHL	C2B-C3B-CAB-CBB
33	R	608	CHL	C2B-C3B-CAB-CBB
33	U	308	CHL	C2B-C3B-CAB-CBB
33	6	617	CHL	C2B-C3B-CAB-CBB
27	A	844	LHG	O9-C7-O7-C5
25	A	804	CLA	C8-C10-C11-C12
25	B	810	CLA	C4-C3-C5-C6
25	a	311	CLA	C2-C3-C5-C6
25	T	610	CLA	C2C-C3C-CAC-CBC
25	A	823	CLA	C1-C2-C3-C4
25	B	829	CLA	C1-C2-C3-C4
33	P	606	CHL	C1-C2-C3-C4
33	Q	606	CHL	C1-C2-C3-C4
33	R	606	CHL	C1-C2-C3-C4
33	S	307	CHL	C1-C2-C3-C4
33	T	601	CHL	C1-C2-C3-C4
33	T	605	CHL	C1-C2-C3-C4
33	U	306	CHL	C1-C2-C3-C4
25	A	810	CLA	C3-C5-C6-C7
25	A	837	CLA	C10-C11-C12-C13
25	B	815	CLA	O1D-CGD-O2D-CED
25	A	820	CLA	C2A-CAA-CBA-CGA
25	B	802	CLA	C2A-CAA-CBA-CGA
25	B	804	CLA	C2A-CAA-CBA-CGA
25	B	834	CLA	C2A-CAA-CBA-CGA
25	Q	612	CLA	C2A-CAA-CBA-CGA
25	R	613	CLA	C2A-CAA-CBA-CGA
25	T	611	CLA	C2A-CAA-CBA-CGA
25	U	312	CLA	C2A-CAA-CBA-CGA
25	8	304	CLA	C2A-CAA-CBA-CGA
25	8	310	CLA	C2A-CAA-CBA-CGA
25	a	301	CLA	C2A-CAA-CBA-CGA
25	P	613	CLA	CBA-CGA-O2A-C1
25	A	826	CLA	C2-C1-O2A-CGA
25	B	815	CLA	C2-C1-O2A-CGA
25	R	603	CLA	C2-C1-O2A-CGA
25	1	613	CLA	C2-C1-O2A-CGA
25	9	310	CLA	C2-C1-O2A-CGA
25	a	312	CLA	C2-C1-O2A-CGA
33	S	302	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
33	T	607	CHL	C2-C1-O2A-CGA
25	5	319	CLA	O1D-CGD-O2D-CED
25	9	308	CLA	O1D-CGD-O2D-CED
32	7	318	LMG	C29-C30-C31-C32
25	3	314	CLA	CBD-CGD-O2D-CED
28	B	843	BCR	C19-C20-C21-C22
25	P	613	CLA	O1A-CGA-O2A-C1
25	a	307	CLA	O1A-CGA-O2A-C1
27	6	618	LHG	O10-C23-O8-C6
25	R	610	CLA	C8-C10-C11-C12
25	a	307	CLA	C4-C3-C5-C6
25	A	805	CLA	O1D-CGD-O2D-CED
25	B	824	CLA	O1D-CGD-O2D-CED
28	B	843	BCR	C23-C24-C25-C26
28	3	317	BCR	C1-C6-C7-C8
34	P	615	LUT	C5-C6-C7-C8
34	R	616	LUT	C5-C6-C7-C8
34	U	315	LUT	C5-C6-C7-C8
34	2	315	LUT	C1-C6-C7-C8
34	9	312	LUT	C1-C6-C7-C8
34	9	313	LUT	C5-C6-C7-C8
25	A	853	CLA	C2-C3-C5-C6
25	1	612	CLA	C2-C3-C5-C6
25	2	304	CLA	C2-C3-C5-C6
25	4	308	CLA	C2-C3-C5-C6
33	P	622	CHL	C2-C3-C5-C6
25	B	802	CLA	O1A-CGA-O2A-C1
27	8	319	LHG	C17-C18-C19-C20
25	Q	611	CLA	C4C-C3C-CAC-CBC
25	S	311	CLA	C11-C12-C13-C14
25	1	612	CLA	C16-C17-C18-C20
25	3	308	CLA	C16-C17-C18-C20
25	a	311	CLA	C16-C17-C18-C20
27	2	317	LHG	C13-C14-C15-C16
32	J	102	LMG	C10-C11-C12-C13
25	A	802	CLA	C2A-CAA-CBA-CGA
25	G	201	CLA	C2A-CAA-CBA-CGA
25	R	604	CLA	C2A-CAA-CBA-CGA
25	2	303	CLA	C2A-CAA-CBA-CGA
27	8	319	LHG	O7-C5-C6-O8
30	B	846	DGD	O2G-C2G-C3G-O3G
32	J	107	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
32	2	301	LMG	O1-C7-C8-O7
27	A	843	LHG	C3-O3-P-O6
27	P	618	LHG	C3-O3-P-O6
27	P	624	LHG	C3-O3-P-O6
27	Q	617	LHG	C3-O3-P-O6
27	R	618	LHG	C3-O3-P-O6
27	S	319	LHG	C3-O3-P-O6
27	T	617	LHG	C3-O3-P-O6
27	1	618	LHG	C3-O3-P-O6
27	1	618	LHG	C4-O6-P-O3
27	2	317	LHG	C3-O3-P-O6
27	4	318	LHG	C3-O3-P-O6
27	4	318	LHG	C4-O6-P-O3
27	4	319	LHG	C3-O3-P-O6
27	4	319	LHG	C4-O6-P-O3
27	a	317	LHG	C3-O3-P-O6
27	a	317	LHG	C4-O6-P-O3
27	7	317	LHG	C4-C5-C6-O8
25	B	805	CLA	C4-C3-C5-C6
25	B	816	CLA	C5-C6-C7-C8
25	B	826	CLA	C5-C6-C7-C8
25	B	830	CLA	C12-C13-C15-C16
25	Q	602	CLA	C6-C7-C8-C10
25	R	602	CLA	C6-C7-C8-C10
25	T	608	CLA	C12-C13-C15-C16
25	T	609	CLA	C11-C10-C8-C7
25	3	302	CLA	C11-C12-C13-C15
25	5	304	CLA	O1A-CGA-O2A-C1
27	A	843	LHG	C10-C11-C12-C13
25	A	851	CLA	C14-C13-C15-C16
25	B	801	CLA	C6-C7-C8-C9
25	B	806	CLA	C11-C10-C8-C9
25	B	806	CLA	C14-C13-C15-C16
25	B	813	CLA	C11-C10-C8-C9
25	B	822	CLA	C14-C13-C15-C16
25	B	830	CLA	C14-C13-C15-C16
25	B	837	CLA	C14-C13-C15-C16
25	B	849	CLA	C11-C10-C8-C9
25	Q	602	CLA	C6-C7-C8-C9
25	R	613	CLA	C11-C12-C13-C14
25	1	612	CLA	C6-C7-C8-C9
25	5	324	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	6	603	CLA	C11-C10-C8-C9
25	a	307	CLA	C11-C10-C8-C9
25	6	604	CLA	O1D-CGD-O2D-CED
35	P	620	XAT	C9-C10-C11-C12
35	Q	616	XAT	C9-C10-C11-C12
25	B	836	CLA	C16-C17-C18-C20
25	U	311	CLA	C2C-C3C-CAC-CBC
25	B	802	CLA	CBA-CGA-O2A-C1
25	T	611	CLA	CBA-CGA-O2A-C1
25	B	802	CLA	C8-C10-C11-C12
25	B	827	CLA	O1A-CGA-O2A-C1
27	2	317	LHG	C26-C27-C28-C29
32	J	102	LMG	C31-C32-C33-C34
25	4	307	CLA	C2A-CAA-CBA-CGA
25	7	313	CLA	C2A-CAA-CBA-CGA
27	6	618	LHG	C17-C18-C19-C20
28	6	621	BCR	C11-C12-C13-C35
27	B	847	LHG	C2-C3-O3-P
27	4	318	LHG	C2-C3-O3-P
25	T	611	CLA	O1A-CGA-O2A-C1
25	U	302	CLA	C10-C11-C12-C13
28	O	204	BCR	C7-C8-C9-C10
28	4	317	BCR	C17-C18-C19-C20
32	1	619	LMG	C20-C21-C22-C23
25	6	611	CLA	C5-C6-C7-C8
25	T	610	CLA	C4C-C3C-CAC-CBC
25	A	829	CLA	C4-C3-C5-C6
25	7	303	CLA	C4-C3-C5-C6
32	J	107	LMG	C28-C29-C30-C31
27	5	301	LHG	O1-C1-C2-O2
27	6	618	LHG	O1-C1-C2-O2
25	S	314	CLA	C16-C17-C18-C19
25	4	308	CLA	C11-C12-C13-C15
25	B	827	CLA	CBA-CGA-O2A-C1
25	S	305	CLA	CBA-CGA-O2A-C1
25	U	312	CLA	CBA-CGA-O2A-C1
25	1	608	CLA	CBA-CGA-O2A-C1
25	8	310	CLA	CBA-CGA-O2A-C1
27	7	317	LHG	C7-C8-C9-C10
25	B	820	CLA	C11-C12-C13-C14
25	A	831	CLA	C4B-C3B-CAB-CBB
25	B	802	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	B	816	CLA	C4B-C3B-CAB-CBB
25	P	613	CLA	C4B-C3B-CAB-CBB
25	R	604	CLA	C4B-C3B-CAB-CBB
25	S	311	CLA	C4B-C3B-CAB-CBB
25	T	603	CLA	C4B-C3B-CAB-CBB
25	T	611	CLA	C4B-C3B-CAB-CBB
25	U	304	CLA	C4B-C3B-CAB-CBB
25	U	312	CLA	C4B-C3B-CAB-CBB
25	5	305	CLA	C4B-C3B-CAB-CBB
25	6	614	CLA	C4B-C3B-CAB-CBB
25	a	311	CLA	C4B-C3B-CAB-CBB
25	R	602	CLA	C2A-CAA-CBA-CGA
25	S	311	CLA	C2A-CAA-CBA-CGA
25	3	301	CLA	C2A-CAA-CBA-CGA
25	9	303	CLA	C2A-CAA-CBA-CGA
25	B	836	CLA	C16-C17-C18-C19
25	5	310	CLA	C11-C12-C13-C14
25	B	810	CLA	C5-C6-C7-C8
27	Q	617	LHG	C28-C29-C30-C31
25	U	312	CLA	O1A-CGA-O2A-C1
25	8	310	CLA	O1A-CGA-O2A-C1
25	R	602	CLA	C10-C11-C12-C13
25	A	819	CLA	CAA-CBA-CGA-O2A
25	1	604	CLA	C4-C3-C5-C6
25	5	324	CLA	C4-C3-C5-C6
25	8	312	CLA	C4-C3-C5-C6
25	B	826	CLA	C2-C3-C5-C6
25	S	305	CLA	O1A-CGA-O2A-C1
25	B	811	CLA	O1D-CGD-O2D-CED
25	6	603	CLA	C10-C11-C12-C13
25	a	308	CLA	C8-C10-C11-C12
35	P	623	XAT	C7-C8-C9-C10
35	P	623	XAT	C9-C10-C11-C12
25	A	811	CLA	C2-C1-O2A-CGA
25	A	814	CLA	C2-C1-O2A-CGA
25	B	809	CLA	C2-C1-O2A-CGA
25	B	829	CLA	C2-C1-O2A-CGA
25	B	837	CLA	C2-C1-O2A-CGA
25	P	603	CLA	C2-C1-O2A-CGA
25	Q	603	CLA	C2-C1-O2A-CGA
25	S	320	CLA	C2-C1-O2A-CGA
25	U	303	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	1	603	CLA	C2-C1-O2A-CGA
33	P	609	CHL	C2-C1-O2A-CGA
33	Q	608	CHL	C2-C1-O2A-CGA
33	R	609	CHL	C2-C1-O2A-CGA
33	T	607	CHL	C2C-C3C-CAC-CBC
25	T	609	CLA	C10-C11-C12-C13
25	A	816	CLA	C8-C10-C11-C12
25	A	828	CLA	C5-C6-C7-C8
25	B	812	CLA	C2A-CAA-CBA-CGA
25	P	602	CLA	C2A-CAA-CBA-CGA
25	Q	602	CLA	C2A-CAA-CBA-CGA
25	T	602	CLA	C2A-CAA-CBA-CGA
25	U	302	CLA	C2A-CAA-CBA-CGA
25	6	610	CLA	C2A-CAA-CBA-CGA
25	7	301	CLA	C2A-CAA-CBA-CGA
25	a	311	CLA	C2A-CAA-CBA-CGA
33	R	606	CHL	C2A-CAA-CBA-CGA
25	A	801	CLA	CAA-CBA-CGA-O2A
25	B	834	CLA	CBD-CGD-O2D-CED
25	U	311	CLA	C4C-C3C-CAC-CBC
27	A	844	LHG	C11-C12-C13-C14
27	5	321	LHG	C28-C29-C30-C31
25	B	803	CLA	C3A-C2A-CAA-CBA
25	B	815	CLA	C3A-C2A-CAA-CBA
25	R	604	CLA	C3A-C2A-CAA-CBA
25	5	324	CLA	C3A-C2A-CAA-CBA
25	8	302	CLA	C3A-C2A-CAA-CBA
25	A	838	CLA	C13-C15-C16-C17
25	A	832	CLA	C16-C17-C18-C19
25	3	302	CLA	C16-C17-C18-C19
31	B	850	SQD	O47-C7-C8-C9
32	6	602	LMG	C29-C30-C31-C32
27	S	319	LHG	C16-C17-C18-C19
25	B	826	CLA	C4-C3-C5-C6
25	L	205	CLA	C4-C3-C5-C6
32	6	602	LMG	C12-C13-C14-C15
25	1	608	CLA	C2-C3-C5-C6
25	7	302	CLA	CAA-CBA-CGA-O2A
25	A	810	CLA	C11-C10-C8-C9
25	A	818	CLA	C14-C13-C15-C16
25	L	205	CLA	C11-C10-C8-C9
25	P	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	Q	603	CLA	C11-C12-C13-C14
25	R	610	CLA	C14-C13-C15-C16
25	S	320	CLA	C11-C12-C13-C14
25	U	302	CLA	C6-C7-C8-C9
25	U	303	CLA	C11-C12-C13-C14
25	5	302	CLA	C11-C10-C8-C9
25	A	822	CLA	C13-C15-C16-C17
30	B	846	DGD	CEA-CFA-CGA-CHA
28	A	849	BCR	C11-C10-C9-C34
28	A	849	BCR	C16-C17-C18-C36
28	B	842	BCR	C11-C10-C9-C34
28	B	842	BCR	C20-C21-C22-C37
28	F	803	BCR	C35-C13-C14-C15
28	L	204	BCR	C11-C10-C9-C34
28	3	318	BCR	C35-C13-C14-C15
28	3	318	BCR	C16-C17-C18-C36
28	3	319	BCR	C35-C13-C14-C15
28	3	319	BCR	C16-C17-C18-C36
28	4	321	BCR	C20-C21-C22-C37
30	B	846	DGD	C1G-C2G-C3G-O3G
36	P	617	NEX	C39-C29-C30-C31
36	P	621	NEX	C39-C29-C30-C31
36	R	617	NEX	C39-C29-C30-C31
36	T	616	NEX	C39-C29-C30-C31
36	U	301	NEX	C39-C29-C30-C31
36	U	316	NEX	C39-C29-C30-C31
25	T	603	CLA	C2A-CAA-CBA-CGA
25	2	302	CLA	C2A-CAA-CBA-CGA
33	P	606	CHL	C2A-CAA-CBA-CGA
27	A	852	LHG	C13-C14-C15-C16
27	Q	617	LHG	C13-C14-C15-C16
25	R	611	CLA	C11-C12-C13-C14
25	S	311	CLA	C11-C12-C13-C15
25	B	836	CLA	O1D-CGD-O2D-CED
25	B	824	CLA	C2C-C3C-CAC-CBC
25	a	306	CLA	C3-C5-C6-C7
25	B	824	CLA	CBD-CGD-O2D-CED
27	P	624	LHG	C31-C32-C33-C34
32	7	318	LMG	C7-C8-O7-C10
25	B	815	CLA	C1A-C2A-CAA-CBA
25	B	830	CLA	C1A-C2A-CAA-CBA
25	B	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	R	604	CLA	C1A-C2A-CAA-CBA
25	S	315	CLA	C1A-C2A-CAA-CBA
25	3	305	CLA	C1A-C2A-CAA-CBA
25	5	319	CLA	C1A-C2A-CAA-CBA
25	5	324	CLA	C1A-C2A-CAA-CBA
25	8	302	CLA	C1A-C2A-CAA-CBA
25	8	311	CLA	C1A-C2A-CAA-CBA
33	6	606	CHL	C1A-C2A-CAA-CBA
33	6	608	CHL	C1A-C2A-CAA-CBA
33	7	305	CHL	C1A-C2A-CAA-CBA
25	A	814	CLA	C11-C10-C8-C7
25	B	824	CLA	C11-C12-C13-C15
25	B	826	CLA	C11-C10-C8-C7
25	L	201	CLA	C11-C10-C8-C7
25	P	612	CLA	C6-C7-C8-C10
25	R	612	CLA	C6-C7-C8-C10
25	1	603	CLA	C11-C12-C13-C15
25	2	304	CLA	C12-C13-C15-C16
25	6	601	CLA	C2-C3-C5-C6
25	7	308	CLA	C11-C10-C8-C7
25	1	609	CLA	C8-C10-C11-C12
32	2	301	LMG	C4-C5-C6-O5
25	A	834	CLA	CAA-CBA-CGA-O1A
34	S	316	LUT	C33-C34-C35-C15
35	T	615	XAT	C9-C10-C11-C12
33	P	605	CHL	C3C-C2C-CMC-OMC
33	Q	605	CHL	C3C-C2C-CMC-OMC
33	T	604	CHL	C3C-C2C-CMC-OMC
33	U	308	CHL	C3C-C2C-CMC-OMC
25	B	834	CLA	C3-C5-C6-C7
25	1	612	CLA	C3-C5-C6-C7
33	T	607	CHL	O1D-CGD-O2D-CED
25	B	811	CLA	C2A-CAA-CBA-CGA
25	B	815	CLA	C2A-CAA-CBA-CGA
25	1	612	CLA	C2A-CAA-CBA-CGA
33	T	605	CHL	C2A-CAA-CBA-CGA
33	U	306	CHL	C2A-CAA-CBA-CGA
25	A	801	CLA	C5-C6-C7-C8
25	A	807	CLA	C10-C11-C12-C13
25	P	602	CLA	C10-C11-C12-C13
33	U	306	CHL	O1A-CGA-O2A-C1
25	A	828	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	B	815	CLA	CAA-CBA-CGA-O2A
25	7	303	CLA	CBA-CGA-O2A-C1
27	8	319	LHG	C13-C14-C15-C16
33	U	309	CHL	C4C-C3C-CAC-CBC
32	H	204	LMG	C32-C33-C34-C35
27	A	844	LHG	C8-C7-O7-C5
25	1	607	CLA	C3-C5-C6-C7
25	Q	602	CLA	C10-C11-C12-C13
25	A	806	CLA	C4-C3-C5-C6
32	1	619	LMG	C12-C13-C14-C15
25	B	805	CLA	C2-C3-C5-C6
25	7	303	CLA	C2-C3-C5-C6
25	a	307	CLA	C2-C3-C5-C6
25	A	806	CLA	C2B-C3B-CAB-CBB
25	B	804	CLA	C2B-C3B-CAB-CBB
25	B	811	CLA	C2B-C3B-CAB-CBB
25	B	816	CLA	C2B-C3B-CAB-CBB
25	B	818	CLA	C2B-C3B-CAB-CBB
25	P	613	CLA	C2B-C3B-CAB-CBB
25	Q	604	CLA	C2B-C3B-CAB-CBB
25	Q	611	CLA	C2B-C3B-CAB-CBB
25	R	613	CLA	C2B-C3B-CAB-CBB
25	S	304	CLA	C2B-C3B-CAB-CBB
25	T	610	CLA	C2B-C3B-CAB-CBB
25	T	611	CLA	C2B-C3B-CAB-CBB
25	U	311	CLA	C2B-C3B-CAB-CBB
25	1	608	CLA	C2B-C3B-CAB-CBB
25	4	302	CLA	C2B-C3B-CAB-CBB
25	6	605	CLA	C2B-C3B-CAB-CBB
25	a	307	CLA	C2B-C3B-CAB-CBB
33	T	606	CHL	C2B-C3B-CAB-CBB
33	4	314	CHL	C2B-C3B-CAB-CBB
33	4	322	CHL	C2B-C3B-CAB-CBB
33	5	307	CHL	C2B-C3B-CAB-CBB
33	5	317	CHL	C2B-C3B-CAB-CBB
33	7	305	CHL	C2B-C3B-CAB-CBB
27	P	618	LHG	C31-C32-C33-C34
25	A	832	CLA	C16-C17-C18-C20
28	A	849	BCR	C11-C10-C9-C8
28	A	849	BCR	C16-C17-C18-C19
28	B	842	BCR	C11-C10-C9-C8
28	B	842	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
28	F	803	BCR	C12-C13-C14-C15
28	L	204	BCR	C11-C10-C9-C8
28	3	318	BCR	C12-C13-C14-C15
28	3	318	BCR	C16-C17-C18-C19
28	3	319	BCR	C12-C13-C14-C15
28	3	319	BCR	C16-C17-C18-C19
28	4	321	BCR	C20-C21-C22-C23
36	P	617	NEX	C28-C29-C30-C31
36	P	621	NEX	C28-C29-C30-C31
36	R	617	NEX	C28-C29-C30-C31
36	T	616	NEX	C28-C29-C30-C31
36	U	301	NEX	C28-C29-C30-C31
36	U	316	NEX	C28-C29-C30-C31
27	4	319	LHG	O7-C5-C6-O8
32	H	204	LMG	O7-C8-C9-O8
25	B	838	CLA	CBA-CGA-O2A-C1
25	5	309	CLA	O1D-CGD-O2D-CED
25	A	825	CLA	C2C-C3C-CAC-CBC
27	T	617	LHG	C31-C32-C33-C34
28	G	203	BCR	C9-C10-C11-C12
28	J	101	BCR	C19-C20-C21-C22
35	P	620	XAT	C29-C30-C31-C32
35	Q	616	XAT	C29-C30-C31-C32
35	T	615	XAT	C29-C30-C31-C32
25	7	303	CLA	O1A-CGA-O2A-C1
25	B	807	CLA	C16-C17-C18-C20
25	Q	612	CLA	C11-C12-C13-C14
27	R	618	LHG	C31-C32-C33-C34
27	4	319	LHG	C9-C10-C11-C12
33	T	607	CHL	CBD-CGD-O2D-CED
25	B	838	CLA	O1A-CGA-O2A-C1
25	1	608	CLA	O1A-CGA-O2A-C1
33	P	606	CHL	O1A-CGA-O2A-C1
27	S	319	LHG	C1-C2-C3-O3
25	A	834	CLA	CAA-CBA-CGA-O2A
25	A	805	CLA	C3-C5-C6-C7
25	B	808	CLA	C4-C3-C5-C6
33	1	606	CHL	C2-C1-O2A-CGA
25	A	804	CLA	C2-C1-O2A-CGA
25	A	836	CLA	C2-C1-O2A-CGA
25	B	802	CLA	C2-C1-O2A-CGA
25	B	826	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	a	302	CLA	C2-C1-O2A-CGA
33	P	606	CHL	C2-C1-O2A-CGA
33	Q	606	CHL	C2-C1-O2A-CGA
33	R	606	CHL	C2-C1-O2A-CGA
33	S	307	CHL	C2-C1-O2A-CGA
33	S	309	CHL	C2-C1-O2A-CGA
33	U	306	CHL	C2-C1-O2A-CGA
33	4	322	CHL	C2-C1-O2A-CGA
25	8	315	CLA	O1D-CGD-O2D-CED
25	A	829	CLA	C2-C3-C5-C6
33	a	305	CHL	C2-C1-O2A-CGA
33	R	606	CHL	O1A-CGA-O2A-C1
33	T	605	CHL	O1A-CGA-O2A-C1
25	A	807	CLA	C11-C10-C8-C9
25	A	837	CLA	C14-C13-C15-C16
25	B	807	CLA	C14-C13-C15-C16
25	P	602	CLA	C6-C7-C8-C9
25	S	313	CLA	C11-C10-C8-C9
25	T	602	CLA	C6-C7-C8-C9
25	5	302	CLA	C6-C7-C8-C9
25	6	603	CLA	C14-C13-C15-C16
25	U	310	CLA	C15-C16-C17-C18
33	Q	606	CHL	O1A-CGA-O2A-C1
33	Q	608	CHL	C2C-C3C-CAC-CBC
33	S	310	CHL	C4-C3-C5-C6
33	T	607	CHL	C4-C3-C5-C6
25	3	309	CLA	O1D-CGD-O2D-CED
27	B	847	LHG	O2-C2-C3-O3
33	R	609	CHL	C2C-C3C-CAC-CBC
33	Q	606	CHL	C2A-CAA-CBA-CGA
25	T	611	CLA	C11-C12-C13-C14
25	A	829	CLA	O1A-CGA-O2A-C1
25	4	303	CLA	O1A-CGA-O2A-C1
28	B	840	BCR	C23-C24-C25-C30
28	O	204	BCR	C1-C6-C7-C8
28	3	319	BCR	C1-C6-C7-C8
28	4	317	BCR	C1-C6-C7-C8
28	4	317	BCR	C5-C6-C7-C8
28	8	301	BCR	C23-C24-C25-C30
34	R	615	LUT	C1-C6-C7-C8
34	R	615	LUT	C5-C6-C7-C8
34	S	316	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	S	317	LUT	C1-C6-C7-C8
34	6	619	LUT	C1-C6-C7-C8
34	6	622	LUT	C1-C6-C7-C8
34	8	316	LUT	C1-C6-C7-C8
34	8	317	LUT	C1-C6-C7-C8
34	9	312	LUT	C5-C6-C7-C8
26	A	841	PQN	C18-C20-C21-C22
25	8	304	CLA	CAA-CBA-CGA-O2A
27	7	317	LHG	O1-C1-C2-C3
27	8	319	LHG	O1-C1-C2-C3
35	P	616	XAT	C9-C10-C11-C12
25	Q	612	CLA	CBA-CGA-O2A-C1
33	P	609	CHL	C2C-C3C-CAC-CBC
25	A	805	CLA	C4-C3-C5-C6
25	B	815	CLA	C4-C3-C5-C6
25	5	312	CLA	C4-C3-C5-C6
25	7	304	CLA	C1A-C2A-CAA-CBA
28	A	846	BCR	C7-C8-C9-C10
34	4	316	LUT	C11-C12-C13-C14
35	Q	616	XAT	C7-C8-C9-C10
35	T	615	XAT	C7-C8-C9-C10
36	R	617	NEX	C11-C12-C13-C14
25	A	837	CLA	C2-C3-C5-C6
25	B	810	CLA	C2-C3-C5-C6
25	3	307	CLA	CAA-CBA-CGA-O2A
25	L	205	CLA	C13-C15-C16-C17
25	T	602	CLA	C10-C11-C12-C13
32	4	320	LMG	C8-C7-O1-C1
25	Q	612	CLA	O1A-CGA-O2A-C1
25	A	809	CLA	C8-C10-C11-C12
25	4	308	CLA	C10-C11-C12-C13
25	L	206	CLA	O1D-CGD-O2D-CED
25	R	611	CLA	CAA-CBA-CGA-O1A
33	R	605	CHL	CAA-CBA-CGA-O2A
25	B	803	CLA	C2A-CAA-CBA-CGA
25	3	307	CLA	C2A-CAA-CBA-CGA
25	B	801	CLA	CAA-CBA-CGA-O2A
25	A	829	CLA	CBA-CGA-O2A-C1
25	B	837	CLA	CBA-CGA-O2A-C1
33	R	606	CHL	CBA-CGA-O2A-C1
27	Q	617	LHG	C31-C32-C33-C34
25	3	312	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	B	810	CLA	C4B-C3B-CAB-CBB
25	B	811	CLA	C4B-C3B-CAB-CBB
25	K	202	CLA	C4B-C3B-CAB-CBB
25	L	201	CLA	C4B-C3B-CAB-CBB
25	P	604	CLA	C4B-C3B-CAB-CBB
25	Q	604	CLA	C4B-C3B-CAB-CBB
25	Q	612	CLA	C4B-C3B-CAB-CBB
25	R	613	CLA	C4B-C3B-CAB-CBB
25	1	612	CLA	C4B-C3B-CAB-CBB
25	5	310	CLA	C4B-C3B-CAB-CBB
25	3	307	CLA	O1A-CGA-O2A-C1
26	B	839	PQN	C14-C13-C15-C16
25	A	807	CLA	C11-C10-C8-C7
25	A	812	CLA	C12-C13-C15-C16
25	B	825	CLA	C12-C13-C15-C16
25	L	205	CLA	C2-C3-C5-C6
25	P	602	CLA	C6-C7-C8-C10
25	R	610	CLA	C12-C13-C15-C16
25	T	602	CLA	C6-C7-C8-C10
25	U	302	CLA	C6-C7-C8-C10
25	5	302	CLA	C6-C7-C8-C10
25	7	301	CLA	C11-C12-C13-C15
25	K	204	CLA	CAA-CBA-CGA-O2A
25	B	836	CLA	CBA-CGA-O2A-C1
33	P	606	CHL	CBA-CGA-O2A-C1
33	U	306	CHL	CBA-CGA-O2A-C1
25	A	818	CLA	C8-C10-C11-C12
25	A	827	CLA	O1A-CGA-O2A-C1
25	B	836	CLA	O1A-CGA-O2A-C1
27	A	843	LHG	C16-C17-C18-C19
27	A	852	LHG	C11-C12-C13-C14
25	a	303	CLA	C1-C2-C3-C4
25	a	302	CLA	CAA-CBA-CGA-O2A
25	B	807	CLA	C16-C17-C18-C19
25	B	837	CLA	O1A-CGA-O2A-C1
25	4	303	CLA	CBA-CGA-O2A-C1
25	9	309	CLA	CBA-CGA-O2A-C1
33	T	605	CHL	CBA-CGA-O2A-C1
25	3	314	CLA	O1D-CGD-O2D-CED
32	J	102	LMG	C33-C34-C35-C36
32	J	104	LMG	C30-C31-C32-C33
25	S	313	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	1	603	CLA	CAA-CBA-CGA-O2A
25	1	614	CLA	CAA-CBA-CGA-O2A
25	a	313	CLA	CAA-CBA-CGA-O2A
27	8	319	LHG	O8-C23-C24-C25
30	B	848	DGD	C4A-C5A-C6A-C7A
25	A	812	CLA	C16-C17-C18-C20
25	B	811	CLA	C16-C17-C18-C19
25	4	308	CLA	C11-C12-C13-C14
25	B	834	CLA	O1D-CGD-O2D-CED
30	B	846	DGD	C6B-C7B-C8B-C9B
25	3	312	CLA	CAA-CBA-CGA-O2A
25	A	827	CLA	CBA-CGA-O2A-C1
33	Q	606	CHL	CBA-CGA-O2A-C1
27	T	617	LHG	C13-C14-C15-C16
25	a	310	CLA	CAA-CBA-CGA-O2A
27	6	618	LHG	O8-C23-C24-C25
33	6	606	CHL	C4-C3-C5-C6
25	A	806	CLA	C2-C3-C5-C6
25	5	311	CLA	C2-C3-C5-C6
27	1	618	LHG	O7-C7-C8-C9
25	A	809	CLA	C6-C7-C8-C9
25	B	804	CLA	C6-C7-C8-C9
25	B	809	CLA	C6-C7-C8-C9
25	B	824	CLA	C11-C12-C13-C14
25	B	830	CLA	C11-C10-C8-C9
25	B	834	CLA	C11-C12-C13-C14
25	R	603	CLA	C11-C12-C13-C14
25	S	312	CLA	C6-C7-C8-C9
25	1	602	CLA	C6-C7-C8-C9
25	6	605	CLA	C11-C10-C8-C9
25	6	605	CLA	C14-C13-C15-C16
25	a	301	CLA	C6-C7-C8-C9
33	P	609	CHL	C11-C12-C13-C14
33	Q	608	CHL	C11-C12-C13-C14
33	R	609	CHL	C11-C12-C13-C14
27	A	843	LHG	C26-C27-C28-C29
25	A	853	CLA	C3A-C2A-CAA-CBA
25	B	834	CLA	C3A-C2A-CAA-CBA
25	S	314	CLA	C3A-C2A-CAA-CBA
33	6	606	CHL	C3A-C2A-CAA-CBA
33	6	608	CHL	C3A-C2A-CAA-CBA
25	P	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	3	310	CLA	CAA-CBA-CGA-O2A
27	a	317	LHG	O7-C7-C8-C9
33	9	307	CHL	CAA-CBA-CGA-O2A
25	A	807	CLA	CAD-CBD-CGD-O2D
25	A	831	CLA	CAD-CBD-CGD-O2D
25	A	837	CLA	CAD-CBD-CGD-O2D
25	B	808	CLA	CAD-CBD-CGD-O2D
25	B	818	CLA	CAD-CBD-CGD-O2D
25	B	822	CLA	CAD-CBD-CGD-O2D
25	B	823	CLA	CAD-CBD-CGD-O2D
25	B	827	CLA	CAD-CBD-CGD-O2D
25	B	828	CLA	CAD-CBD-CGD-O2D
25	B	834	CLA	CAD-CBD-CGD-O2D
25	B	835	CLA	CAD-CBD-CGD-O2D
25	B	838	CLA	CAD-CBD-CGD-O2D
25	K	205	CLA	CAD-CBD-CGD-O2D
25	L	201	CLA	CAD-CBD-CGD-O2D
25	R	604	CLA	CAD-CBD-CGD-O2D
25	1	603	CLA	CAD-CBD-CGD-O2D
25	1	605	CLA	CAD-CBD-CGD-O2D
25	3	310	CLA	CAD-CBD-CGD-O2D
25	4	302	CLA	CAD-CBD-CGD-O2D
25	4	308	CLA	CAD-CBD-CGD-O2D
25	4	312	CLA	CAD-CBD-CGD-O2D
25	5	303	CLA	CAD-CBD-CGD-O2D
25	5	313	CLA	CAD-CBD-CGD-O2D
25	6	605	CLA	CAD-CBD-CGD-O2D
25	7	304	CLA	CAD-CBD-CGD-O2D
25	7	310	CLA	CAD-CBD-CGD-O2D
25	7	312	CLA	CAD-CBD-CGD-O2D
25	9	302	CLA	CAD-CBD-CGD-O2D
25	9	305	CLA	CAD-CBD-CGD-O2D
25	a	302	CLA	CAD-CBD-CGD-O2D
25	a	303	CLA	CAD-CBD-CGD-O2D
25	a	304	CLA	CAD-CBD-CGD-O2D
33	S	306	CHL	CAD-CBD-CGD-O2D
33	9	306	CHL	CAD-CBD-CGD-O2D
32	J	107	LMG	C29-C30-C31-C32
33	U	305	CHL	CAA-CBA-CGA-O2A
25	B	835	CLA	CAA-CBA-CGA-O2A
25	T	609	CLA	CAA-CBA-CGA-O2A
27	2	317	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	B	846	DGD	C7B-C8B-C9B-CAB
31	B	850	SQD	C25-C26-C27-C28
25	B	814	CLA	C3-C5-C6-C7
25	A	810	CLA	CAA-CBA-CGA-O2A
25	1	611	CLA	CAA-CBA-CGA-O2A
25	2	304	CLA	CAA-CBA-CGA-O2A
25	5	309	CLA	CAA-CBA-CGA-O2A
30	B	848	DGD	C8B-C9B-CAB-CBB
28	B	840	BCR	C21-C22-C23-C24
28	B	842	BCR	C7-C8-C9-C10
28	I	201	BCR	C7-C8-C9-C10
28	6	621	BCR	C11-C12-C13-C14
36	P	617	NEX	O24-C26-C27-C28
36	R	617	NEX	O24-C26-C27-C28
36	T	616	NEX	O24-C26-C27-C28
36	U	301	NEX	O24-C26-C27-C28
36	U	316	NEX	O24-C26-C27-C28
27	P	624	LHG	C13-C14-C15-C16
27	A	852	LHG	O6-C4-C5-O7
25	B	830	CLA	C13-C15-C16-C17
25	A	806	CLA	CAA-CBA-CGA-O2A
25	A	823	CLA	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
33	R	606	CHL	O2A-C1-C2-C3
25	8	304	CLA	CAA-CBA-CGA-O1A
27	P	618	LHG	C13-C14-C15-C16
25	A	806	CLA	O2A-C1-C2-C3
25	A	851	CLA	O2A-C1-C2-C3
25	P	603	CLA	O2A-C1-C2-C3
25	Q	603	CLA	O2A-C1-C2-C3
25	R	603	CLA	O2A-C1-C2-C3
25	S	320	CLA	O2A-C1-C2-C3
25	U	303	CLA	O2A-C1-C2-C3
25	9	305	CLA	O2A-C1-C2-C3
33	P	607	CHL	O2A-C1-C2-C3
33	P	619	CHL	O2A-C1-C2-C3
33	R	607	CHL	O2A-C1-C2-C3
33	S	308	CHL	O2A-C1-C2-C3
33	S	321	CHL	O2A-C1-C2-C3
33	U	307	CHL	O2A-C1-C2-C3
33	6	608	CHL	O2A-C1-C2-C3
27	8	319	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	A	813	CLA	C6-C7-C8-C9
25	J	103	CLA	CAA-CBA-CGA-O2A
25	U	303	CLA	CAA-CBA-CGA-O2A
25	4	302	CLA	CAA-CBA-CGA-O2A
25	7	313	CLA	CAA-CBA-CGA-O2A
25	A	809	CLA	C13-C15-C16-C17
25	A	804	CLA	CHA-CBD-CGD-O1D
25	A	804	CLA	CHA-CBD-CGD-O2D
25	A	835	CLA	CHA-CBD-CGD-O1D
25	A	837	CLA	CHA-CBD-CGD-O1D
25	A	851	CLA	CHA-CBD-CGD-O1D
25	A	851	CLA	CHA-CBD-CGD-O2D
25	B	819	CLA	CHA-CBD-CGD-O1D
25	B	819	CLA	CHA-CBD-CGD-O2D
25	G	202	CLA	CHA-CBD-CGD-O2D
25	J	103	CLA	CHA-CBD-CGD-O1D
25	K	202	CLA	CHA-CBD-CGD-O2D
25	Q	613	CLA	CHA-CBD-CGD-O1D
25	Q	613	CLA	CHA-CBD-CGD-O2D
25	R	614	CLA	CHA-CBD-CGD-O1D
25	R	614	CLA	CHA-CBD-CGD-O2D
25	S	301	CLA	CHA-CBD-CGD-O1D
25	S	301	CLA	CHA-CBD-CGD-O2D
25	S	303	CLA	CHA-CBD-CGD-O2D
25	S	304	CLA	CHA-CBD-CGD-O2D
25	S	305	CLA	CHA-CBD-CGD-O2D
25	T	612	CLA	CHA-CBD-CGD-O1D
25	T	612	CLA	CHA-CBD-CGD-O2D
25	U	313	CLA	CHA-CBD-CGD-O1D
25	U	313	CLA	CHA-CBD-CGD-O2D
25	1	612	CLA	CHA-CBD-CGD-O2D
25	2	304	CLA	CHA-CBD-CGD-O2D
25	2	311	CLA	CHA-CBD-CGD-O1D
25	2	311	CLA	CHA-CBD-CGD-O2D
25	3	301	CLA	CHA-CBD-CGD-O1D
25	3	301	CLA	CHA-CBD-CGD-O2D
25	3	314	CLA	CHA-CBD-CGD-O1D
25	3	314	CLA	CHA-CBD-CGD-O2D
25	4	303	CLA	CHA-CBD-CGD-O1D
25	4	303	CLA	CHA-CBD-CGD-O2D
25	5	311	CLA	CHA-CBD-CGD-O2D
25	5	315	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	5	315	CLA	CHA-CBD-CGD-O2D
25	7	301	CLA	CHA-CBD-CGD-O1D
25	8	304	CLA	CHA-CBD-CGD-O1D
25	8	304	CLA	CHA-CBD-CGD-O2D
25	8	306	CLA	CHA-CBD-CGD-O1D
25	9	303	CLA	CHA-CBD-CGD-O1D
25	9	304	CLA	CHA-CBD-CGD-O1D
25	9	304	CLA	CHA-CBD-CGD-O2D
25	9	310	CLA	CHA-CBD-CGD-O1D
25	9	310	CLA	CHA-CBD-CGD-O2D
25	a	301	CLA	CHA-CBD-CGD-O1D
33	P	607	CHL	CHA-CBD-CGD-O1D
33	P	607	CHL	CHA-CBD-CGD-O2D
33	P	619	CHL	CHA-CBD-CGD-O1D
33	P	619	CHL	CHA-CBD-CGD-O2D
33	R	607	CHL	CHA-CBD-CGD-O1D
33	R	607	CHL	CHA-CBD-CGD-O2D
33	S	309	CHL	CHA-CBD-CGD-O1D
33	S	309	CHL	CHA-CBD-CGD-O2D
33	S	321	CHL	CHA-CBD-CGD-O1D
33	S	321	CHL	CHA-CBD-CGD-O2D
33	U	307	CHL	CHA-CBD-CGD-O1D
33	U	307	CHL	CHA-CBD-CGD-O2D
33	6	608	CHL	CHA-CBD-CGD-O1D
33	6	608	CHL	CHA-CBD-CGD-O2D
35	P	616	XAT	C29-C30-C31-C32
33	U	305	CHL	CAA-CBA-CGA-O1A
25	S	320	CLA	CAA-CBA-CGA-O2A
25	9	309	CLA	CAA-CBA-CGA-O2A
27	A	852	LHG	O7-C7-C8-C9
25	A	805	CLA	C2-C3-C5-C6
25	K	205	CLA	CAA-CBA-CGA-O2A
25	Q	603	CLA	CAA-CBA-CGA-O2A
25	6	616	CLA	CAA-CBA-CGA-O2A
25	9	304	CLA	CAA-CBA-CGA-O2A
25	A	831	CLA	O1A-CGA-O2A-C1
25	1	610	CLA	C4C-C3C-CAC-CBC
33	T	607	CHL	C4C-C3C-CAC-CBC
25	2	303	CLA	CAA-CBA-CGA-O2A
25	4	311	CLA	CAA-CBA-CGA-O2A
27	Q	617	LHG	O8-C23-C24-C25
27	S	319	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	810	CLA	C2A-CAA-CBA-CGA
25	3	308	CLA	C2A-CAA-CBA-CGA
27	a	317	LHG	C11-C10-C9-C8
25	A	831	CLA	CBA-CGA-O2A-C1
25	3	307	CLA	CBA-CGA-O2A-C1
25	B	818	CLA	O1A-CGA-O2A-C1
25	B	826	CLA	CAA-CBA-CGA-O2A
25	H	203	CLA	CAA-CBA-CGA-O2A
25	9	305	CLA	CAA-CBA-CGA-O2A
33	5	307	CHL	CAA-CBA-CGA-O2A
25	A	818	CLA	C6-C7-C8-C10
25	B	802	CLA	C11-C12-C13-C15
25	7	311	CLA	C6-C7-C8-C10
25	B	811	CLA	C16-C17-C18-C20
25	Q	609	CLA	C16-C17-C18-C19
27	5	301	LHG	O8-C23-C24-C25
25	A	832	CLA	C6-C7-C8-C9
25	B	826	CLA	C11-C10-C8-C9
25	B	830	CLA	C11-C12-C13-C14
25	L	201	CLA	C11-C10-C8-C9
25	U	312	CLA	C11-C12-C13-C14
25	1	603	CLA	C11-C12-C13-C14
25	P	604	CLA	C2B-C3B-CAB-CBB
25	Q	612	CLA	C2B-C3B-CAB-CBB
33	T	601	CHL	O2A-C1-C2-C3
25	7	311	CLA	CBA-CGA-O2A-C1
25	7	311	CLA	O1A-CGA-O2A-C1
33	R	605	CHL	CAA-CBA-CGA-O1A
25	A	806	CLA	C2A-CAA-CBA-CGA
25	5	310	CLA	C2A-CAA-CBA-CGA
25	a	313	CLA	CAA-CBA-CGA-O1A
25	a	309	CLA	C4C-C3C-CAC-CBC
25	A	814	CLA	CAA-CBA-CGA-O2A
25	B	818	CLA	CBA-CGA-O2A-C1
28	B	840	BCR	C36-C18-C19-C20
25	A	823	CLA	CAA-CBA-CGA-O1A
25	1	611	CLA	CAA-CBA-CGA-O1A
25	a	310	CLA	CAA-CBA-CGA-O1A
25	B	805	CLA	C16-C17-C18-C19
25	S	312	CLA	C4-C3-C5-C6
25	K	204	CLA	CAA-CBA-CGA-O1A
25	4	312	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	a	317	LHG	O9-C7-C8-C9
25	A	814	CLA	C1A-C2A-CAA-CBA
25	A	825	CLA	C1A-C2A-CAA-CBA
25	A	826	CLA	C1A-C2A-CAA-CBA
25	A	851	CLA	C1A-C2A-CAA-CBA
25	A	853	CLA	C1A-C2A-CAA-CBA
25	B	803	CLA	C1A-C2A-CAA-CBA
25	S	314	CLA	C1A-C2A-CAA-CBA
25	2	303	CLA	C1A-C2A-CAA-CBA
25	4	310	CLA	C1A-C2A-CAA-CBA
25	6	613	CLA	C1A-C2A-CAA-CBA
25	7	313	CLA	C1A-C2A-CAA-CBA
25	9	309	CLA	C1A-C2A-CAA-CBA
25	a	309	CLA	C1A-C2A-CAA-CBA
33	4	306	CHL	C1A-C2A-CAA-CBA
25	1	603	CLA	CAA-CBA-CGA-O1A
25	3	310	CLA	CAA-CBA-CGA-O1A
25	a	302	CLA	CAA-CBA-CGA-O1A
25	5	314	CLA	CAA-CBA-CGA-O2A
25	9	309	CLA	O1A-CGA-O2A-C1
25	A	808	CLA	C2-C1-O2A-CGA
33	T	605	CHL	C2-C1-O2A-CGA
25	1	614	CLA	CAA-CBA-CGA-O1A
25	9	309	CLA	CAA-CBA-CGA-O1A
27	6	618	LHG	O10-C23-C24-C25
25	a	301	CLA	CAA-CBA-CGA-O2A
25	H	203	CLA	C2A-CAA-CBA-CGA
25	2	309	CLA	C2A-CAA-CBA-CGA
25	8	315	CLA	C2A-CAA-CBA-CGA
25	L	206	CLA	CBD-CGD-O2D-CED
32	J	104	LMG	C29-C30-C31-C32
25	B	830	CLA	C16-C17-C18-C20
25	P	603	CLA	CAA-CBA-CGA-O1A
27	1	618	LHG	O9-C7-C8-C9
33	9	307	CHL	CAA-CBA-CGA-O1A
25	5	319	CLA	C4C-C3C-CAC-CBC
31	B	850	SQD	C34-C35-C36-C37
25	S	313	CLA	CAA-CBA-CGA-O1A
25	4	311	CLA	CAA-CBA-CGA-O1A
25	5	324	CLA	C2-C3-C5-C6
25	8	312	CLA	C2-C3-C5-C6
25	6	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	A	806	CLA	C4B-C3B-CAB-CBB
25	B	809	CLA	C4B-C3B-CAB-CBB
25	3	313	CLA	C4B-C3B-CAB-CBB
27	1	618	LHG	C3-O3-P-O5
27	1	618	LHG	C4-O6-P-O5
27	4	318	LHG	C4-O6-P-O5
27	4	319	LHG	C3-O3-P-O5
27	6	618	LHG	C4-O6-P-O4
27	a	317	LHG	C3-O3-P-O5
27	a	317	LHG	C4-O6-P-O5
33	Q	605	CHL	C4B-C3B-CAB-CBB
33	R	605	CHL	C4B-C3B-CAB-CBB
33	S	308	CHL	C4B-C3B-CAB-CBB
33	T	604	CHL	C4B-C3B-CAB-CBB
33	U	305	CHL	C4B-C3B-CAB-CBB
33	4	322	CHL	C4B-C3B-CAB-CBB
33	5	308	CHL	C4B-C3B-CAB-CBB
33	6	607	CHL	C4B-C3B-CAB-CBB
33	7	305	CHL	C4B-C3B-CAB-CBB
25	3	308	CLA	O1D-CGD-O2D-CED
33	P	609	CHL	C4C-C3C-CAC-CBC
33	Q	608	CHL	C4C-C3C-CAC-CBC
33	R	609	CHL	C4C-C3C-CAC-CBC
25	A	806	CLA	CAA-CBA-CGA-O1A
25	A	810	CLA	CAA-CBA-CGA-O1A
25	S	320	CLA	CAA-CBA-CGA-O1A
25	T	609	CLA	CAA-CBA-CGA-O1A
25	6	616	CLA	CAA-CBA-CGA-O1A
25	7	313	CLA	CAA-CBA-CGA-O1A
25	9	304	CLA	CAA-CBA-CGA-O1A
25	K	205	CLA	CAA-CBA-CGA-O1A
28	B	840	BCR	C23-C24-C25-C26
28	3	319	BCR	C5-C6-C7-C8
34	S	316	LUT	C5-C6-C7-C8
25	B	835	CLA	CAA-CBA-CGA-O1A
25	J	103	CLA	CAA-CBA-CGA-O1A
25	Q	603	CLA	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
25	U	303	CLA	CAA-CBA-CGA-O1A
25	5	309	CLA	CAA-CBA-CGA-O1A
27	A	852	LHG	O9-C7-C8-C9
27	8	319	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	A	816	CLA	CAA-CBA-CGA-O2A
25	1	602	CLA	CAA-CBA-CGA-O2A
25	8	312	CLA	CAA-CBA-CGA-O2A
27	P	618	LHG	O8-C23-C24-C25
27	P	624	LHG	O8-C23-C24-C25
25	5	310	CLA	C5-C6-C7-C8
25	5	319	CLA	C2C-C3C-CAC-CBC
33	U	309	CHL	C2-C1-O2A-CGA
25	R	613	CLA	CBA-CGA-O2A-C1
25	K	201	CLA	C2A-CAA-CBA-CGA
25	2	304	CLA	CAA-CBA-CGA-O1A
27	Q	617	LHG	O10-C23-C24-C25
27	T	617	LHG	O8-C23-C24-C25
27	7	317	LHG	O8-C23-C24-C25
25	4	302	CLA	CAA-CBA-CGA-O1A
25	B	815	CLA	C2-C3-C5-C6
25	A	807	CLA	C16-C17-C18-C19
25	A	821	CLA	CAD-CBD-CGD-O1D
25	A	834	CLA	CAD-CBD-CGD-O1D
25	A	835	CLA	CAD-CBD-CGD-O1D
25	A	851	CLA	CAD-CBD-CGD-O1D
25	K	201	CLA	C2-C3-C5-C6
25	S	314	CLA	CAD-CBD-CGD-O1D
25	2	308	CLA	CAD-CBD-CGD-O1D
25	5	315	CLA	CAD-CBD-CGD-O1D
25	7	308	CLA	CAD-CBD-CGD-O1D
25	8	304	CLA	CAD-CBD-CGD-O1D
25	9	303	CLA	CAD-CBD-CGD-O1D
32	7	318	LMG	C9-C8-O7-C10
33	4	304	CHL	CAD-CBD-CGD-O1D
33	6	608	CHL	CAD-CBD-CGD-O1D
27	2	317	LHG	C11-C10-C9-C8
25	B	806	CLA	CAA-CBA-CGA-O2A
25	6	601	CLA	CAA-CBA-CGA-O2A
27	R	618	LHG	O8-C23-C24-C25
25	A	807	CLA	C5-C6-C7-C8
25	B	802	CLA	C11-C12-C13-C14
25	4	311	CLA	C6-C7-C8-C9
25	7	311	CLA	C11-C12-C13-C14
27	R	618	LHG	C13-C14-C15-C16
25	5	309	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	L	205	CLA	C3-C5-C6-C7
25	A	822	CLA	CAA-CBA-CGA-O2A
25	A	840	CLA	CAA-CBA-CGA-O2A
25	H	201	CLA	CAA-CBA-CGA-O2A
25	S	314	CLA	CAA-CBA-CGA-O2A
25	3	314	CLA	CAA-CBA-CGA-O2A
25	5	312	CLA	CAA-CBA-CGA-O2A
30	B	848	DGD	O2G-C1B-C2B-C3B
33	U	307	CHL	CAA-CBA-CGA-O2A
33	8	307	CHL	CAA-CBA-CGA-O2A
25	S	304	CLA	C13-C15-C16-C17
25	4	301	CLA	C5-C6-C7-C8
27	R	618	LHG	C28-C29-C30-C31
25	H	203	CLA	CAA-CBA-CGA-O1A
25	A	840	CLA	C5-C6-C7-C8
25	B	807	CLA	C2A-CAA-CBA-CGA
25	4	308	CLA	C2A-CAA-CBA-CGA
25	B	805	CLA	CAA-CBA-CGA-O2A
25	B	822	CLA	CAA-CBA-CGA-O2A
25	R	610	CLA	CAA-CBA-CGA-O2A
25	4	301	CLA	CAA-CBA-CGA-O2A
25	9	302	CLA	CAA-CBA-CGA-O2A
33	R	601	CHL	CAA-CBA-CGA-O2A
33	T	601	CHL	CAA-CBA-CGA-O2A
33	3	306	CHL	CAA-CBA-CGA-O2A
25	S	312	CLA	C8-C10-C11-C12
25	8	313	CLA	C13-C15-C16-C17
25	B	826	CLA	CAA-CBA-CGA-O1A
25	a	301	CLA	CAA-CBA-CGA-O1A
27	4	318	LHG	C29-C30-C31-C32
25	A	809	CLA	C4-C3-C5-C6
25	T	609	CLA	C4-C3-C5-C6
25	B	833	CLA	C10-C11-C12-C13
25	A	808	CLA	C6-C7-C8-C10
25	A	820	CLA	C11-C10-C8-C7
25	A	830	CLA	C6-C7-C8-C10
25	A	832	CLA	C6-C7-C8-C10
25	A	837	CLA	C12-C13-C15-C16
25	A	840	CLA	C11-C10-C8-C7
25	B	802	CLA	C12-C13-C15-C16
25	B	830	CLA	C11-C10-C8-C7
25	B	849	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	L	201	CLA	C11-C12-C13-C15
25	R	602	CLA	C12-C13-C15-C16
25	S	313	CLA	C11-C10-C8-C7
25	U	302	CLA	C12-C13-C15-C16
25	1	604	CLA	C2-C3-C5-C6
25	3	303	CLA	C11-C10-C8-C7
25	3	314	CLA	C6-C7-C8-C10
25	4	310	CLA	C3A-C2A-CAA-CBA
25	9	309	CLA	C6-C7-C8-C10
33	U	308	CHL	C3A-C2A-CAA-CBA
25	2	303	CLA	CAA-CBA-CGA-O1A
25	9	305	CLA	CAA-CBA-CGA-O1A
25	A	815	CLA	CAA-CBA-CGA-O2A
25	P	610	CLA	CAA-CBA-CGA-O2A
25	Q	609	CLA	CAA-CBA-CGA-O2A
25	2	311	CLA	CAA-CBA-CGA-O2A
25	5	311	CLA	CAA-CBA-CGA-O2A
25	9	310	CLA	CAA-CBA-CGA-O2A
33	P	601	CHL	CAA-CBA-CGA-O2A
33	P	607	CHL	CAA-CBA-CGA-O2A
33	P	619	CHL	CAA-CBA-CGA-O2A
33	Q	601	CHL	CAA-CBA-CGA-O2A
33	R	607	CHL	CAA-CBA-CGA-O2A
33	S	321	CHL	CAA-CBA-CGA-O2A
25	6	605	CLA	C3-C5-C6-C7
28	A	845	BCR	C7-C8-C9-C10
28	8	318	BCR	C7-C8-C9-C10
34	4	315	LUT	C11-C12-C13-C14
36	U	301	NEX	C11-C12-C13-C14
25	A	814	CLA	CAA-CBA-CGA-O1A
33	P	601	CHL	CAA-CBA-CGA-O1A
33	P	607	CHL	CAA-CBA-CGA-O1A
33	P	619	CHL	CAA-CBA-CGA-O1A
33	Q	601	CHL	CAA-CBA-CGA-O1A
33	R	607	CHL	CAA-CBA-CGA-O1A
28	L	204	BCR	C15-C16-C17-C18
35	P	623	XAT	C29-C30-C31-C32
36	P	621	NEX	C13-C14-C15-C35
25	S	304	CLA	CAA-CBA-CGA-O2A
25	T	608	CLA	CAA-CBA-CGA-O2A
25	3	305	CLA	CAA-CBA-CGA-O2A
33	P	622	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	3	314	CLA	C5-C6-C7-C8
27	A	852	LHG	C34-C35-C36-C37
25	A	815	CLA	CAA-CBA-CGA-O1A
25	H	201	CLA	CAA-CBA-CGA-O1A
25	S	314	CLA	CAA-CBA-CGA-O1A
25	1	602	CLA	CAA-CBA-CGA-O1A
25	5	311	CLA	CAA-CBA-CGA-O1A
27	P	618	LHG	O10-C23-C24-C25
33	R	601	CHL	CAA-CBA-CGA-O1A
25	B	802	CLA	CAA-CBA-CGA-O2A
25	U	310	CLA	CAA-CBA-CGA-O2A
25	5	324	CLA	CAA-CBA-CGA-O2A
32	J	104	LMG	O7-C10-C11-C12
25	3	314	CLA	CAA-CBA-CGA-O1A
25	4	301	CLA	CAA-CBA-CGA-O1A
27	P	624	LHG	O10-C23-C24-C25
27	R	618	LHG	O10-C23-C24-C25
27	T	617	LHG	O10-C23-C24-C25
33	8	307	CHL	CAA-CBA-CGA-O1A
25	7	308	CLA	C2A-CAA-CBA-CGA
25	8	302	CLA	C2A-CAA-CBA-CGA
25	5	314	CLA	CAA-CBA-CGA-O1A
25	1	608	CLA	C10-C11-C12-C13
25	9	302	CLA	CAA-CBA-CGA-O1A
25	9	310	CLA	CAA-CBA-CGA-O1A
33	U	307	CHL	CAA-CBA-CGA-O1A
33	3	306	CHL	CAA-CBA-CGA-O1A
25	B	821	CLA	CAA-CBA-CGA-O2A
33	S	302	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

390 monomers are involved in 1340 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	301	CLA	1	0
33	R	608	CHL	3	0
33	Q	607	CHL	3	0
25	8	310	CLA	3	0
25	A	811	CLA	4	0
25	R	602	CLA	6	0
27	B	847	LHG	2	0
25	1	609	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Q	613	CLA	2	0
33	P	605	CHL	2	0
25	T	610	CLA	7	0
25	S	301	CLA	15	0
25	2	309	CLA	4	0
25	5	302	CLA	2	0
33	5	317	CHL	1	0
33	8	307	CHL	4	0
35	S	318	XAT	8	0
27	5	321	LHG	1	0
25	1	611	CLA	4	0
28	A	845	BCR	5	0
36	R	617	NEX	3	0
27	A	843	LHG	1	0
25	S	312	CLA	4	0
25	a	304	CLA	5	0
28	3	317	BCR	1	0
25	7	308	CLA	2	0
33	S	302	CHL	5	0
28	G	203	BCR	1	0
33	U	309	CHL	3	0
25	5	306	CLA	2	0
25	B	812	CLA	2	0
28	B	843	BCR	2	0
33	R	605	CHL	2	0
25	A	823	CLA	2	0
32	J	104	LMG	1	0
25	B	827	CLA	1	0
25	B	806	CLA	1	0
25	B	831	CLA	2	0
25	Q	618	CLA	12	0
25	B	820	CLA	1	0
32	4	320	LMG	1	0
25	A	822	CLA	6	0
25	B	817	CLA	1	0
25	6	620	CLA	3	0
25	B	808	CLA	1	0
34	1	615	LUT	8	0
34	S	317	LUT	8	0
27	A	844	LHG	2	0
25	A	814	CLA	6	0
34	R	615	LUT	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	1	606	CHL	1	0
25	S	304	CLA	6	0
34	2	316	LUT	4	0
28	A	854	BCR	7	0
34	9	312	LUT	4	0
25	7	311	CLA	4	0
28	7	316	BCR	2	0
25	6	605	CLA	6	0
28	5	320	BCR	4	0
25	1	610	CLA	5	0
25	A	821	CLA	1	0
25	B	833	CLA	6	0
33	6	617	CHL	2	0
34	2	315	LUT	5	0
33	5	307	CHL	1	0
25	a	310	CLA	3	0
25	4	309	CLA	2	0
25	B	832	CLA	2	0
25	U	304	CLA	1	0
25	9	302	CLA	1	0
25	a	303	CLA	18	0
25	6	612	CLA	1	0
34	U	315	LUT	8	0
25	6	615	CLA	2	0
25	5	304	CLA	1	0
33	6	606	CHL	3	0
25	S	320	CLA	6	0
25	6	601	CLA	2	0
25	B	826	CLA	2	0
25	B	804	CLA	1	0
25	a	312	CLA	3	0
35	P	623	XAT	8	0
28	J	106	BCR	5	0
25	1	604	CLA	3	0
34	T	614	LUT	3	0
34	6	622	LUT	1	0
25	A	836	CLA	2	0
25	B	828	CLA	2	0
25	L	202	CLA	1	0
33	1	601	CHL	3	0
25	P	611	CLA	22	0
25	Q	603	CLA	33	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	U	301	NEX	21	0
25	3	320	CLA	3	0
25	4	307	CLA	1	0
25	7	313	CLA	1	0
25	T	611	CLA	4	0
25	3	301	CLA	1	0
25	1	612	CLA	1	0
33	R	601	CHL	2	0
31	B	850	SQD	5	0
25	A	809	CLA	3	0
25	U	310	CLA	7	0
25	4	308	CLA	6	0
25	2	313	CLA	2	0
25	A	807	CLA	3	0
25	5	310	CLA	1	0
25	B	822	CLA	3	0
25	U	311	CLA	9	0
25	4	302	CLA	1	0
34	P	615	LUT	9	0
34	5	318	LUT	3	0
33	S	321	CHL	5	0
34	5	322	LUT	5	0
33	U	307	CHL	3	0
33	U	305	CHL	2	0
25	K	204	CLA	1	0
33	P	606	CHL	4	0
25	A	820	CLA	3	0
30	B	848	DGD	3	0
28	L	204	BCR	1	0
35	T	615	XAT	6	0
25	B	810	CLA	4	0
34	1	617	LUT	3	0
34	R	616	LUT	5	0
25	B	813	CLA	1	0
34	8	317	LUT	1	0
33	T	605	CHL	2	0
25	L	201	CLA	4	0
25	1	608	CLA	2	0
33	6	607	CHL	1	0
25	a	307	CLA	6	0
32	2	301	LMG	5	0
25	A	830	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	818	CLA	3	0
25	R	612	CLA	62	0
25	S	314	CLA	5	0
33	S	309	CHL	2	0
28	I	201	BCR	5	0
25	5	313	CLA	5	0
25	B	836	CLA	3	0
35	P	616	XAT	7	0
33	R	606	CHL	3	0
27	P	618	LHG	9	0
32	1	619	LMG	1	0
34	S	316	LUT	3	0
34	a	315	LUT	5	0
25	3	308	CLA	3	0
25	A	835	CLA	1	0
33	3	306	CHL	1	0
25	8	303	CLA	1	0
25	2	312	CLA	5	0
25	7	301	CLA	1	0
25	B	825	CLA	3	0
25	T	608	CLA	7	0
25	a	308	CLA	2	0
25	B	837	CLA	4	0
25	1	605	CLA	4	0
25	G	202	CLA	2	0
25	5	324	CLA	4	0
36	T	616	NEX	3	0
25	2	307	CLA	1	0
28	L	208	BCR	1	0
25	P	613	CLA	7	0
25	1	613	CLA	4	0
33	S	306	CHL	7	0
34	7	315	LUT	2	0
33	4	306	CHL	2	0
33	T	601	CHL	1	0
25	2	304	CLA	5	0
25	B	801	CLA	2	0
32	J	107	LMG	2	0
28	B	842	BCR	4	0
25	U	312	CLA	4	0
25	B	824	CLA	1	0
27	Q	617	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	1	616	LUT	1	0
33	P	607	CHL	1	0
34	Q	614	LUT	5	0
25	R	611	CLA	17	0
33	T	604	CHL	1	0
34	Q	615	LUT	7	0
25	6	609	CLA	1	0
28	4	321	BCR	2	0
25	A	834	CLA	1	0
28	F	803	BCR	3	0
33	P	601	CHL	2	0
33	9	306	CHL	1	0
25	a	301	CLA	6	0
25	8	313	CLA	2	0
25	8	302	CLA	3	0
25	A	832	CLA	2	0
25	L	206	CLA	2	0
25	L	209	CLA	1	0
33	Q	608	CHL	50	0
28	3	319	BCR	7	0
34	a	314	LUT	8	0
25	P	602	CLA	6	0
25	6	611	CLA	3	0
27	S	319	LHG	3	0
25	K	203	CLA	2	0
33	R	607	CHL	1	0
35	Q	616	XAT	6	0
25	T	602	CLA	6	0
25	A	826	CLA	2	0
25	H	202	CLA	3	0
25	B	811	CLA	2	0
33	P	622	CHL	8	0
25	R	603	CLA	29	0
34	P	614	LUT	5	0
25	9	304	CLA	2	0
25	A	810	CLA	5	0
25	4	310	CLA	8	0
25	5	315	CLA	3	0
25	B	823	CLA	6	0
25	B	830	CLA	3	0
25	B	803	CLA	1	0
25	K	202	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	813	CLA	2	0
25	6	610	CLA	3	0
33	T	607	CHL	4	0
25	2	314	CLA	3	0
33	7	305	CHL	2	0
25	A	802	CLA	7	0
25	P	603	CLA	28	0
25	2	303	CLA	5	0
33	S	307	CHL	1	0
25	A	839	CLA	3	0
25	A	817	CLA	2	0
25	6	613	CLA	1	0
33	S	308	CHL	2	0
33	Q	605	CHL	2	0
25	A	819	CLA	2	0
25	A	840	CLA	3	0
25	A	831	CLA	1	0
25	a	302	CLA	6	0
25	H	201	CLA	1	0
25	A	851	CLA	4	0
25	F	802	CLA	2	0
27	a	317	LHG	6	0
36	P	617	NEX	3	0
36	U	316	NEX	4	0
25	A	827	CLA	3	0
25	Q	602	CLA	6	0
28	A	846	BCR	4	0
25	T	612	CLA	1	0
25	T	609	CLA	6	0
33	T	606	CHL	4	0
25	B	816	CLA	1	0
25	Q	612	CLA	5	0
27	A	852	LHG	6	0
25	2	306	CLA	2	0
28	A	848	BCR	3	0
25	K	205	CLA	1	0
28	5	323	BCR	4	0
33	S	310	CHL	7	0
25	Q	611	CLA	8	0
33	Q	606	CHL	4	0
25	9	301	CLA	1	0
25	a	309	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	T	613	LUT	5	0
35	P	620	XAT	8	0
25	P	610	CLA	29	0
25	U	303	CLA	6	0
33	5	308	CHL	2	0
25	A	801	CLA	3	0
25	5	303	CLA	8	0
28	O	205	BCR	1	0
34	a	316	LUT	4	0
25	B	818	CLA	2	0
25	3	302	CLA	4	0
28	B	841	BCR	1	0
25	A	833	CLA	1	0
25	9	308	CLA	1	0
34	U	314	LUT	4	0
27	T	617	LHG	5	0
28	B	844	BCR	5	0
33	R	609	CHL	47	0
32	7	319	LMG	2	0
25	U	302	CLA	6	0
25	R	610	CLA	30	0
25	B	809	CLA	2	0
28	B	845	BCR	3	0
27	1	618	LHG	3	0
28	B	840	BCR	3	0
28	A	847	BCR	2	0
25	A	838	CLA	1	0
25	B	807	CLA	3	0
25	T	603	CLA	1	0
25	Q	604	CLA	3	0
34	4	315	LUT	9	0
25	R	613	CLA	6	0
25	2	305	CLA	1	0
33	4	322	CHL	5	0
25	A	812	CLA	3	0
25	A	825	CLA	5	0
34	3	316	LUT	1	0
25	J	103	CLA	6	0
25	a	306	CLA	8	0
25	B	802	CLA	3	0
25	a	311	CLA	2	0
25	Q	609	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	3	318	BCR	2	0
25	A	804	CLA	3	0
33	Q	601	CHL	1	0
36	P	621	NEX	15	0
25	B	835	CLA	1	0
25	7	304	CLA	1	0
25	P	612	CLA	41	0
25	7	310	CLA	1	0
33	a	305	CHL	1	0
25	6	603	CLA	4	0
27	6	618	LHG	5	0
30	B	846	DGD	3	0
25	B	815	CLA	2	0
34	4	316	LUT	2	0
25	1	607	CLA	6	0
25	A	803	CLA	2	0
25	8	309	CLA	1	0
25	8	306	CLA	1	0
25	L	205	CLA	3	0
25	9	309	CLA	1	0
33	U	306	CHL	2	0
28	4	317	BCR	8	0
25	S	315	CLA	4	0
28	8	318	BCR	3	0
25	H	203	CLA	2	0
25	A	828	CLA	6	0
33	6	608	CHL	6	0
25	A	816	CLA	7	0
28	6	621	BCR	2	0
25	7	312	CLA	2	0
25	S	303	CLA	10	0
32	6	602	LMG	1	0
29	C	101	SF4	1	0
25	2	311	CLA	5	0
25	5	316	CLA	1	0
25	2	310	CLA	2	0
25	1	602	CLA	6	0
25	A	837	CLA	2	0
27	P	624	LHG	6	0
28	J	101	BCR	2	0
25	B	834	CLA	6	0
25	S	313	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	7	309	CLA	1	0
27	4	318	LHG	1	0
25	A	853	CLA	2	0
25	3	307	CLA	2	0
25	6	623	CLA	2	0
25	3	303	CLA	2	0
25	3	305	CLA	3	0
25	A	806	CLA	3	0
25	8	314	CLA	3	0
26	B	839	PQN	2	0
28	O	204	BCR	2	0
25	A	842	CLA	2	0
25	A	808	CLA	4	0
28	L	207	BCR	2	0
34	8	316	LUT	8	0
25	B	805	CLA	3	0
33	P	619	CHL	4	0
33	P	609	CHL	48	0
34	3	315	LUT	4	0
25	A	815	CLA	4	0
28	A	849	BCR	4	0
25	B	829	CLA	1	0
34	9	313	LUT	7	0
27	R	618	LHG	7	0
25	K	201	CLA	1	0
33	P	608	CHL	3	0
27	5	301	LHG	5	0
25	O	202	CLA	1	0
28	B	851	BCR	2	0
33	4	314	CHL	3	0
33	U	308	CHL	3	0
25	2	302	CLA	2	0
27	7	317	LHG	1	0
25	3	314	CLA	3	0
25	R	614	CLA	1	0
27	2	317	LHG	1	0
34	6	619	LUT	4	0
25	9	303	CLA	2	0
25	B	838	CLA	3	0
32	J	102	LMG	1	0
34	7	314	LUT	8	0
27	8	319	LHG	1	0

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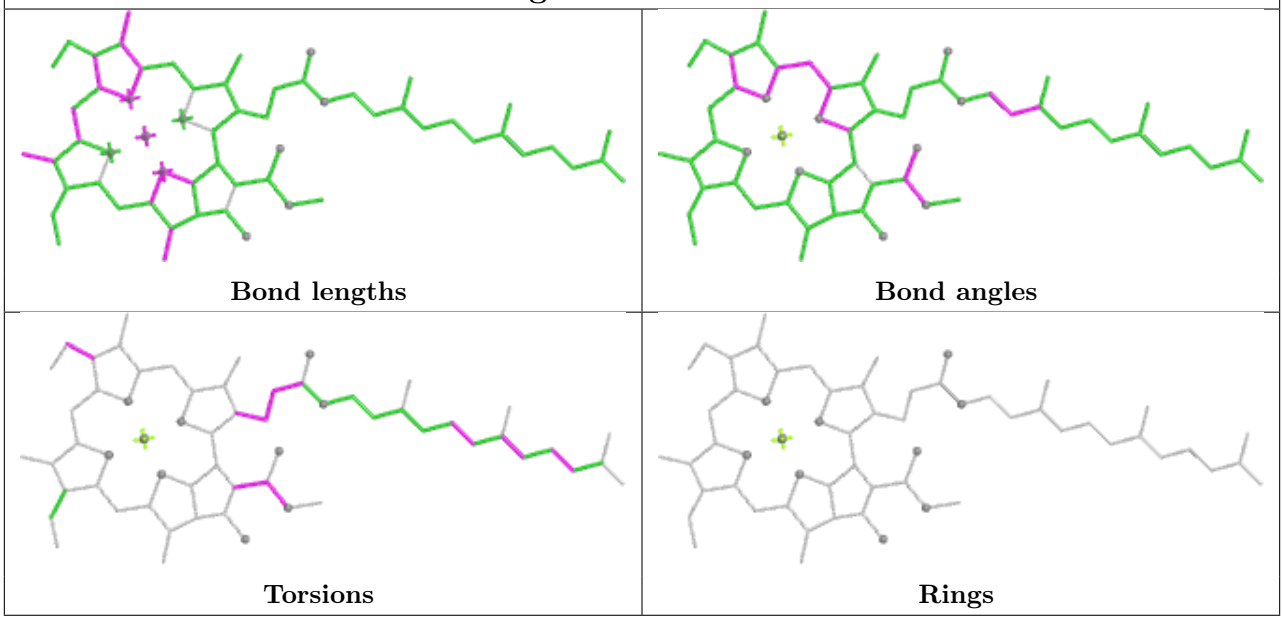
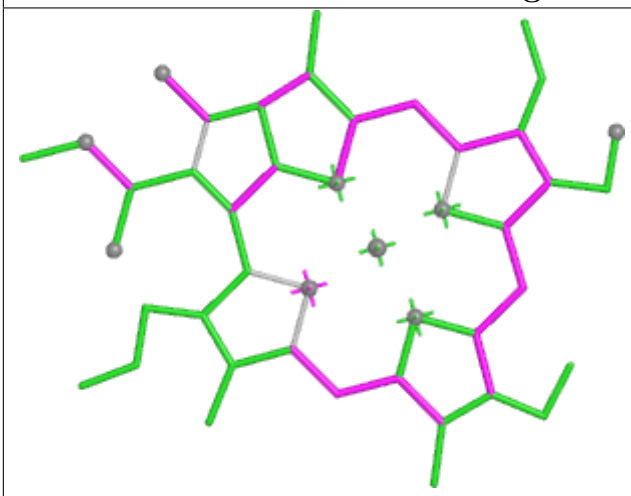
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	821	CLA	1	0
25	Q	610	CLA	3	0
25	U	313	CLA	6	0
32	H	204	LMG	3	0

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.

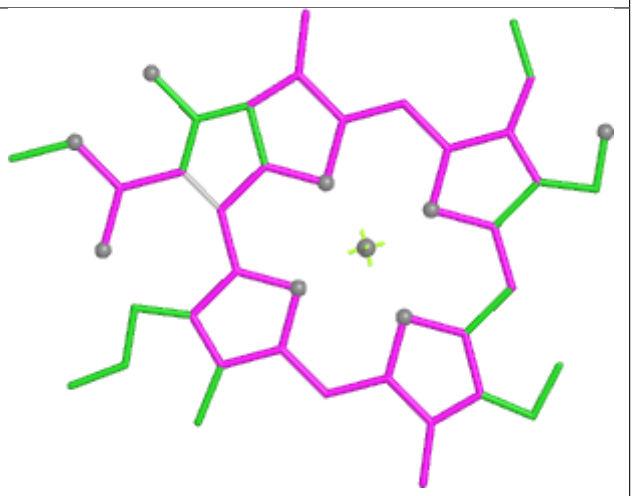
Ligand CLA 4 301



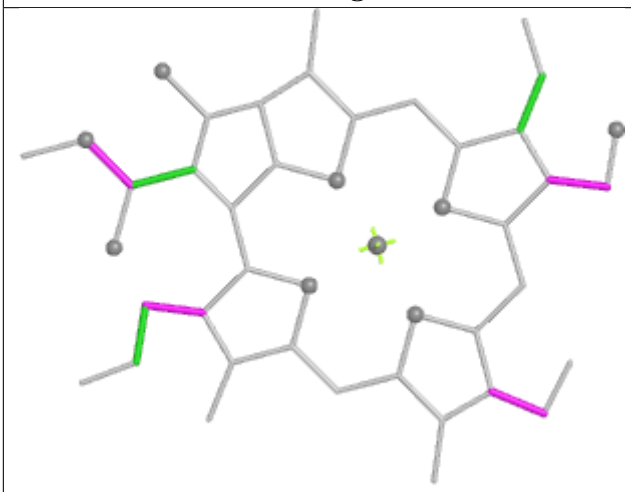
Ligand CHL R 608



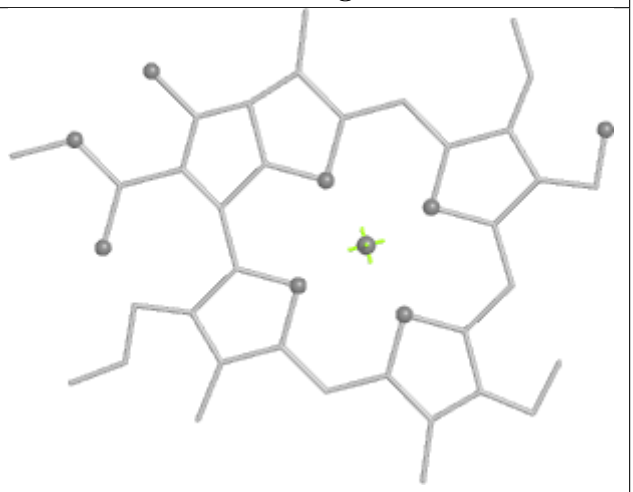
Bond lengths



Bond angles

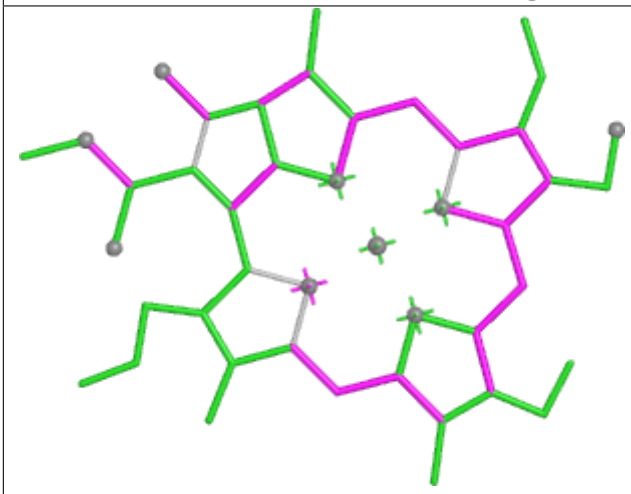


Torsions

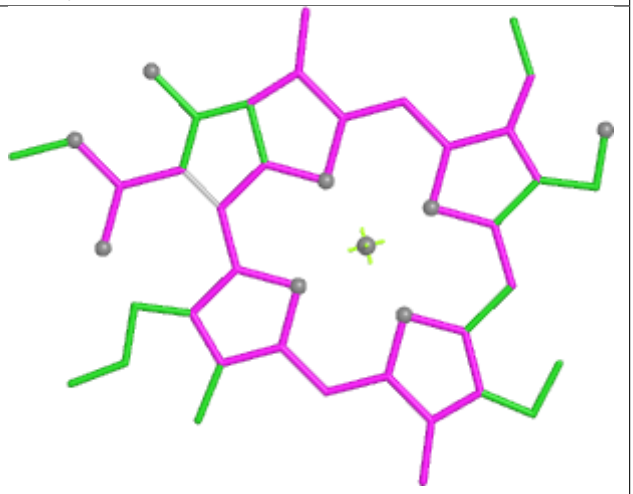


Rings

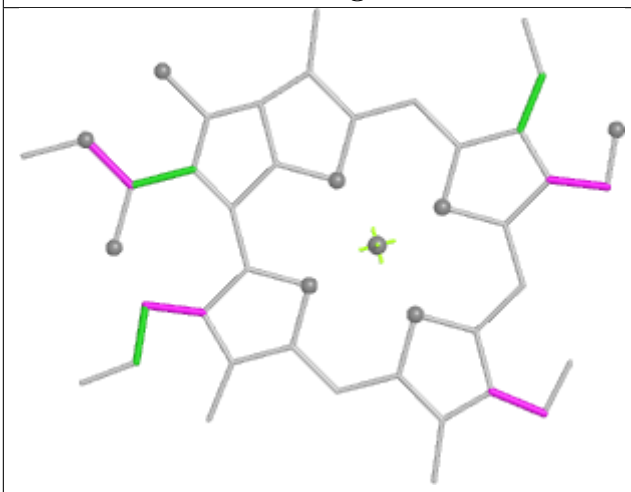
Ligand CHL Q 607



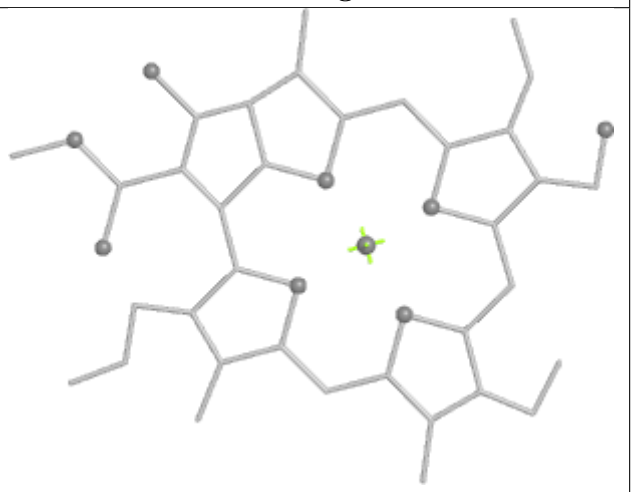
Bond lengths



Bond angles

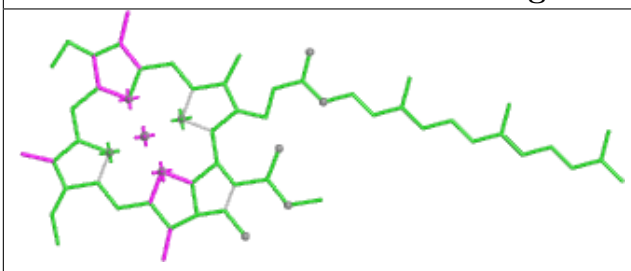


Torsions

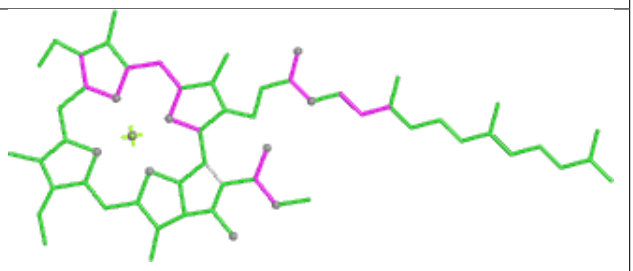


Rings

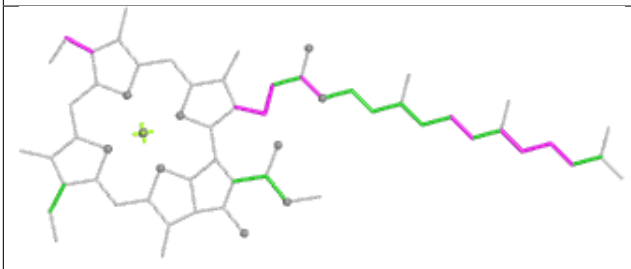
Ligand CLA 8 310



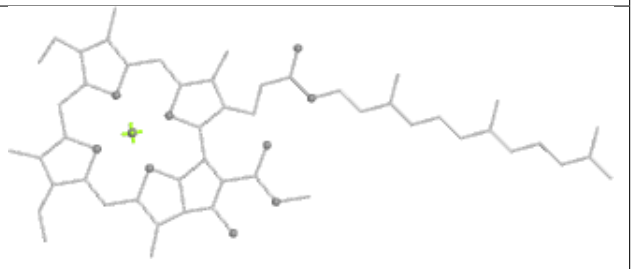
Bond lengths



Bond angles

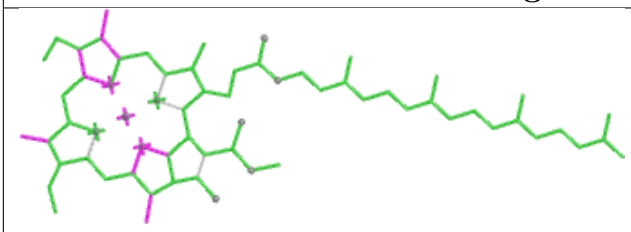


Torsions

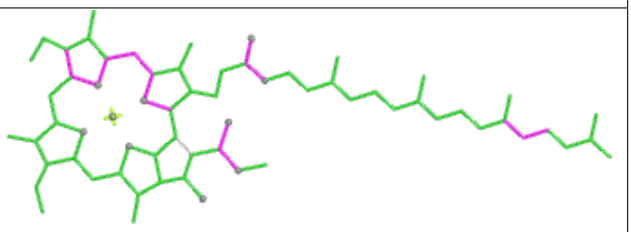


Rings

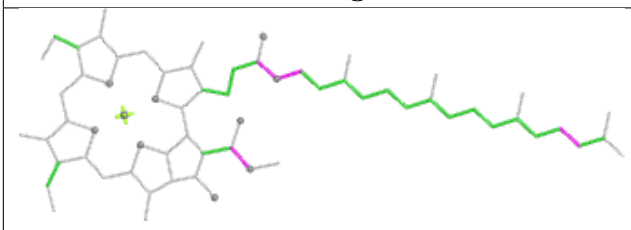
Ligand CLA A 811



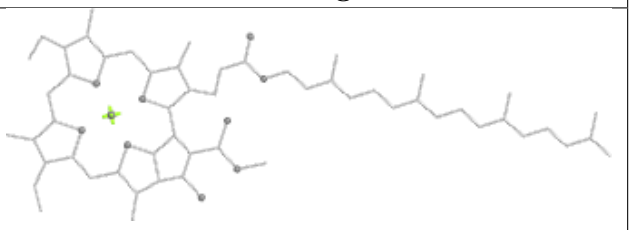
Bond lengths



Bond angles

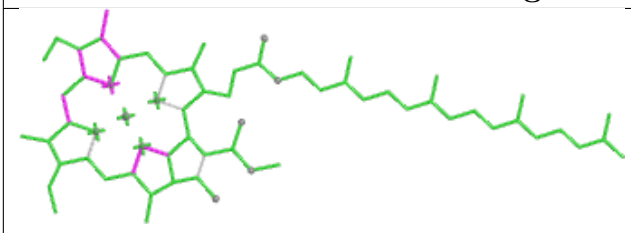


Torsions



Rings

Ligand CLA R 602



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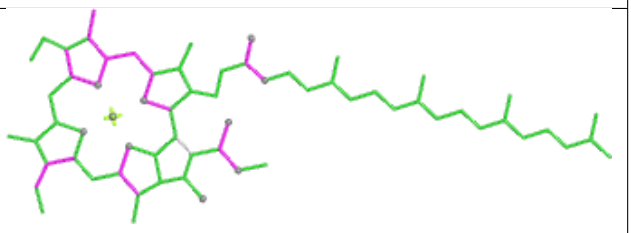

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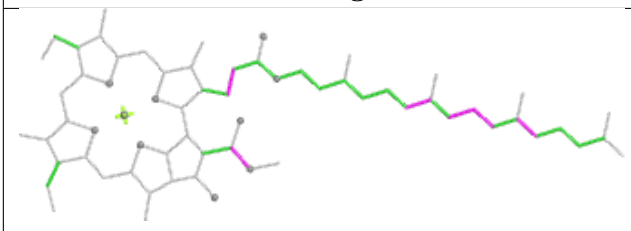

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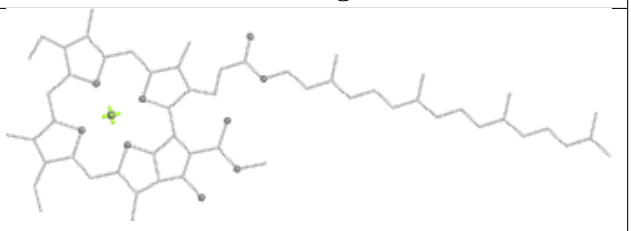
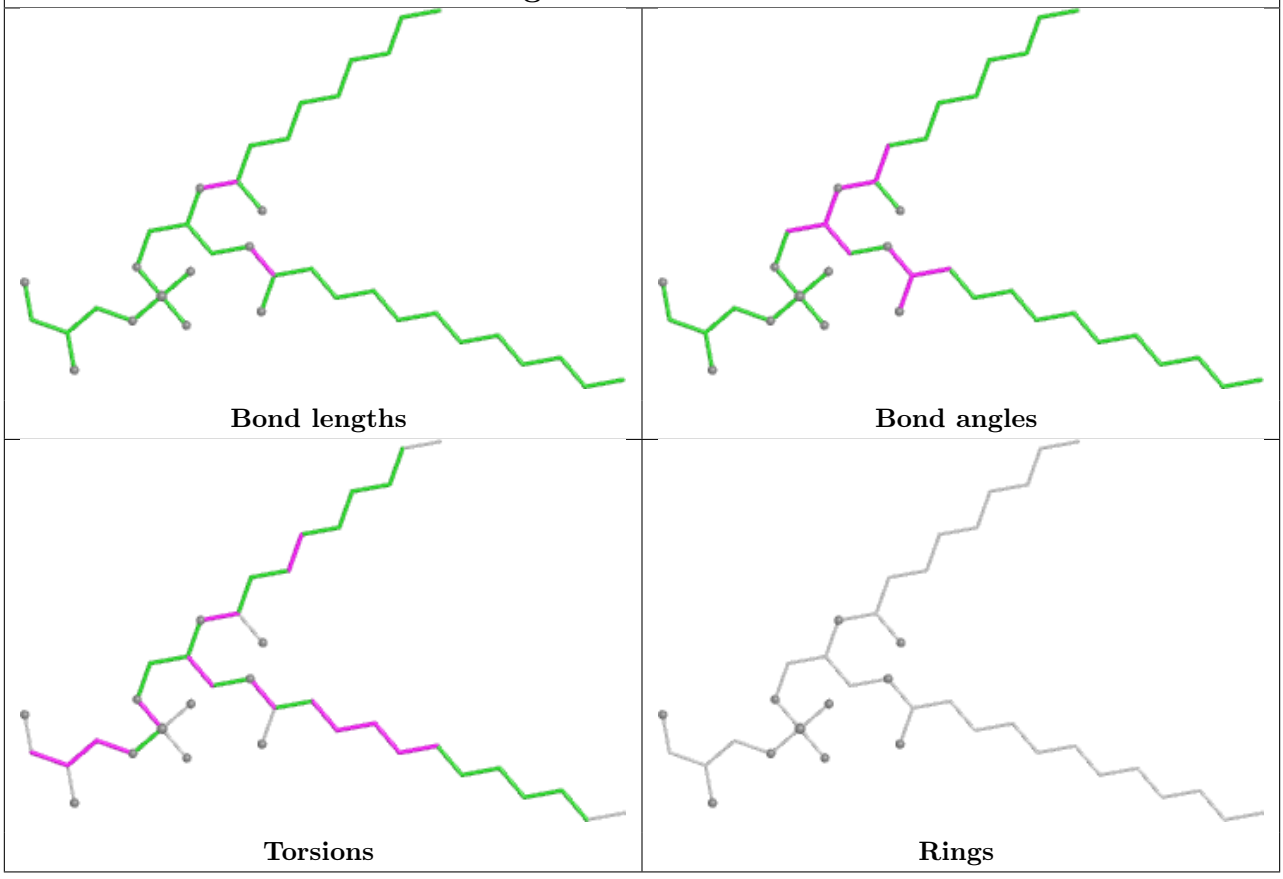
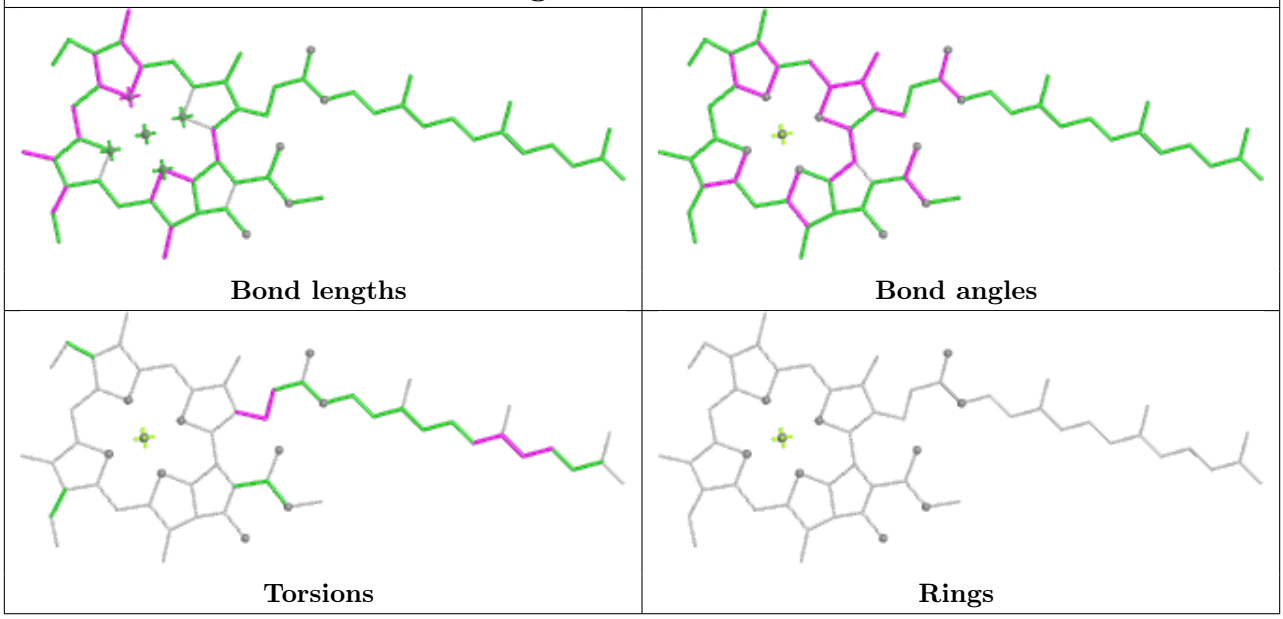


Rings

Ligand LHG B 847



Ligand CLA 1 609



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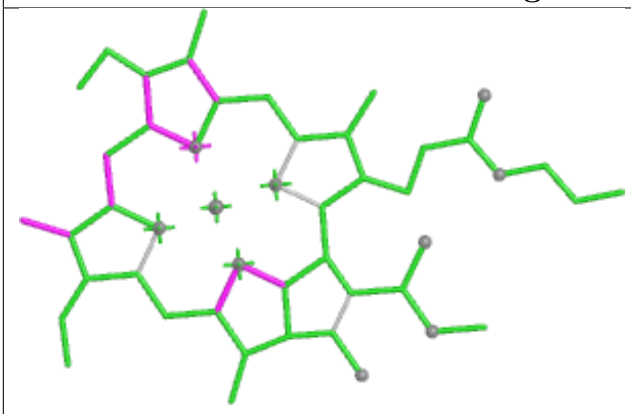
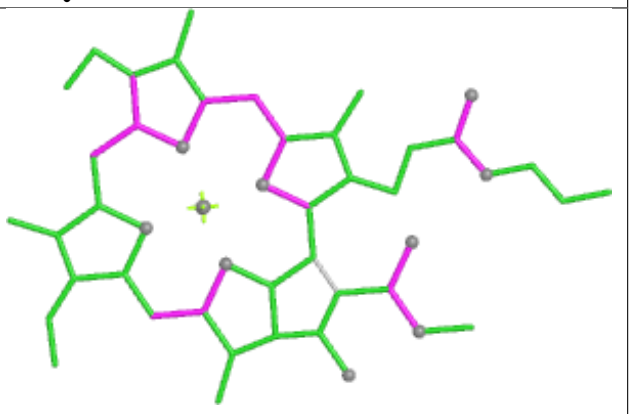


Bond lengths



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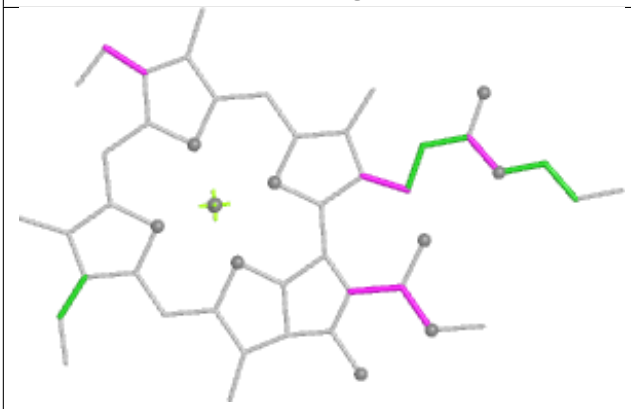

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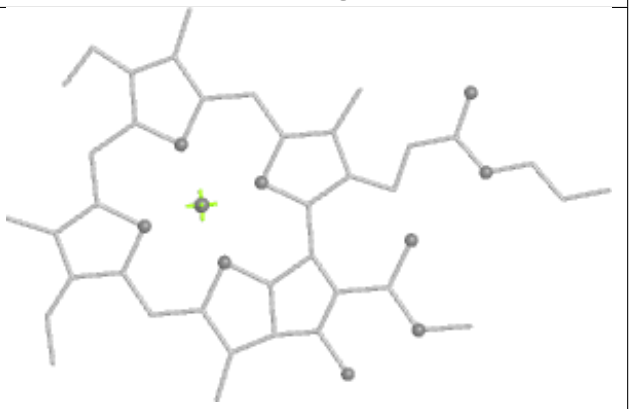
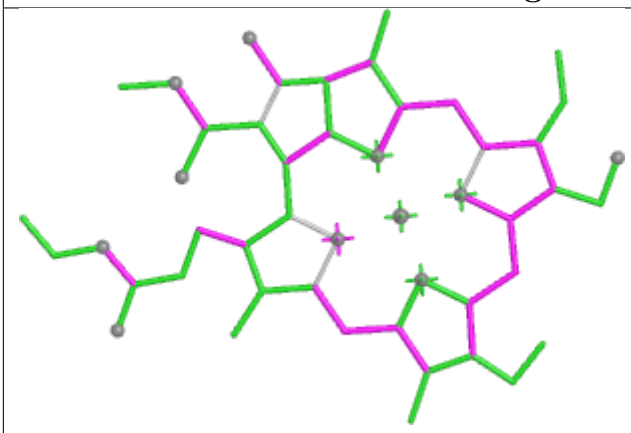


Rings

Ligand CHL P 605



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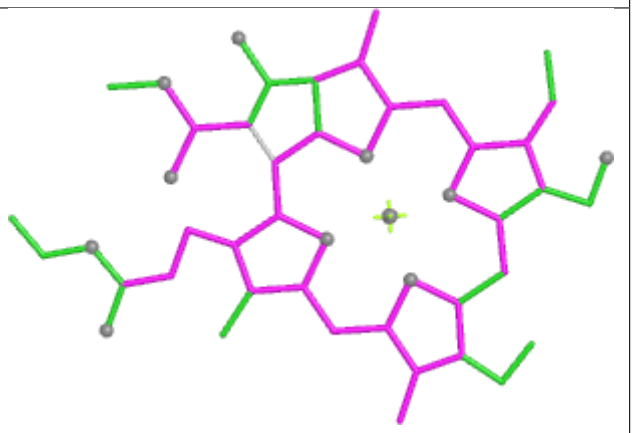
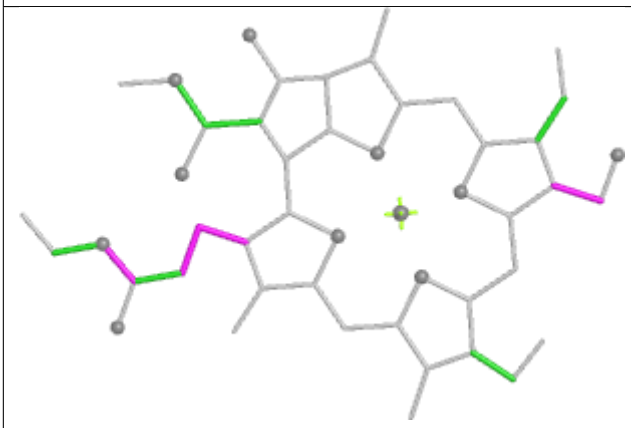


Bond angles



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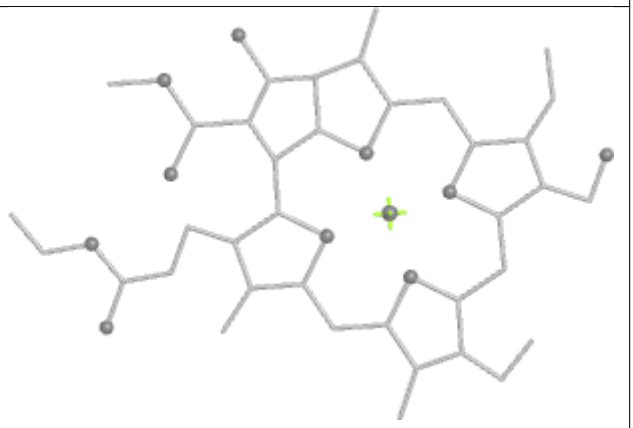
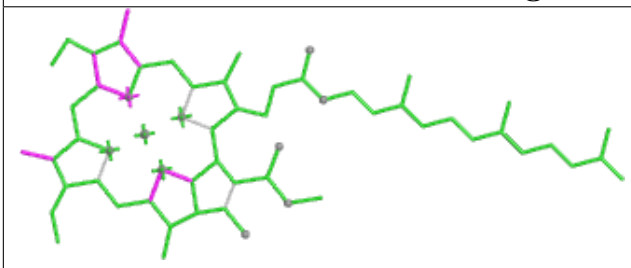


Rings

Ligand CLA T 610



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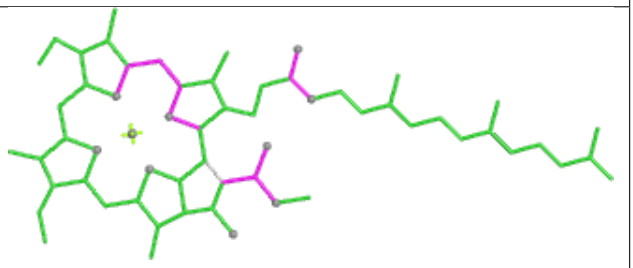
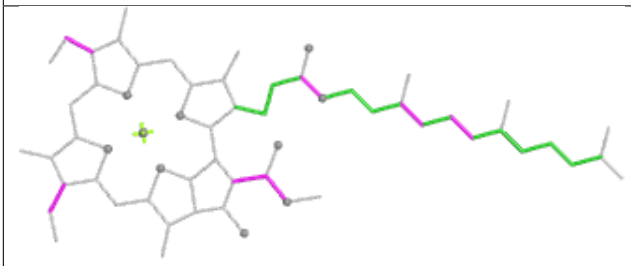


Bond angles



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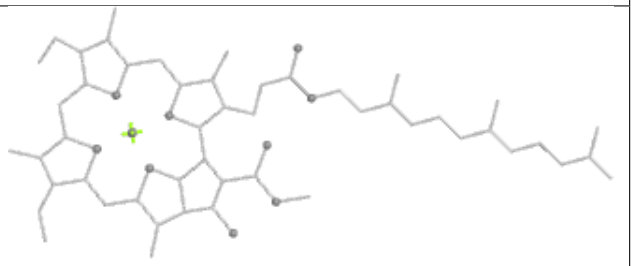
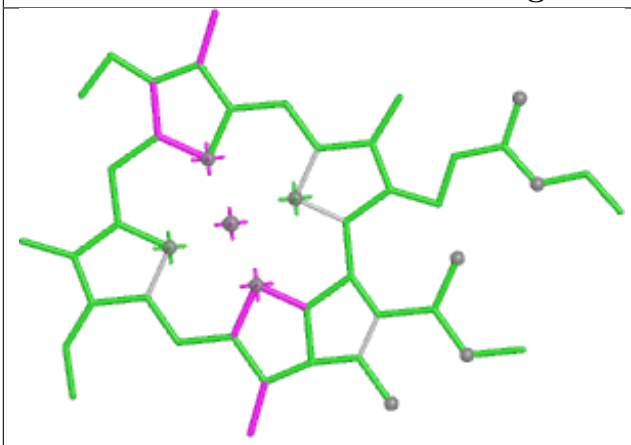


Rings

Ligand CLA S 301



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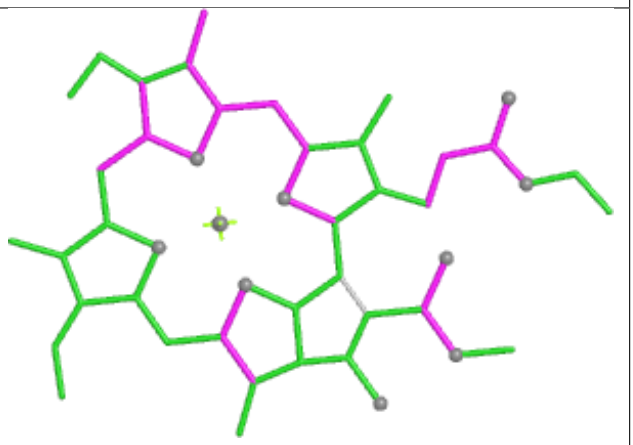

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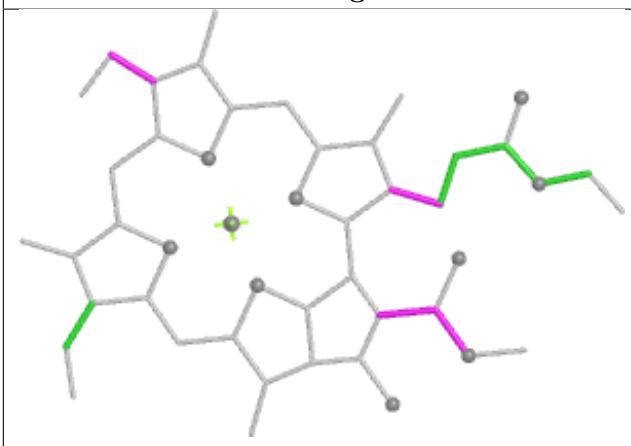

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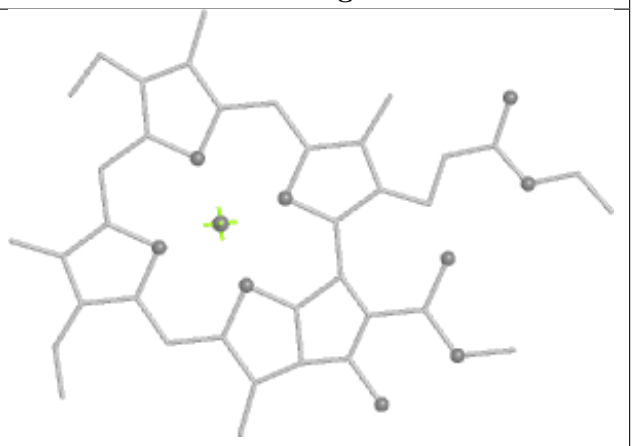
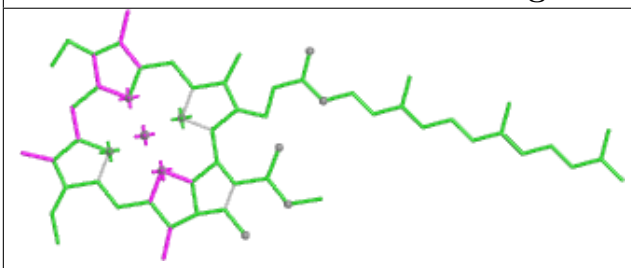


Rings

Ligand CLA 2 309



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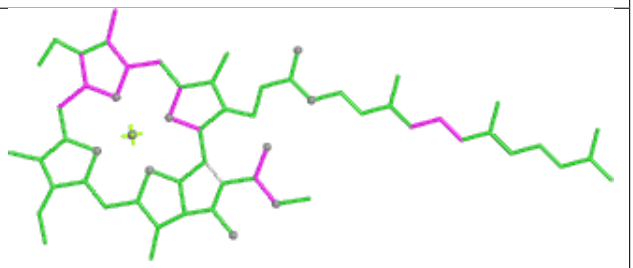

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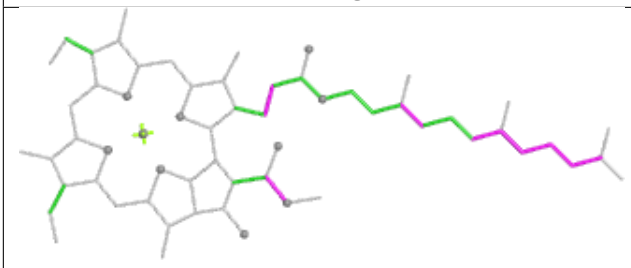

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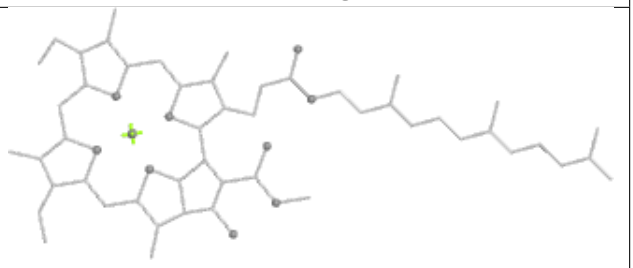
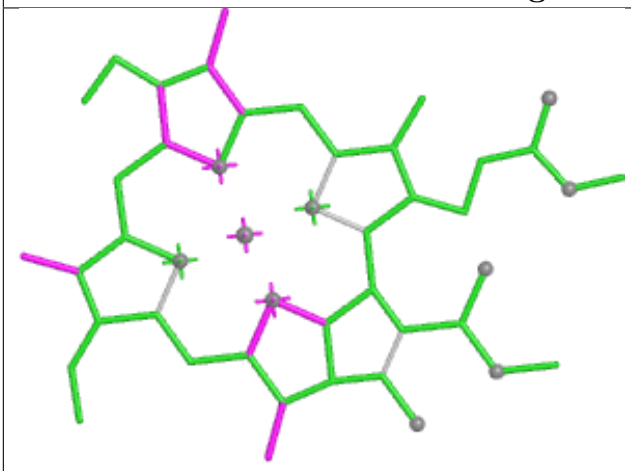


Rings

Ligand CLA 1 614



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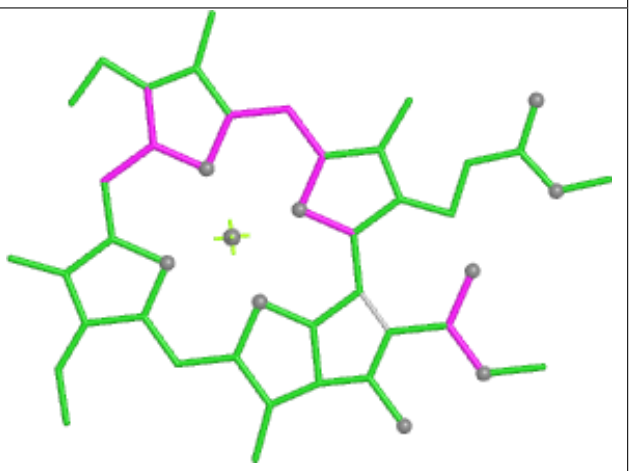

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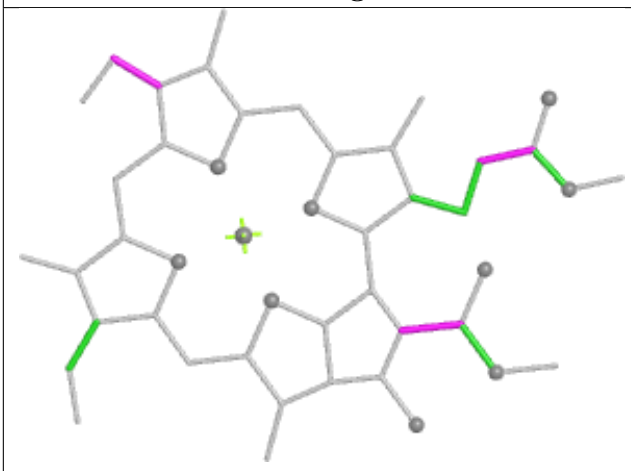

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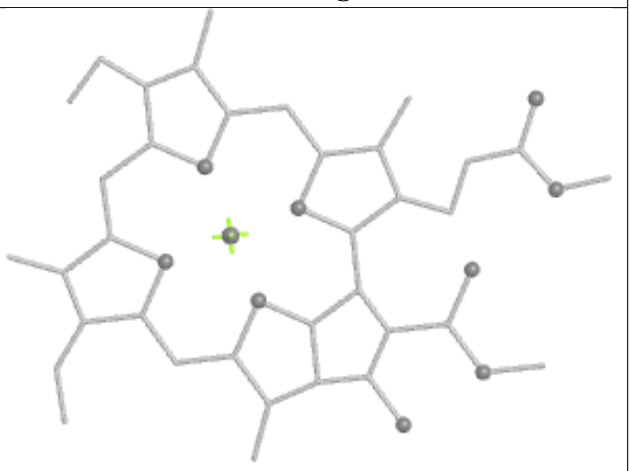
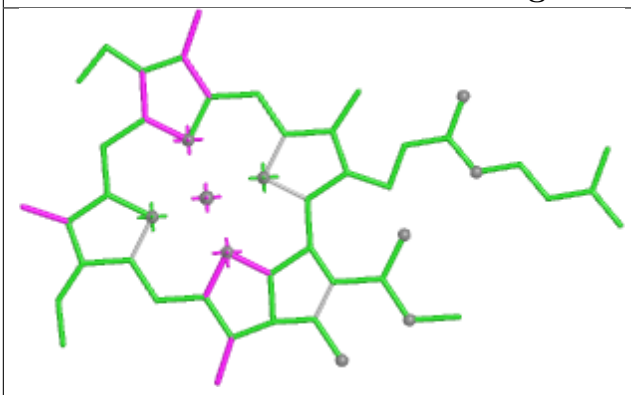


Rings

Ligand CLA 7 307



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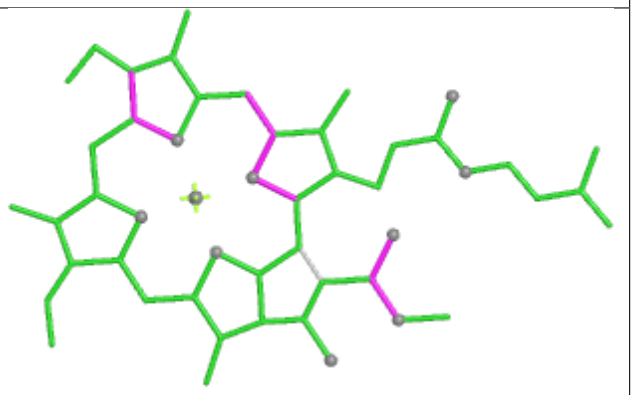

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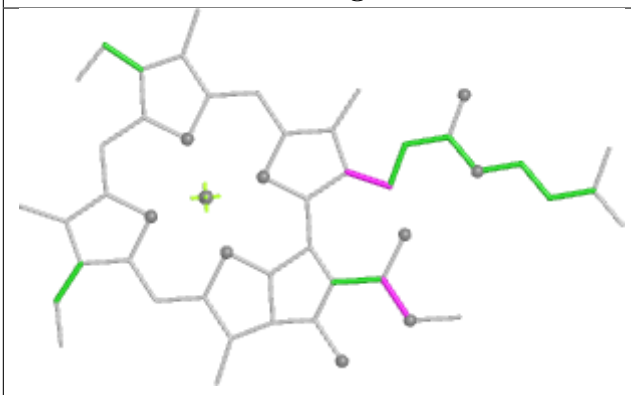

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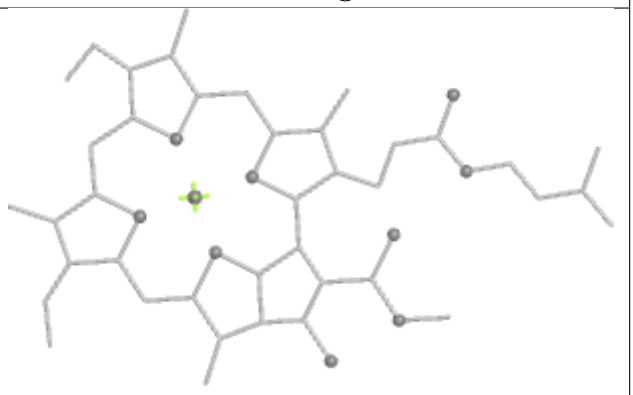
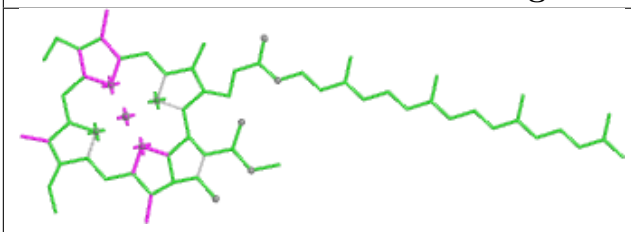


Rings

Ligand CLA 5 302



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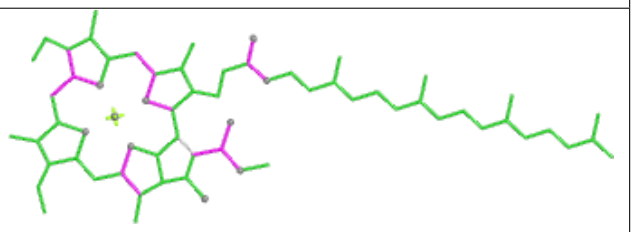

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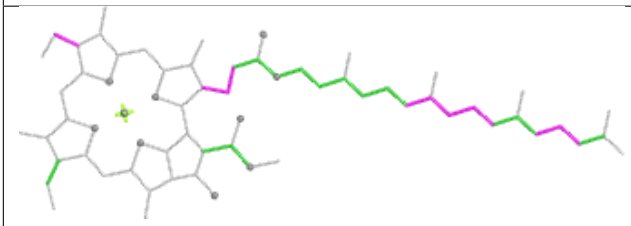

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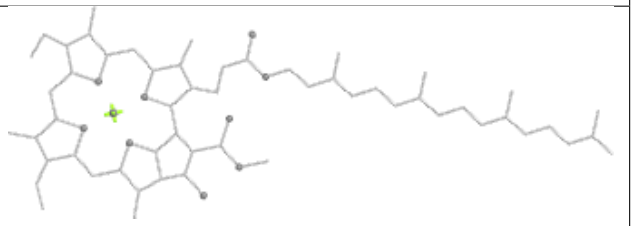
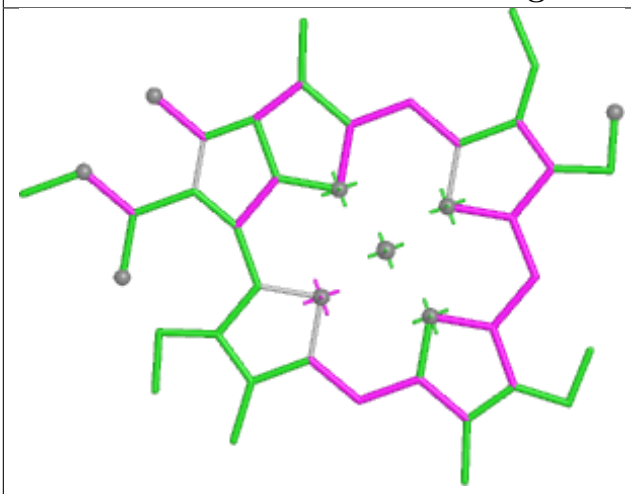


Rings

Ligand CHL 5 317



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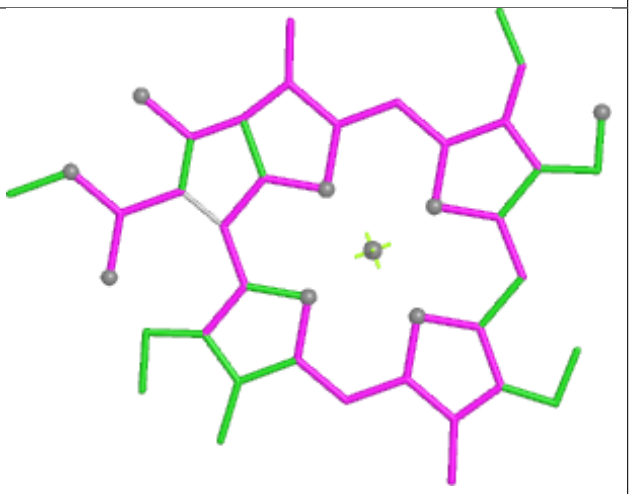

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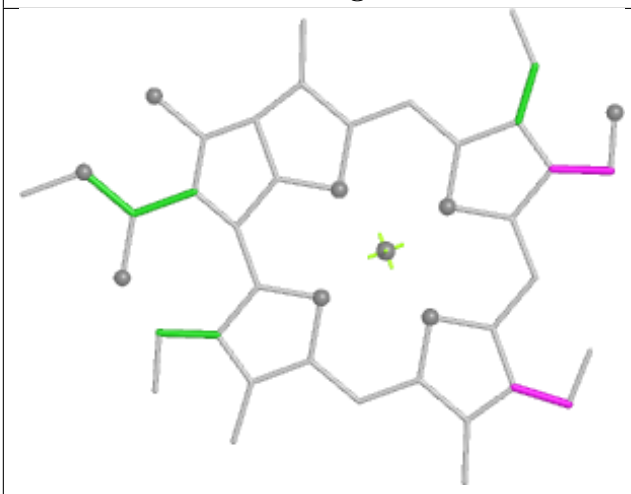
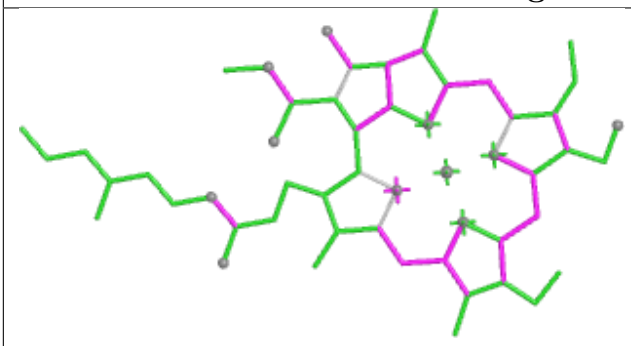


Torsions

Rings

Ligand CHL 8 307



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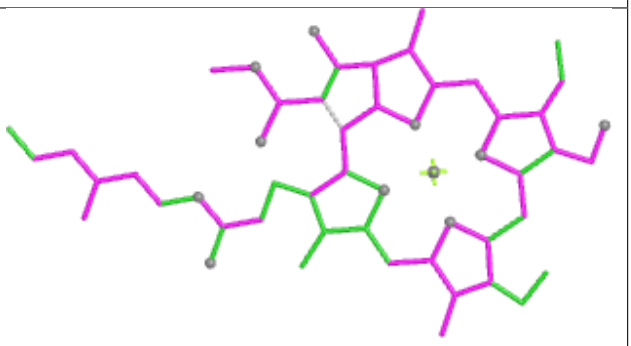

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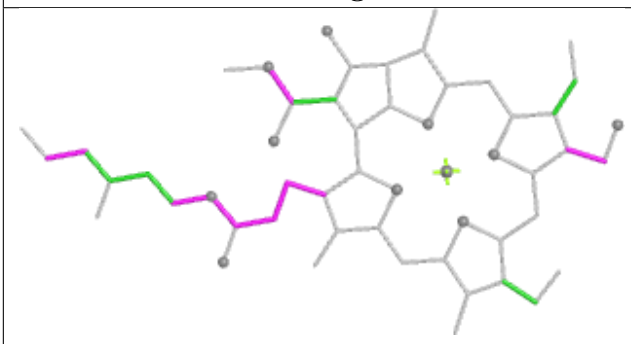

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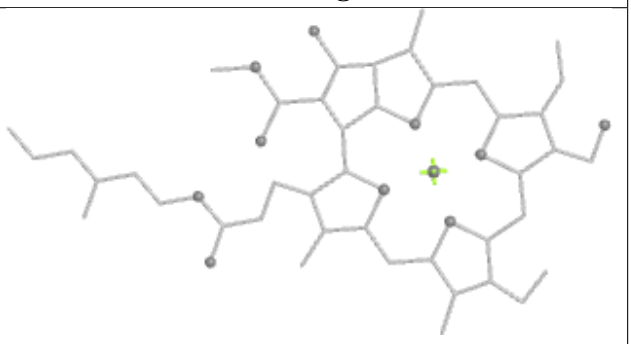
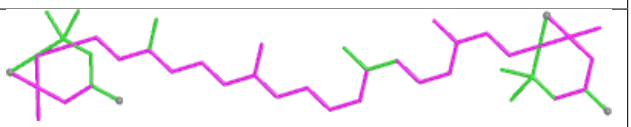


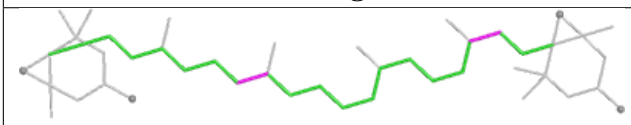
Rings

Ligand XAT S 318

Bond lengths



Bond angles



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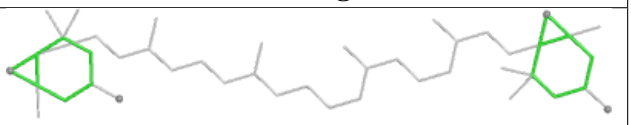
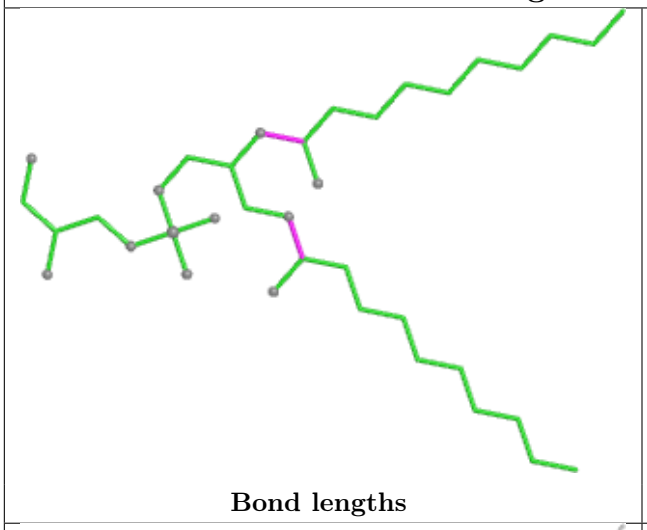


Rings

Ligand LHG 5 321



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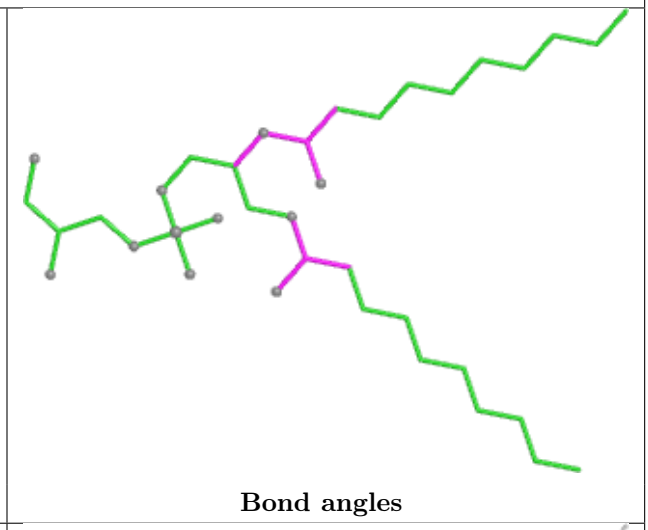
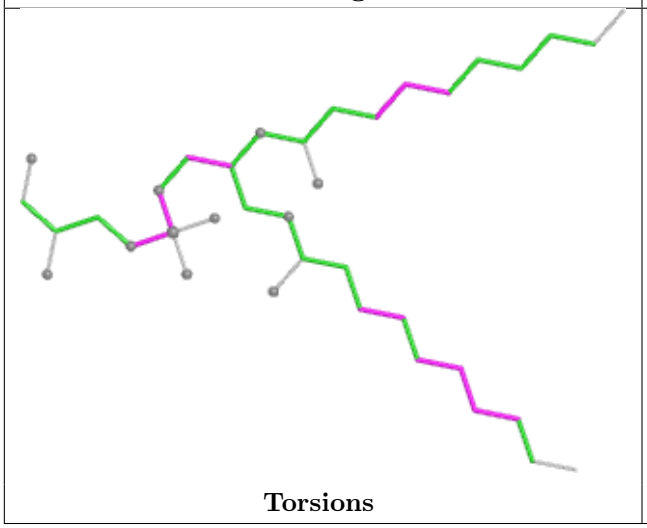


Bond angles



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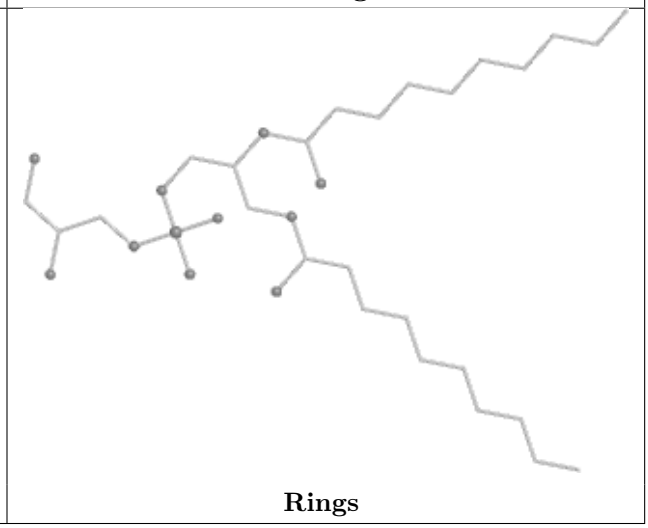
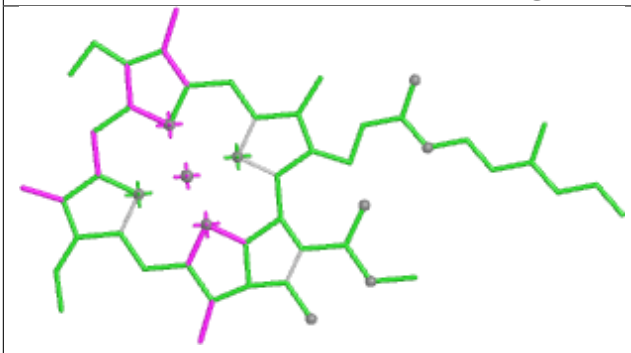
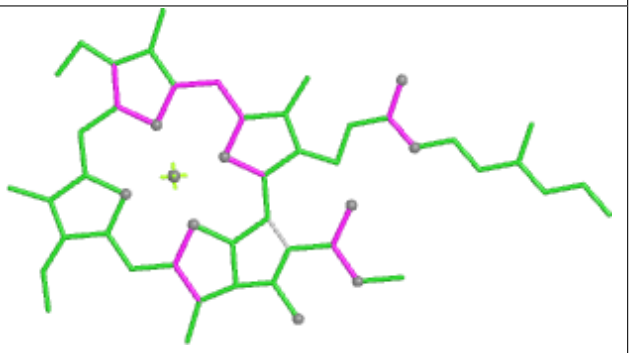


Rings

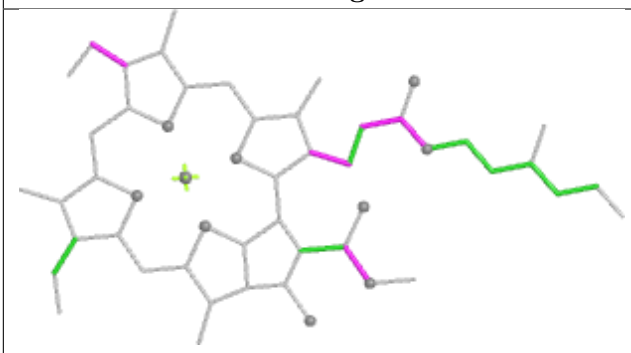
Ligand CLA 1 611



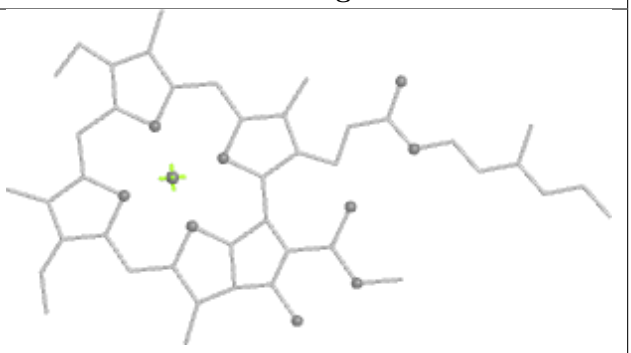
Bond lengths



Bond angles

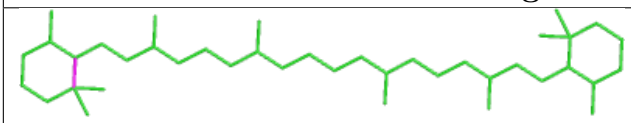


Torsions

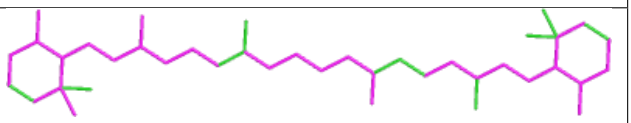


Rings

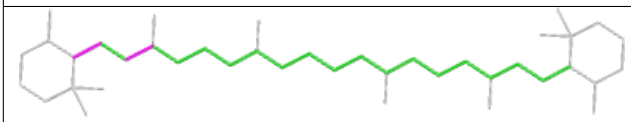
Ligand BCR A 845



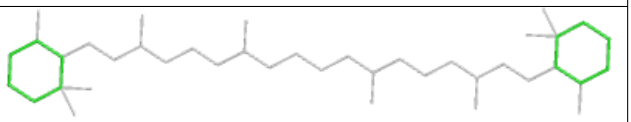
Bond lengths



Bond angles

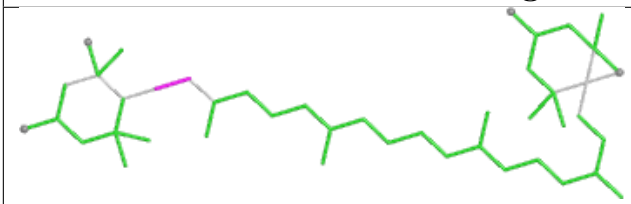


Torsions

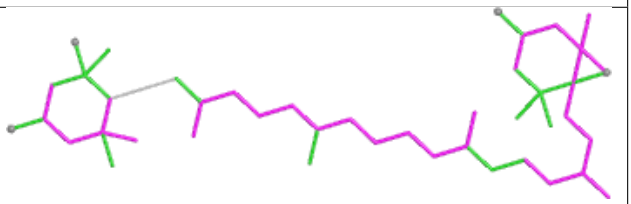


Rings

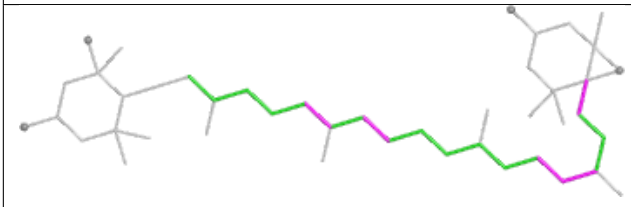
Ligand NEX R 617



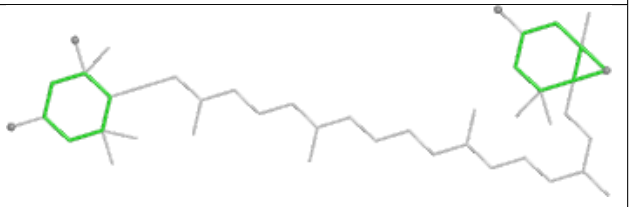
Bond lengths



Bond angles

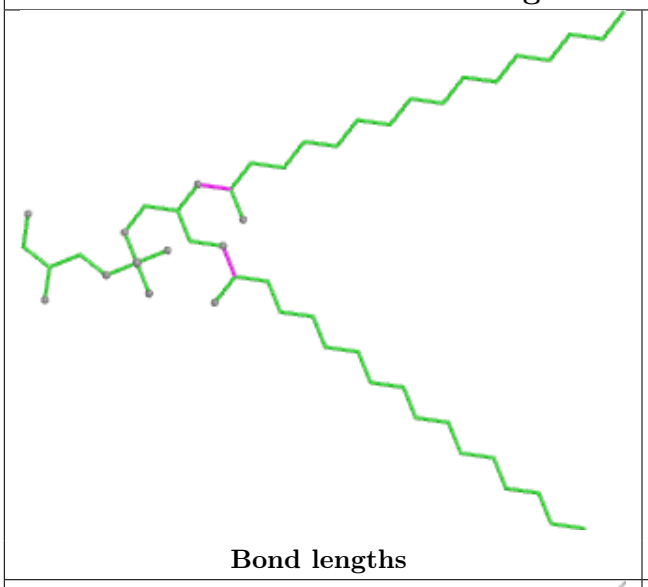


Torsions

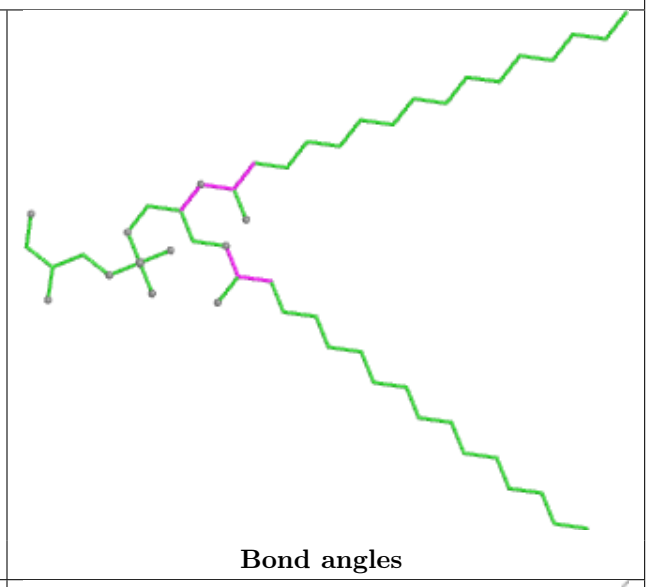


Rings

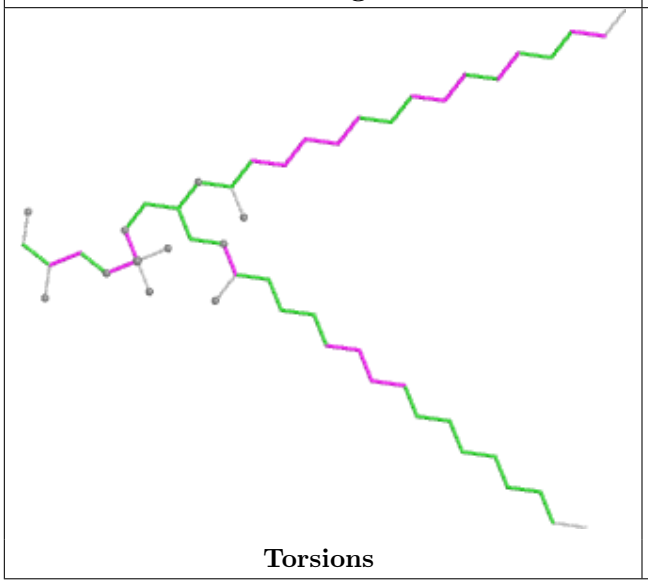
Ligand LHG A 843



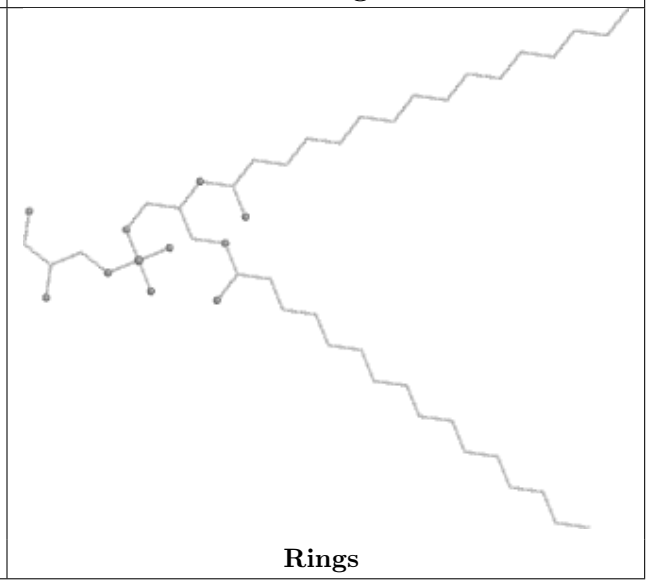
Bond lengths



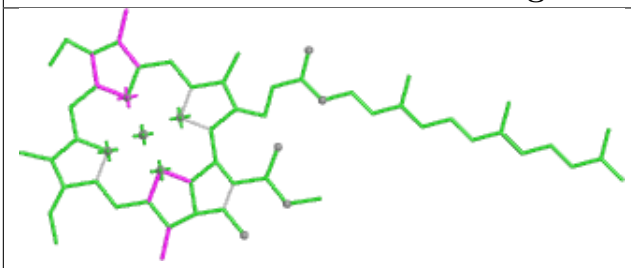
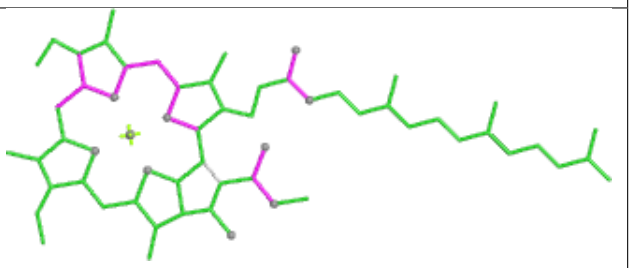
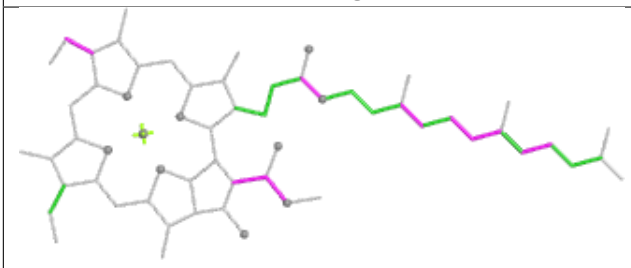
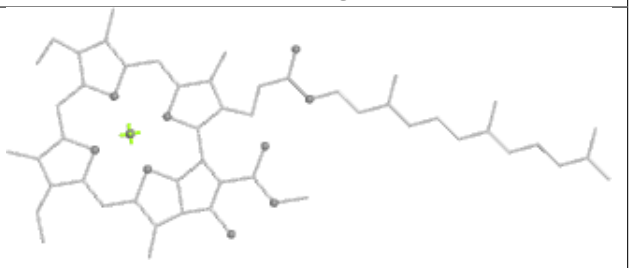
Bond angles

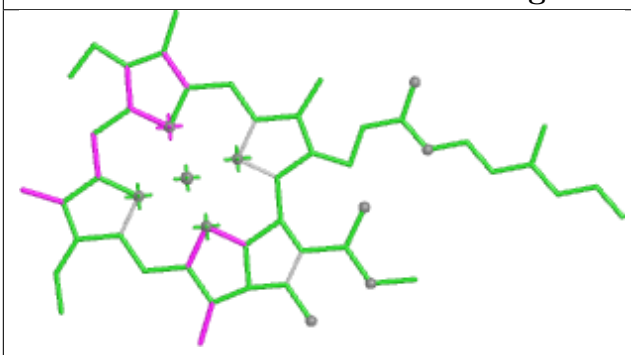
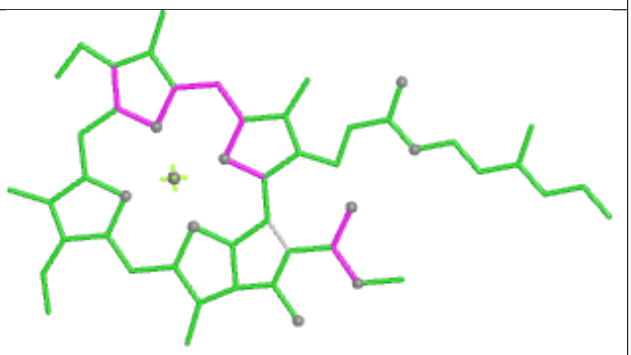
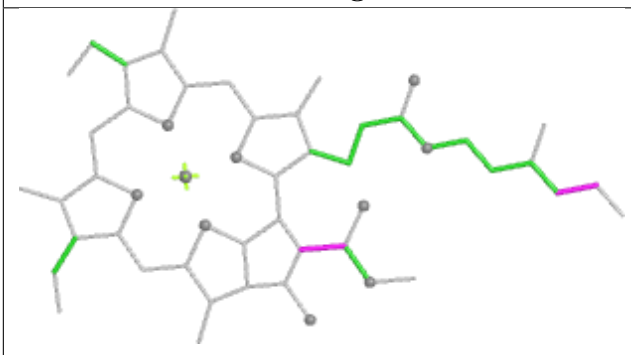
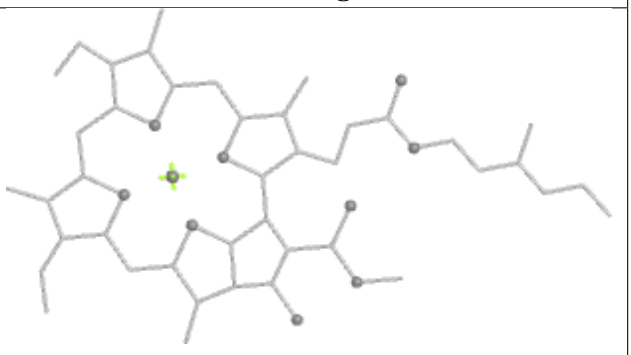


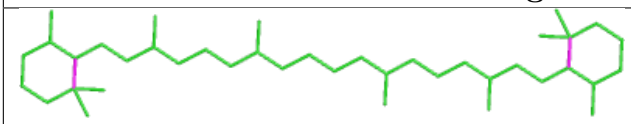
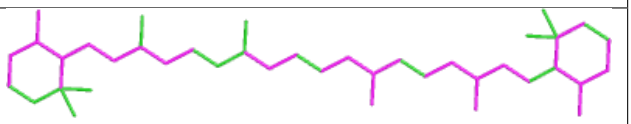
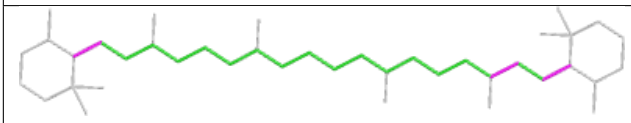
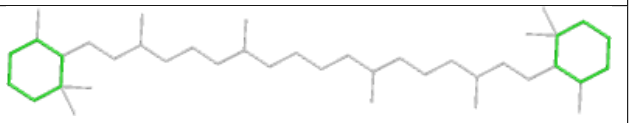
Torsions

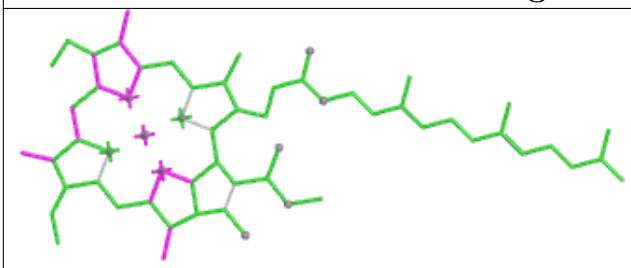
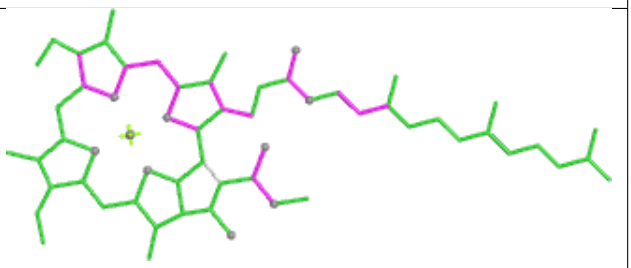
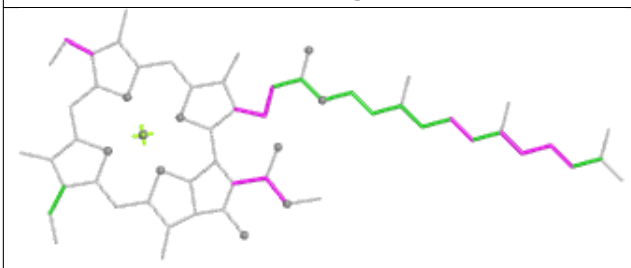
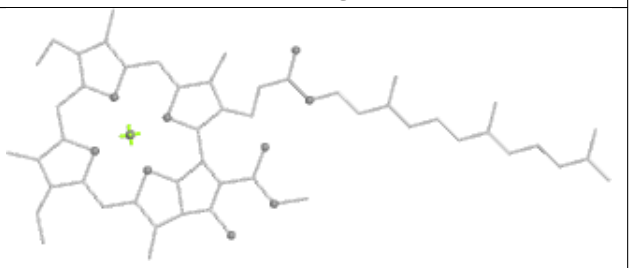


Rings

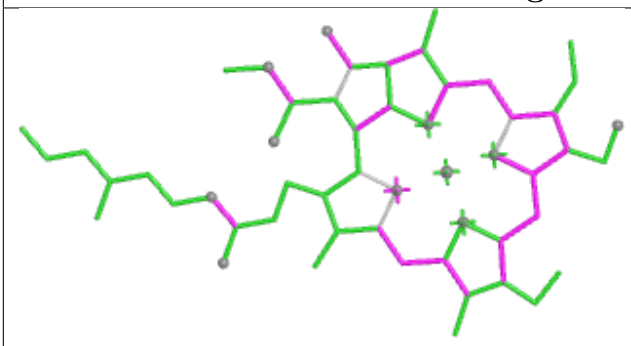
Ligand CLA S 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

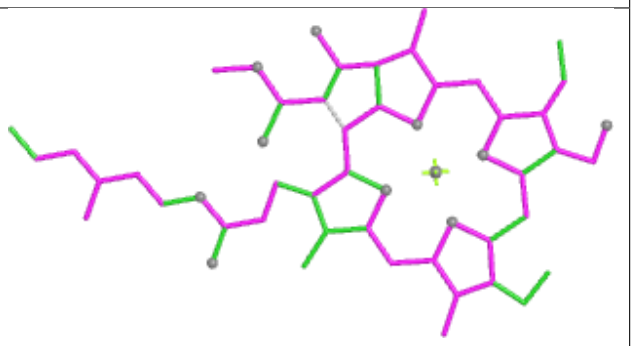
Ligand BCR 3 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

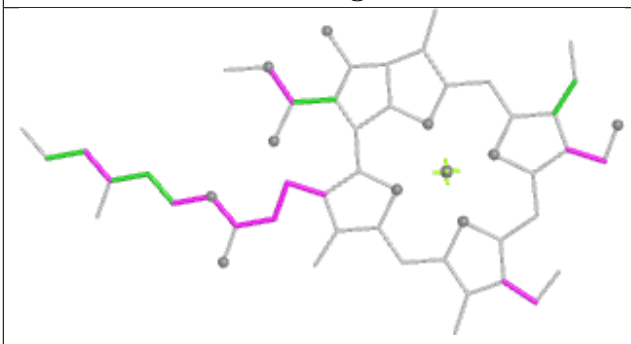
Ligand CHL S 302



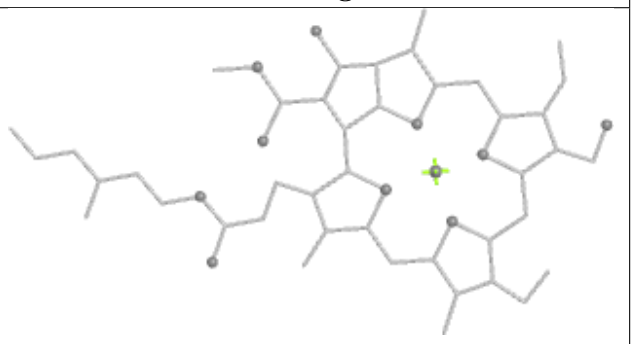
Bond lengths



Bond angles



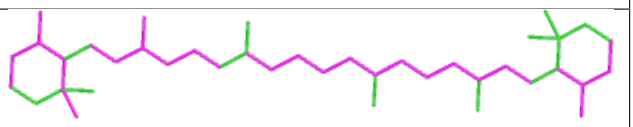
Torsions



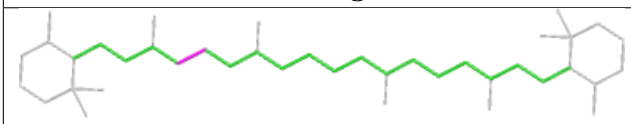
Rings

Ligand BCR G 203

Bond lengths



Bond angles



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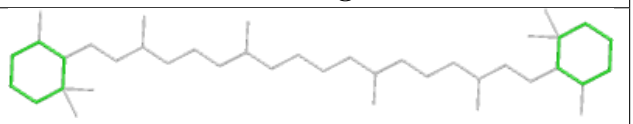
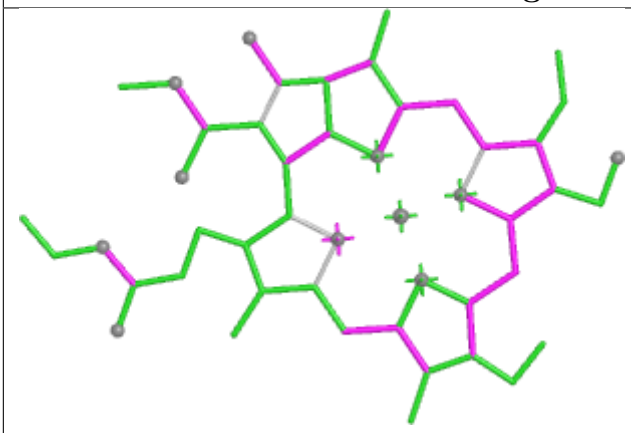


Rings

Ligand CHL U 309



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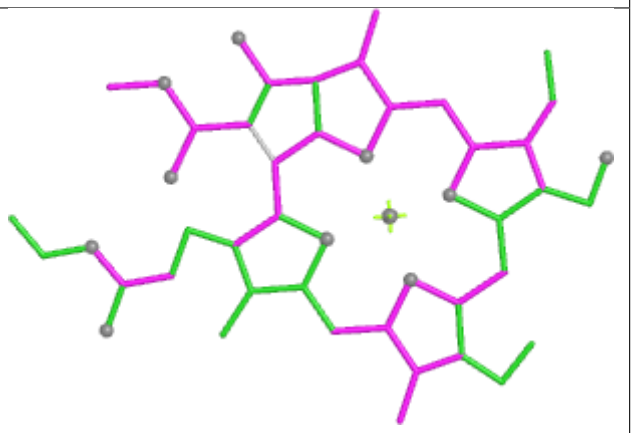
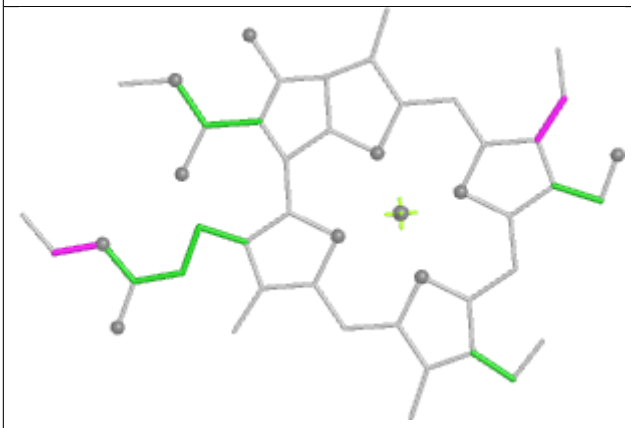
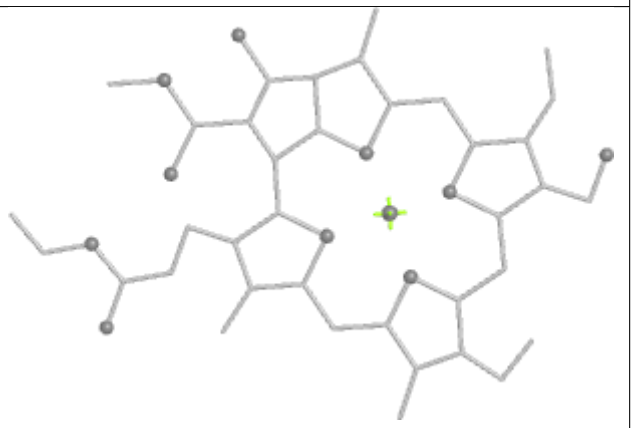


Bond angles

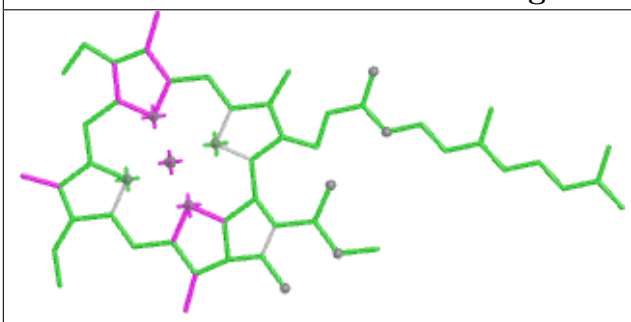


Torsions

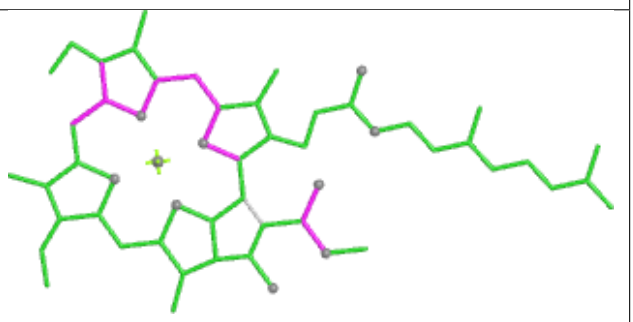


Rings

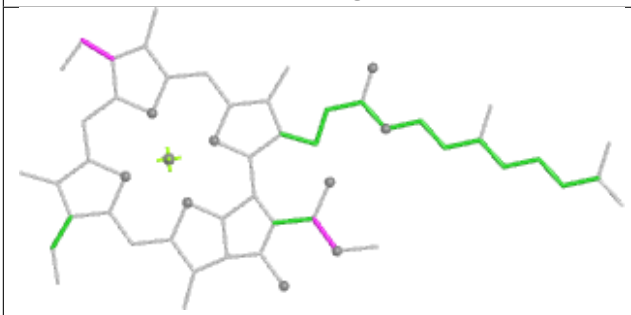
Ligand CLA 5 306



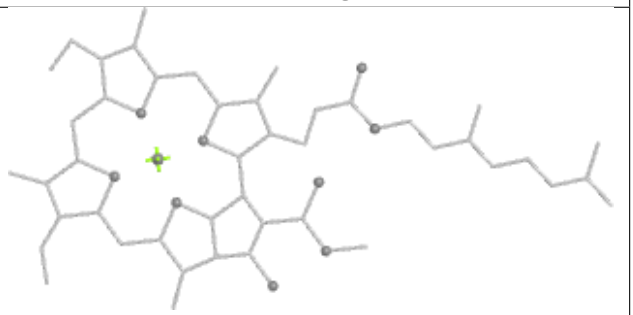
Bond lengths



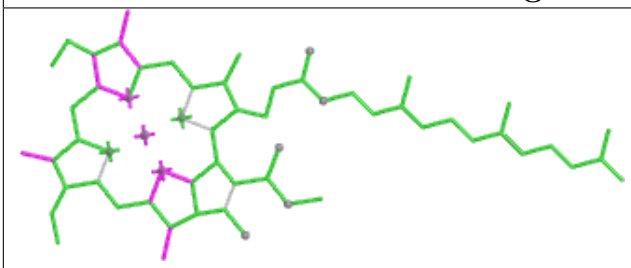
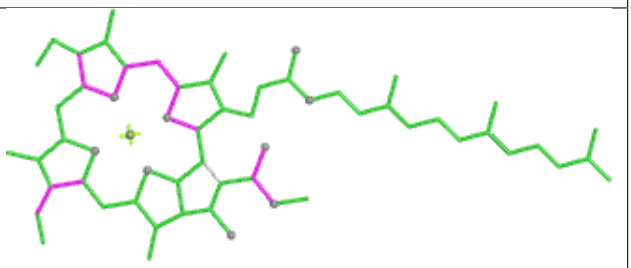
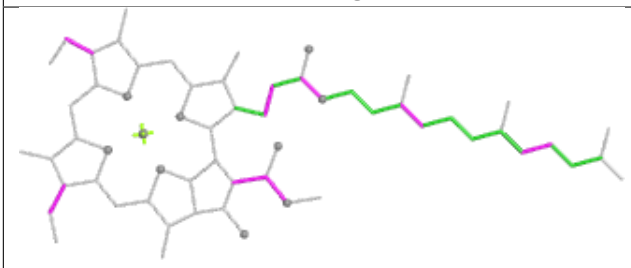
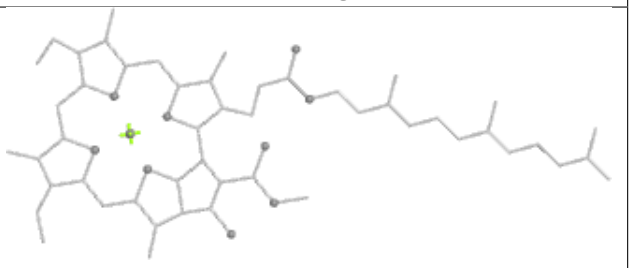
Bond angles

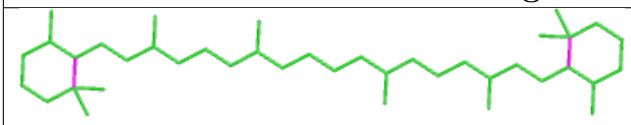
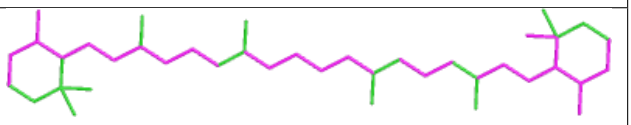
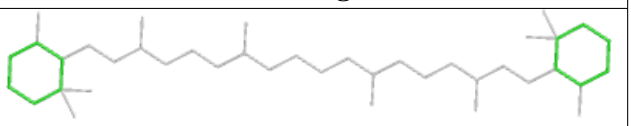


Torsions

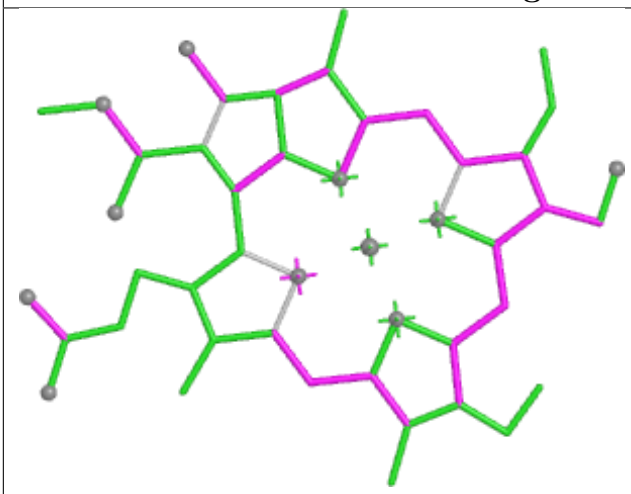


Rings

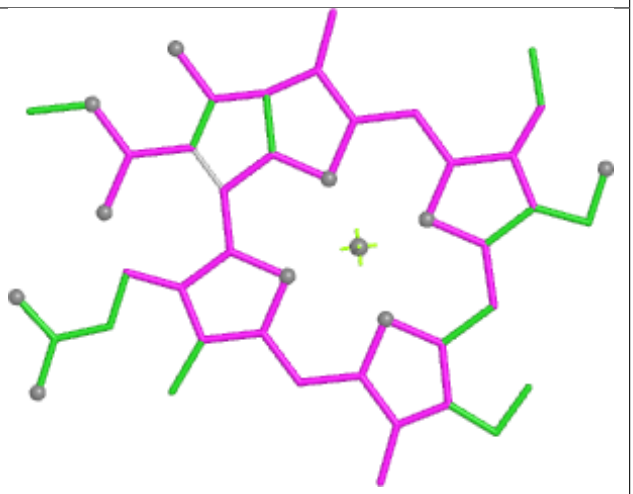
Ligand CLA B 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

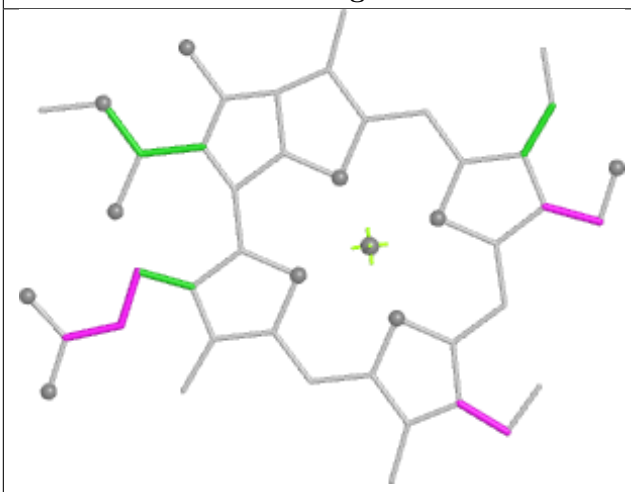
Ligand CHL R 605



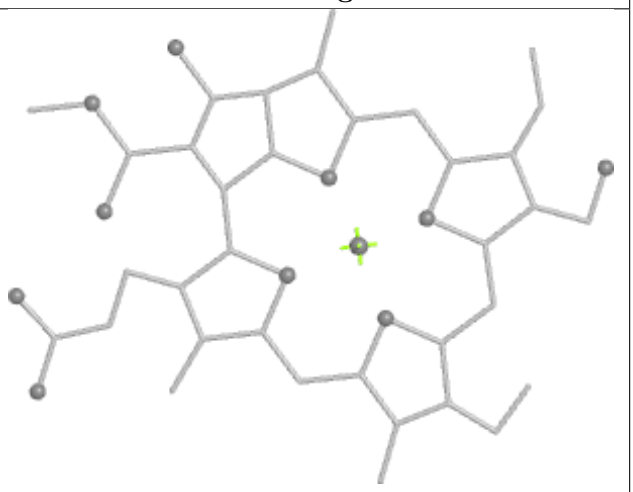
Bond lengths



Bond angles

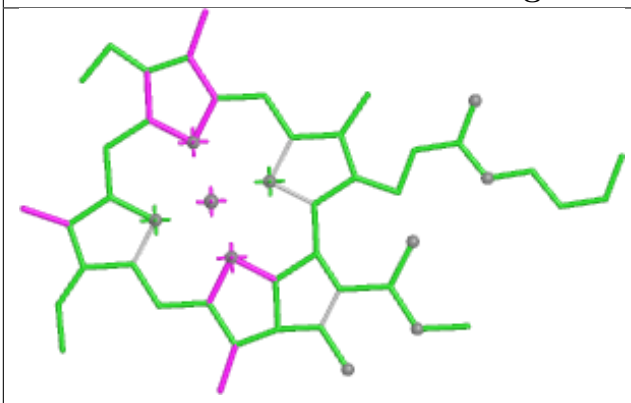


Torsions

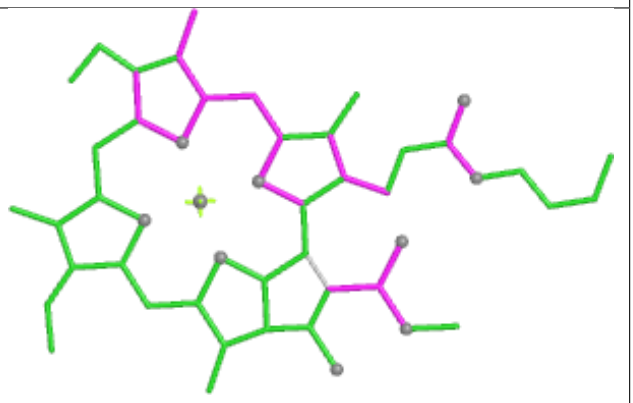


Rings

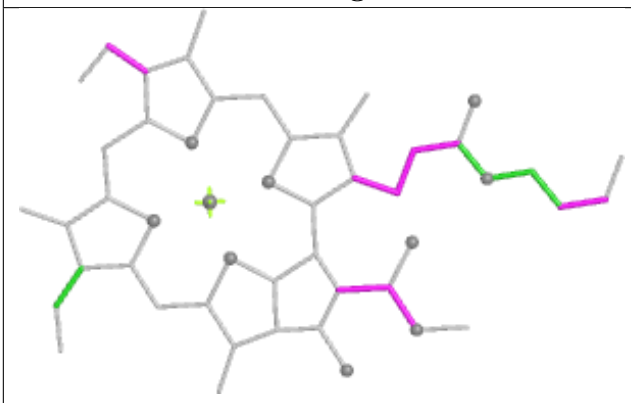
Ligand CLA A 823



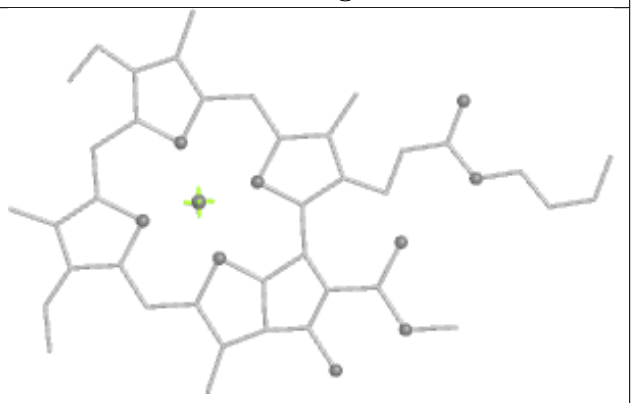
Bond lengths



Bond angles

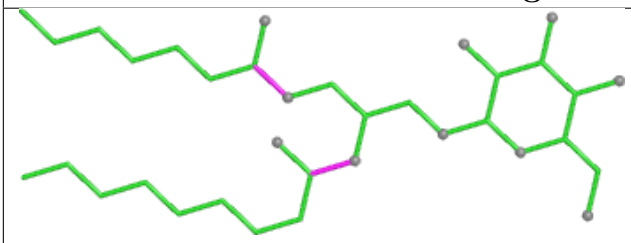


Torsions

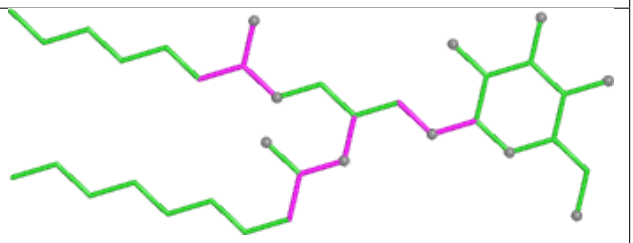


Rings

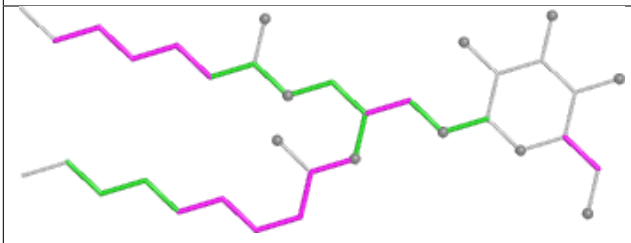
Ligand LMG J 104



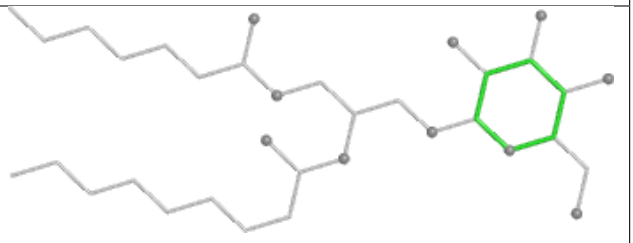
Bond lengths



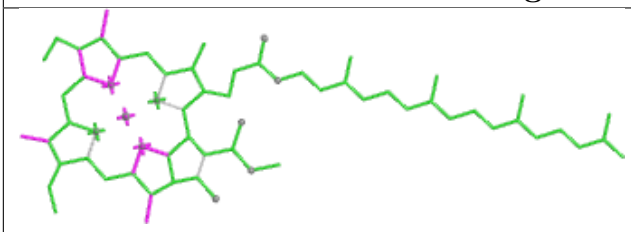
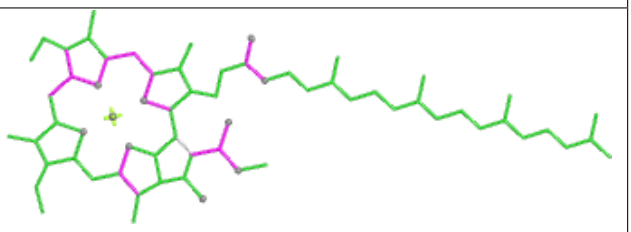
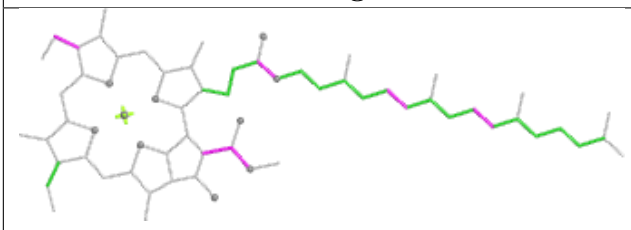
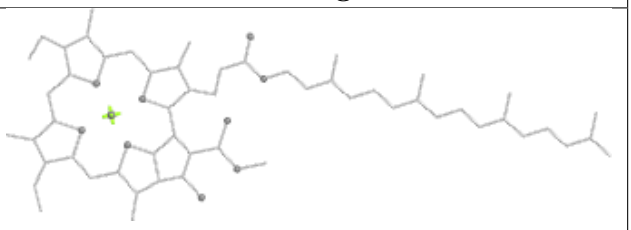
Bond angles

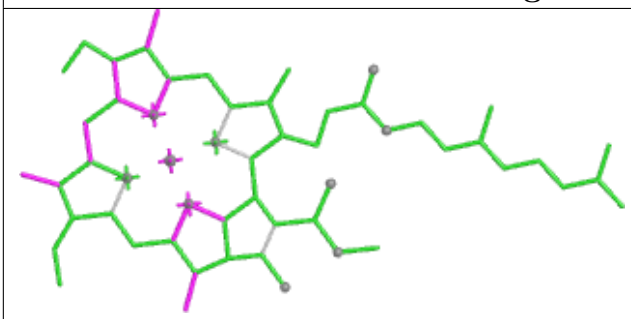
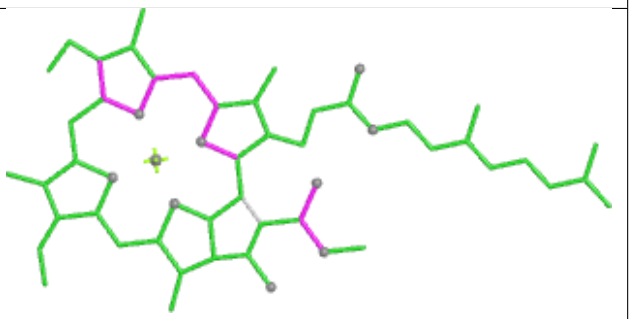
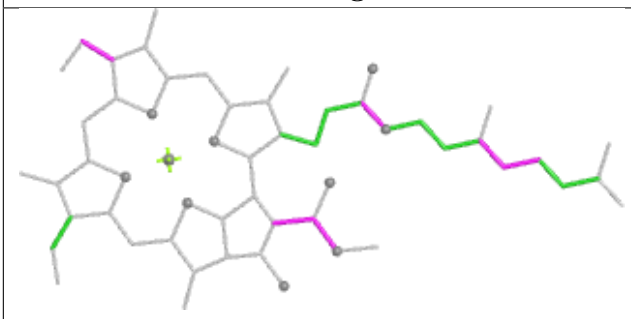
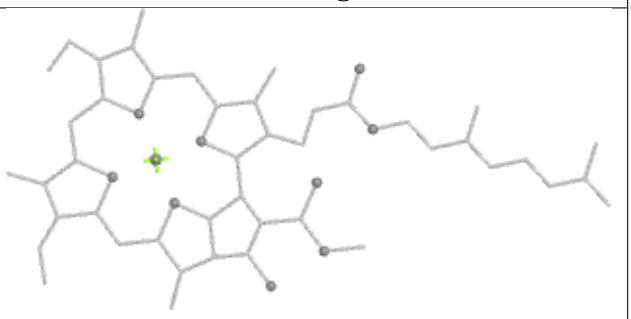


Torsions

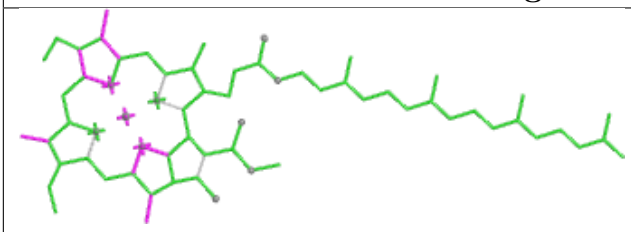


Rings

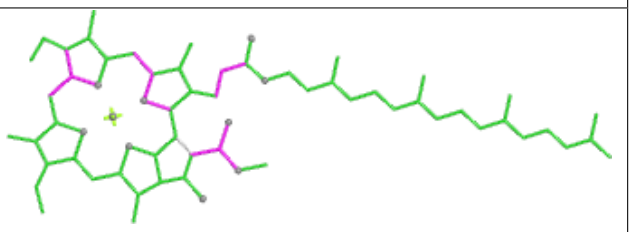
Ligand CLA B 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

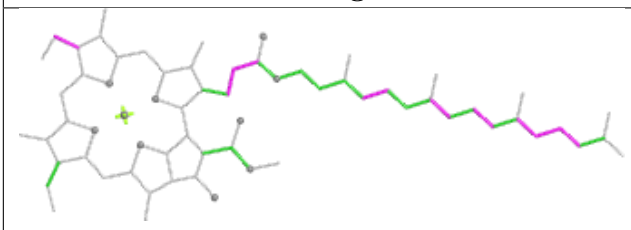
Ligand CLA B 806



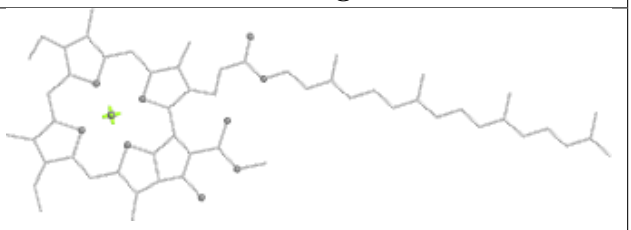
Bond lengths



Bond angles

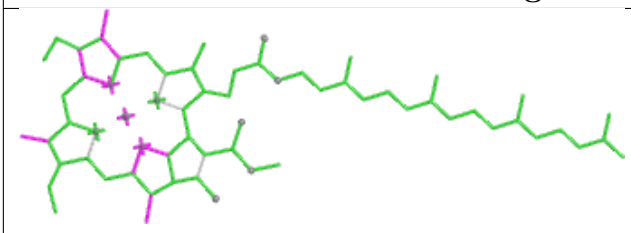


Torsions

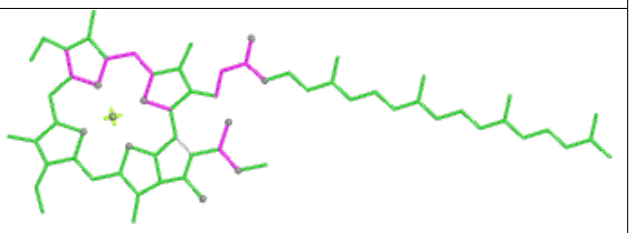


Rings

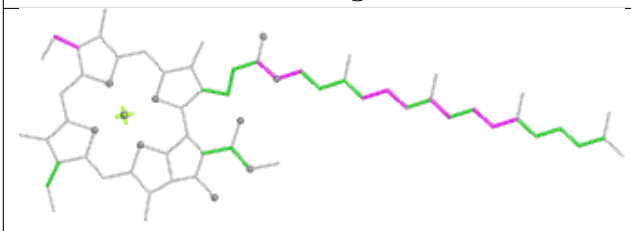
Ligand CLA B 831



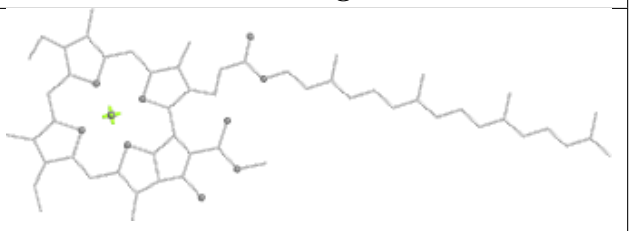
Bond lengths



Bond angles

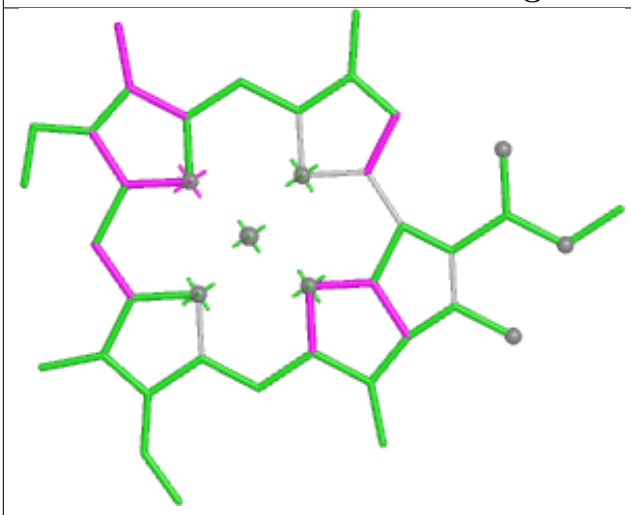


Torsions

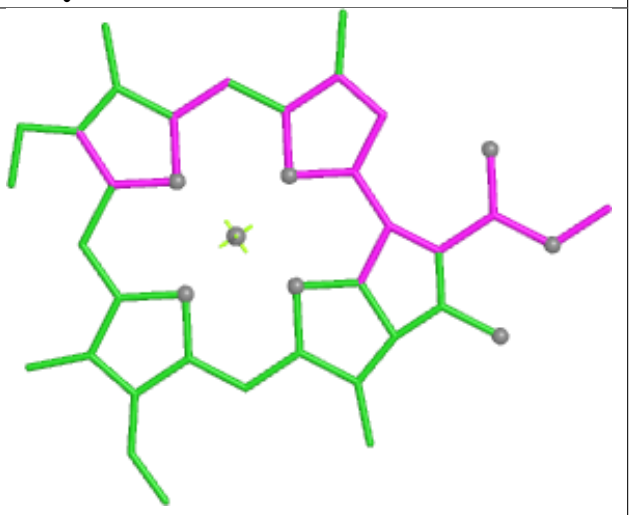


Rings

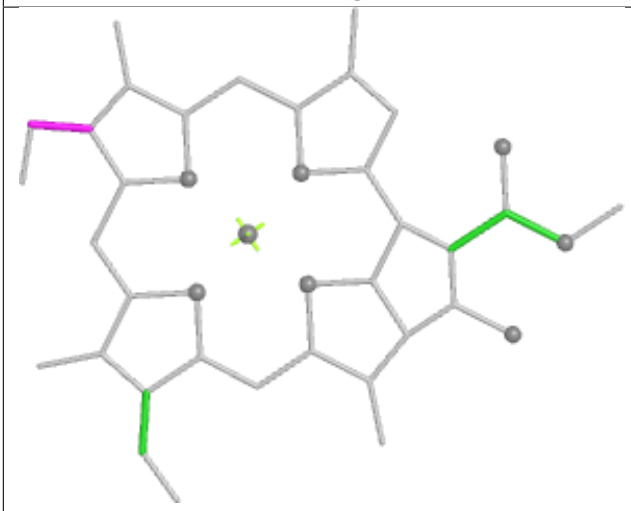
Ligand CLA Q 618



Bond lengths



Bond angles



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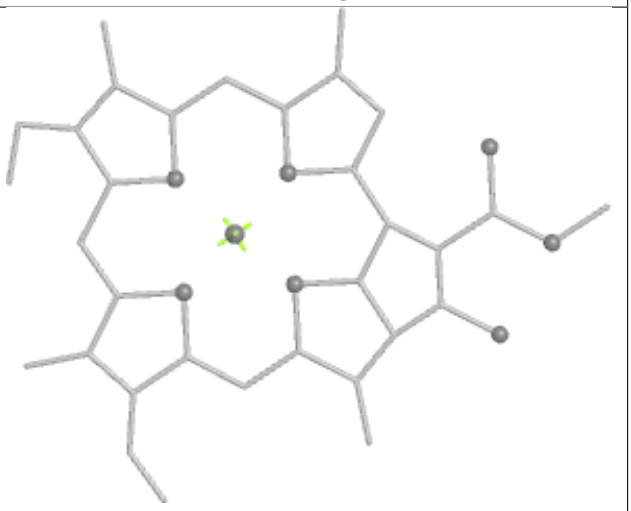
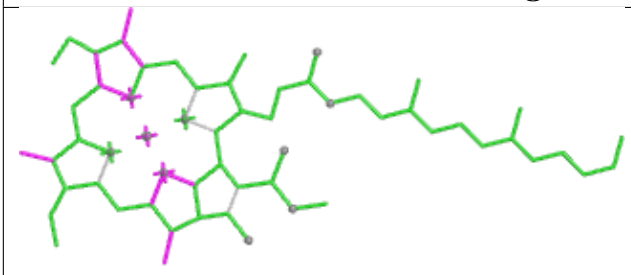
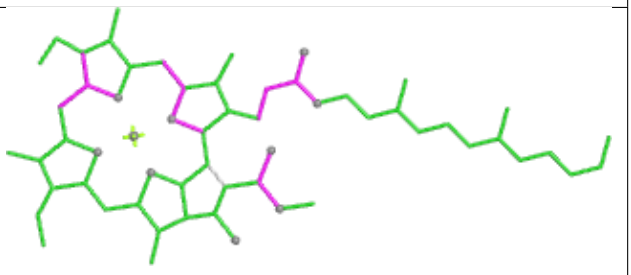


Rings

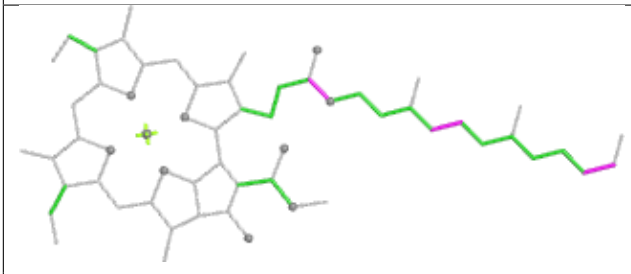
Ligand CLA B 820



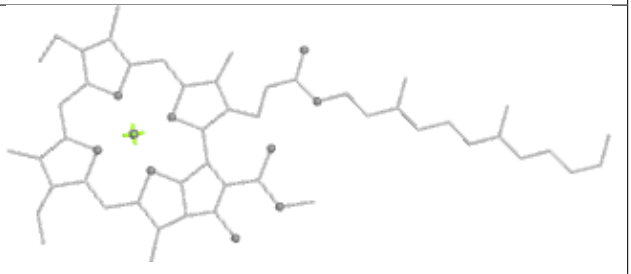
Bond lengths



Bond angles

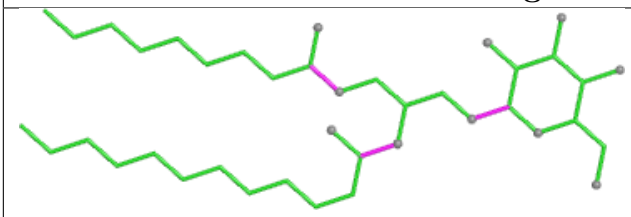


Torsions

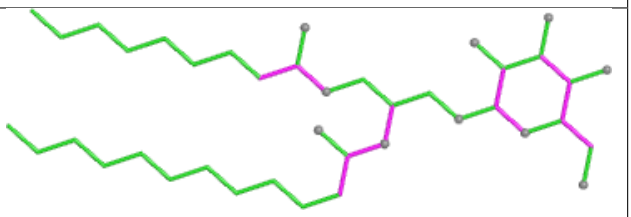


Rings

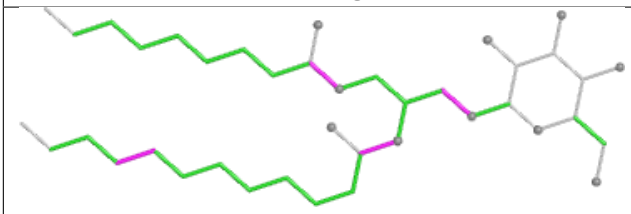
Ligand LMG 4 320



Bond lengths



Bond angles



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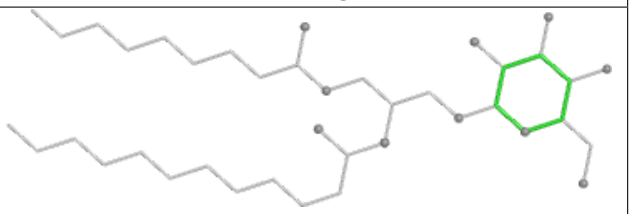
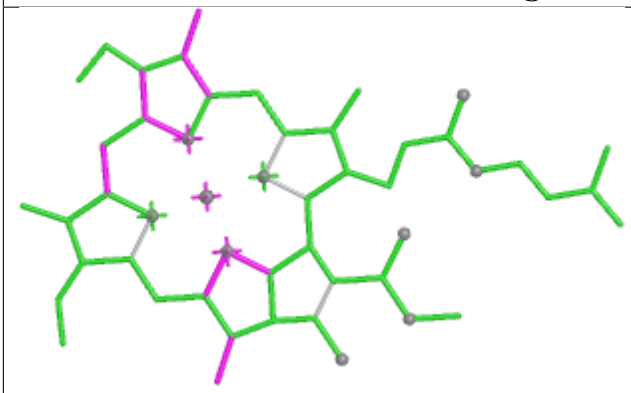


Rings

Ligand CLA G 201



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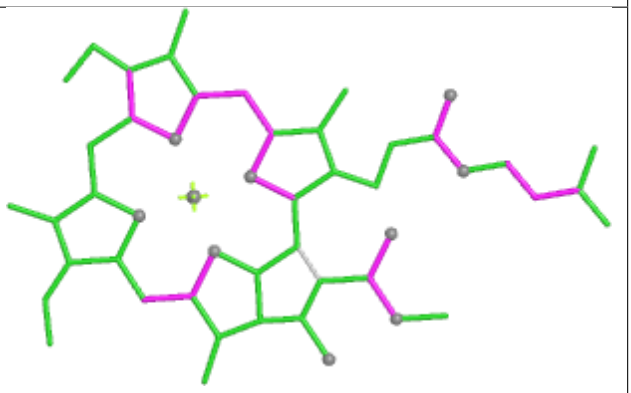
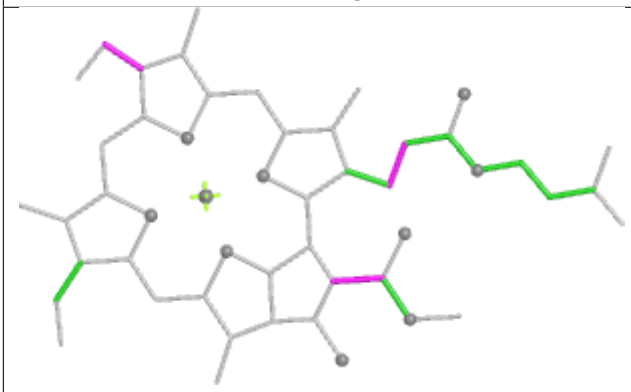
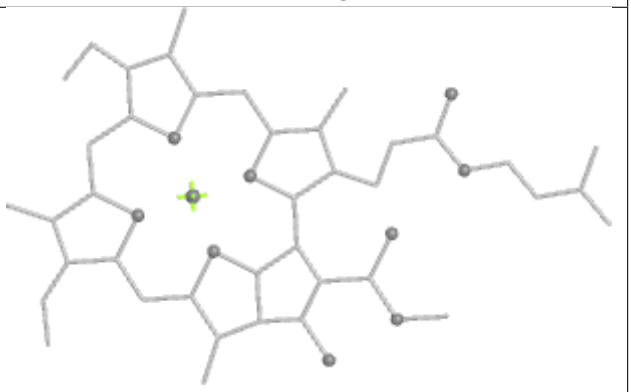


Bond angles

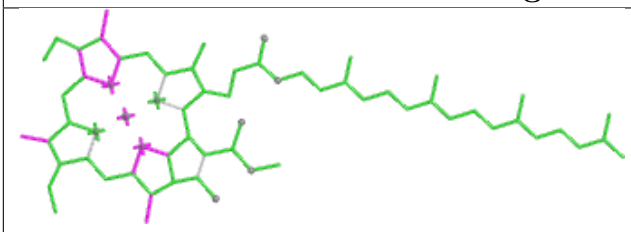


Torsions



Rings

Ligand CLA A 822



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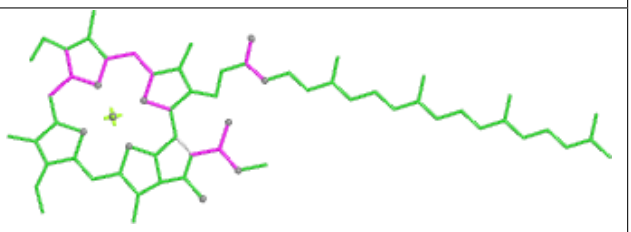
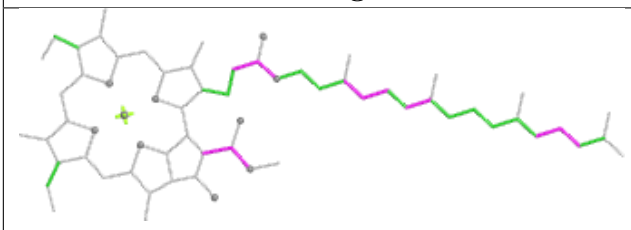
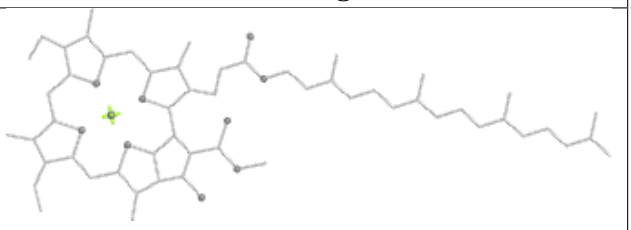


Bond angles

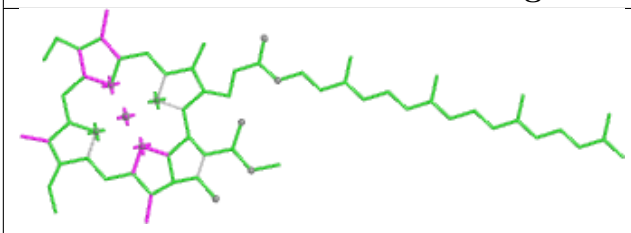


Torsions

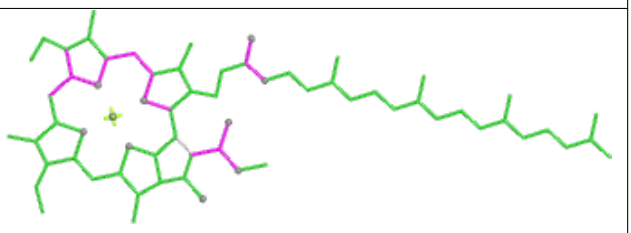


Rings

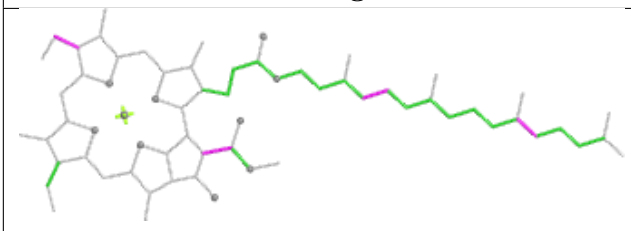
Ligand CLA B 817



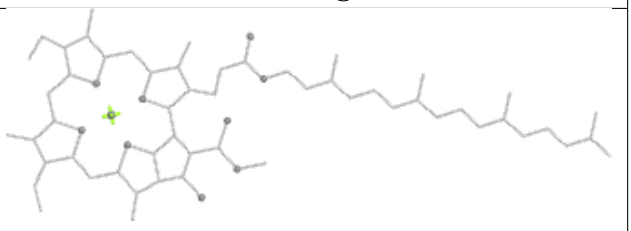
Bond lengths



Bond angles

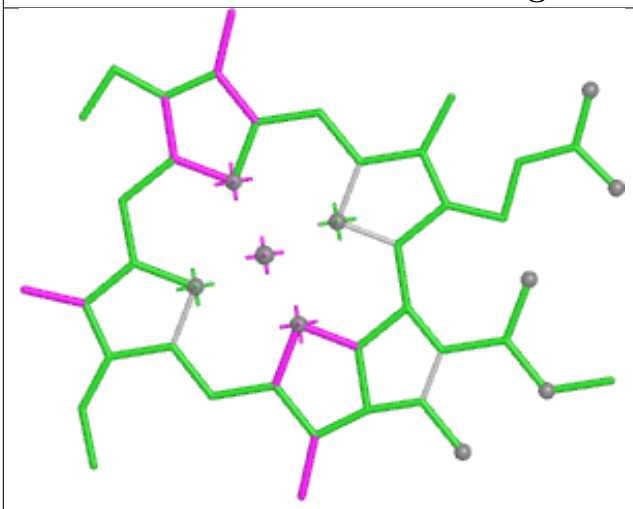


Torsions

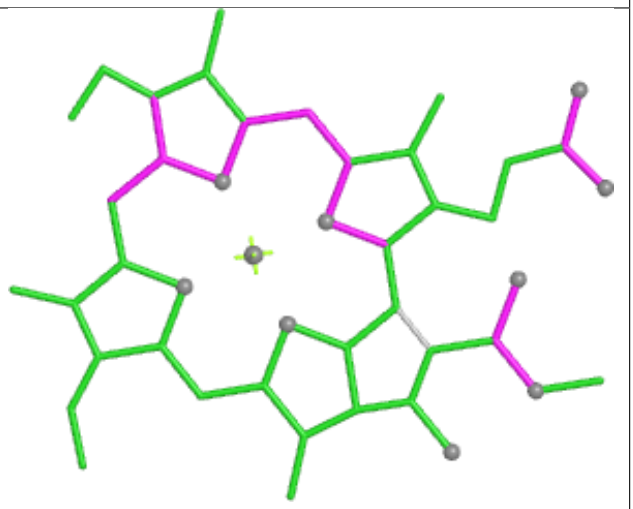


Rings

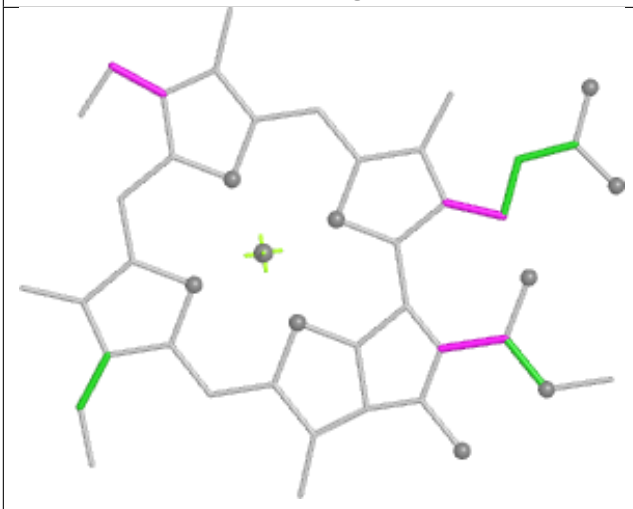
Ligand CLA 6 620



Bond lengths



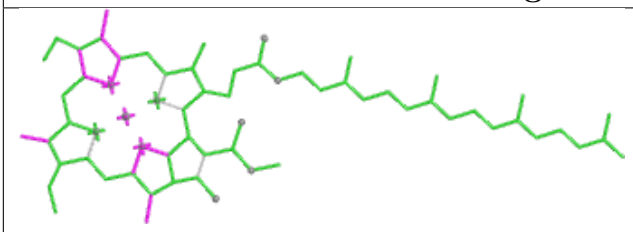
Bond angles



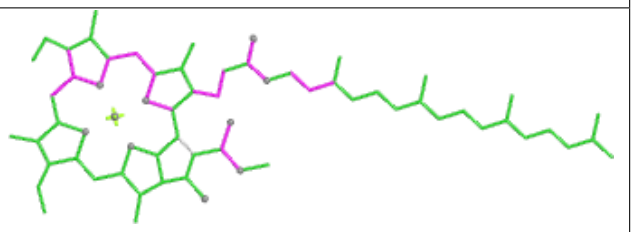
Torsions

Rings

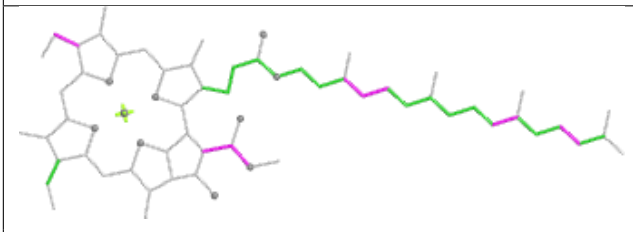
Ligand CLA B 808



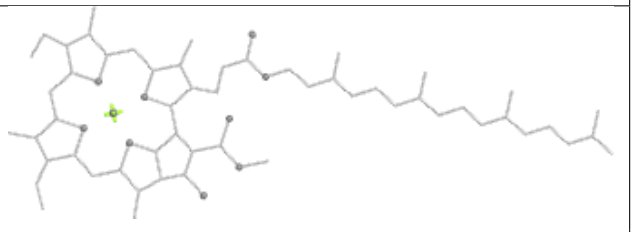
Bond lengths



Bond angles

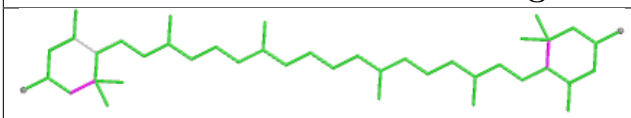


Torsions

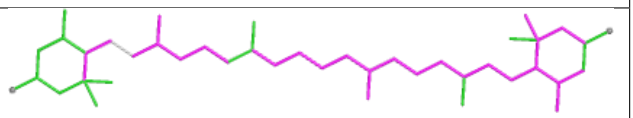


Rings

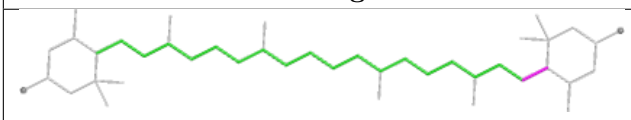
Ligand LUT 1 615



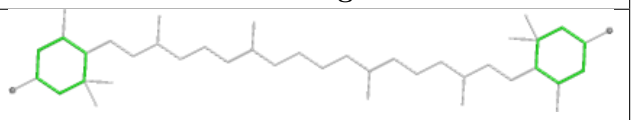
Bond lengths



Bond angles



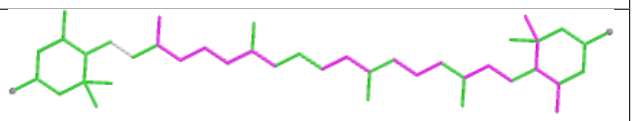
Torsions



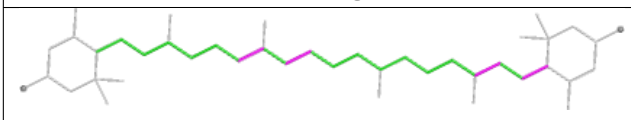
Rings

Ligand LUT S 317

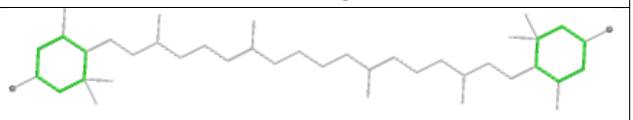
Bond lengths



Bond angles

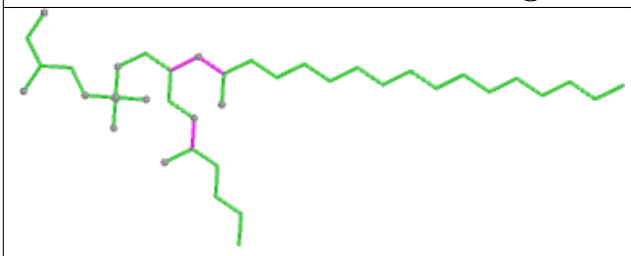


Torsions



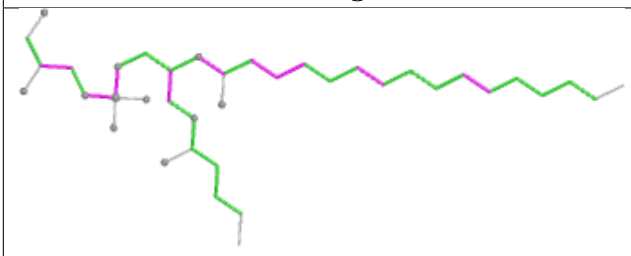
Rings

Ligand LHG A 844

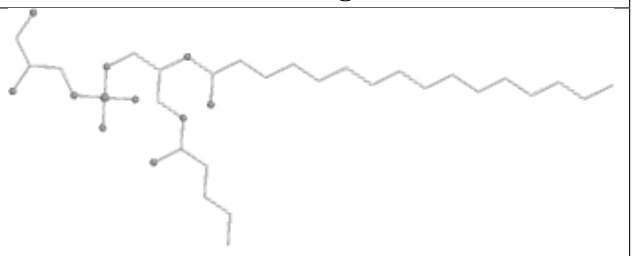


Bond lengths

Bond angles

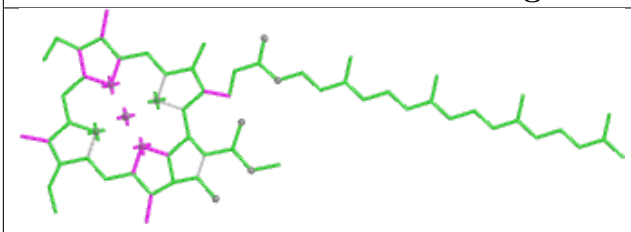


Torsions

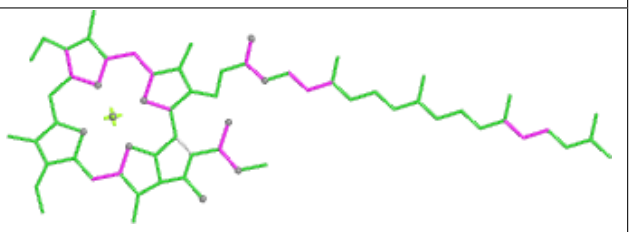


Rings

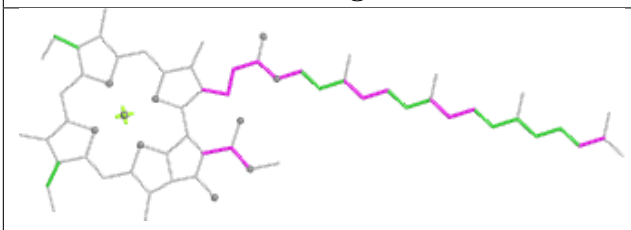
Ligand CLA A 814



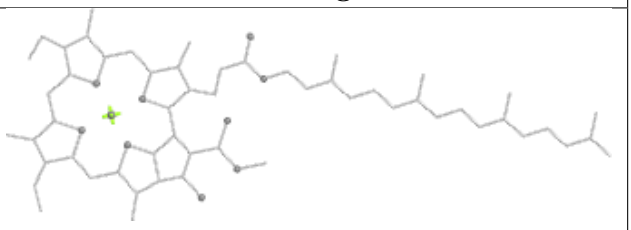
Bond lengths



Bond angles



Torsions

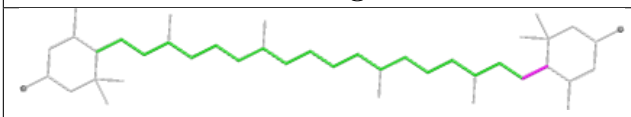


Rings

Ligand LUT R 615

Bond lengths

Bond angles



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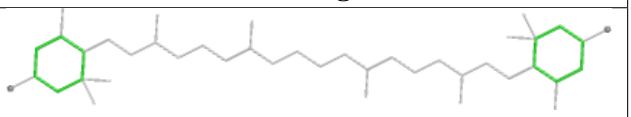
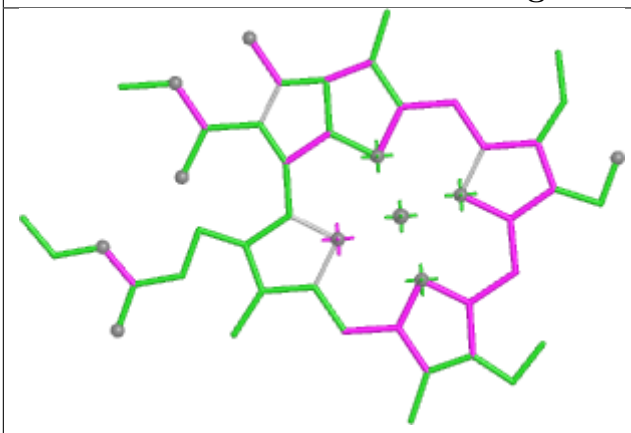
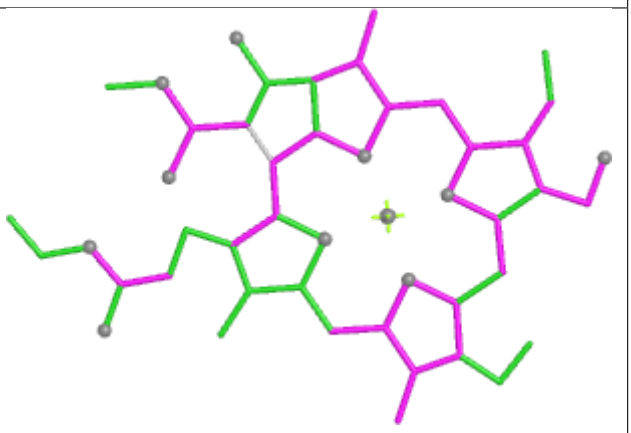


Rings

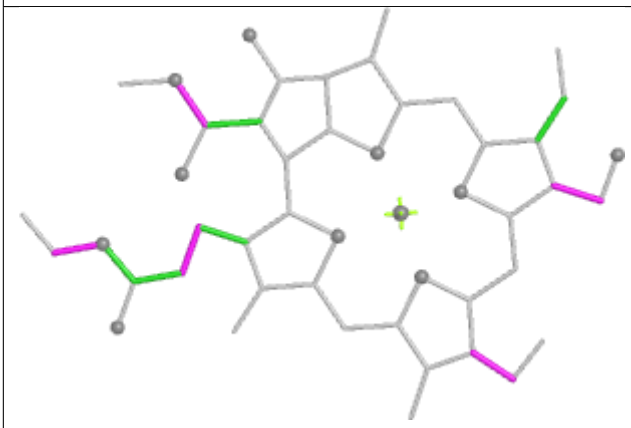
Ligand CHL 1 606



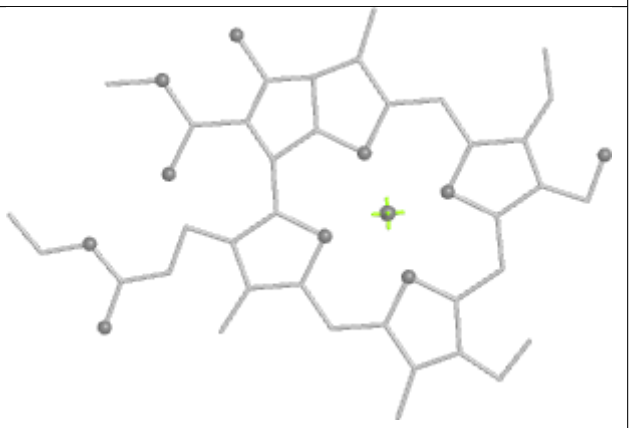
Bond lengths



Bond angles

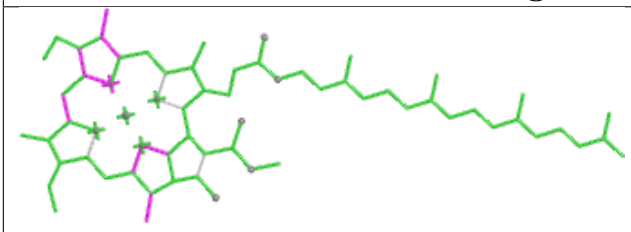


Torsions

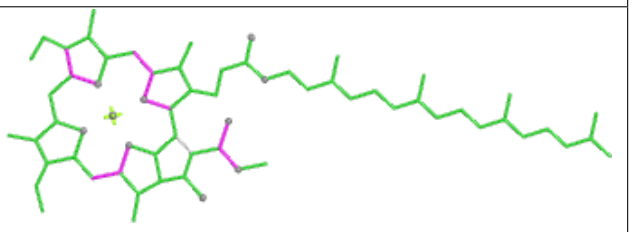


Rings

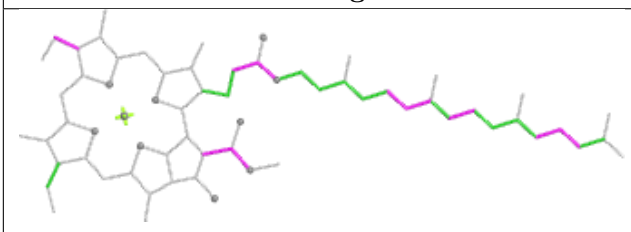
Ligand CLA S 304



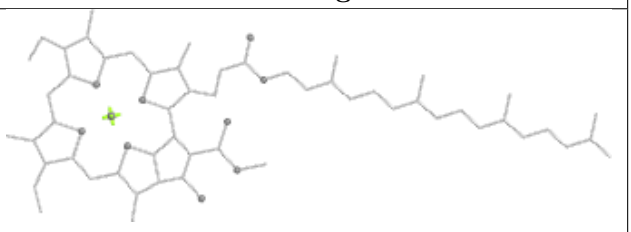
Bond lengths



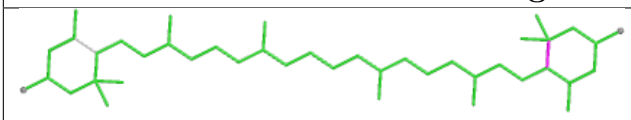
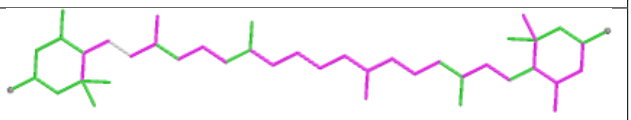
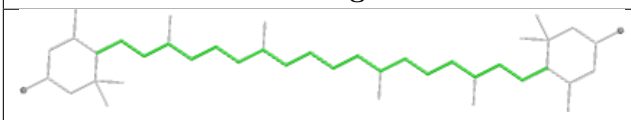
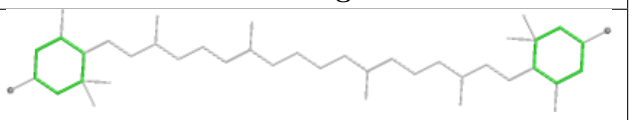
Bond angles

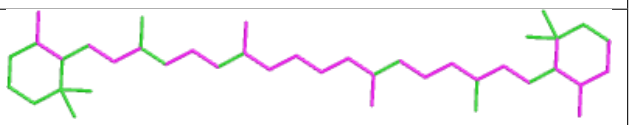
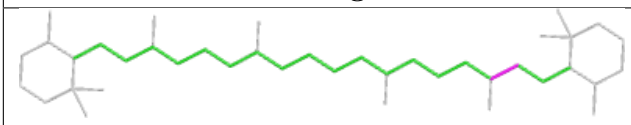
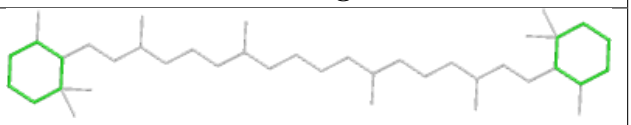


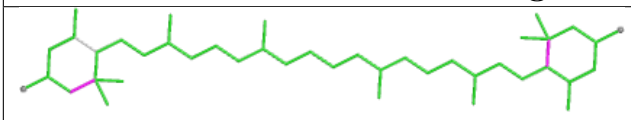
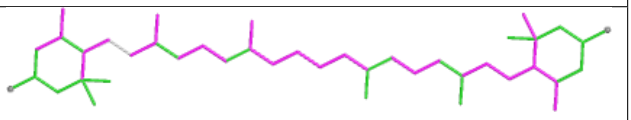
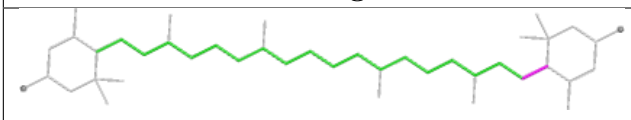
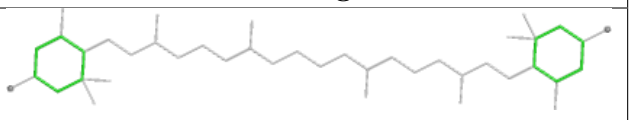
Torsions

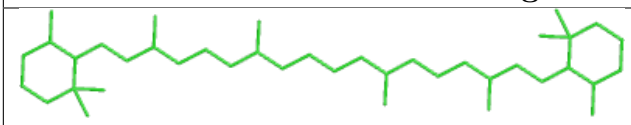
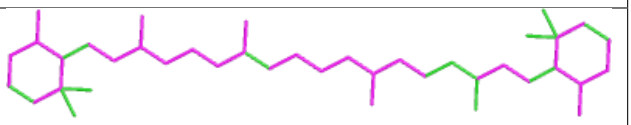
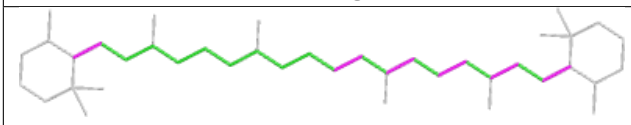
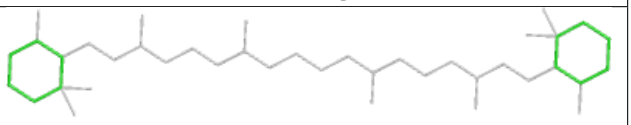


Rings

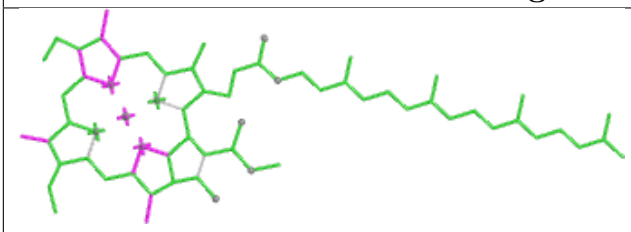
Ligand LUT 2 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 854	
Bond lengths	 Bond angles
 Torsions	 Rings

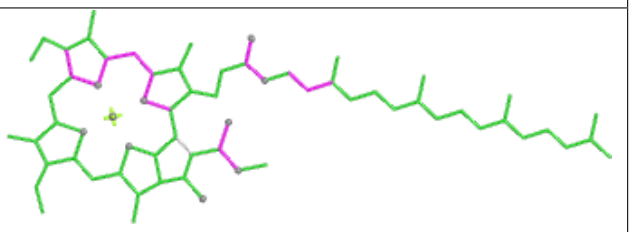
Ligand LUT 9 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

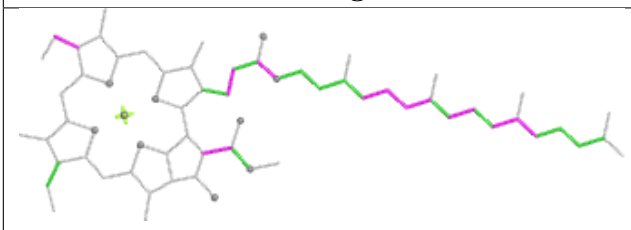
Ligand CLA 7 311



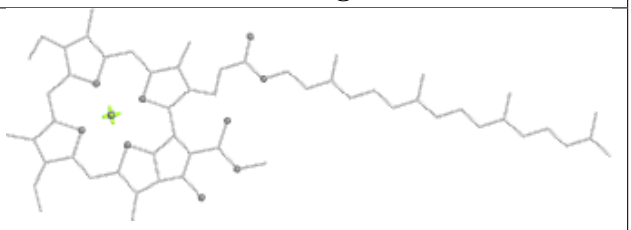
Bond lengths



Bond angles



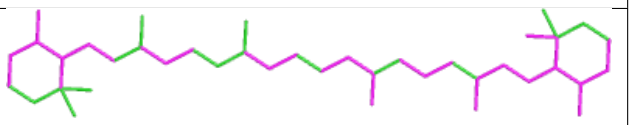
Torsions



Rings

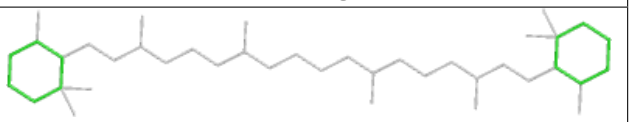
Ligand BCR 7 316

Bond lengths



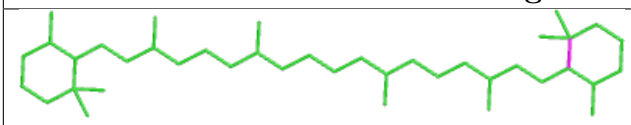
Bond angles

Torsions

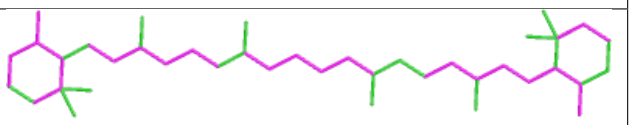


Rings

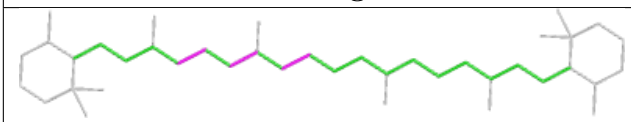
Ligand BCR L 203



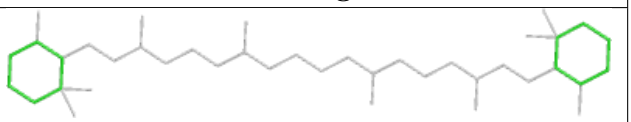
Bond lengths



Bond angles

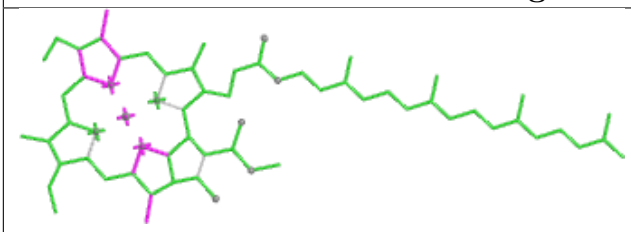


Torsions

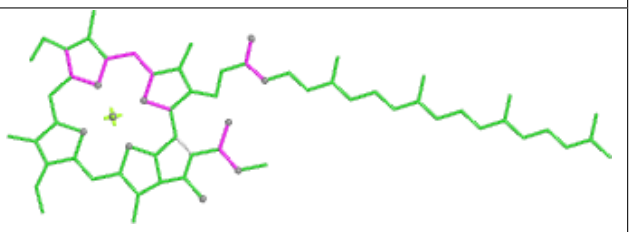


Rings

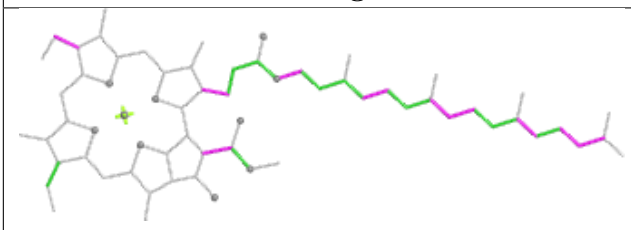
Ligand CLA 6 605



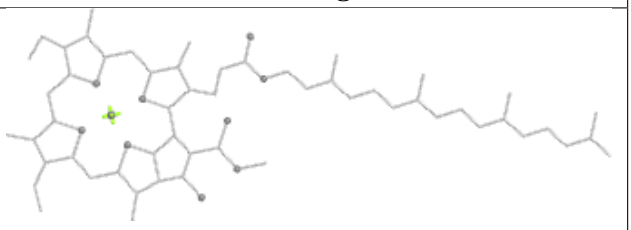
Bond lengths



Bond angles



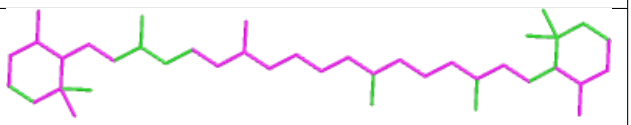
Torsions



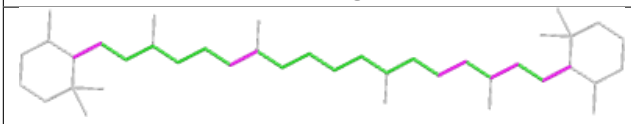
Rings

Ligand BCR 5 320

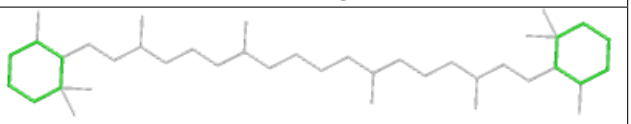
Bond lengths



Bond angles

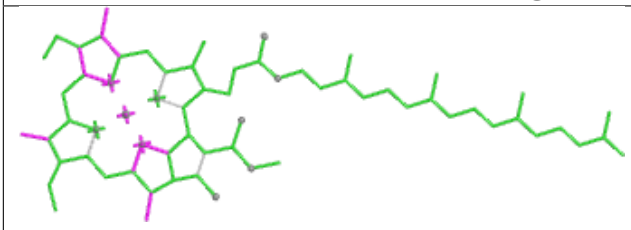


Torsions

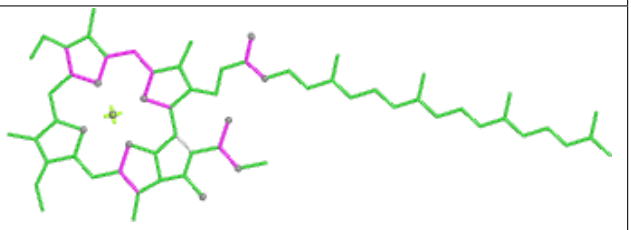


Rings

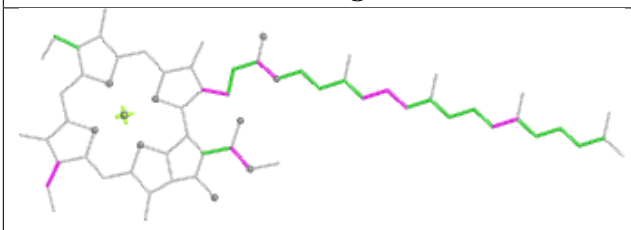
Ligand CLA 1 610



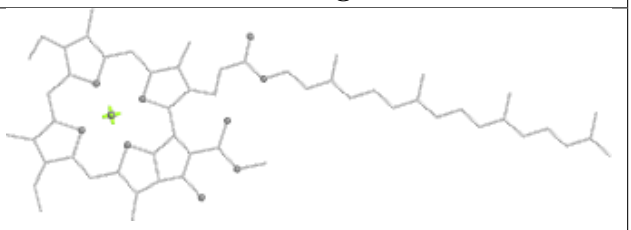
Bond lengths



Bond angles

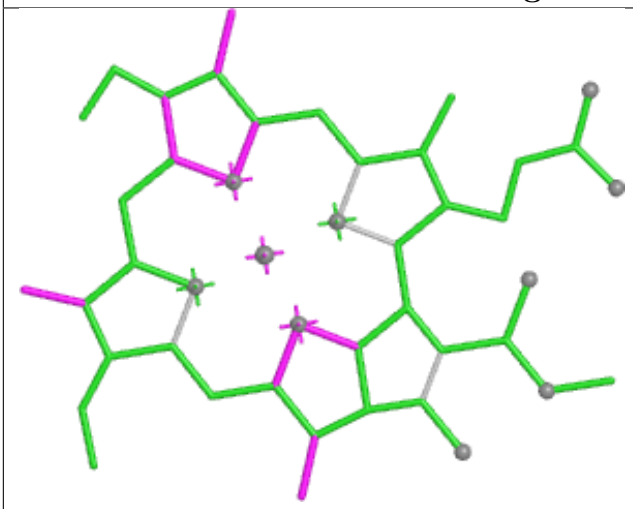


Torsions



Rings

Ligand CLA A 821



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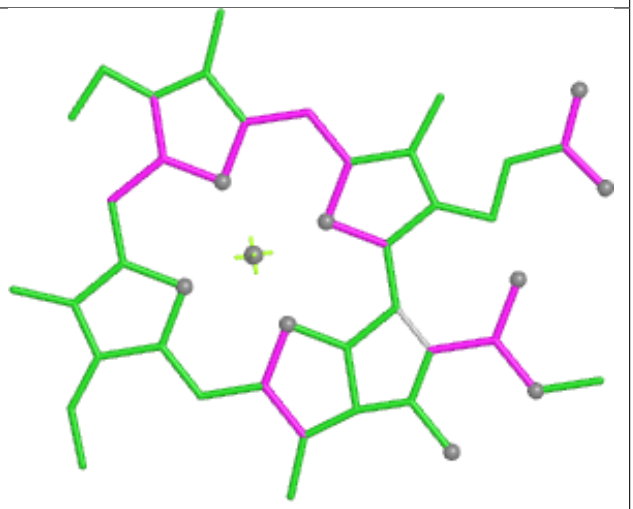
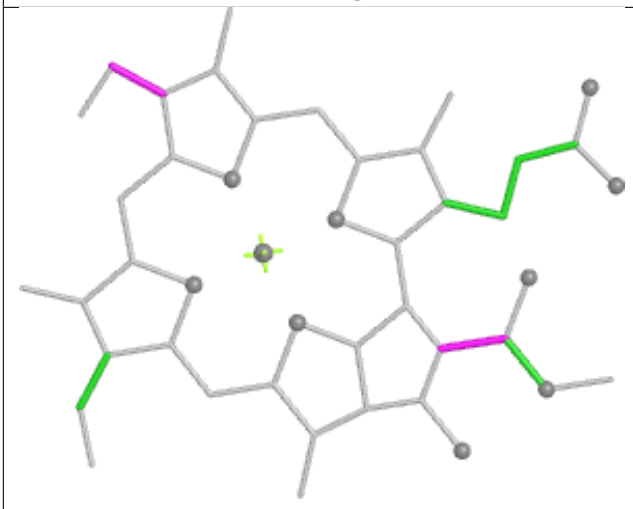


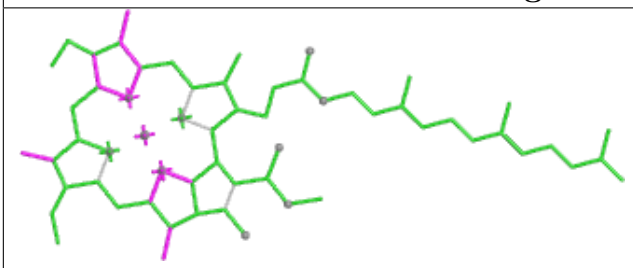
Bond angles



Torsions

Rings

Ligand CLA B 833



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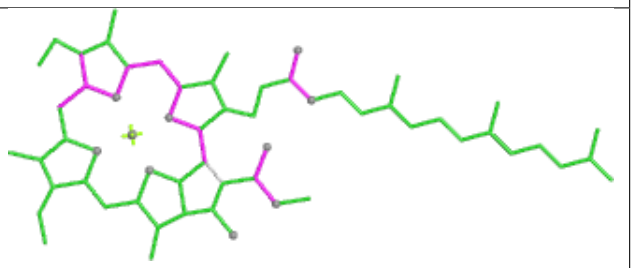
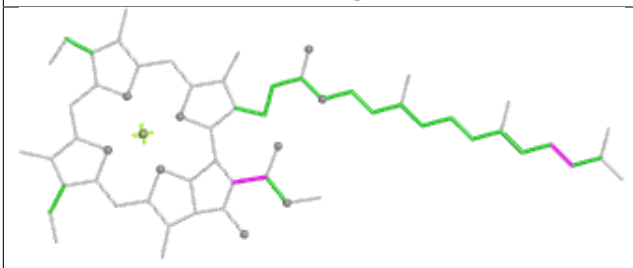
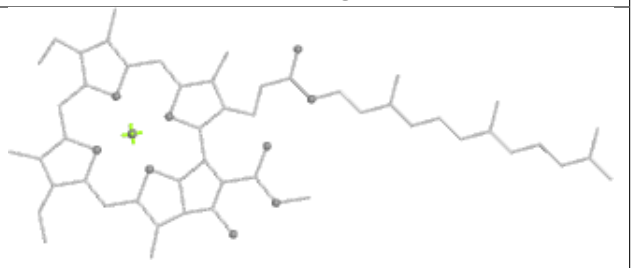


Bond angles

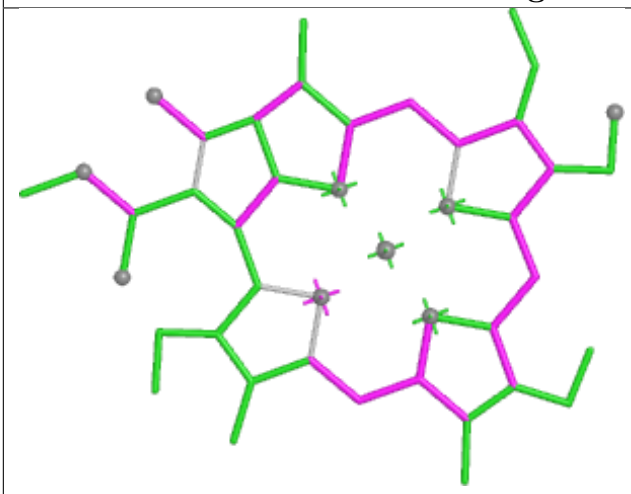


Torsions



Rings

Ligand CHL 6 617



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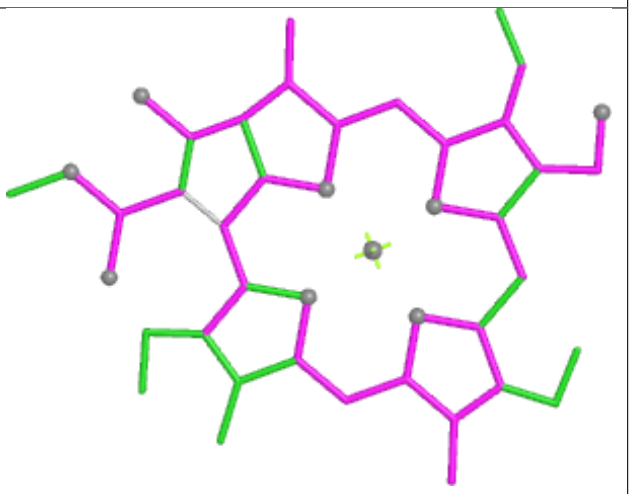
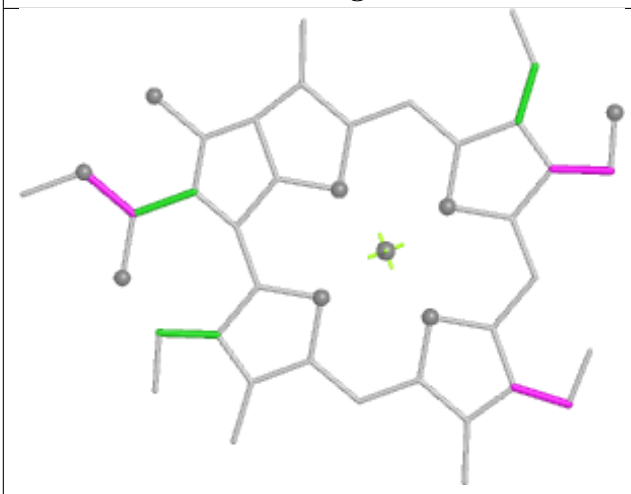


Bond angles



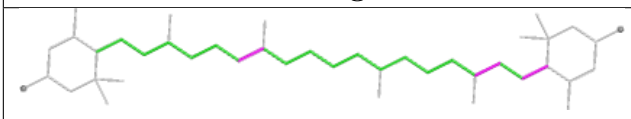
Torsions

Rings

Ligand LUT 2 315

Bond lengths

Bond angles



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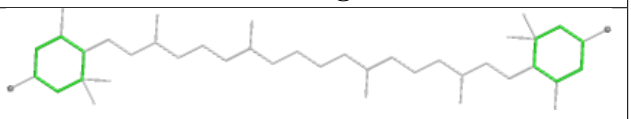
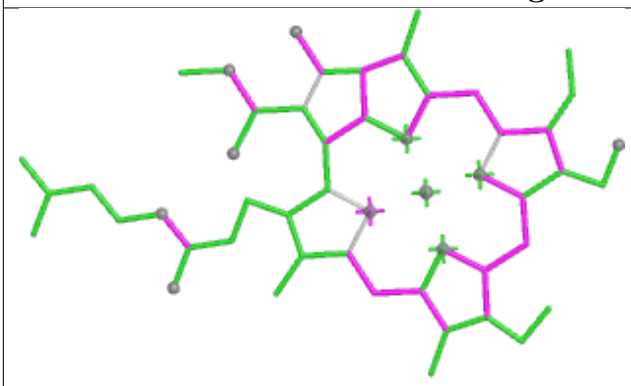
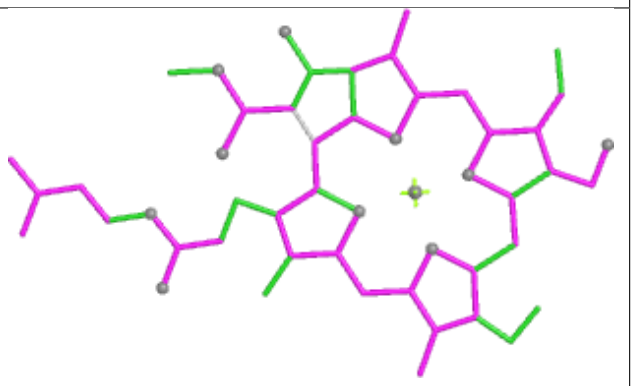


Rings

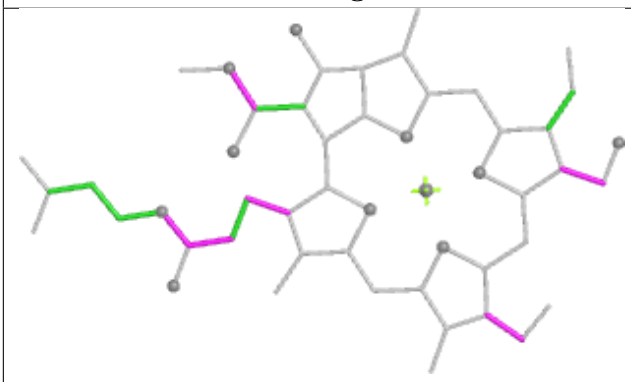
Ligand CHL 5 307



Bond lengths



Bond angles



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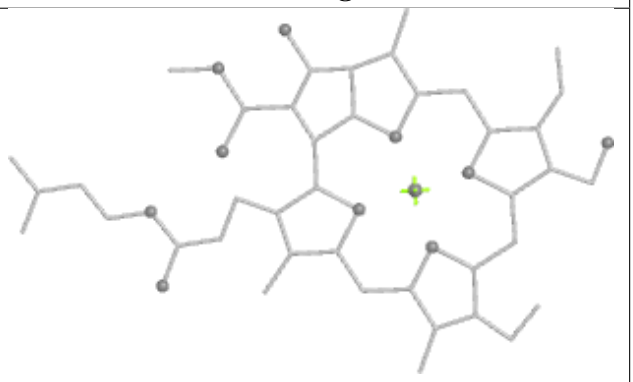
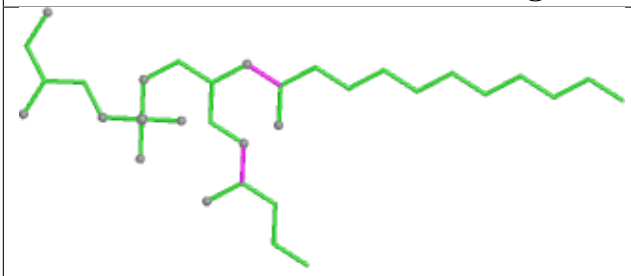


Rings

Ligand LHG 4 319



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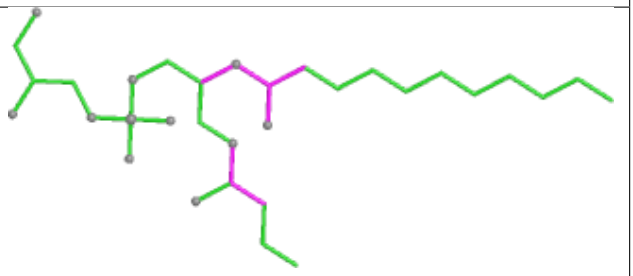
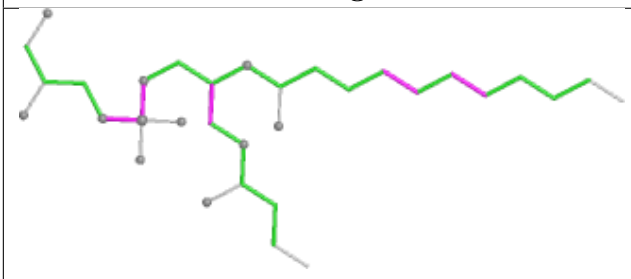


Bond angles



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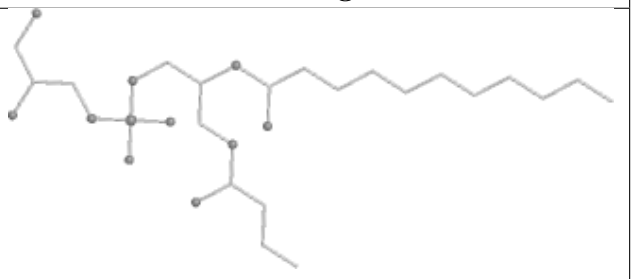
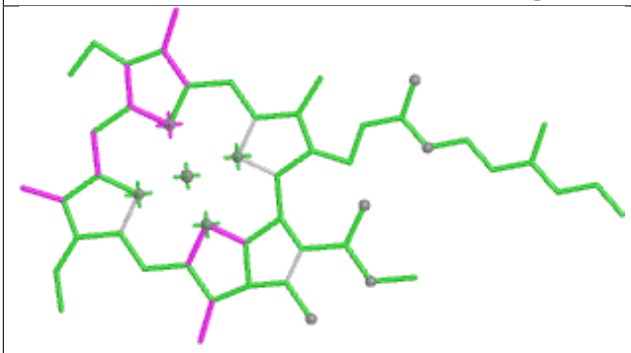
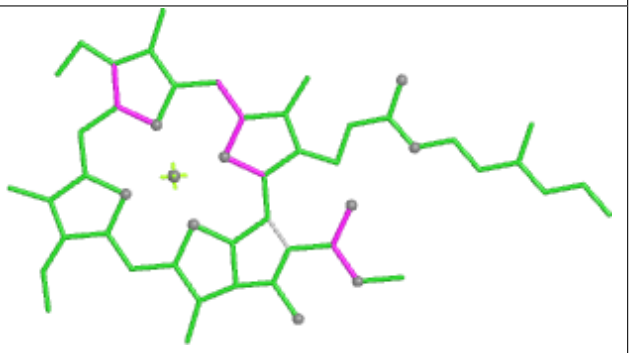
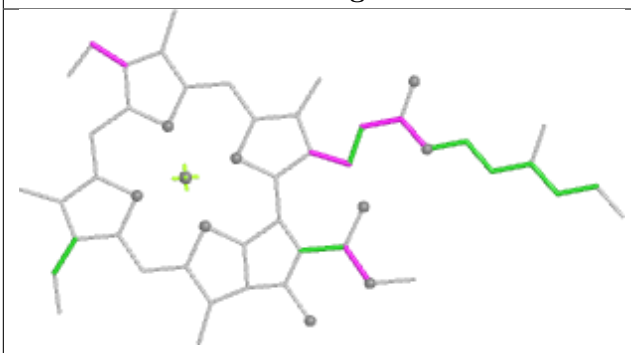
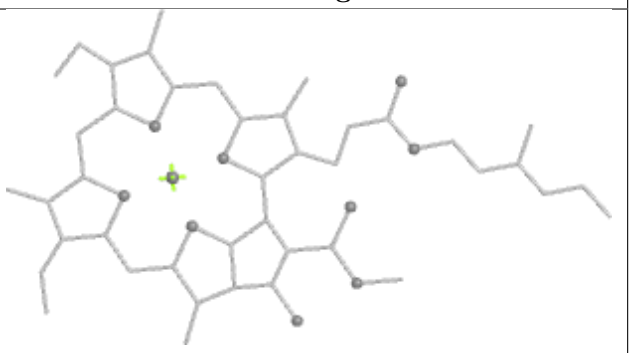
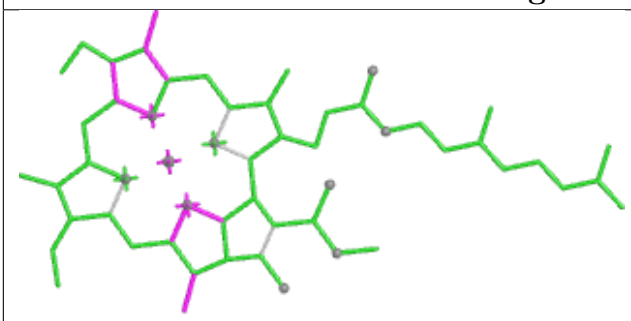
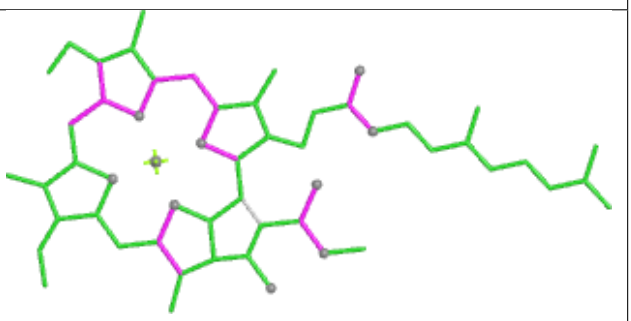
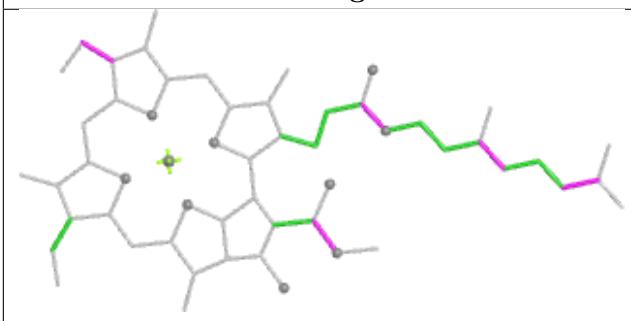
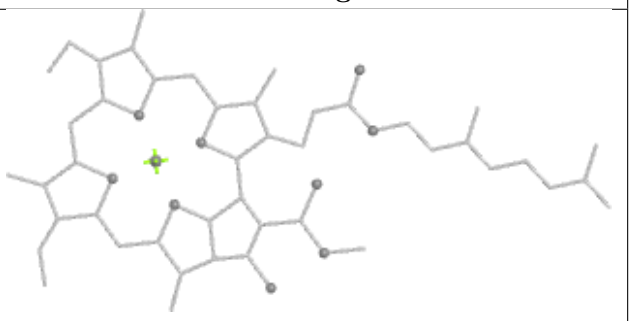
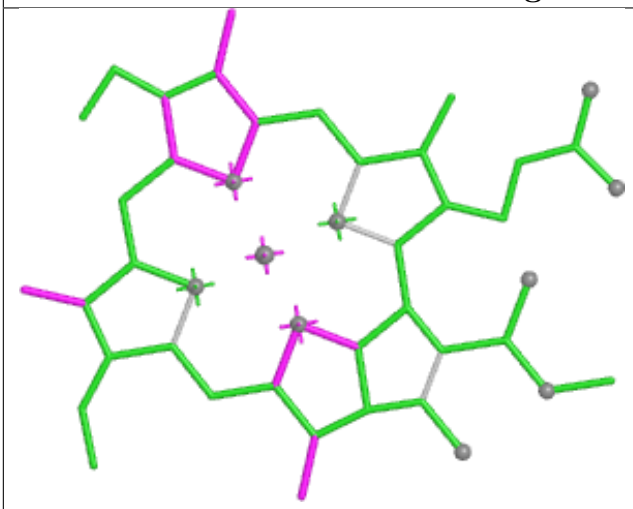


Rings

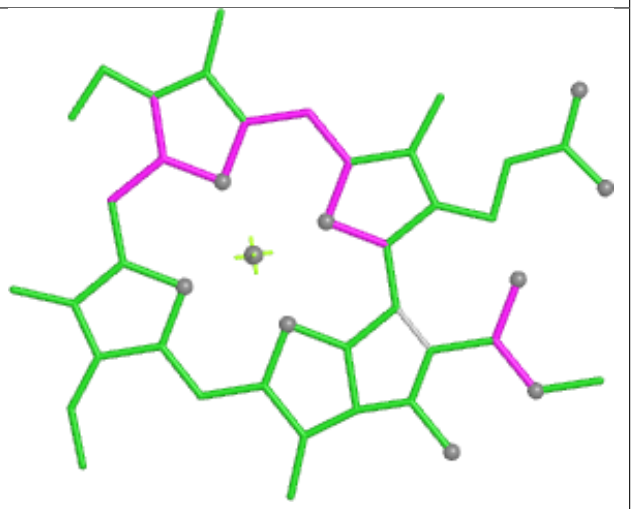
Ligand CLA a 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

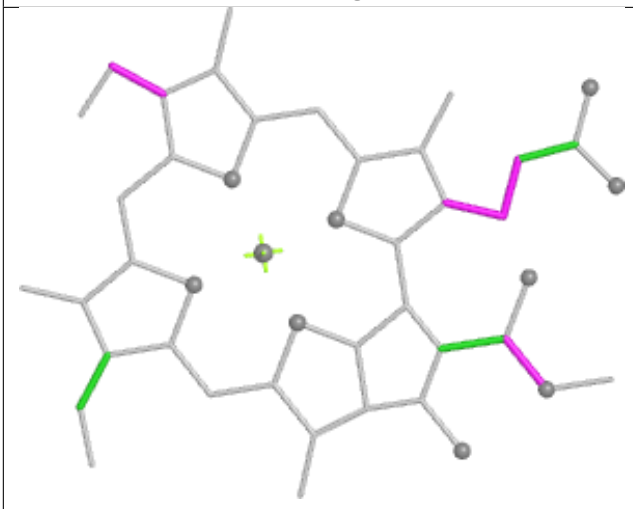
Ligand CLA B 832



Bond lengths



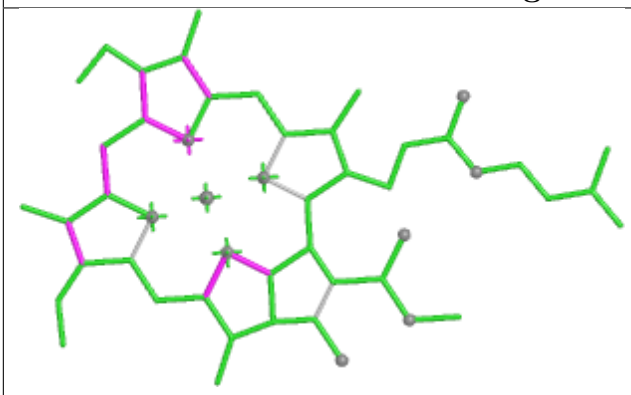
Bond angles



Torsions

Rings

Ligand CLA U 304



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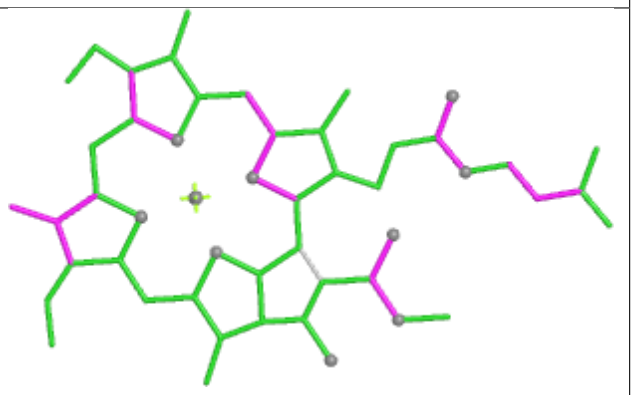
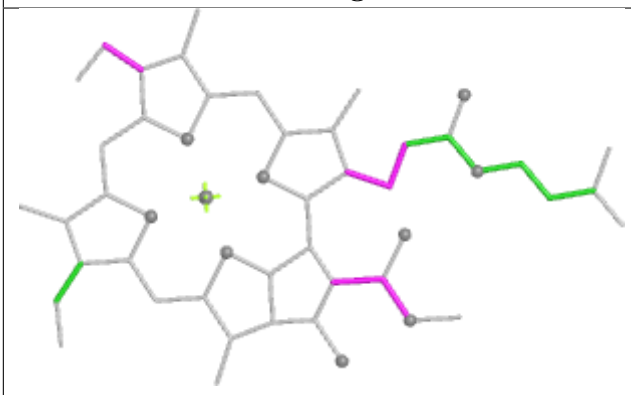
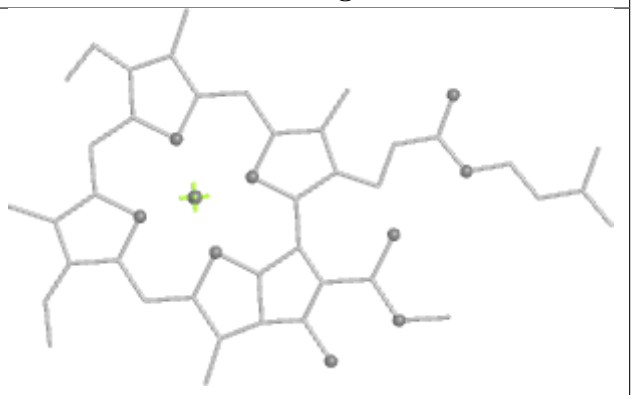


Bond angles

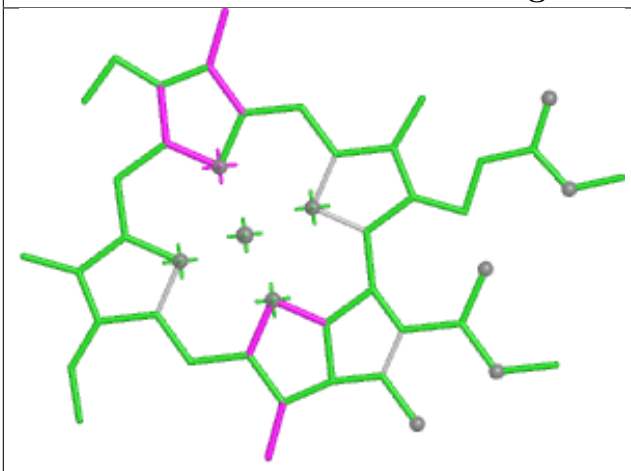


Torsions

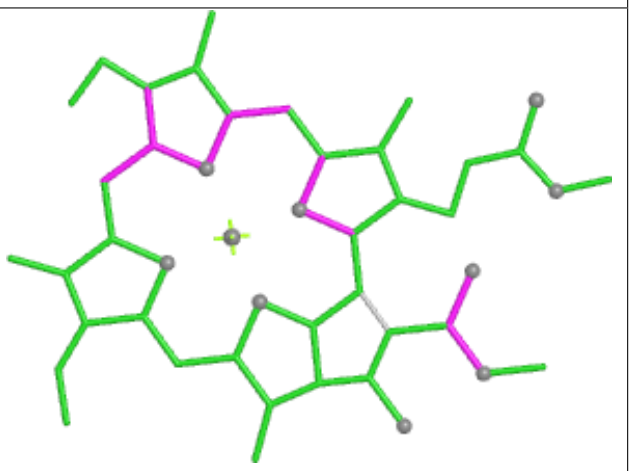


Rings

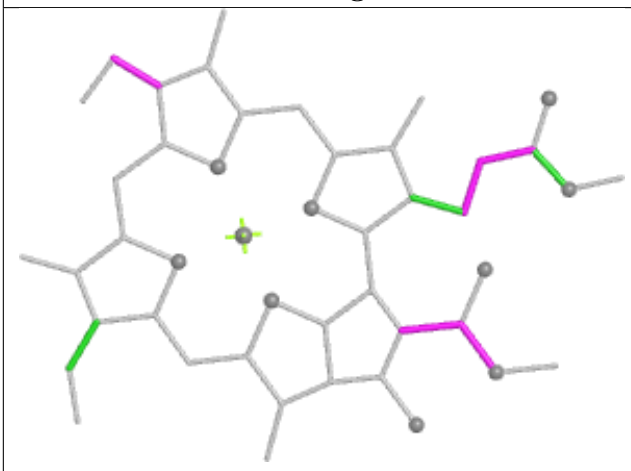
Ligand CLA 9 302



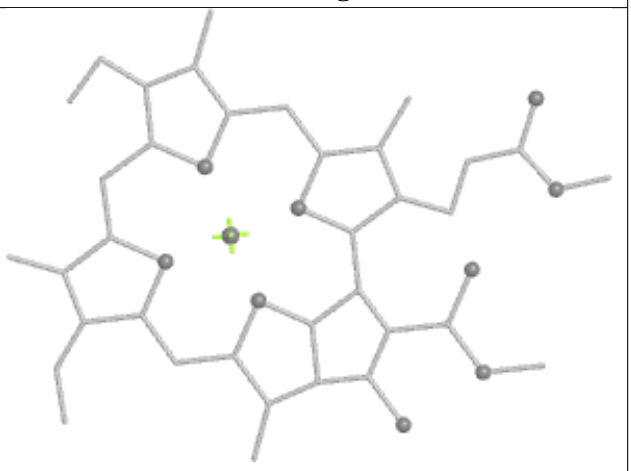
Bond lengths



Bond angles

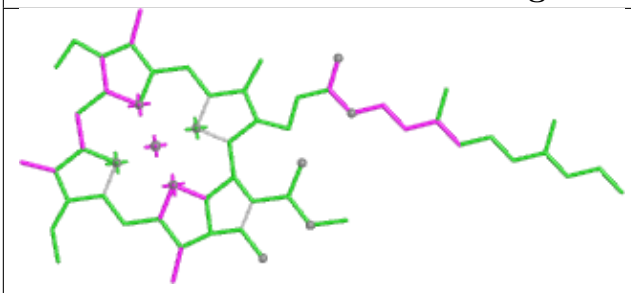


Torsions

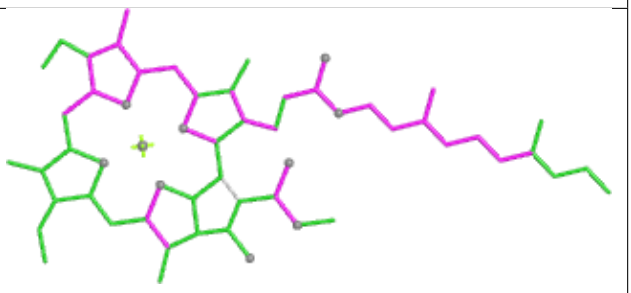


Rings

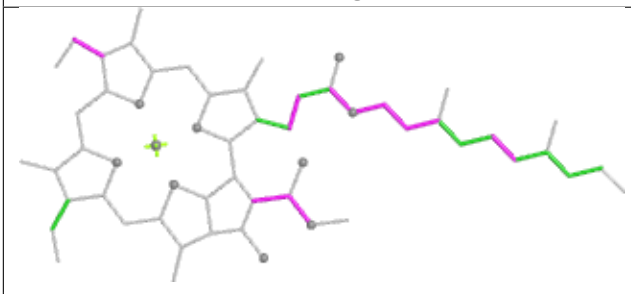
Ligand CLA a 303



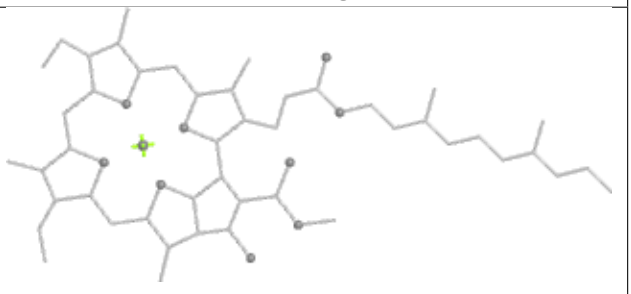
Bond lengths



Bond angles

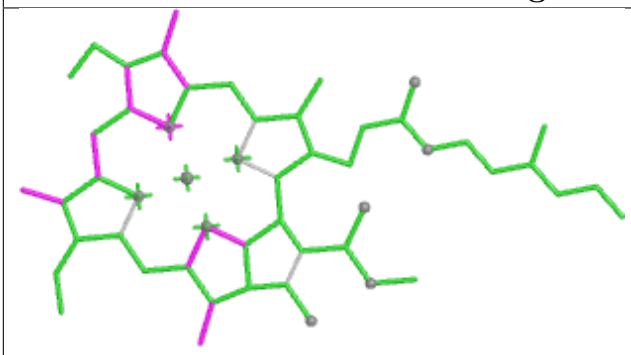


Torsions

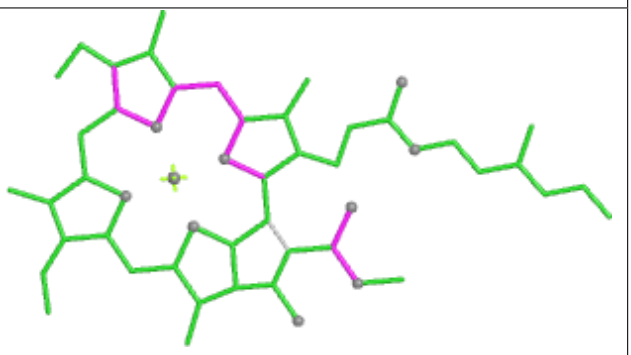


Rings

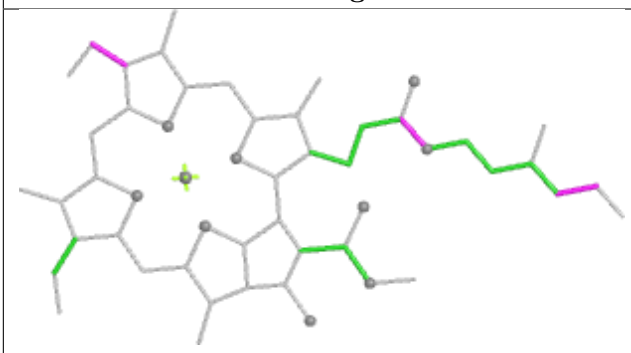
Ligand CLA 6 612



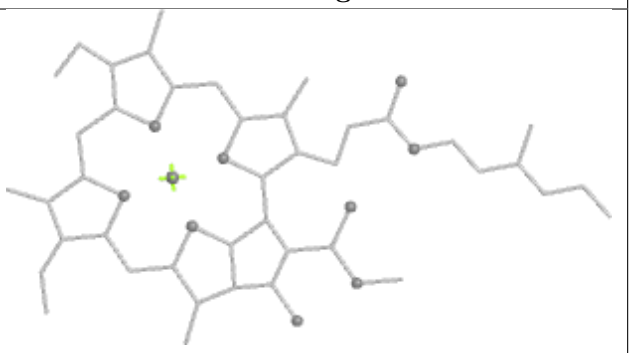
Bond lengths



Bond angles

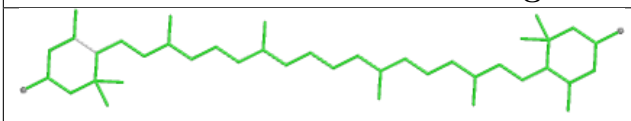


Torsions

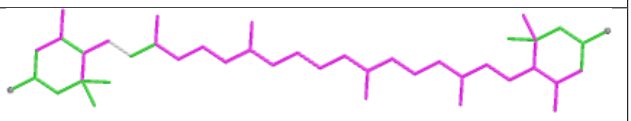


Rings

Ligand LUT U 315



Bond lengths



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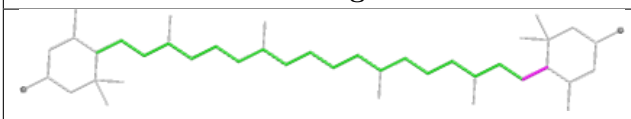

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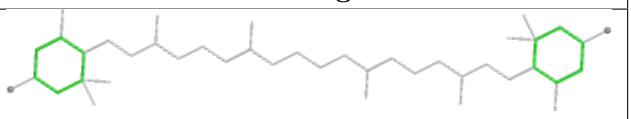
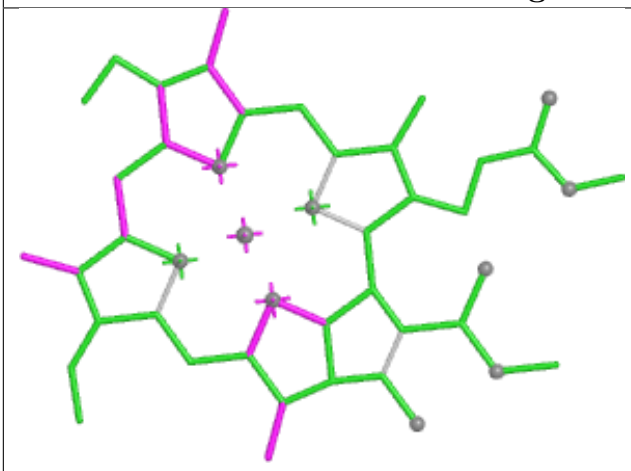


Rings

Ligand CLA 6 615



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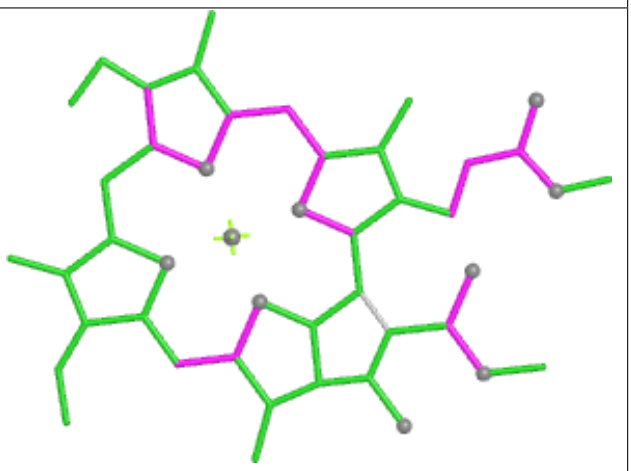

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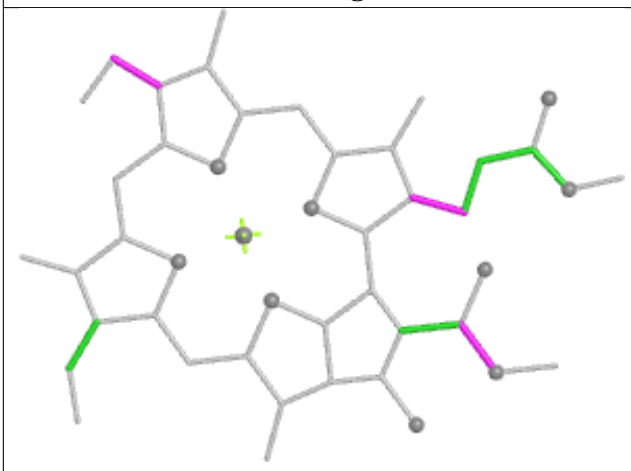

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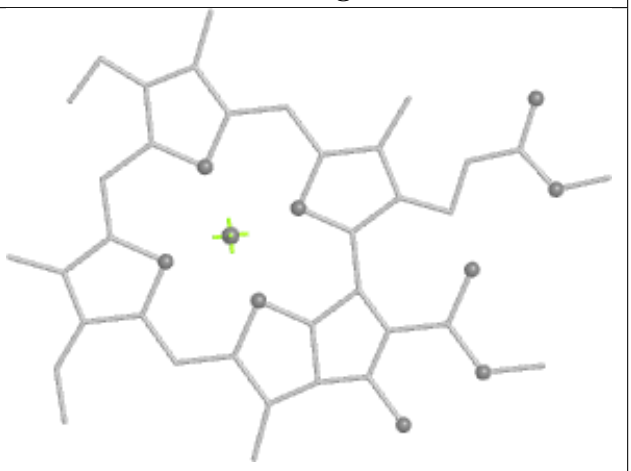
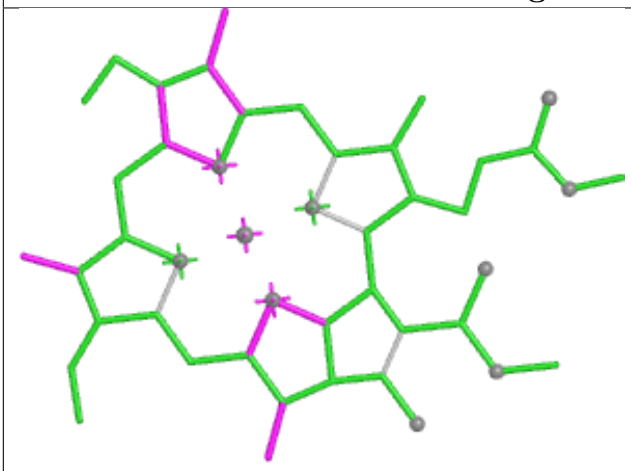


Rings

Ligand CLA 5 304



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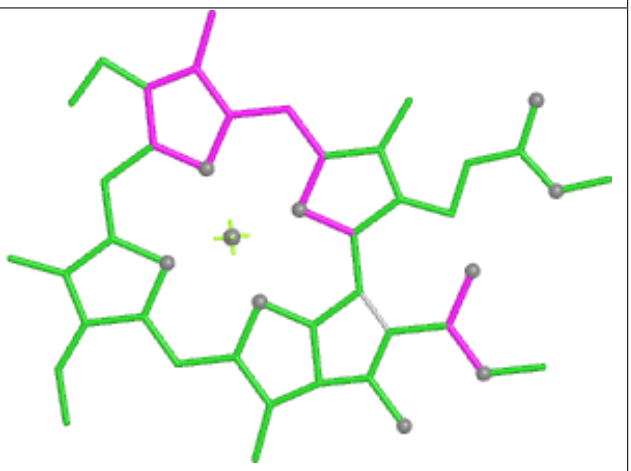
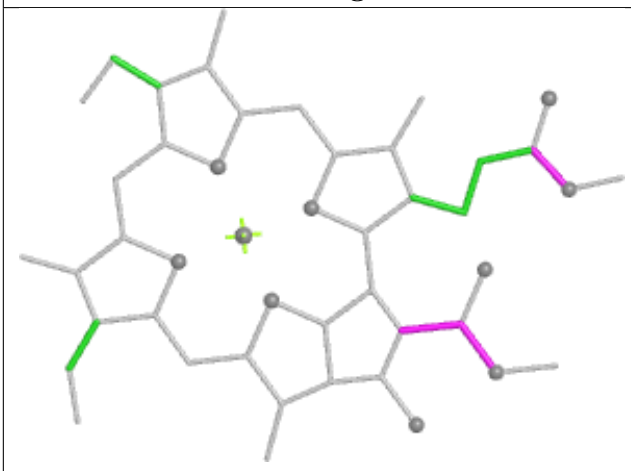


Bond angles



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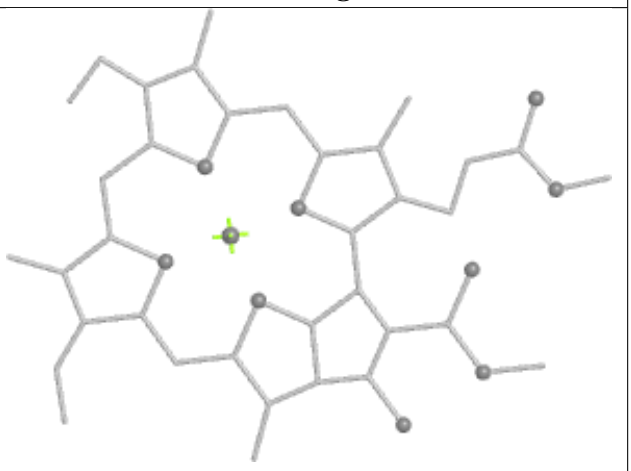
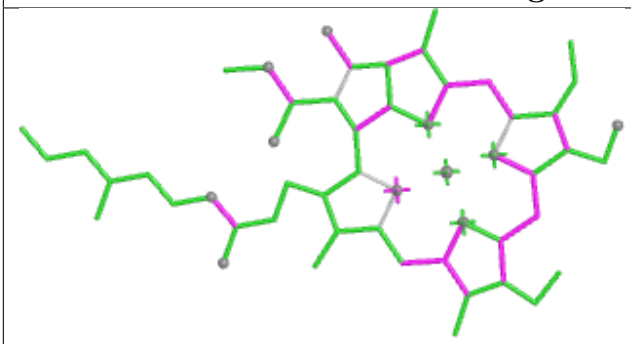


Rings

Ligand CHL 6 606



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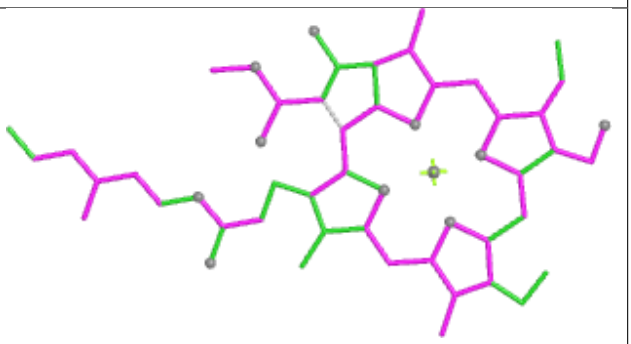
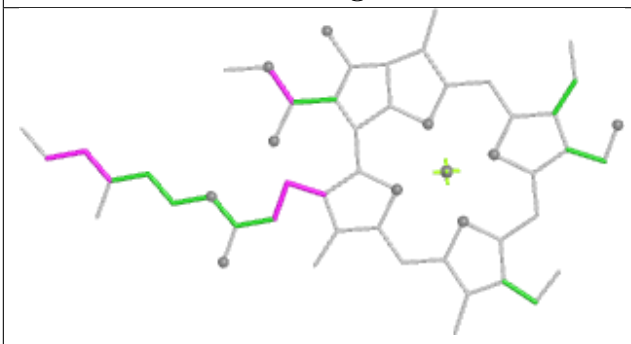


Bond angles



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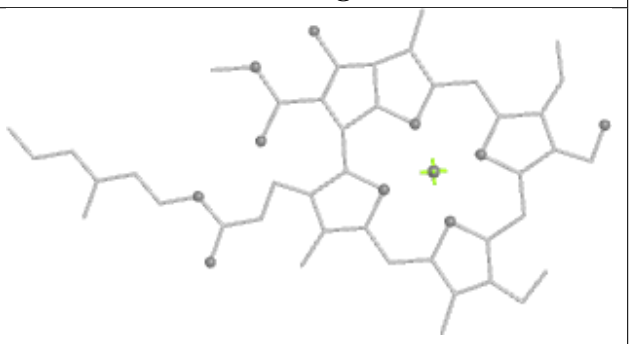
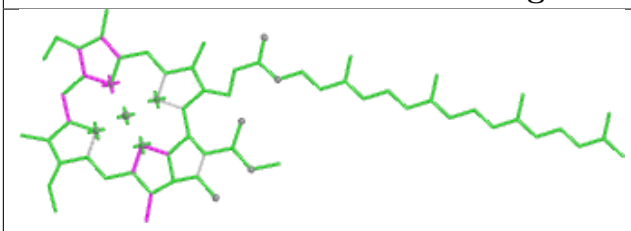


Rings

Ligand CLA S 320



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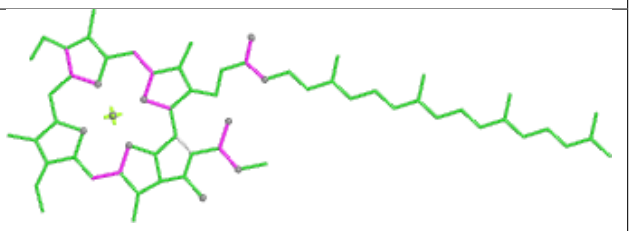
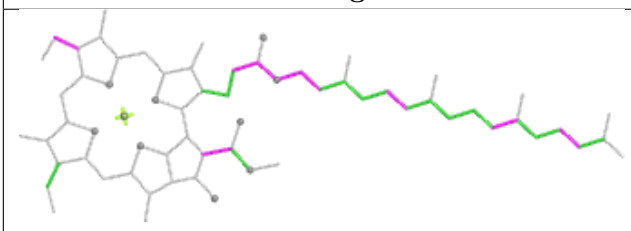


Bond angles



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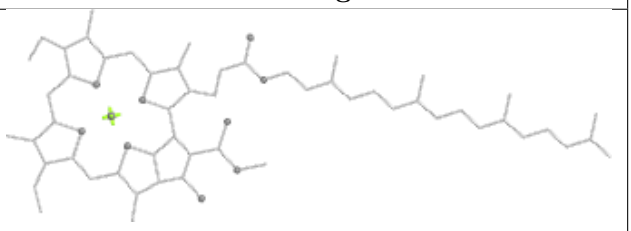
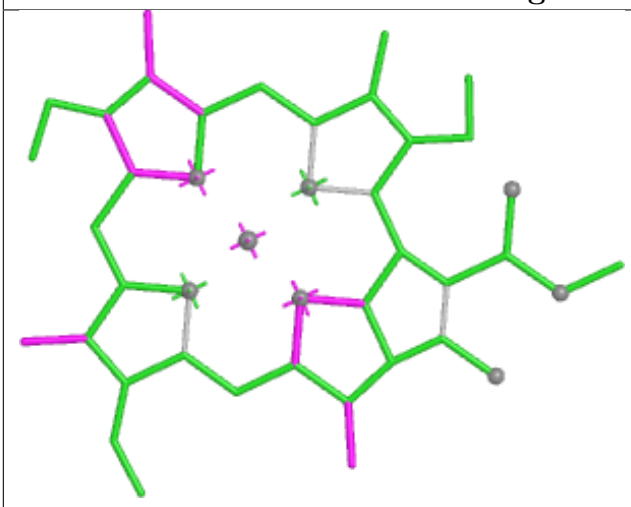


Rings

Ligand CLA J 105



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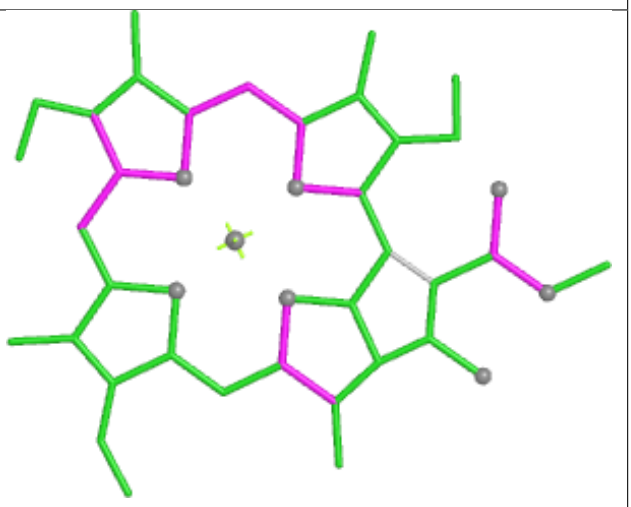

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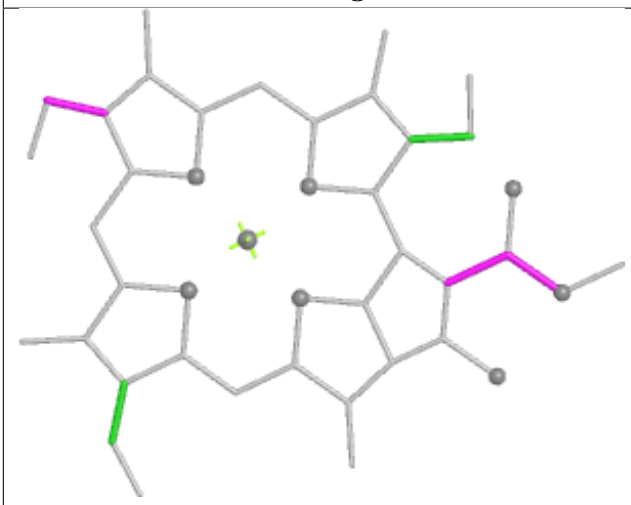
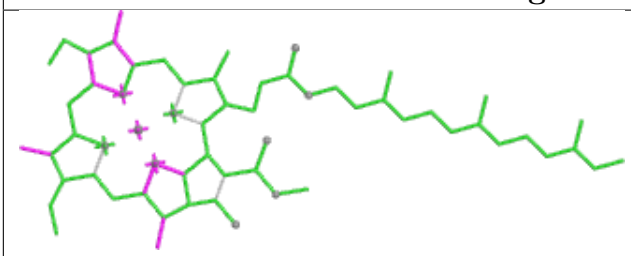


Torsions

Rings

Ligand CLA 6 601



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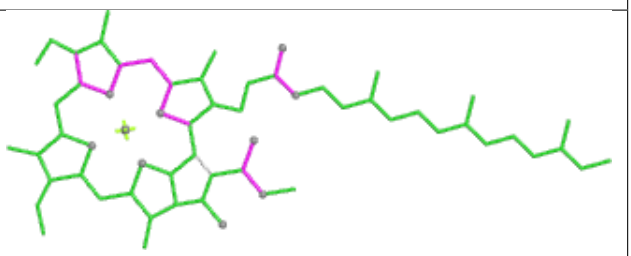

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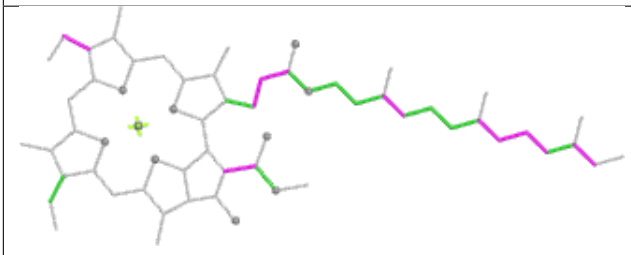

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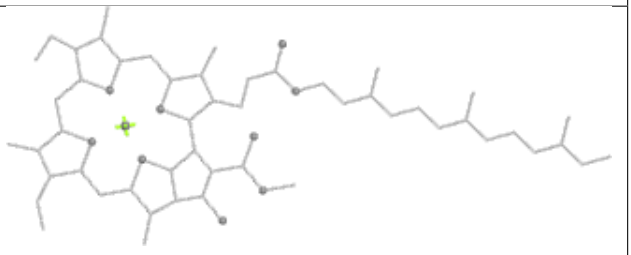
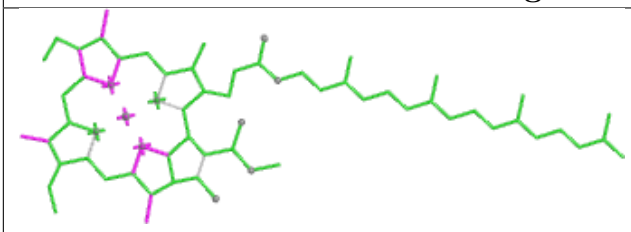
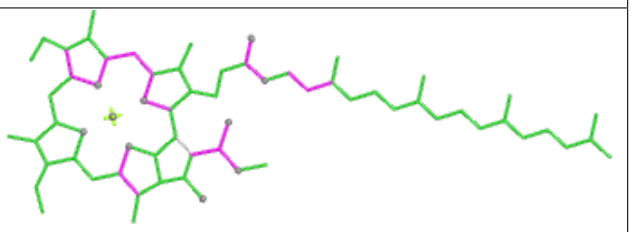


Rings

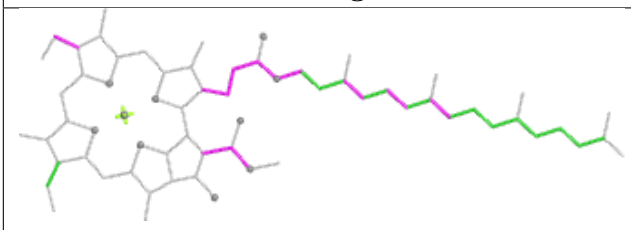
Ligand CLA B 826



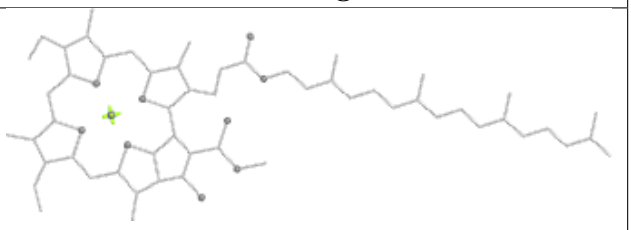
Bond lengths



Bond angles

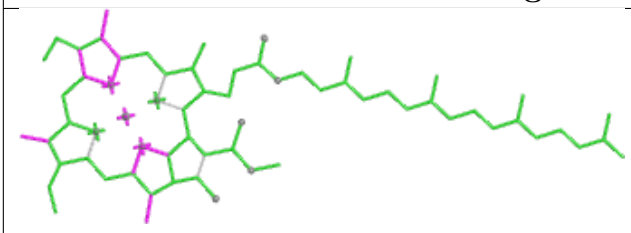


Torsions

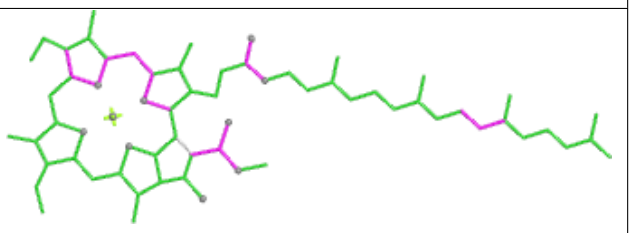


Rings

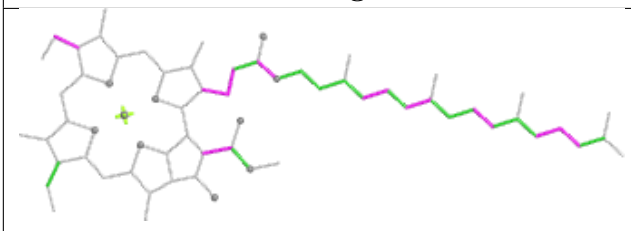
Ligand CLA B 804



Bond lengths



Bond angles



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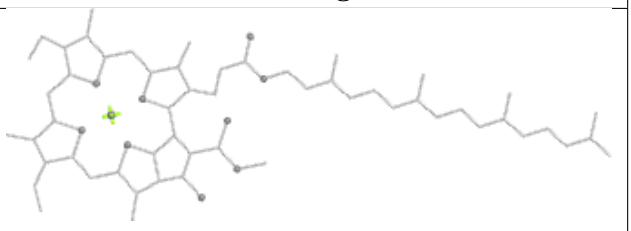
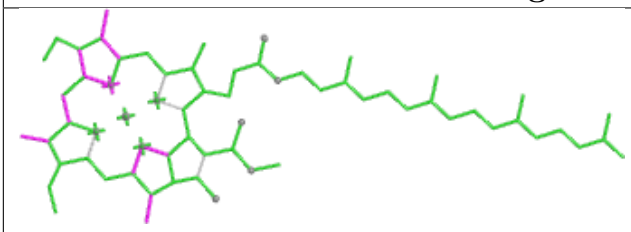


Rings

Ligand CLA a 312



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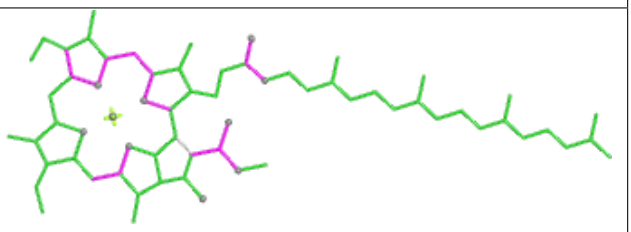
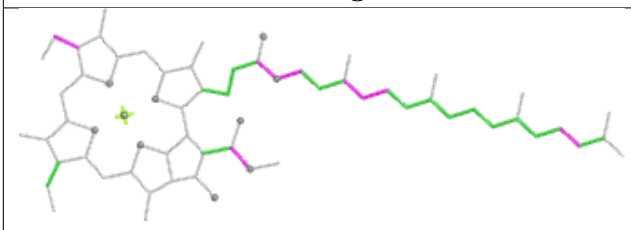


Bond angles



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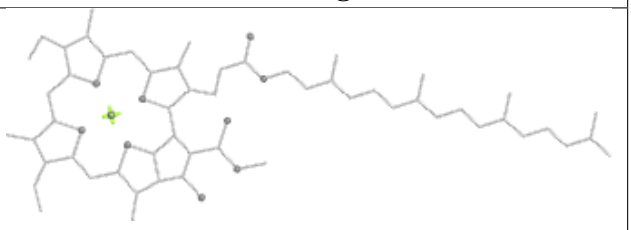
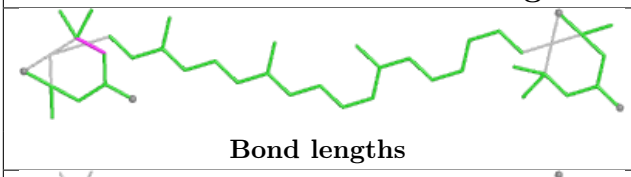


Rings

Ligand XAT P 623



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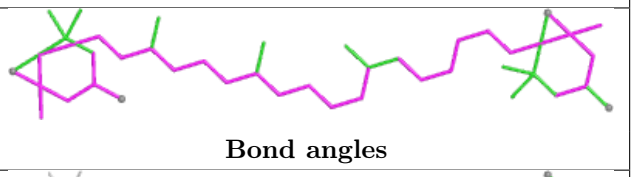
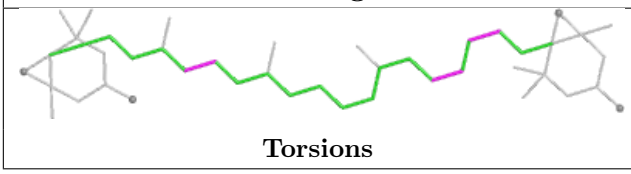


Bond angles



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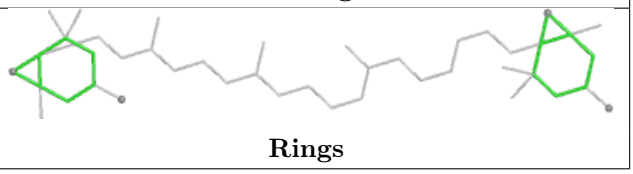
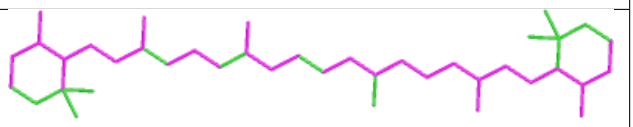


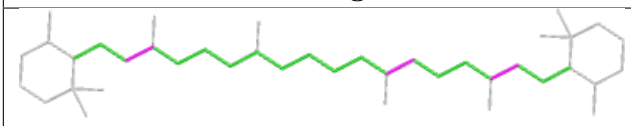
Rings

Ligand BCR J 106

Bond lengths



Bond angles



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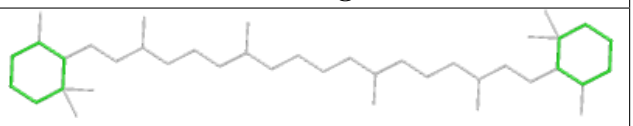
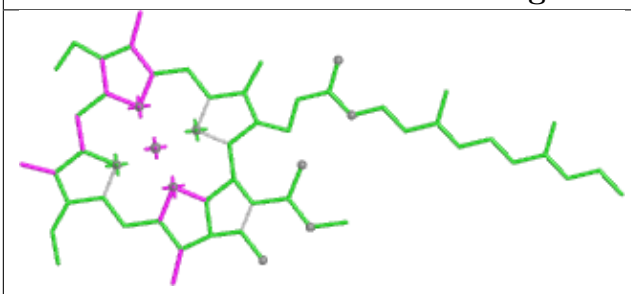


Rings

Ligand CLA 1 604



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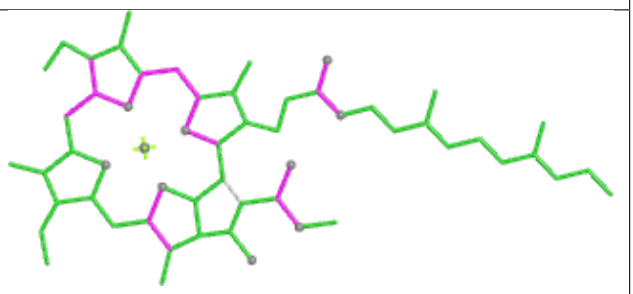
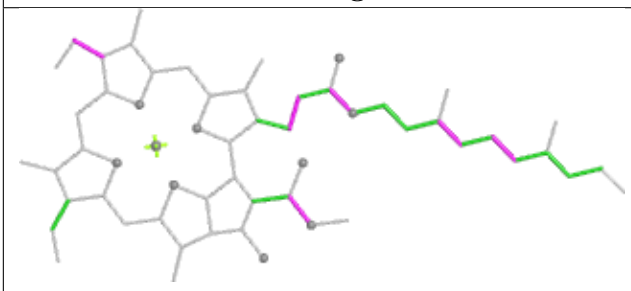
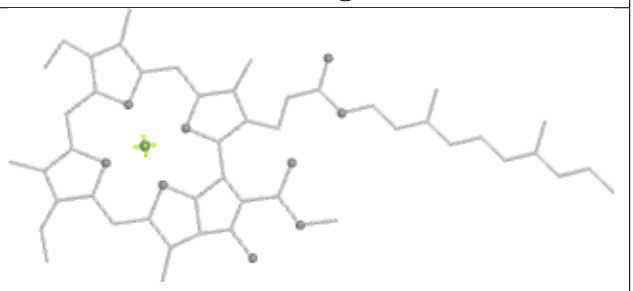


Bond angles

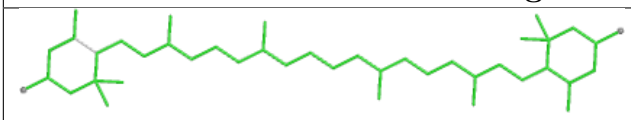


Torsions



Rings

Ligand LUT T 614



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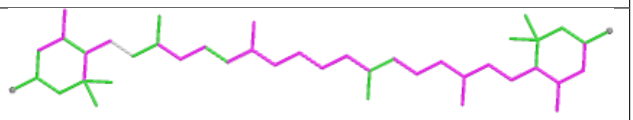
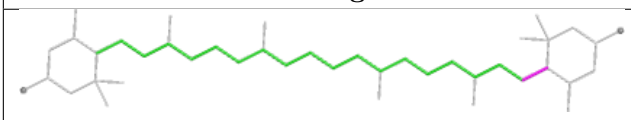
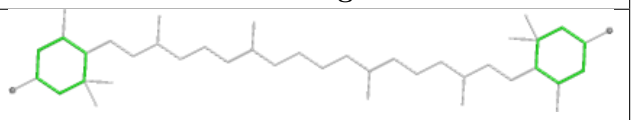


Bond angles

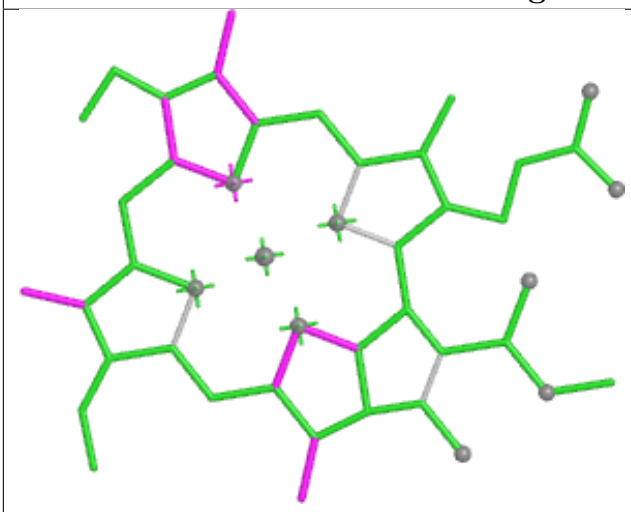


Torsions

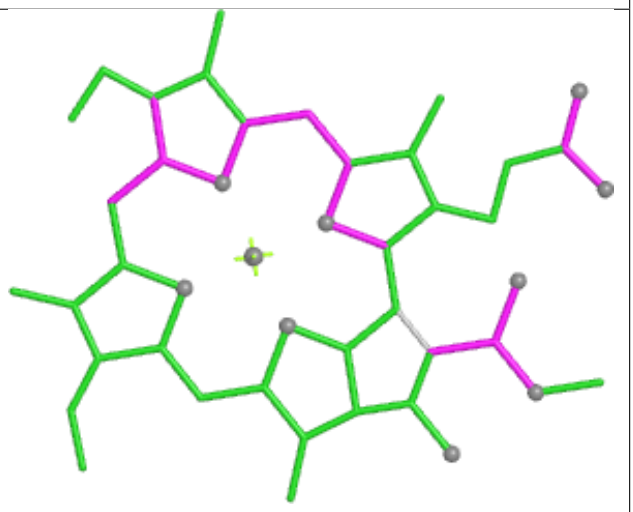


Rings

Ligand CLA 3 312



Bond lengths



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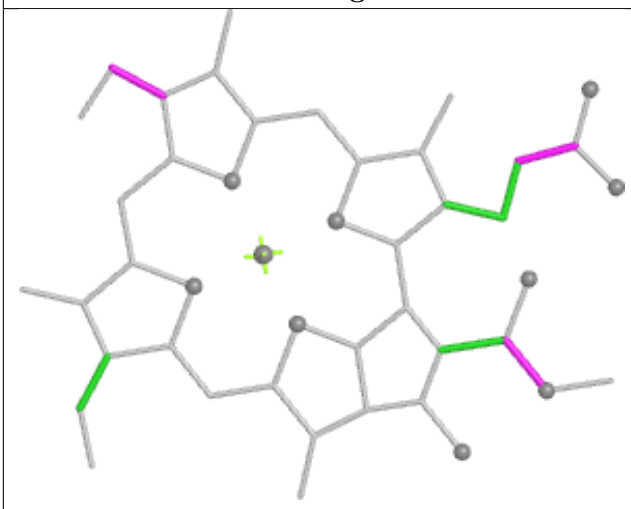

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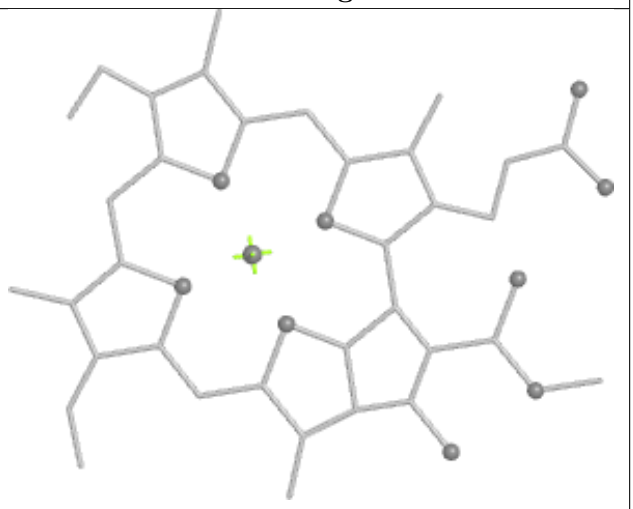
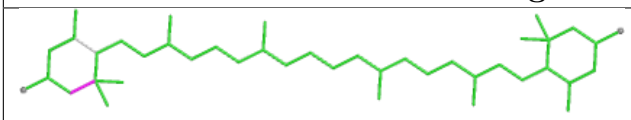


Rings

Ligand LUT 6 622



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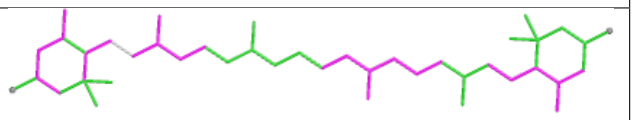
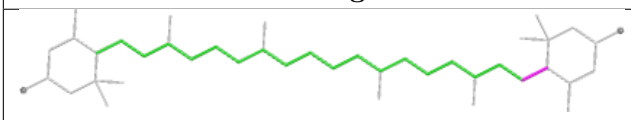


Bond angles



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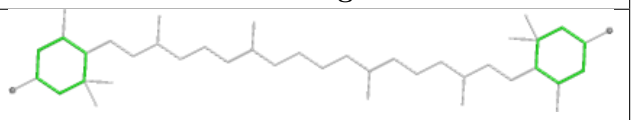
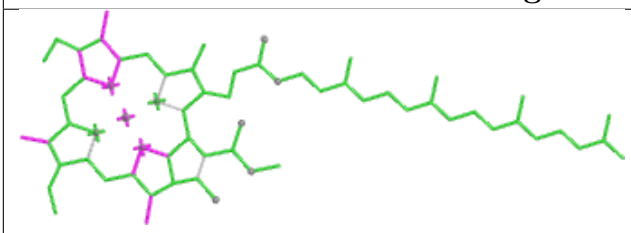


Rings

Ligand CLA A 836



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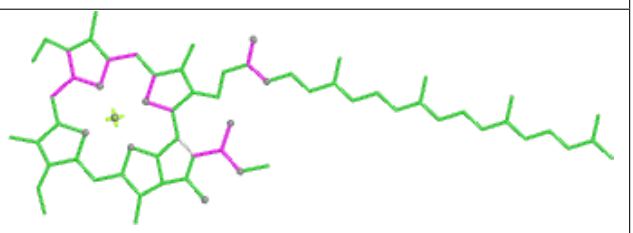
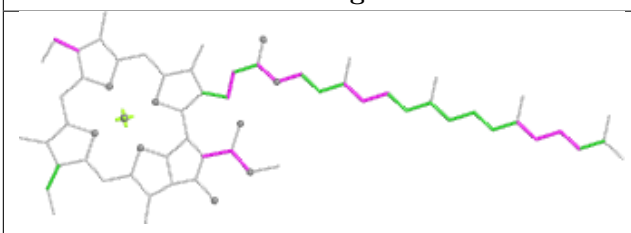


Bond angles



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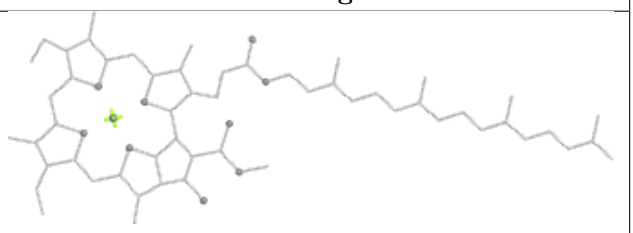
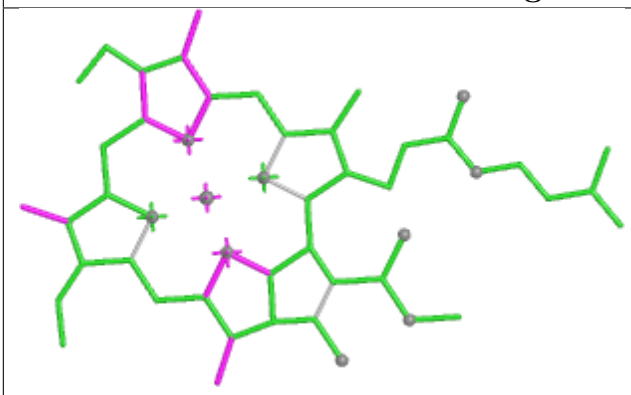
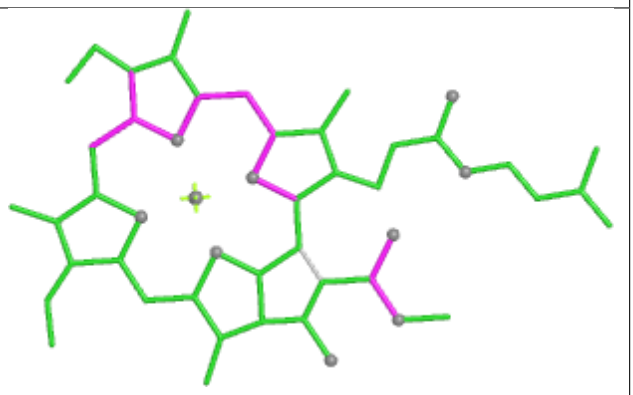


Rings

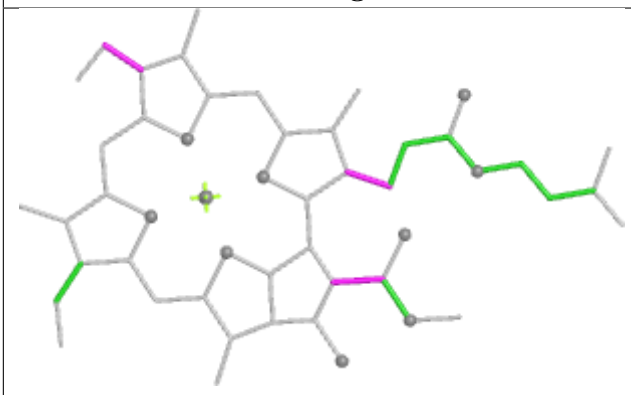
Ligand CLA B 828



Bond lengths



Bond angles



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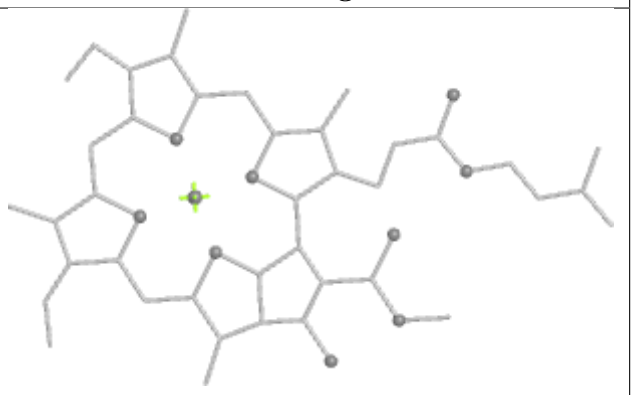
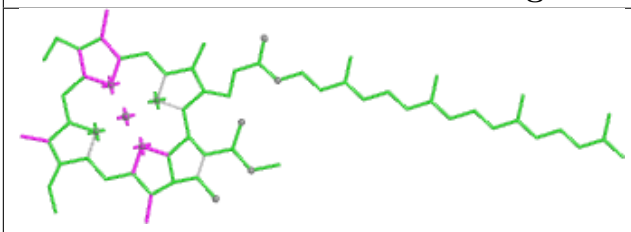


Rings

Ligand CLA L 202



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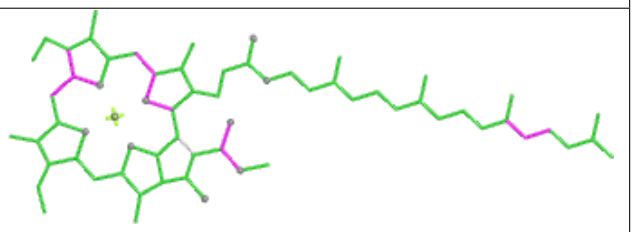
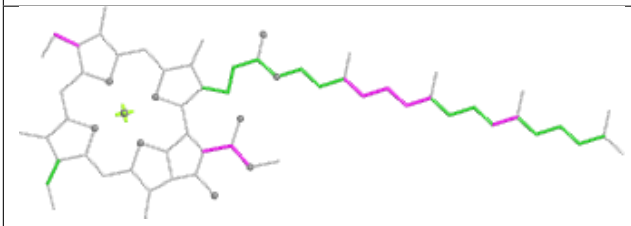


Bond angles



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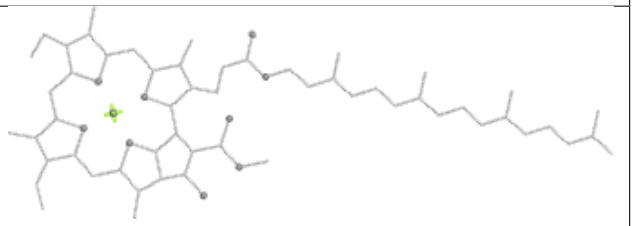
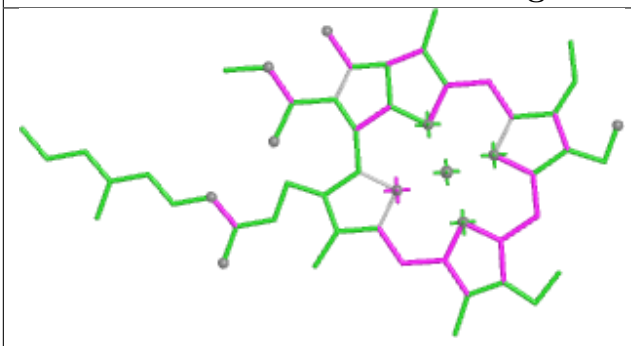


Rings

Ligand CHL 1 601



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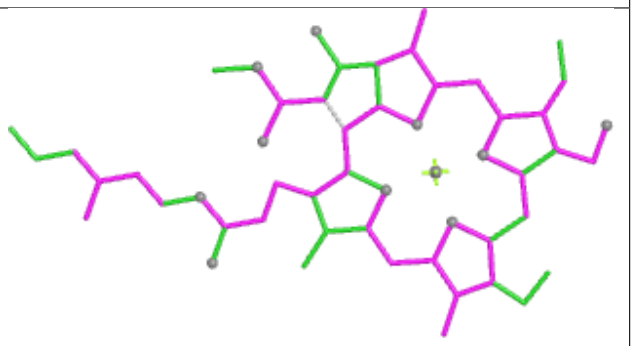
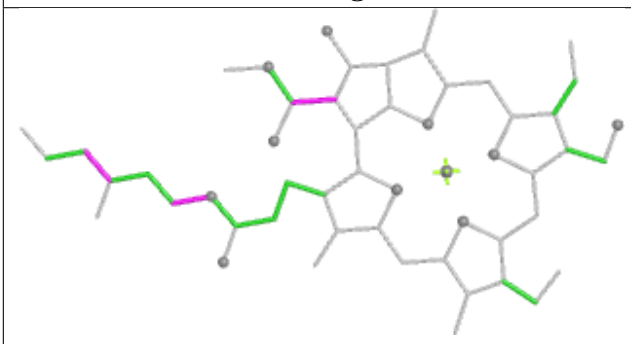


Bond angles



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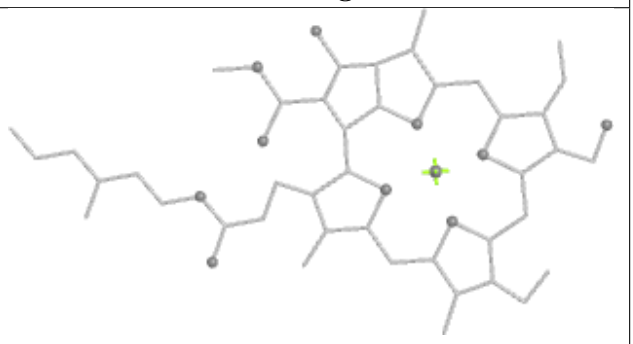
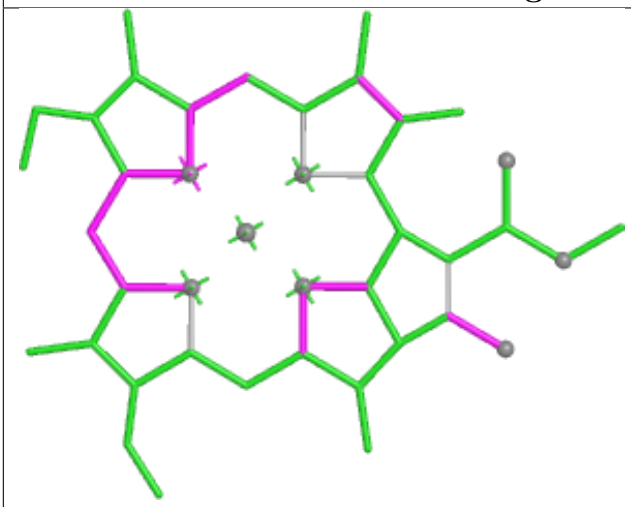


Rings

Ligand CLA P 611



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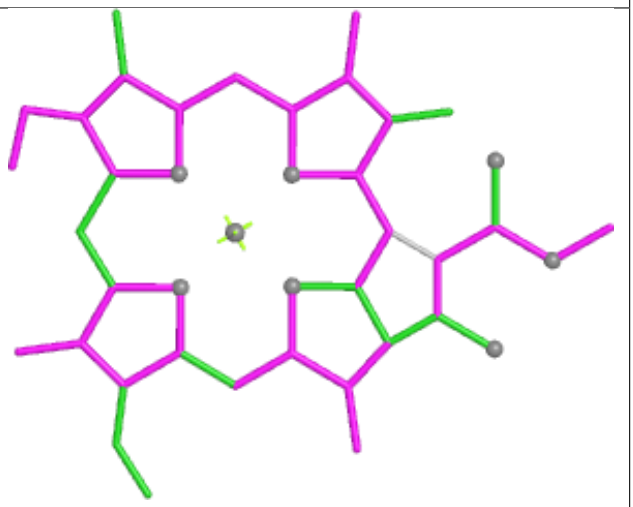
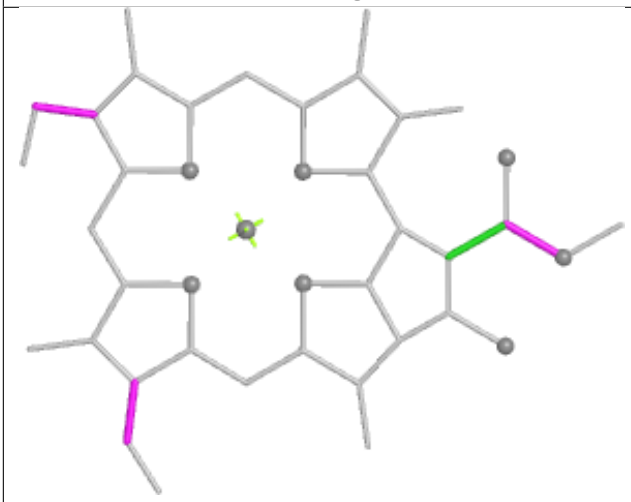


Bond angles



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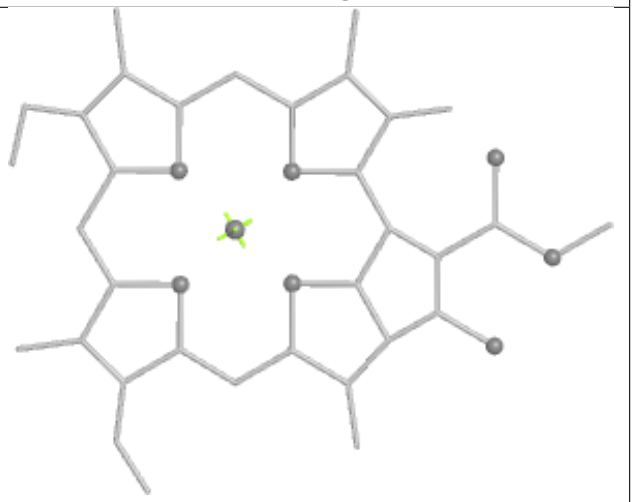
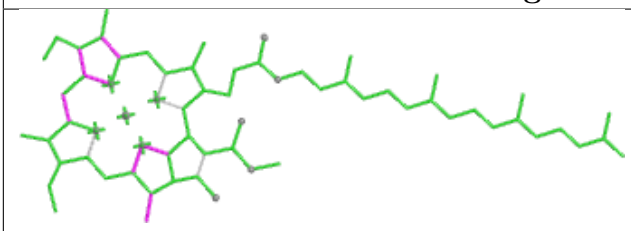


Rings

Ligand CLA Q 603



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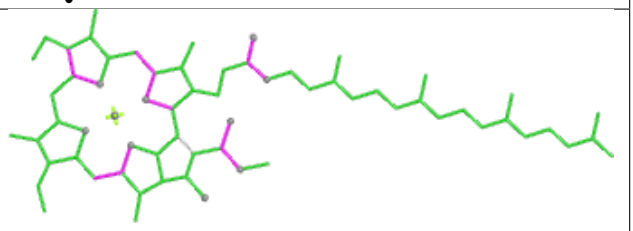
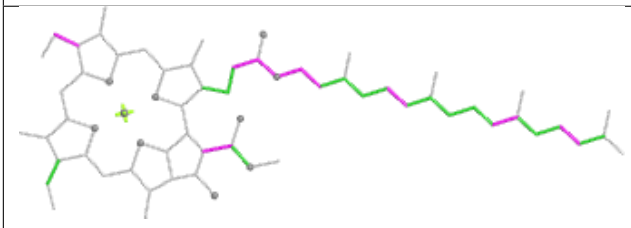
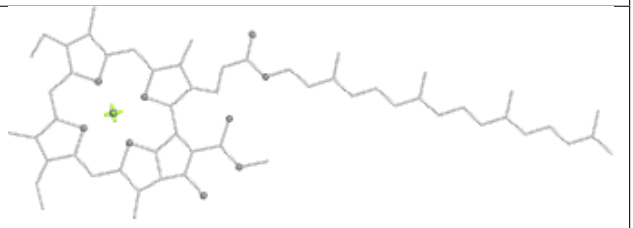


Bond angles

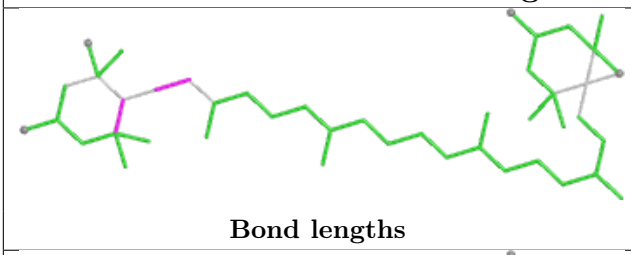


Torsions



Rings

Ligand NEX U 301



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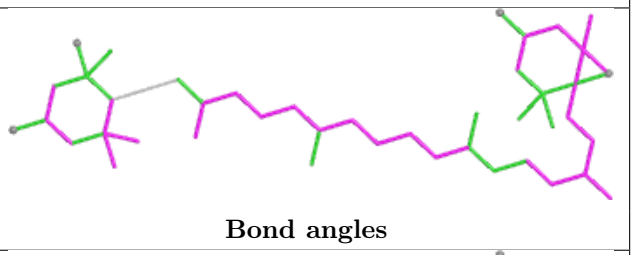
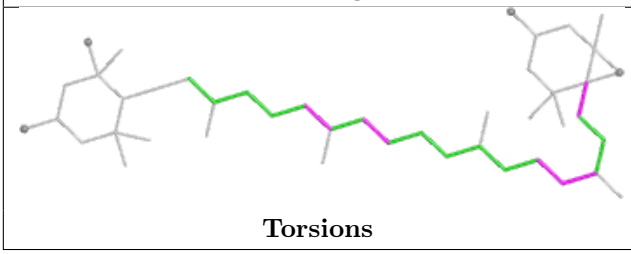


Bond angles



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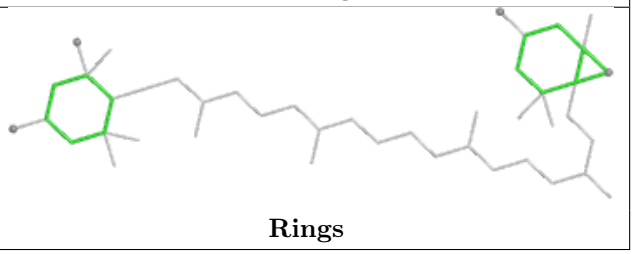
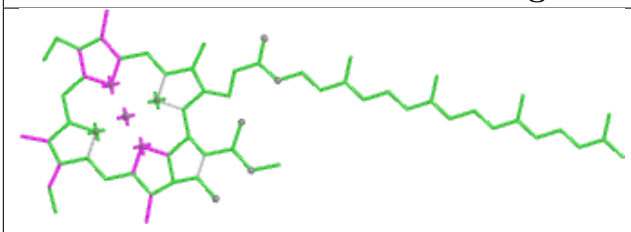


Rings

Ligand CLA 3 320



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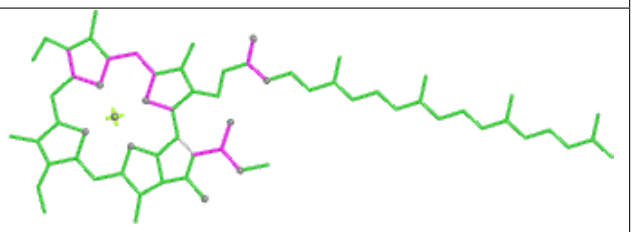

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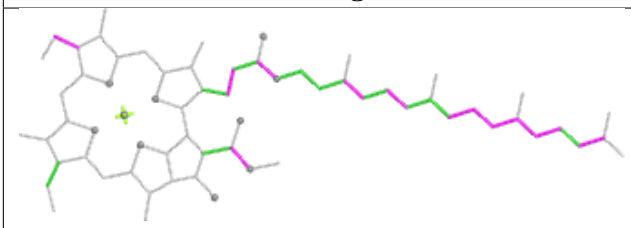

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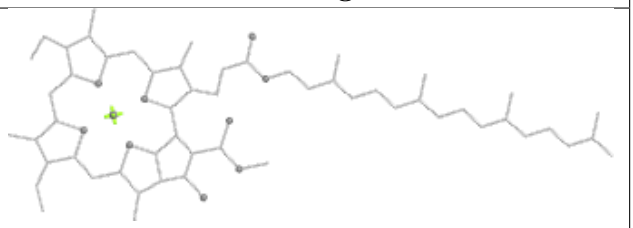
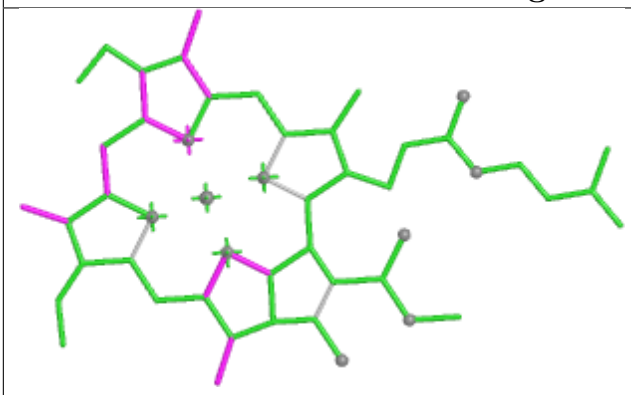


Rings

Ligand CLA 4 307



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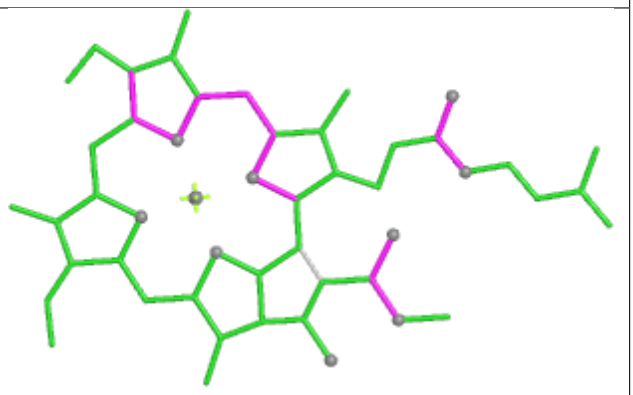
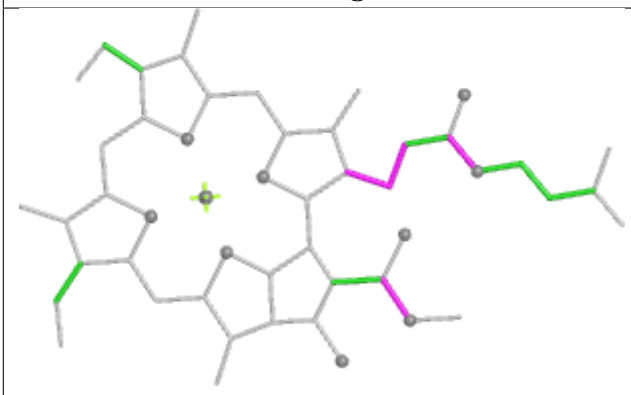


Bond angles



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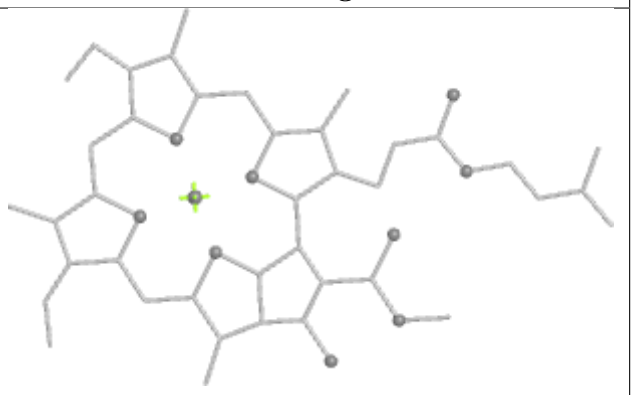
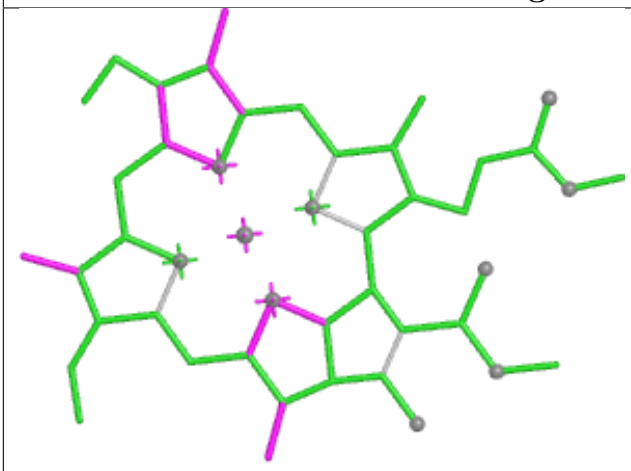


Rings

Ligand CLA 7 313



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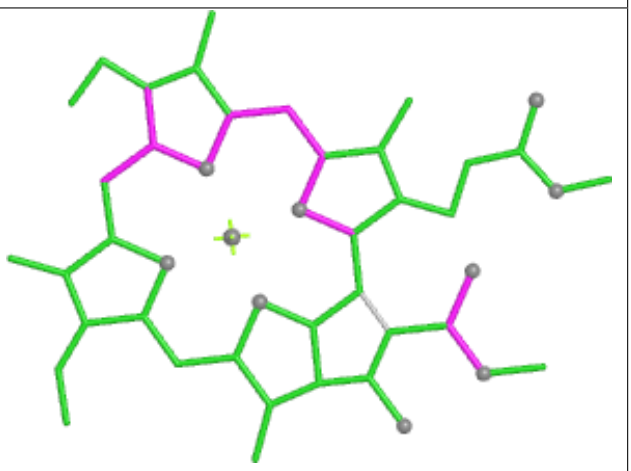
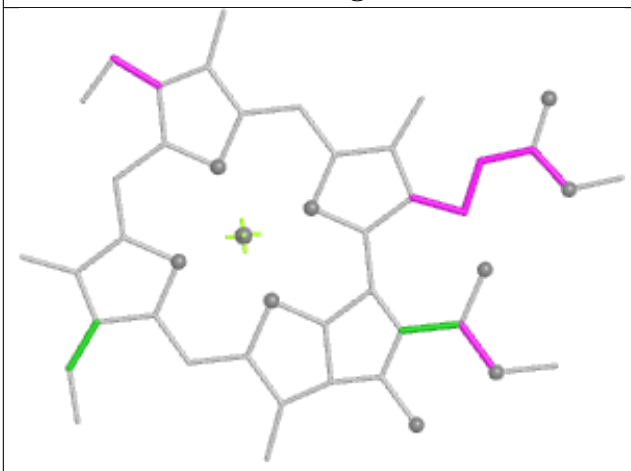


Bond angles



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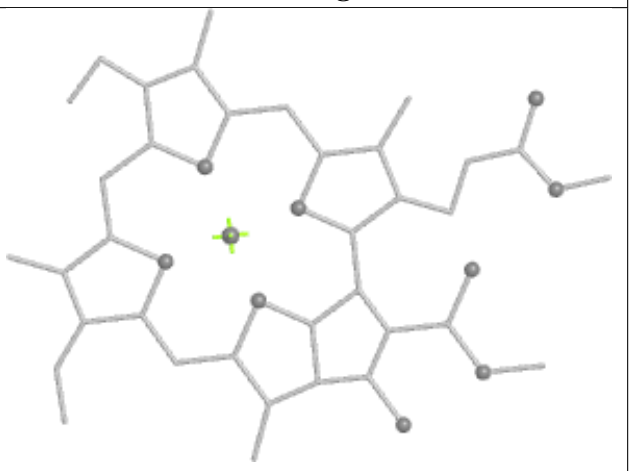
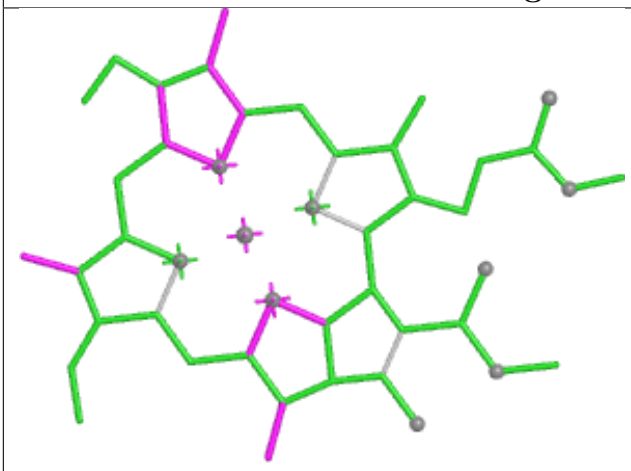
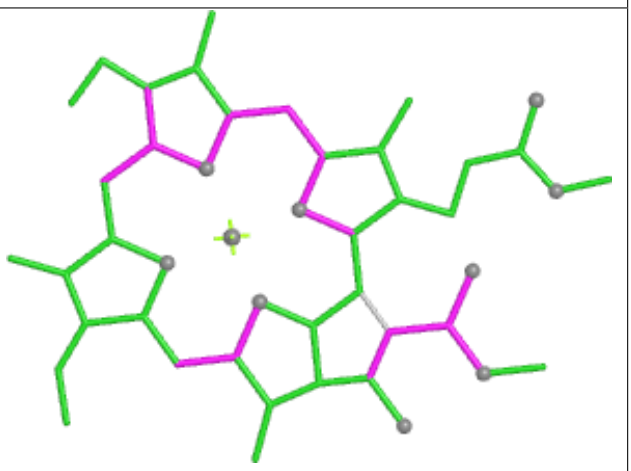


Rings

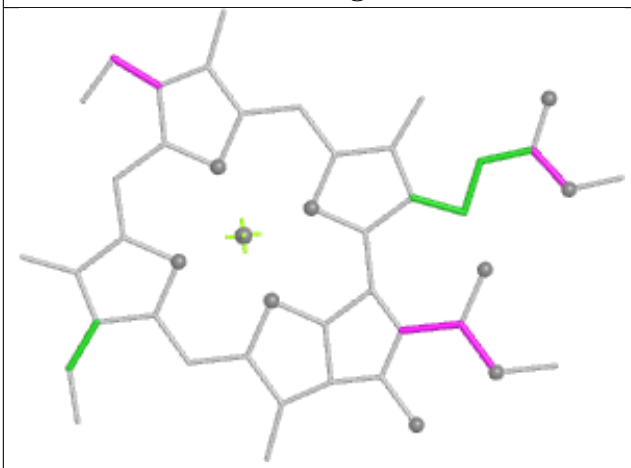
Ligand CLA B 819



Bond lengths



Bond angles



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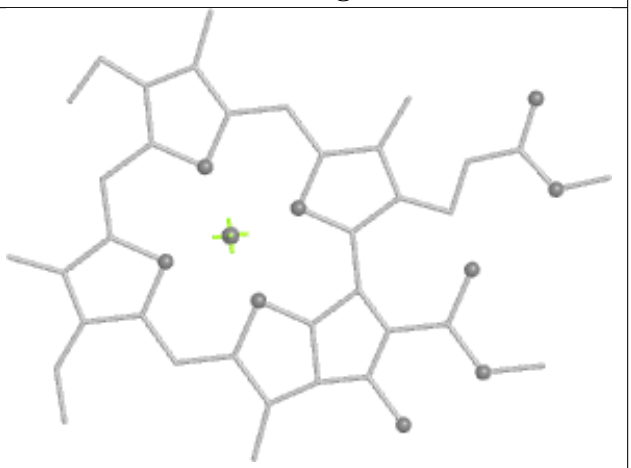
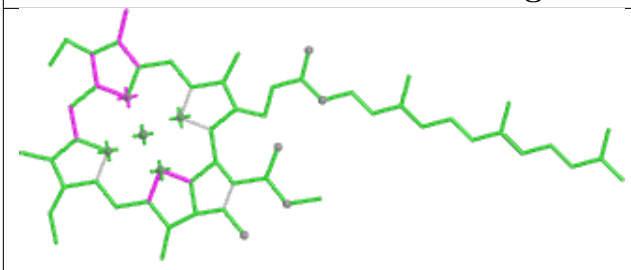
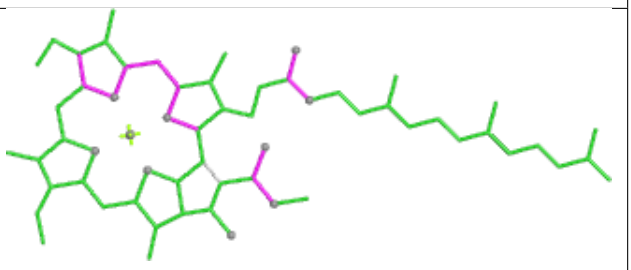


Rings

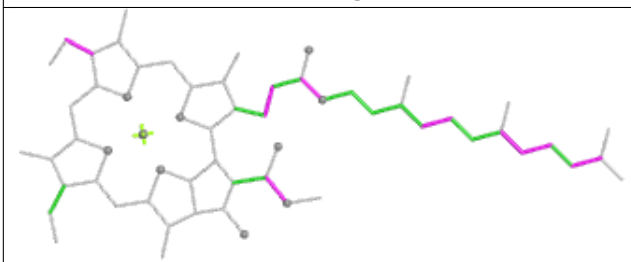
Ligand CLA T 611



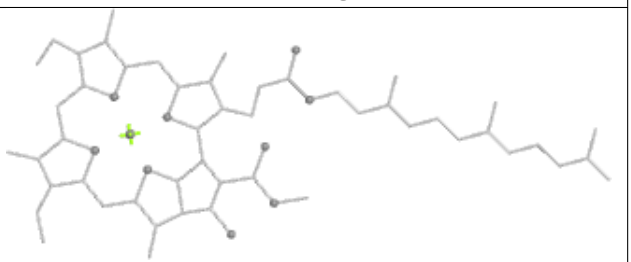
Bond lengths



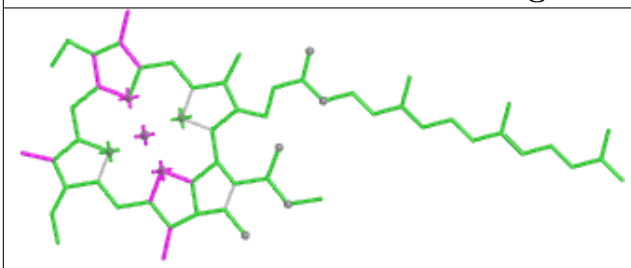
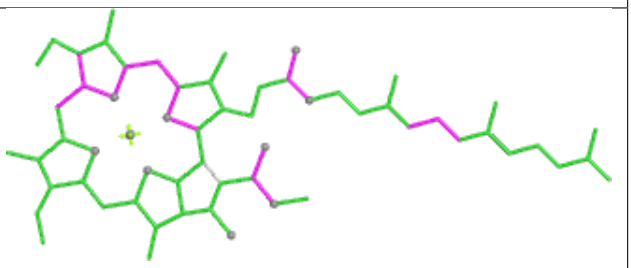
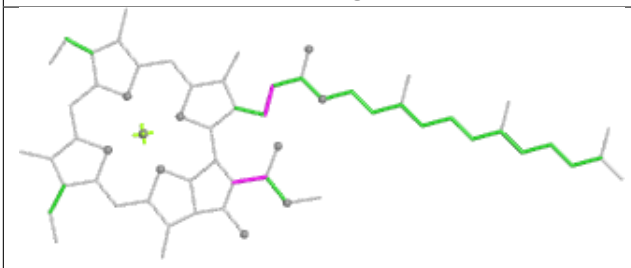
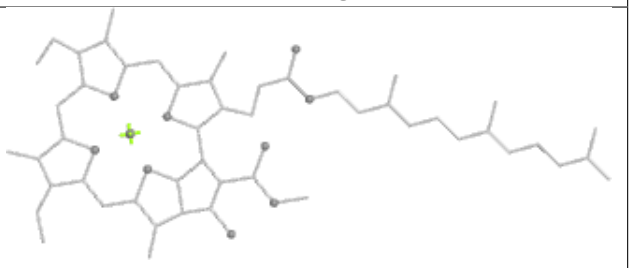
Bond angles

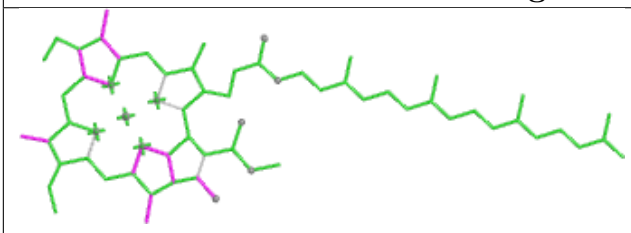
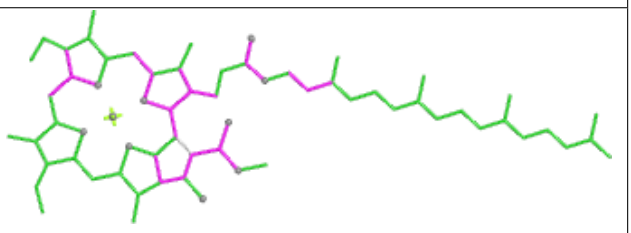
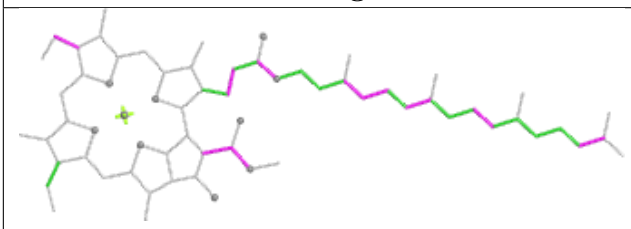
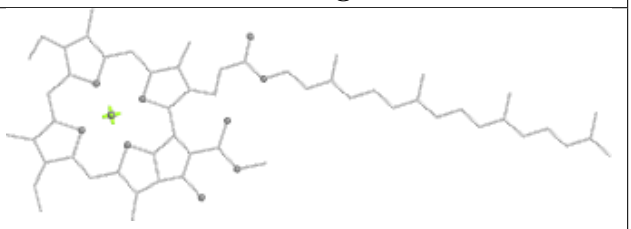


Torsions

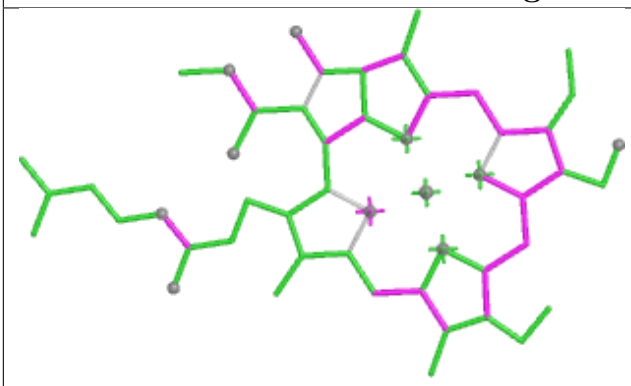


Rings

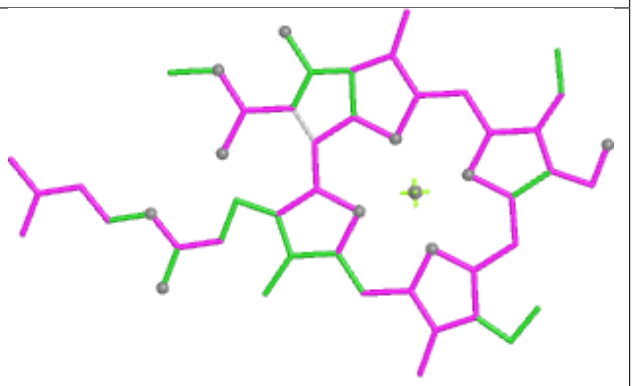
Ligand CLA 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

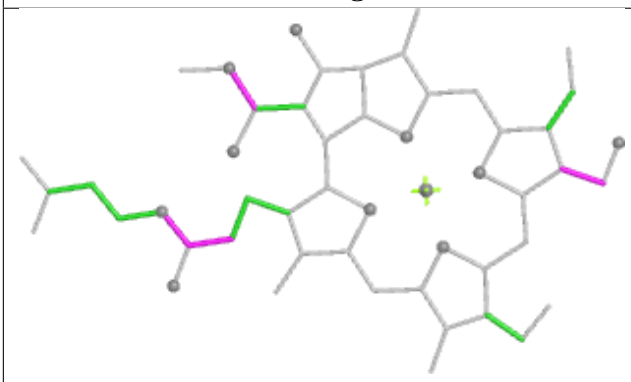
Ligand CHL R 601



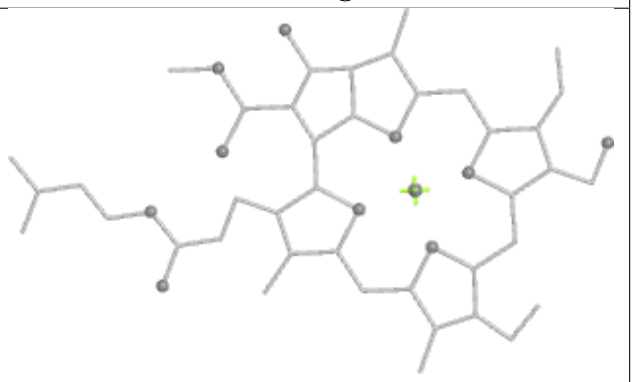
Bond lengths



Bond angles

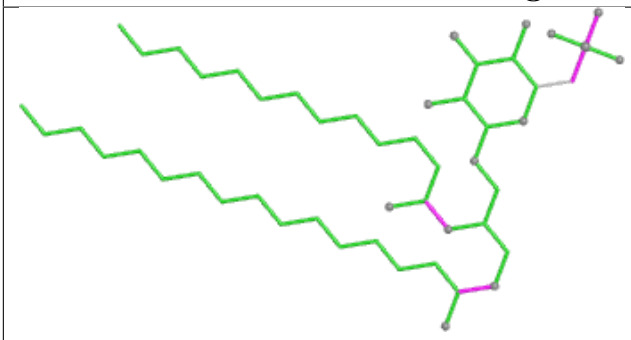


Torsions



Rings

Ligand SQD B 850



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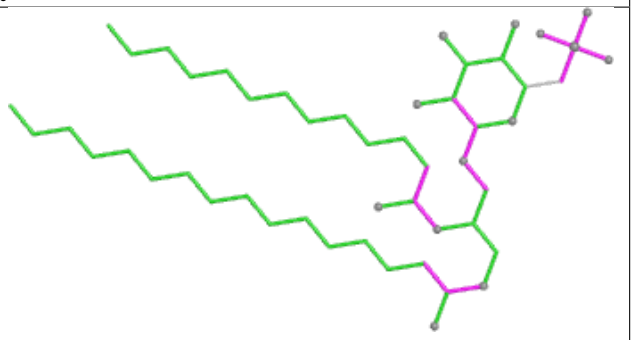
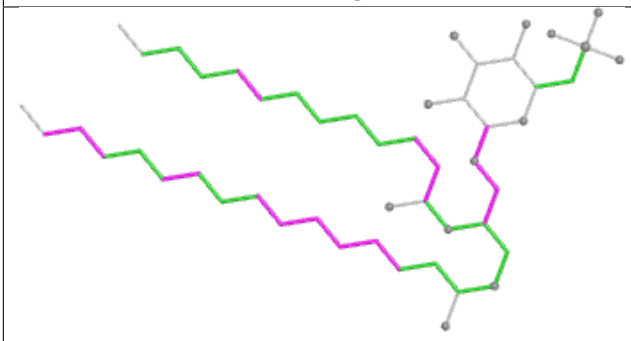


Bond angles



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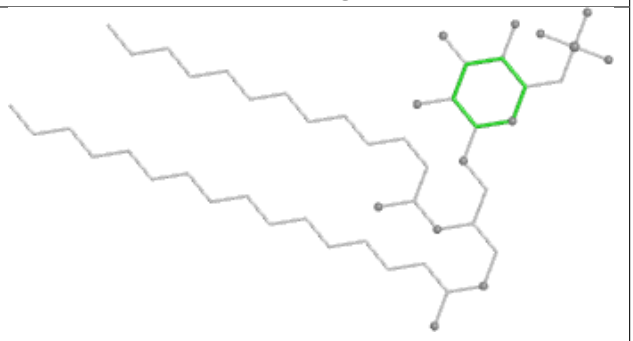
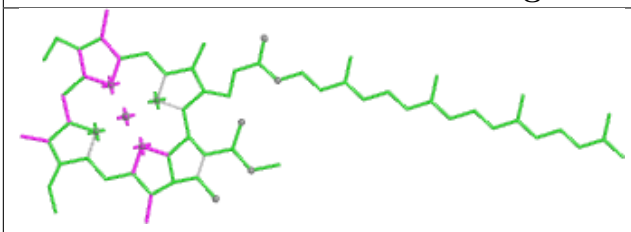


Rings

Ligand CLA A 809



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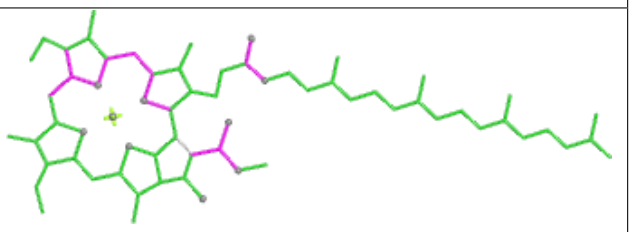
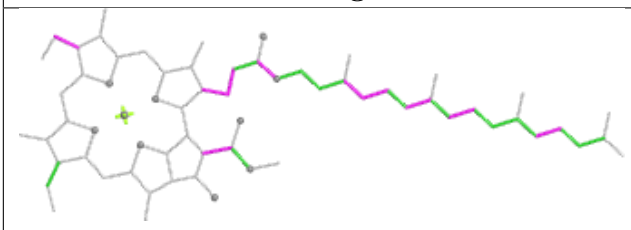


Bond angles



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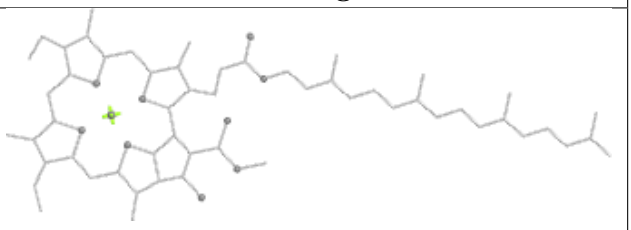
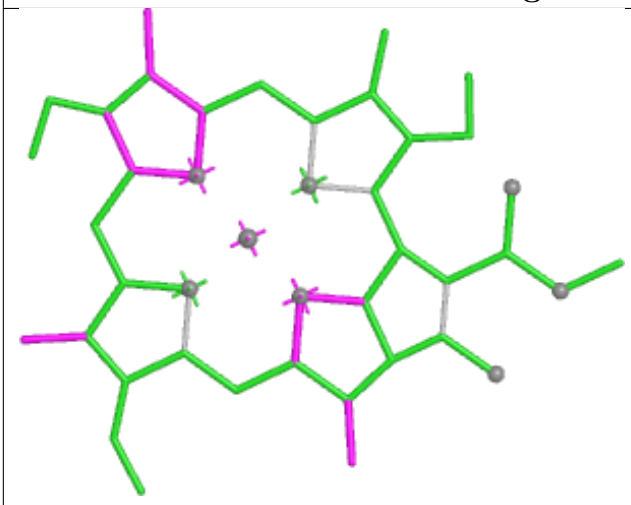


Rings

Ligand CLA H 205



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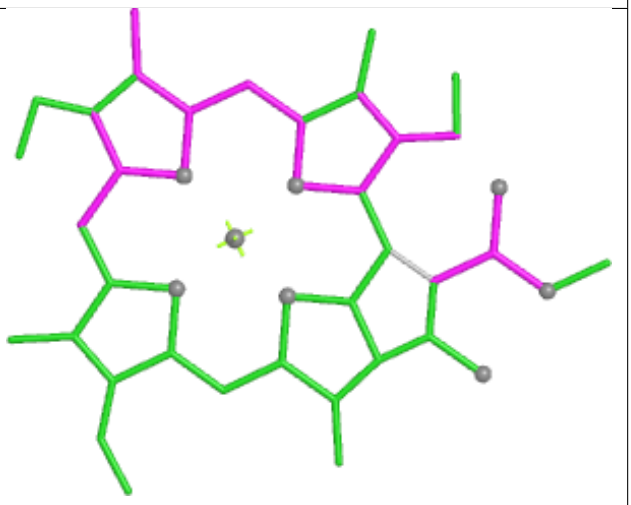

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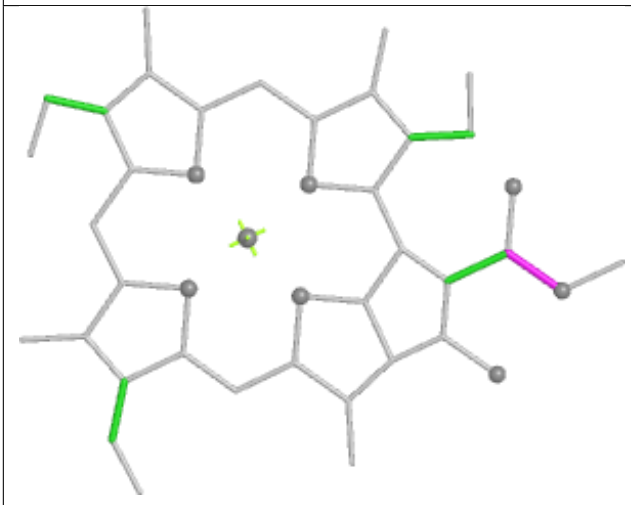

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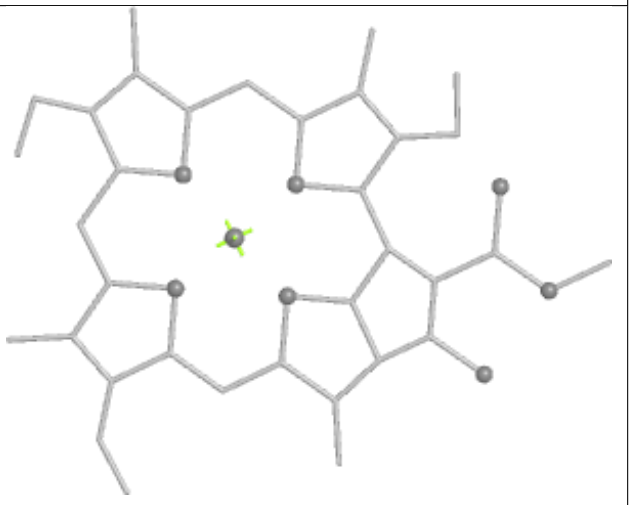
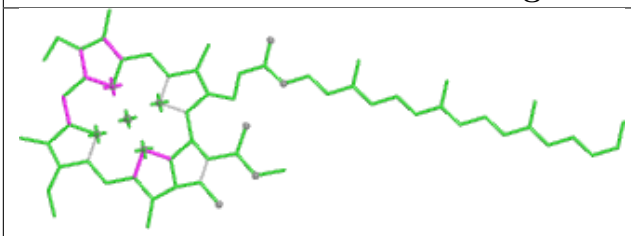


Rings

Ligand CLA U 310



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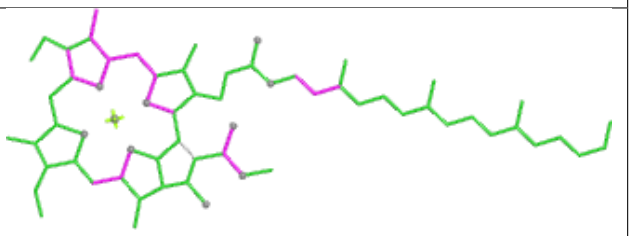
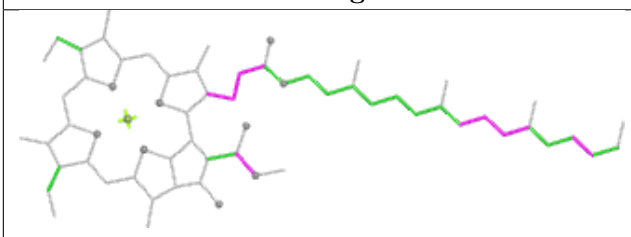


Bond angles



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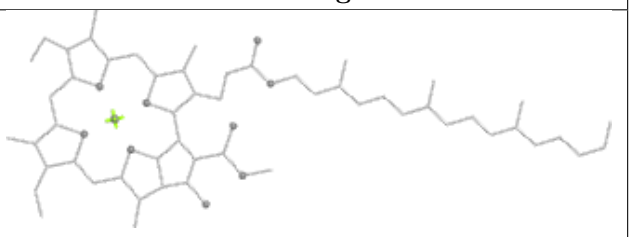
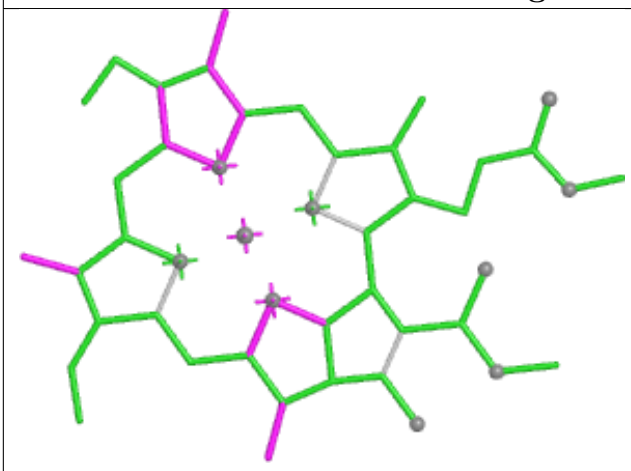


Rings

Ligand CLA 6 604



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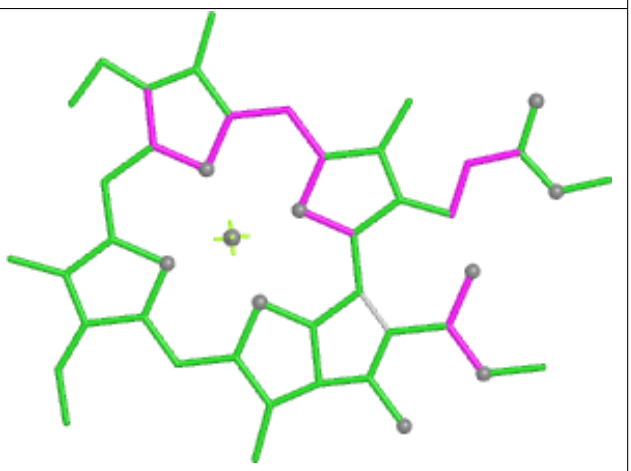
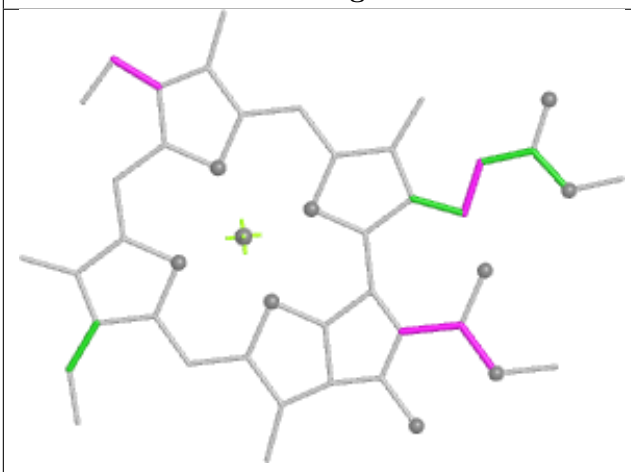
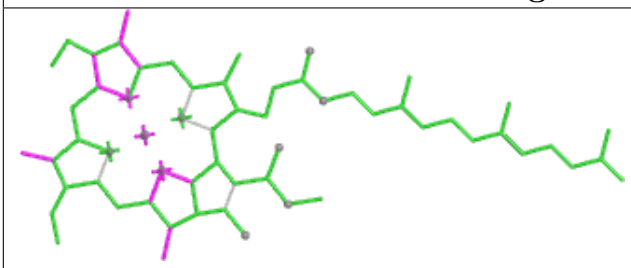
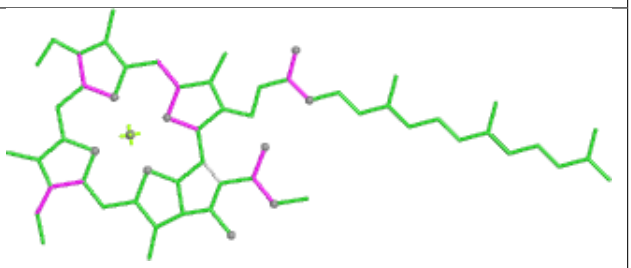
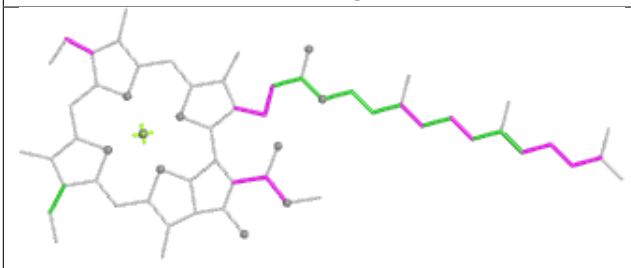
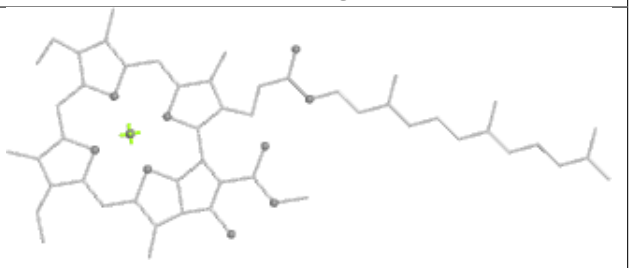


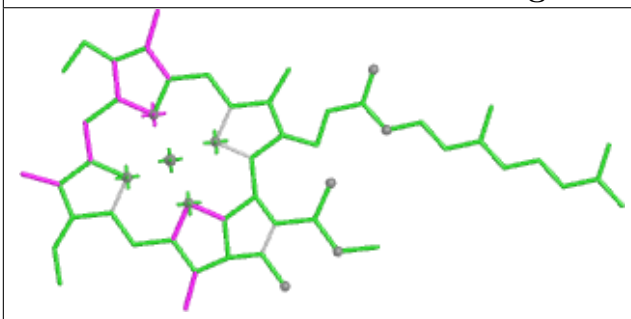
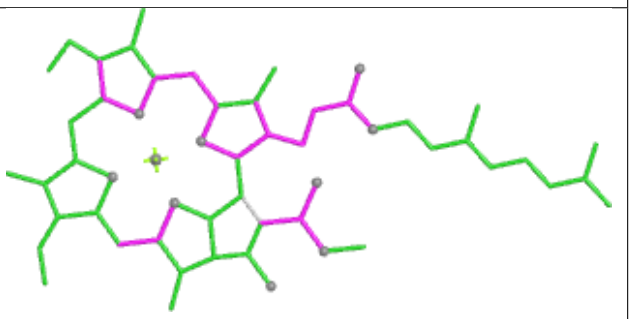
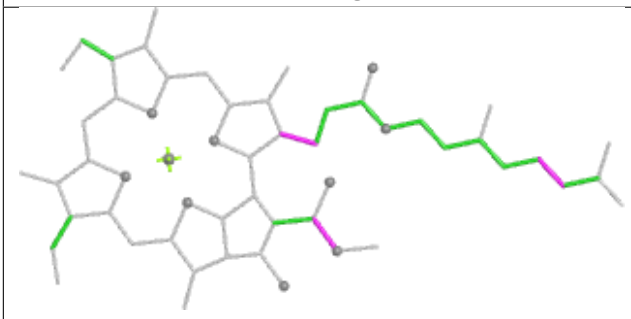
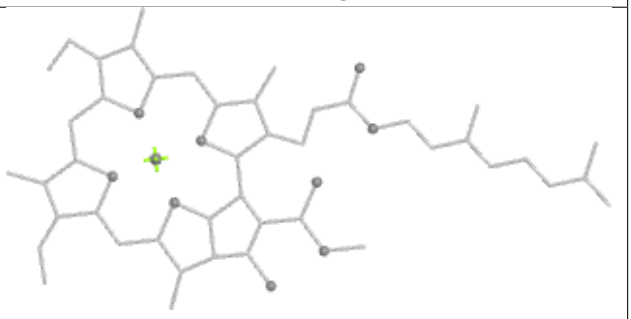
Bond angles



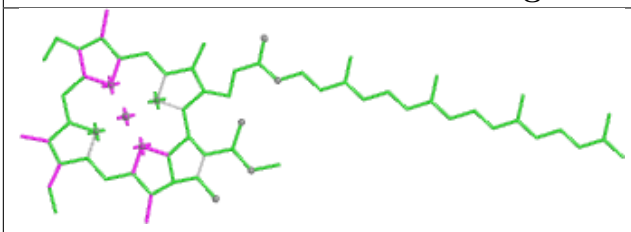
Torsions

Rings

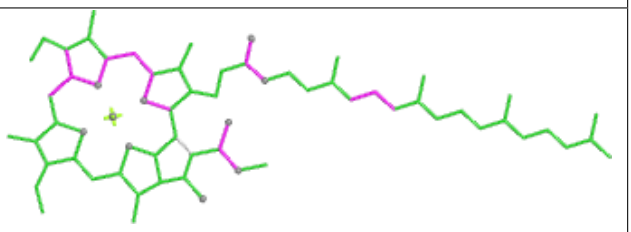
Ligand CLA 4 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

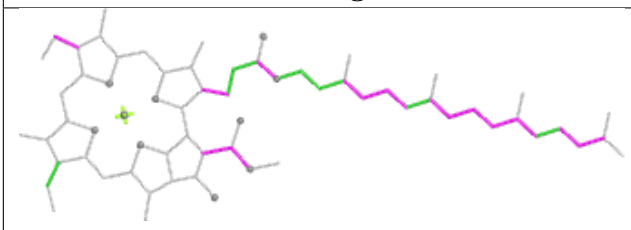
Ligand CLA A 807



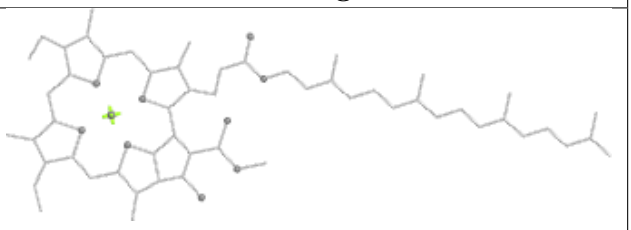
Bond lengths



Bond angles

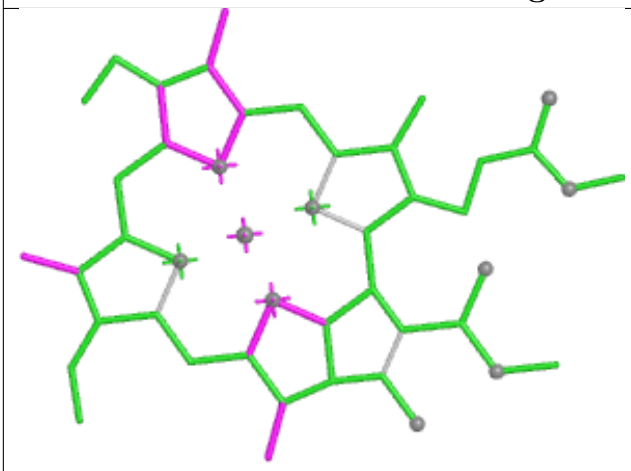


Torsions



Rings

Ligand CLA 8 305



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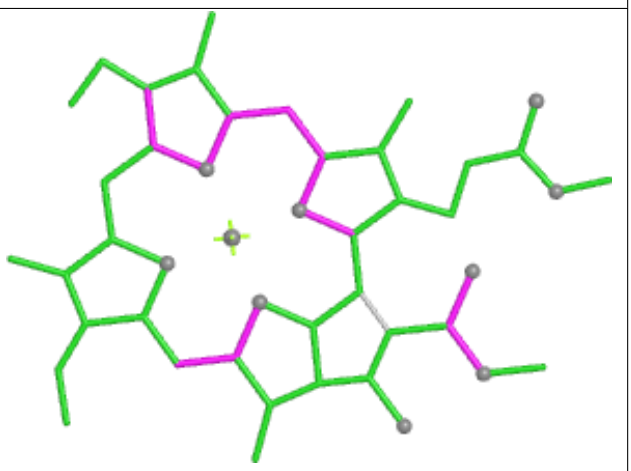
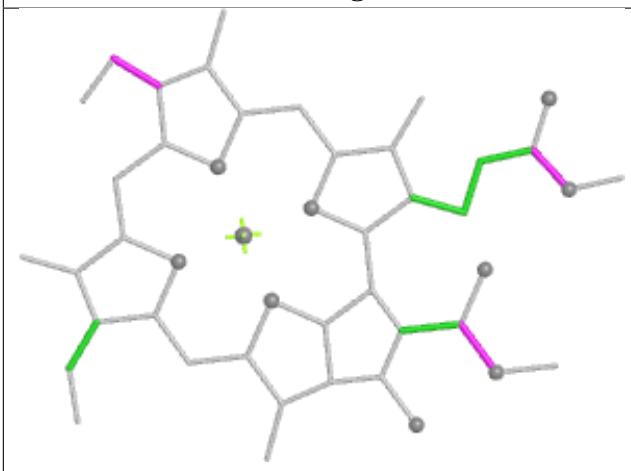
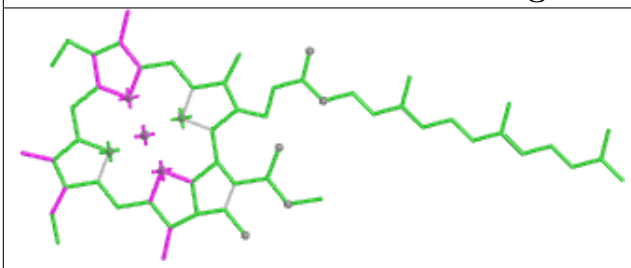
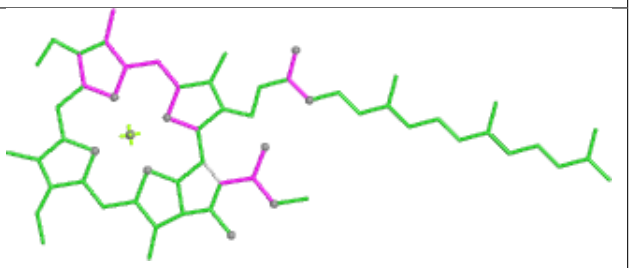
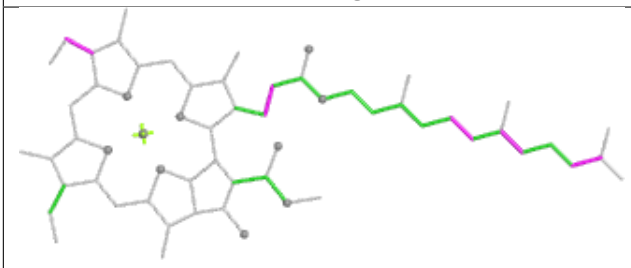
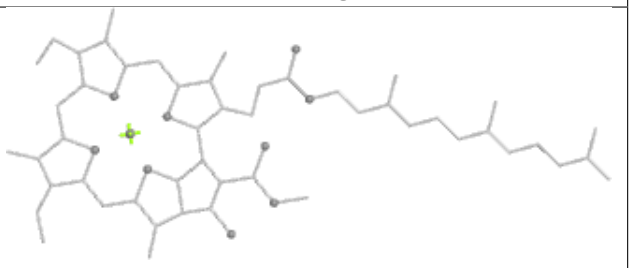


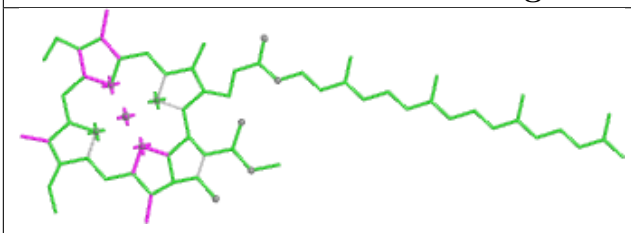
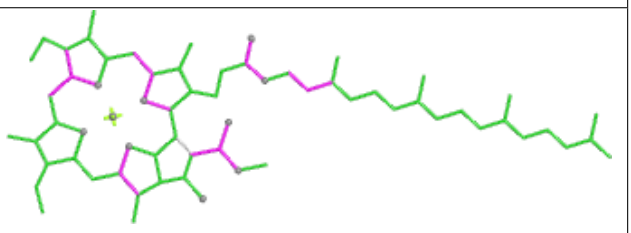
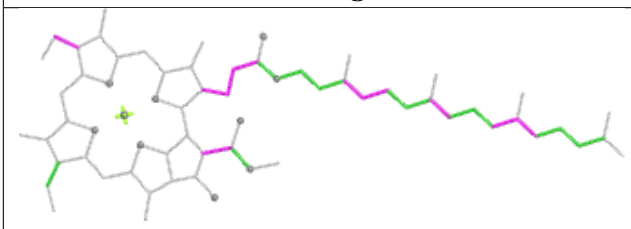
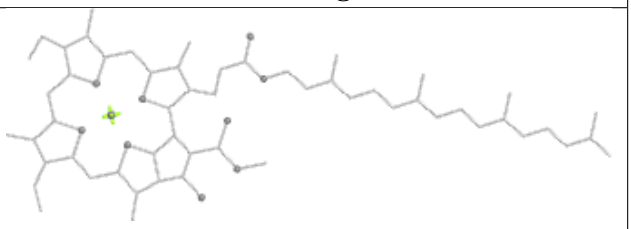
Bond angles



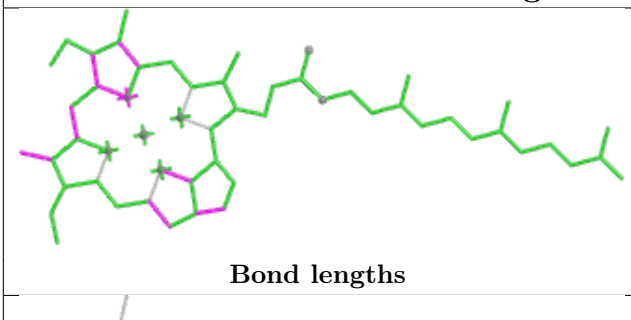
Torsions

Rings

Ligand CLA 5 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA U 311



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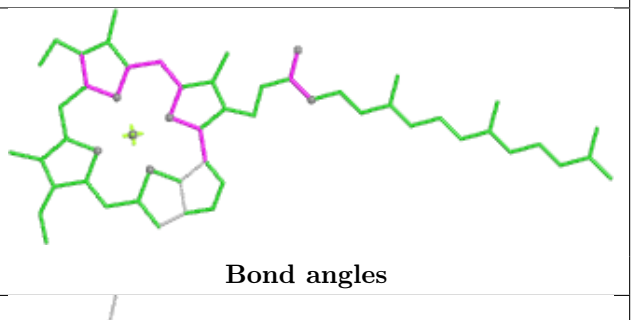

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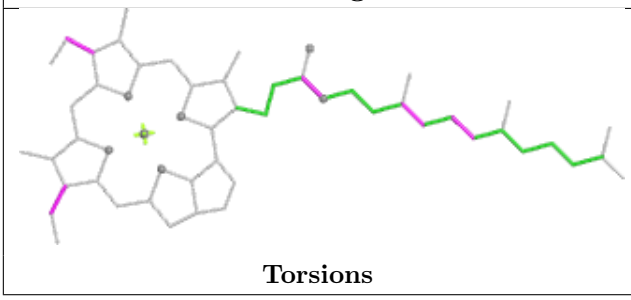
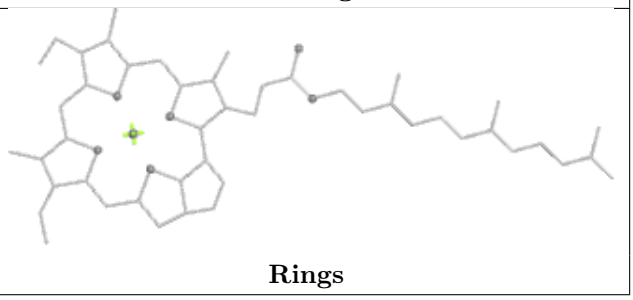
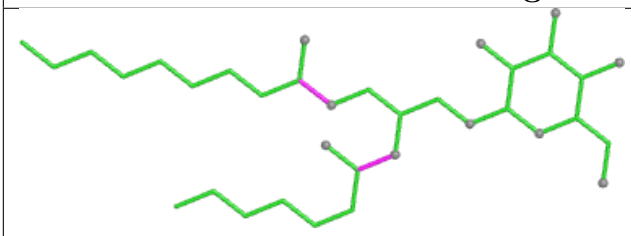


Torsions



Rings

Ligand LMG 7 318



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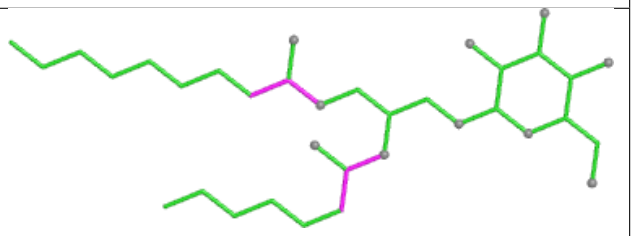

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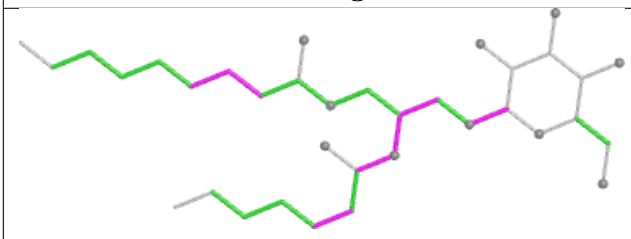

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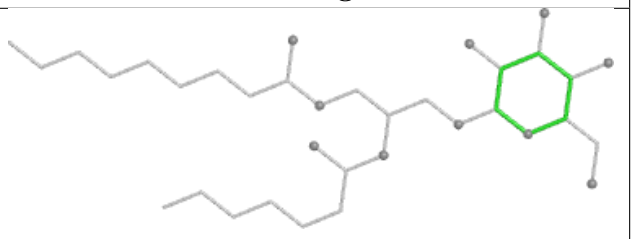
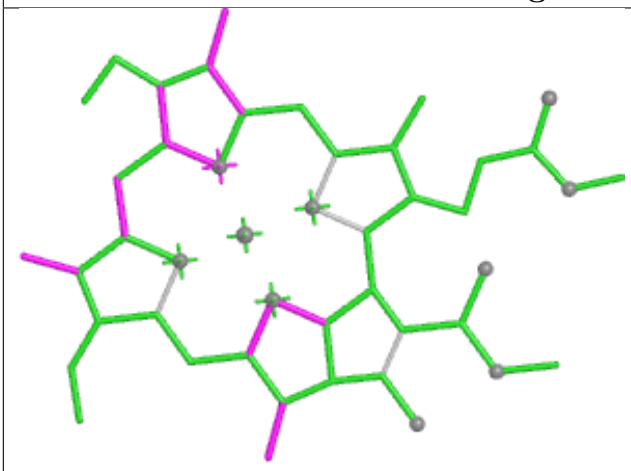


Rings

Ligand CLA 4 302



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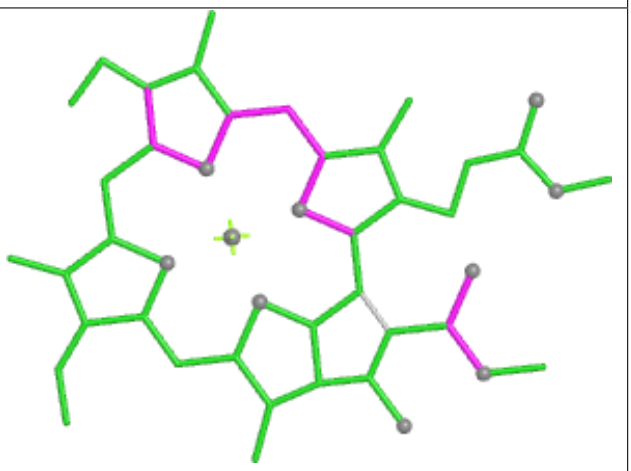

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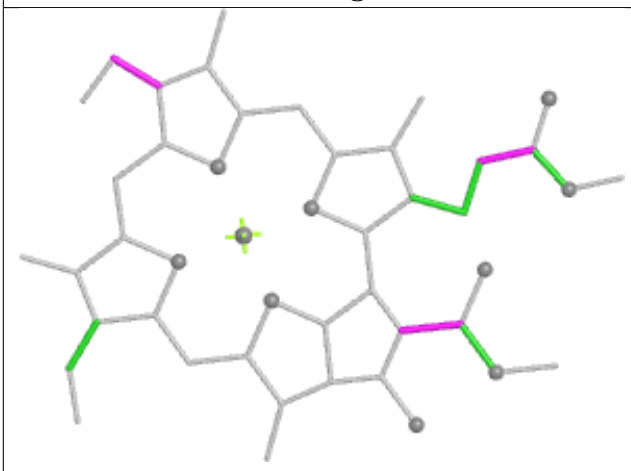

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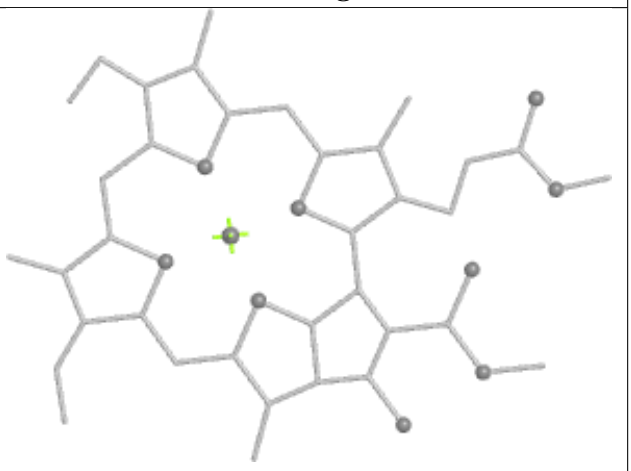
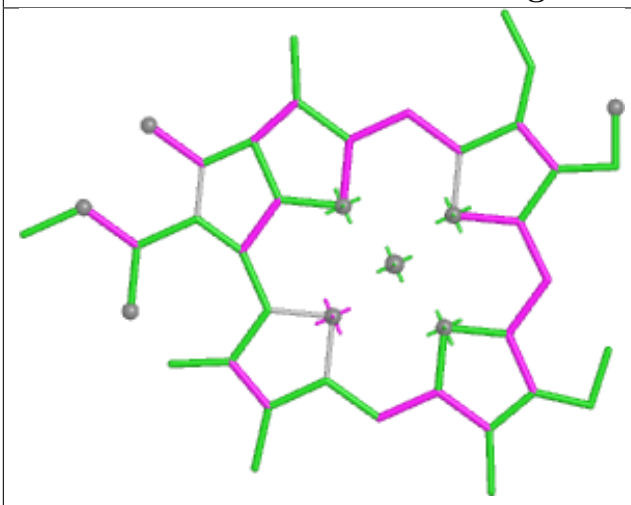


Rings

Ligand CHL 4 304



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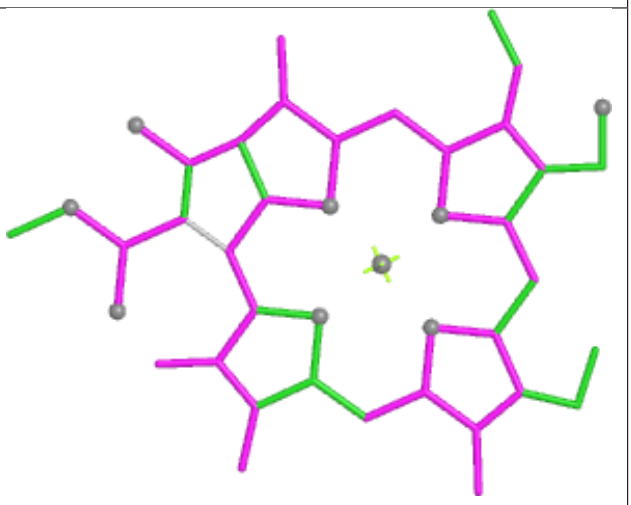

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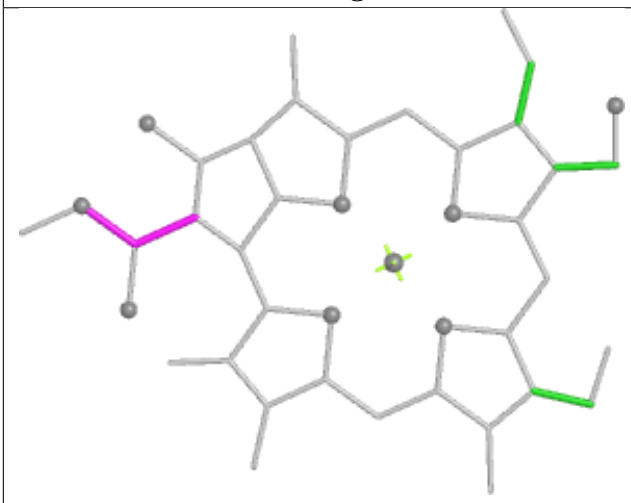

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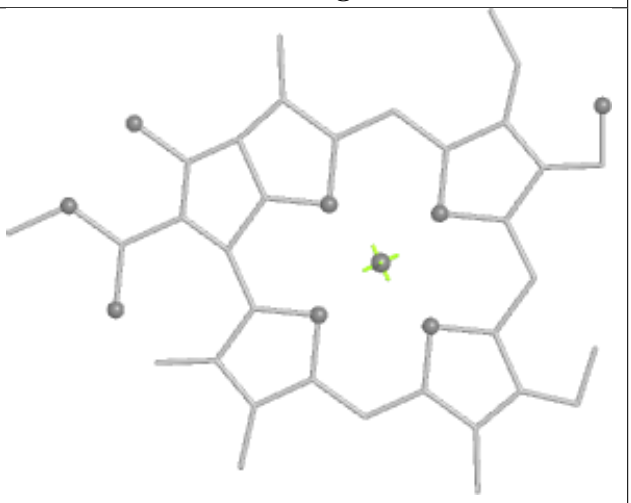
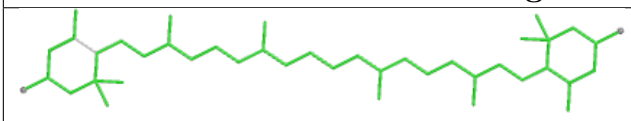


Rings

Ligand LUT P 615



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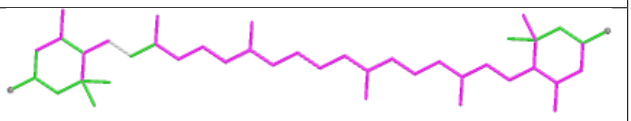
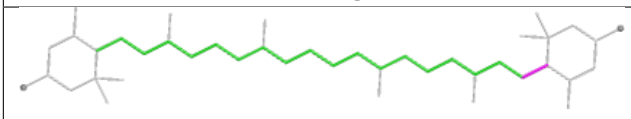


Bond angles



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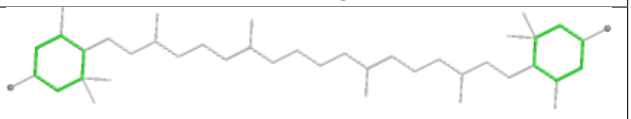
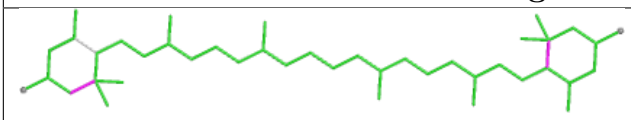


Rings

Ligand LUT 5 318



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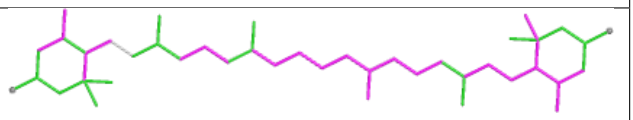
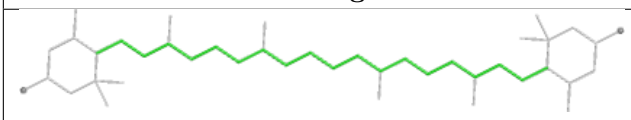


Bond angles



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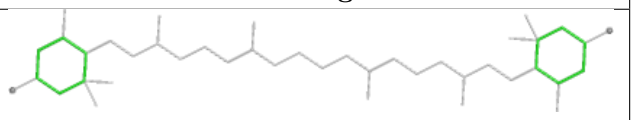
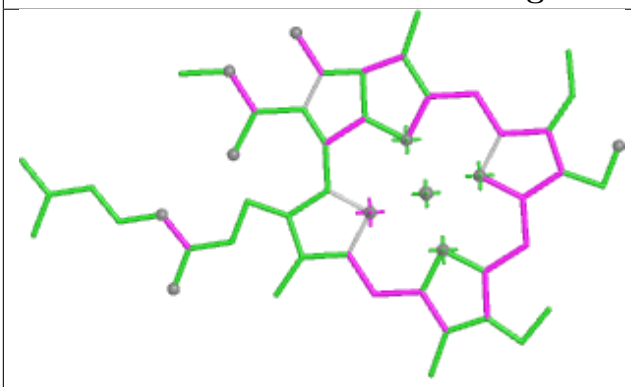


Rings

Ligand CHL S 321



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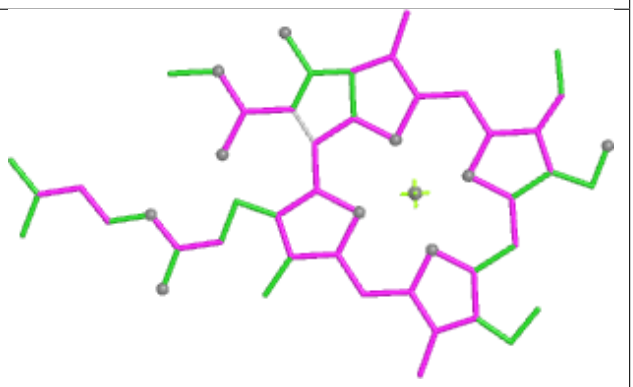
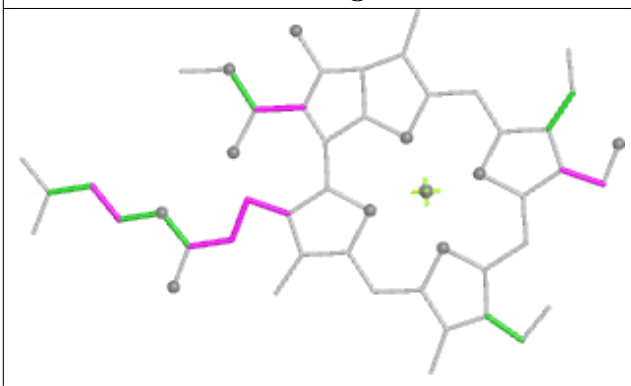


Bond angles



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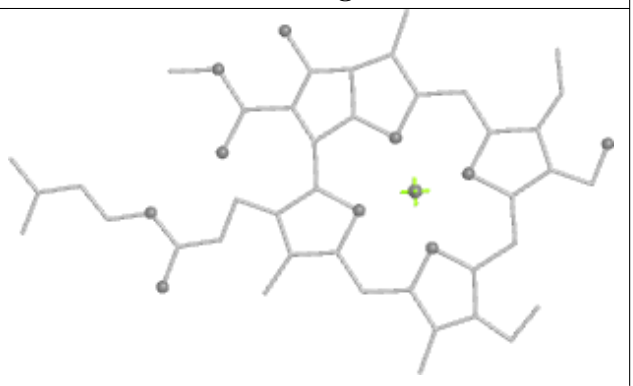
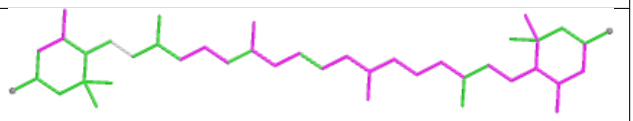


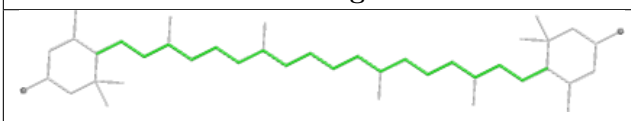
Rings

Ligand LUT 5 322

Bond lengths



Bond angles



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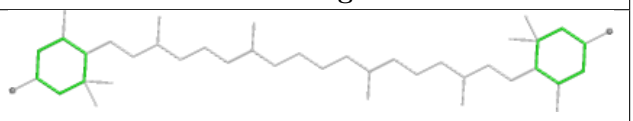
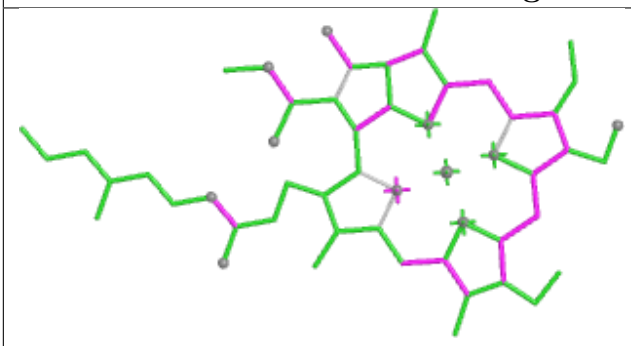


Rings

Ligand CHL U 307



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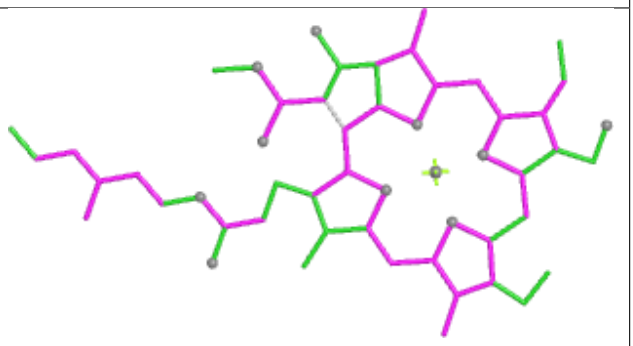
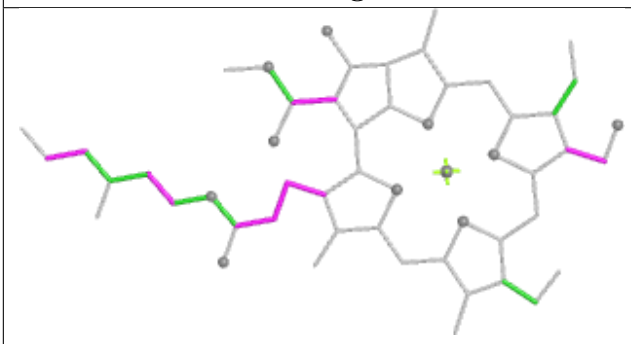
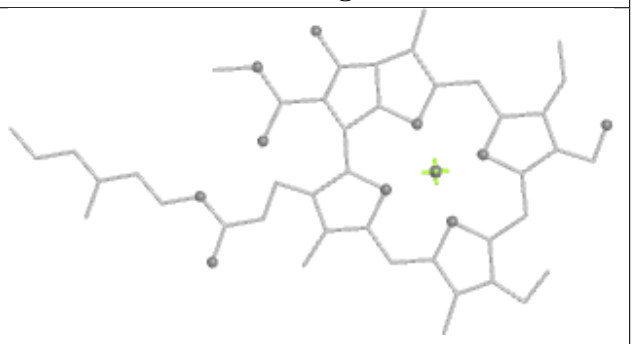


Bond angles

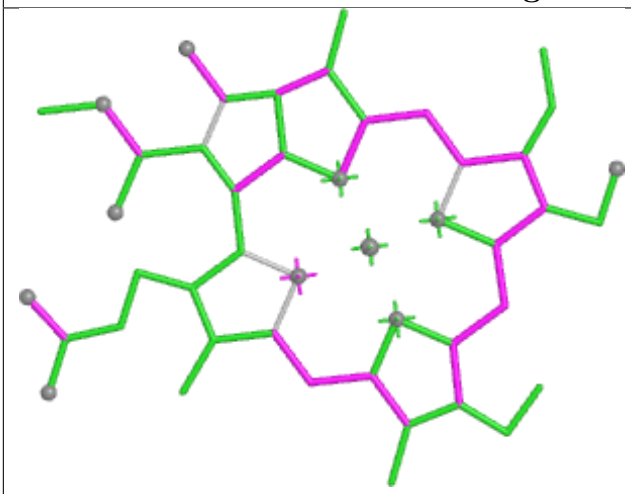


Torsions



Rings

Ligand CHL U 305



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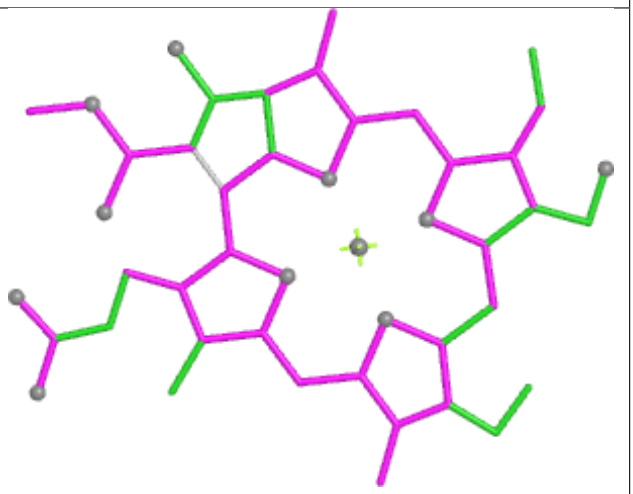
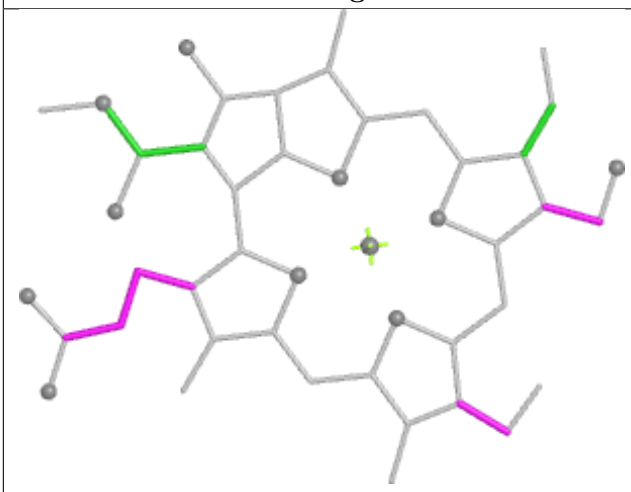


Bond angles



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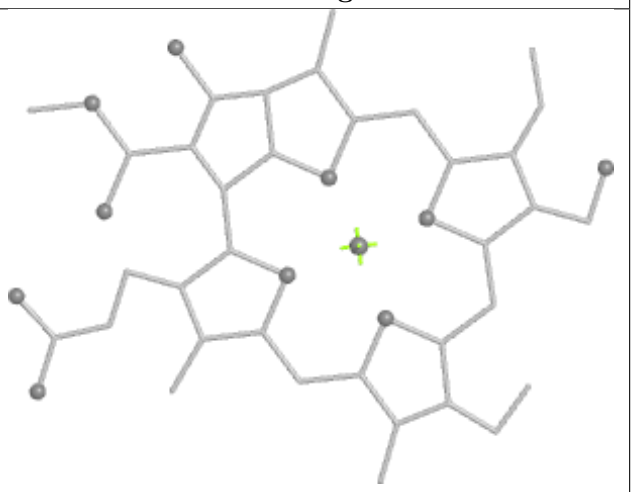
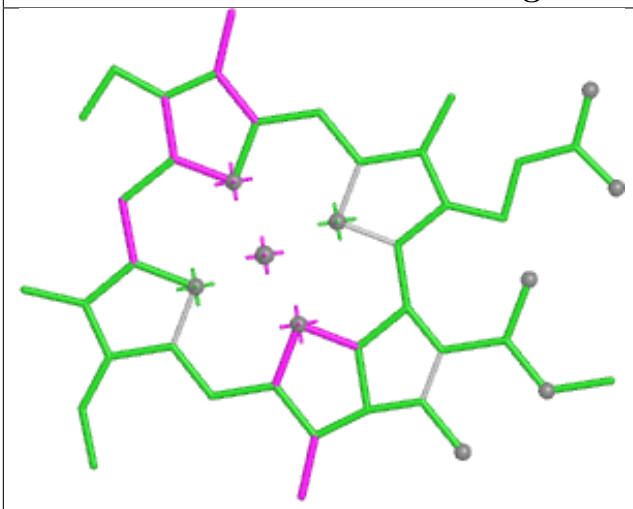


Rings

Ligand CLA K 204



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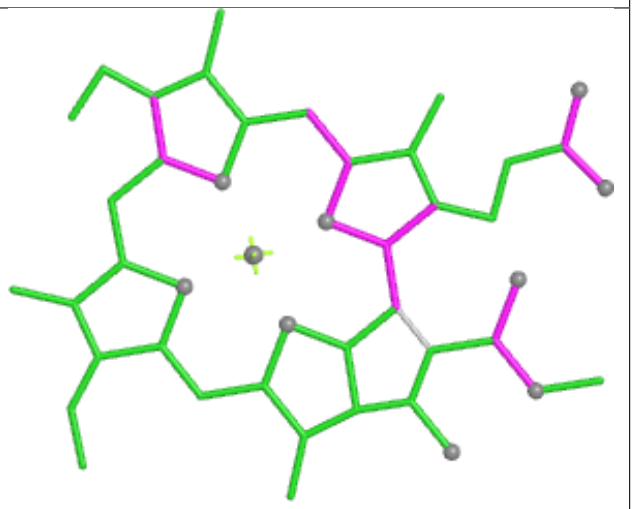
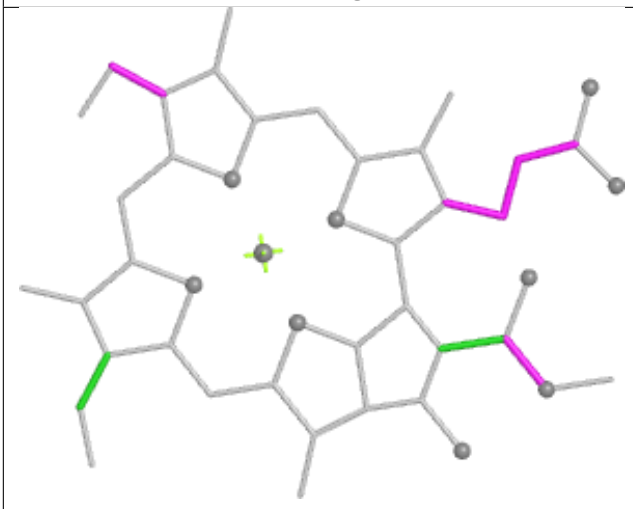


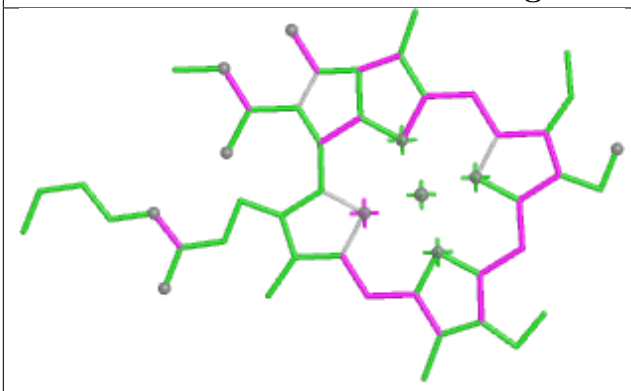
Bond angles



Torsions

Rings

Ligand CHL P 606



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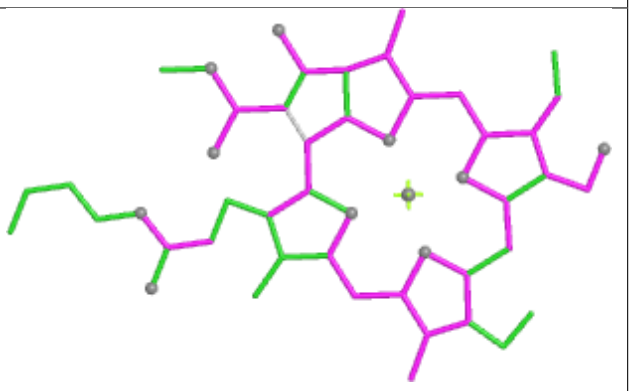
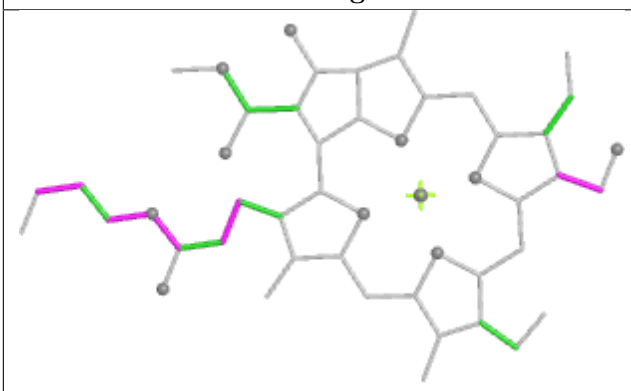
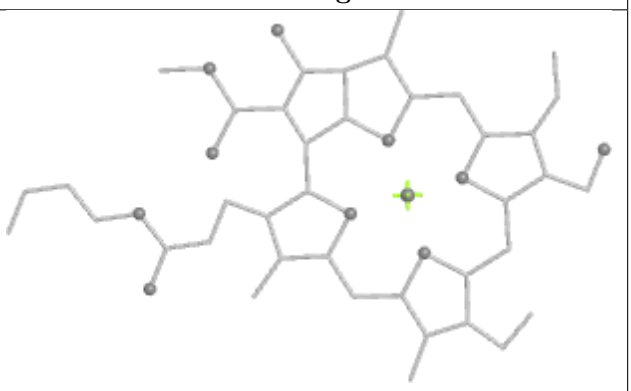


Bond angles

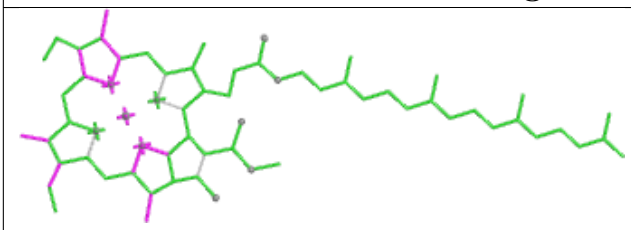


Torsions



Rings

Ligand CLA A 820



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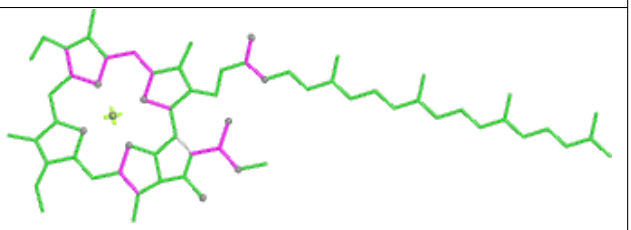
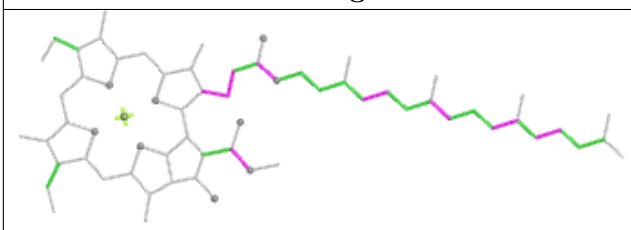


Bond angles



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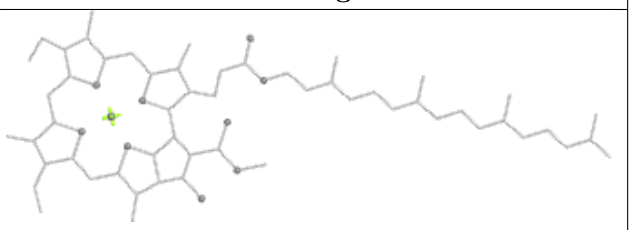
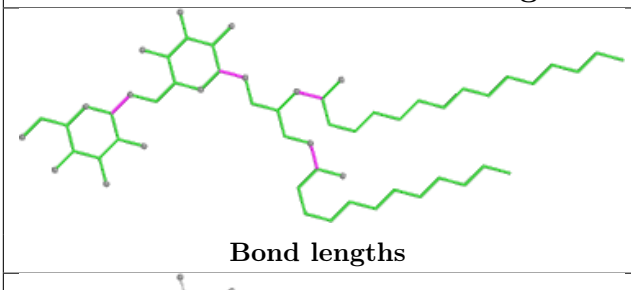
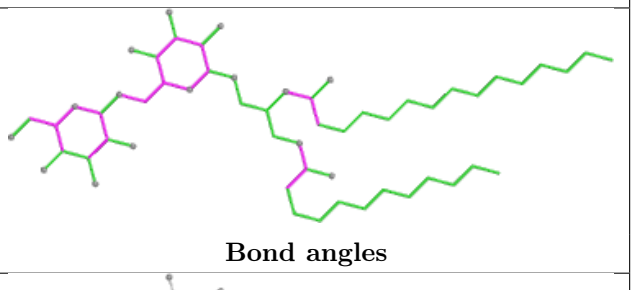


Rings

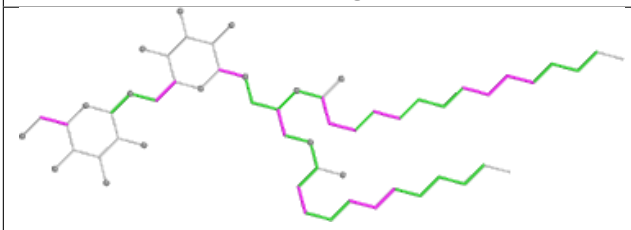
Ligand DGD B 848



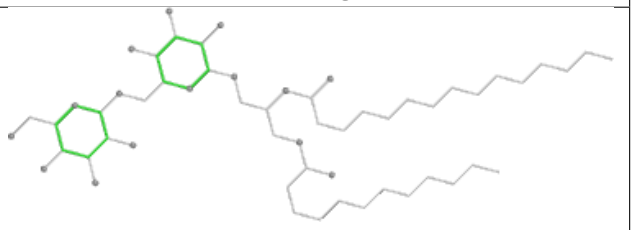
Bond lengths



Bond angles

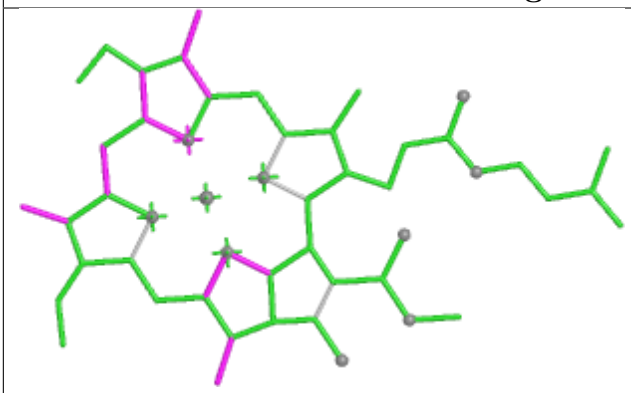


Torsions



Rings

Ligand CLA P 604



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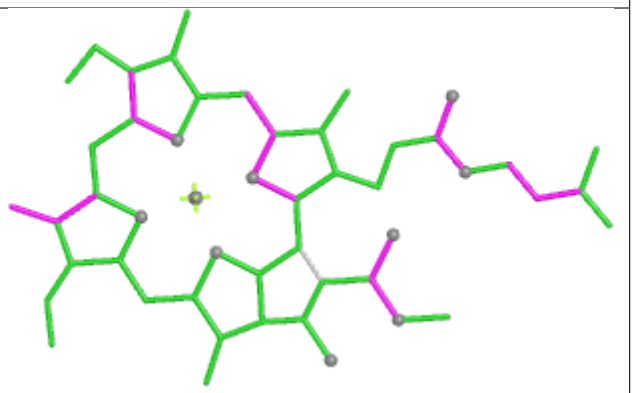
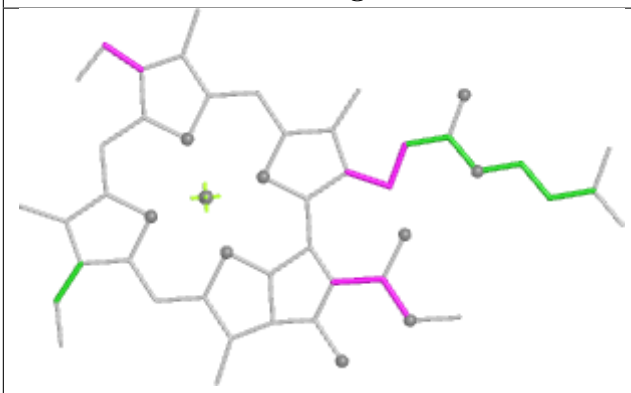


Bond angles



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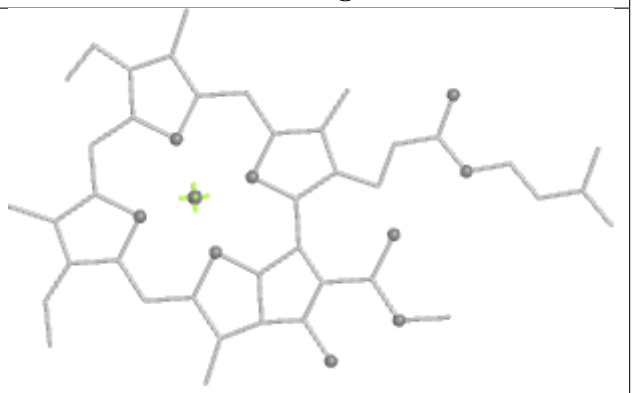
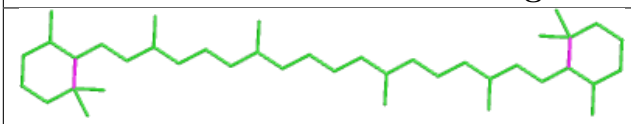


Rings

Ligand BCR L 204



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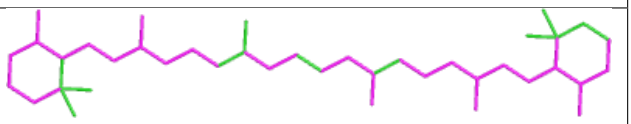

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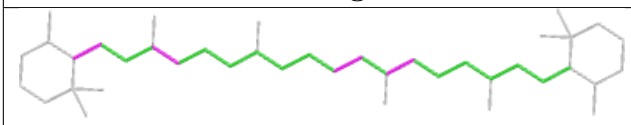

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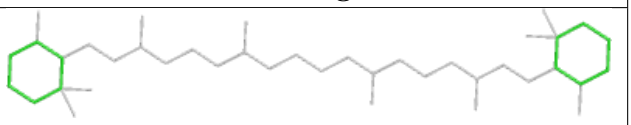

Rings

Ligand XAT T 615

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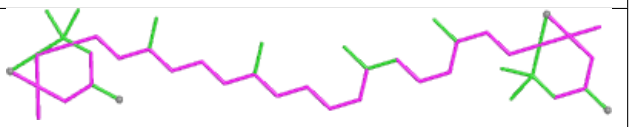
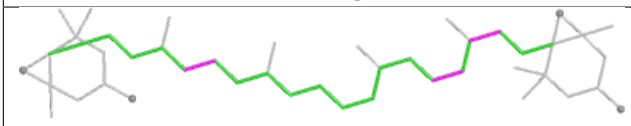
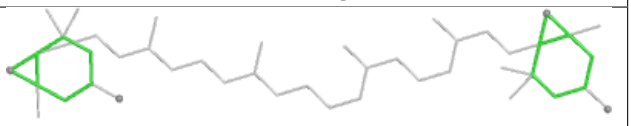


Bond angles

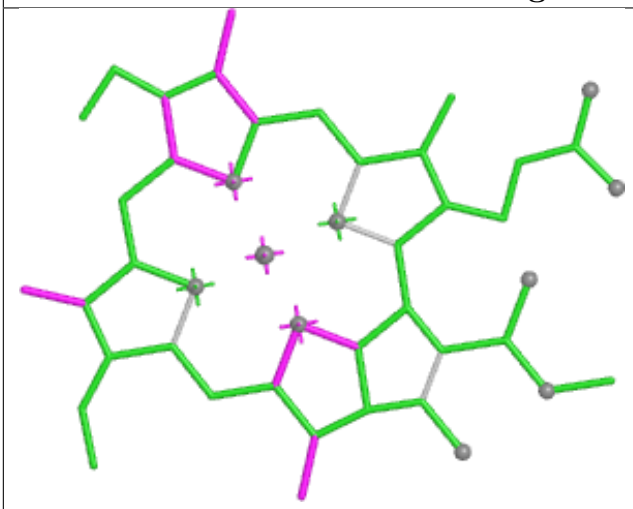


Torsions



Rings

Ligand CLA 8 304



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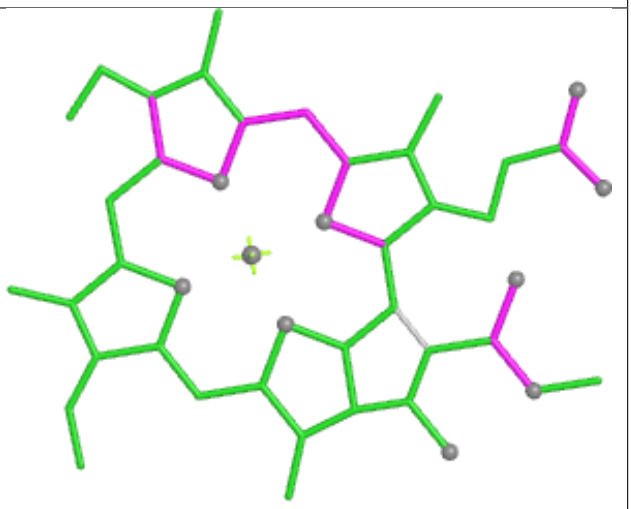
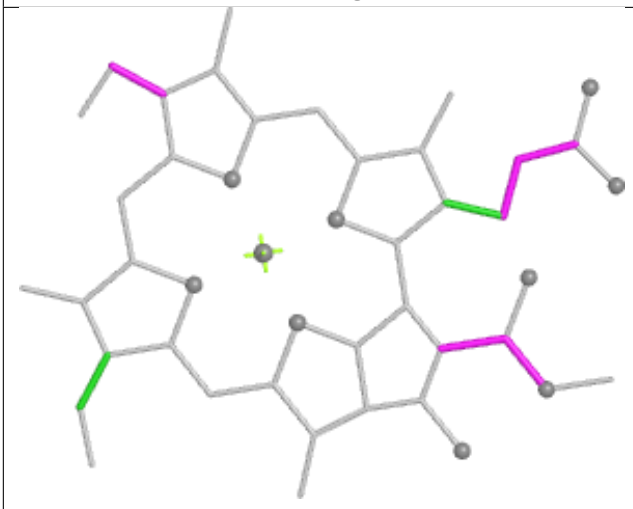


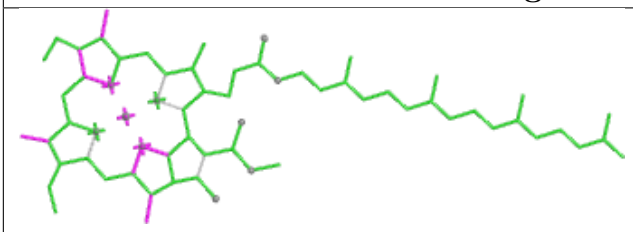
Bond angles



Torsions

Rings

Ligand CLA B 810



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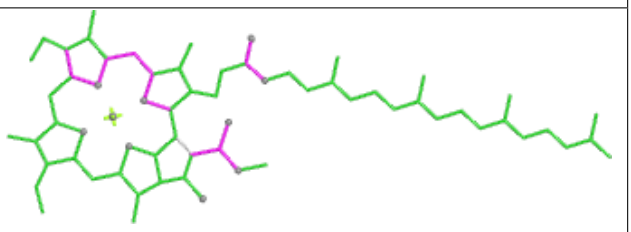

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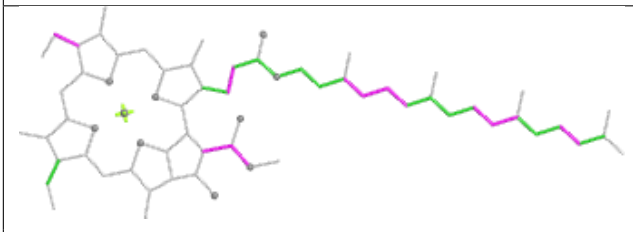

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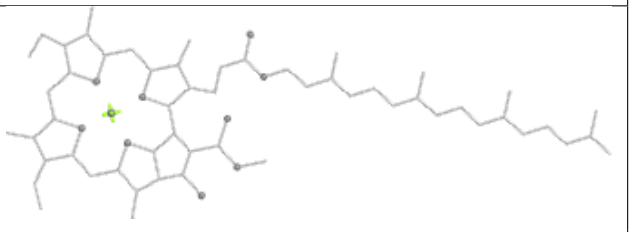
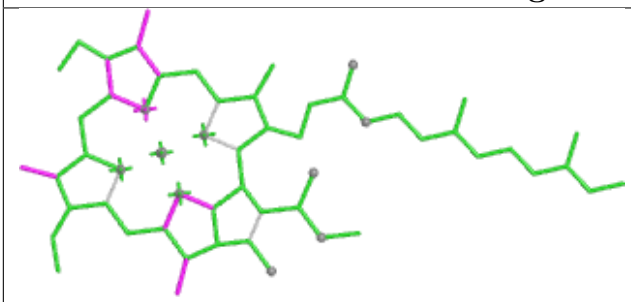


Rings

Ligand CLA 4 311



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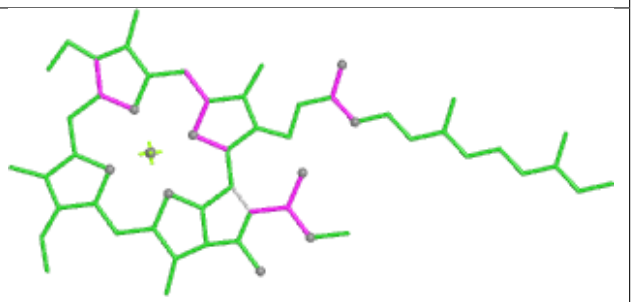
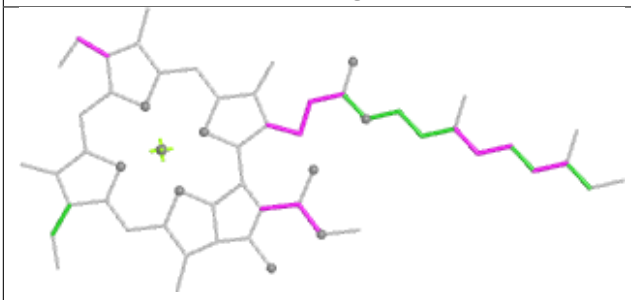


Bond angles



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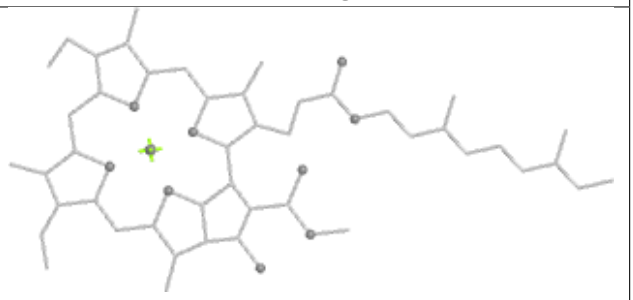
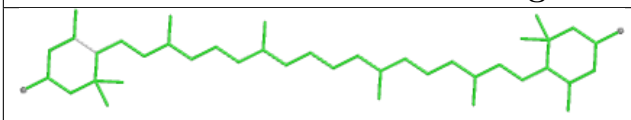


Rings

Ligand LUT 1 617



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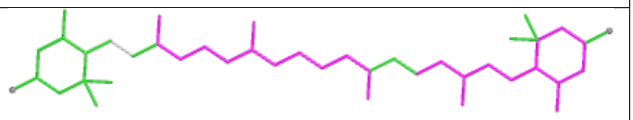

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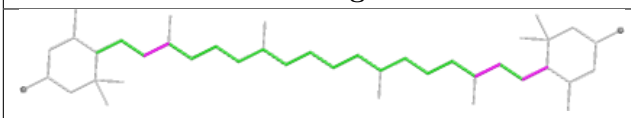

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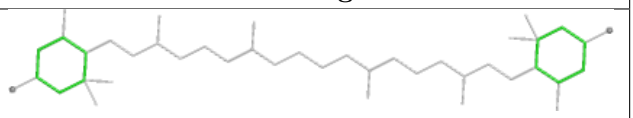
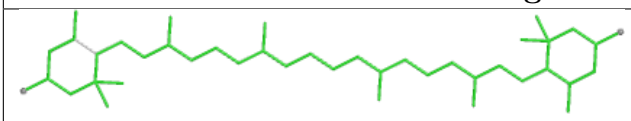


Rings

Ligand LUT R 616



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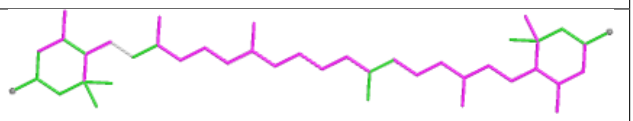
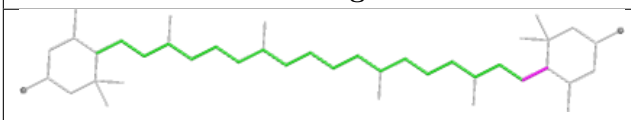


Bond angles



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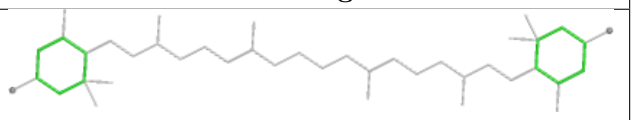
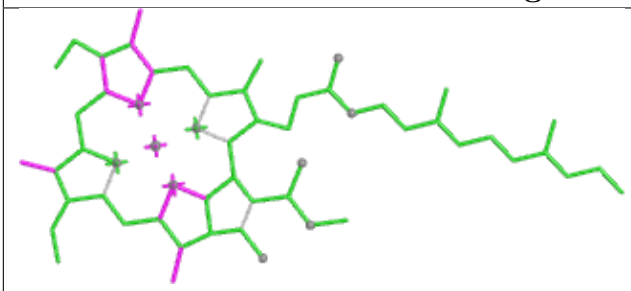


Rings

Ligand CLA B 813



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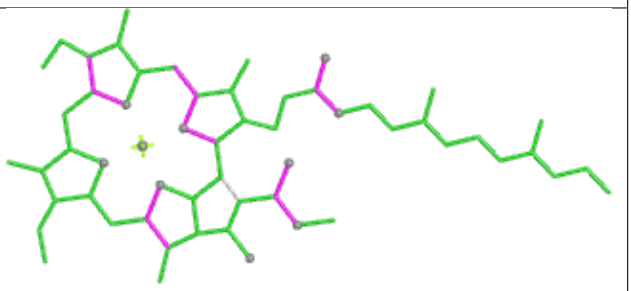
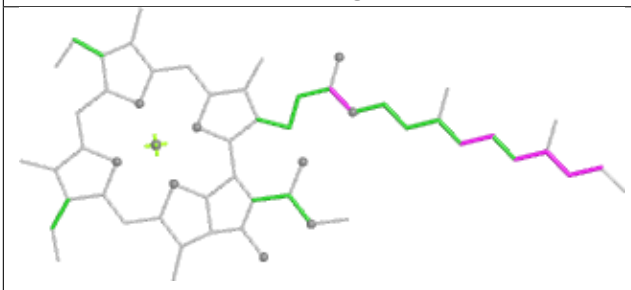


Bond angles



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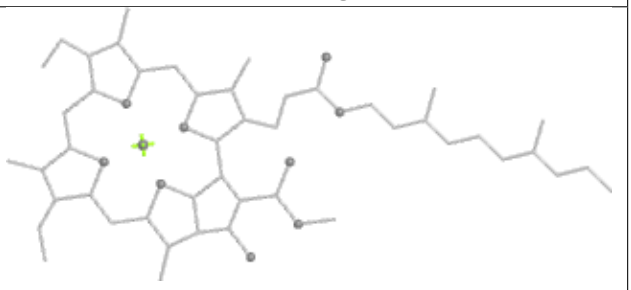
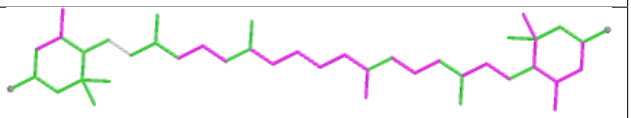


Rings

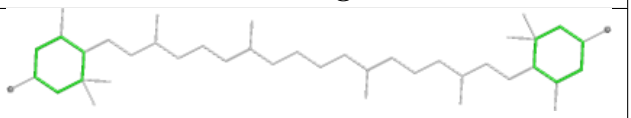
Ligand LUT 8 317

Bond lengths



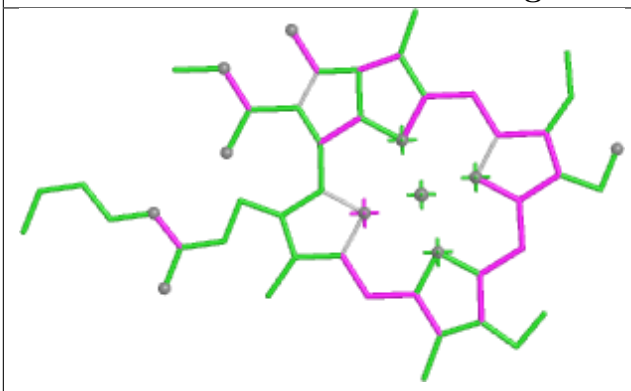
Bond angles

Torsions



Rings

Ligand CHL T 605



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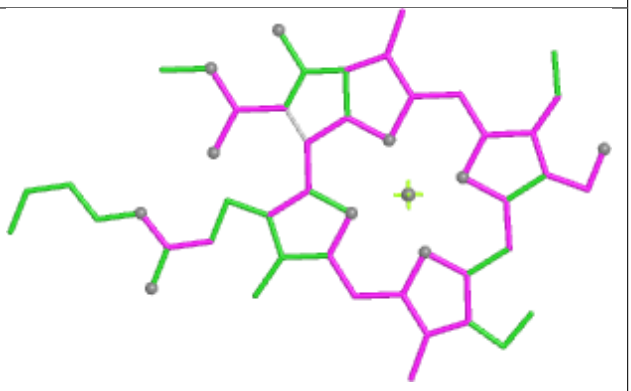
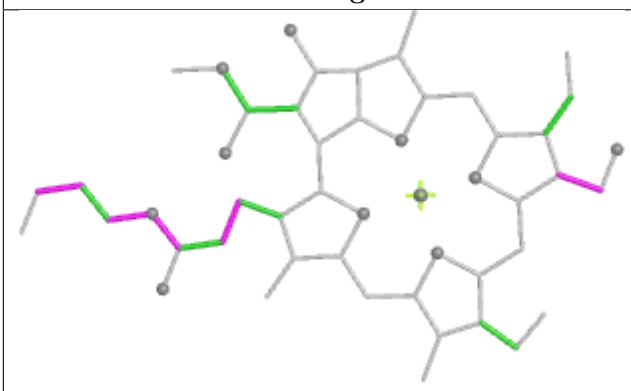


Bond angles



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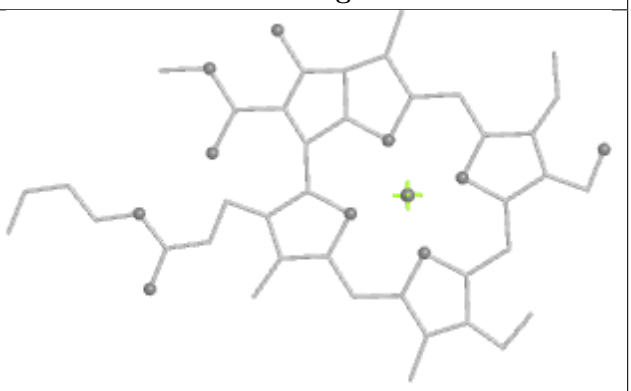
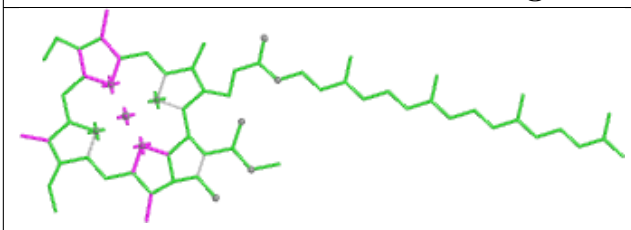
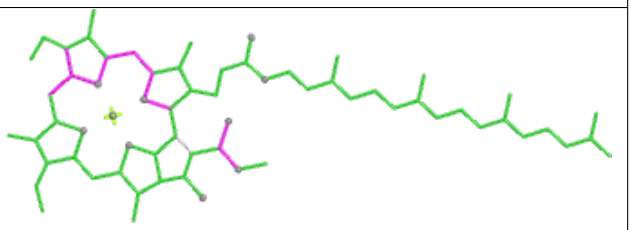


Rings

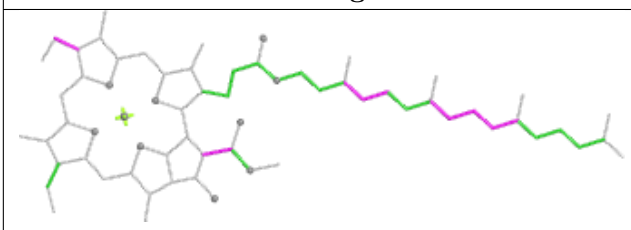
Ligand CLA L 201



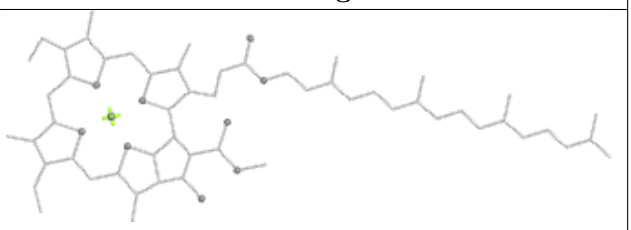
Bond lengths



Bond angles

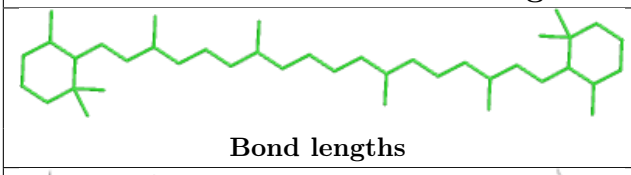


Torsions



Rings

Ligand BCR 8 301



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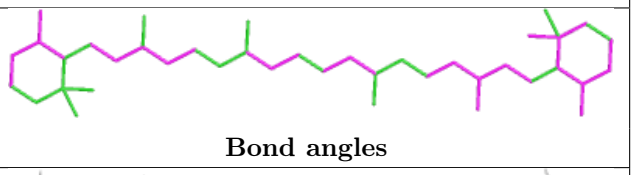
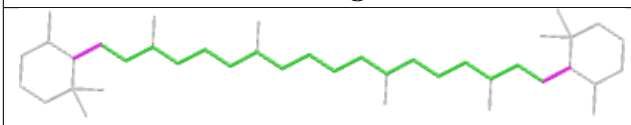


Bond angles



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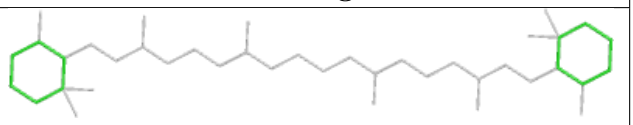
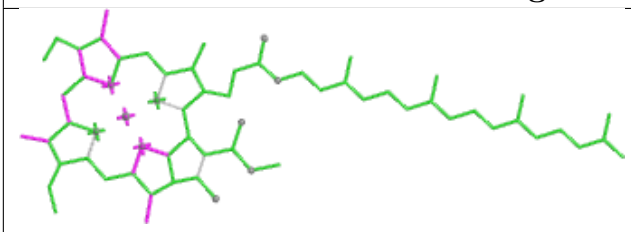


Rings

Ligand CLA 1 608



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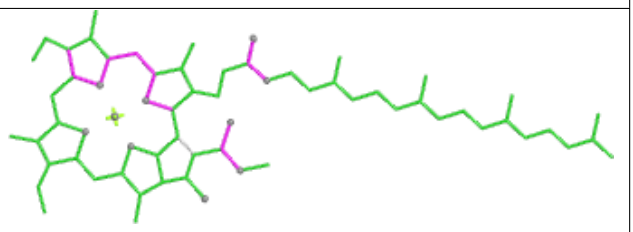
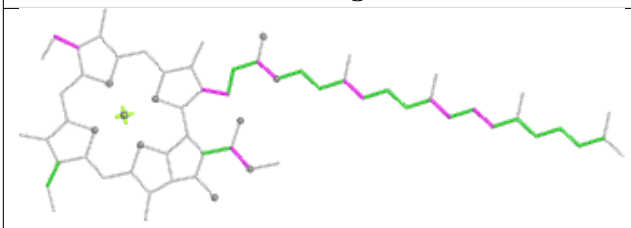
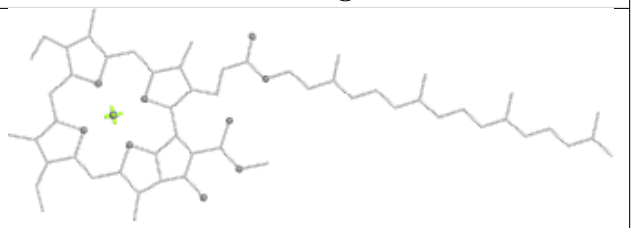


Bond angles

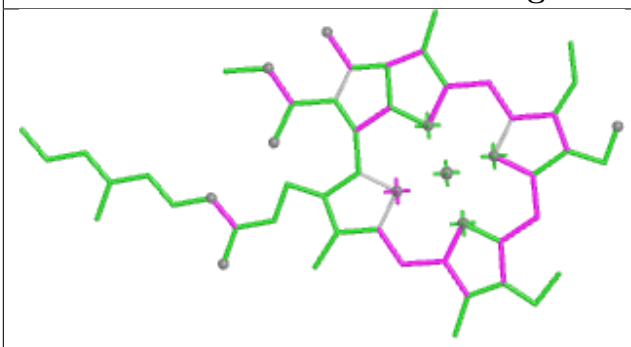


Torsions

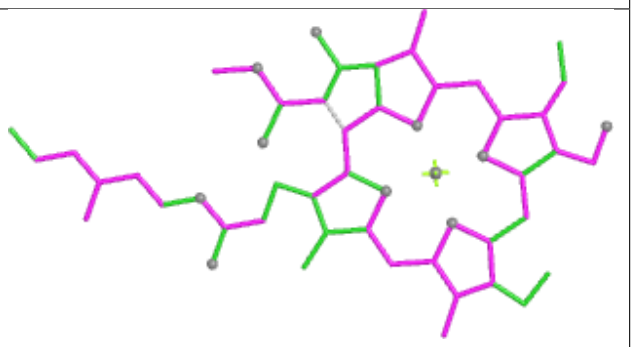


Rings

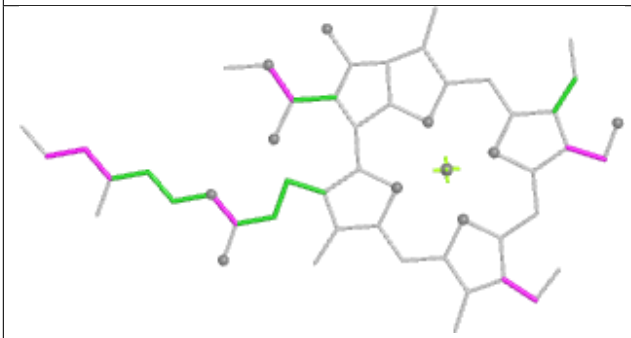
Ligand CHL 6 607



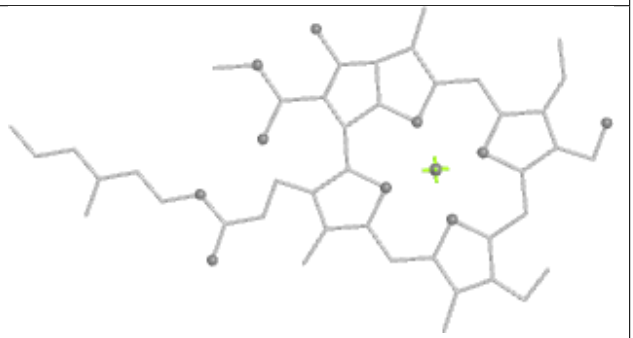
Bond lengths



Bond angles

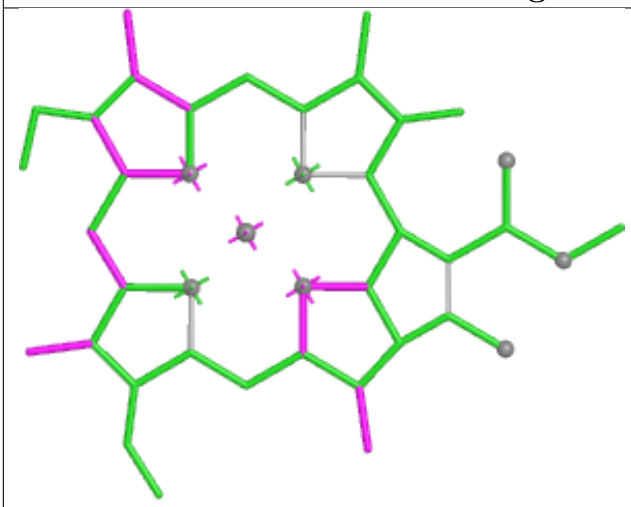


Torsions

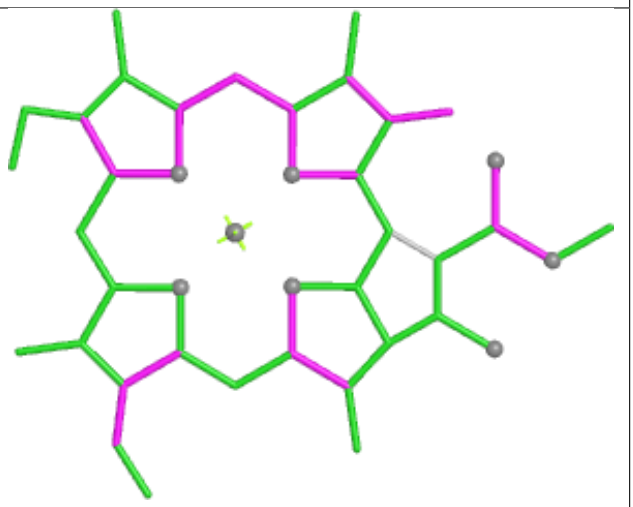


Rings

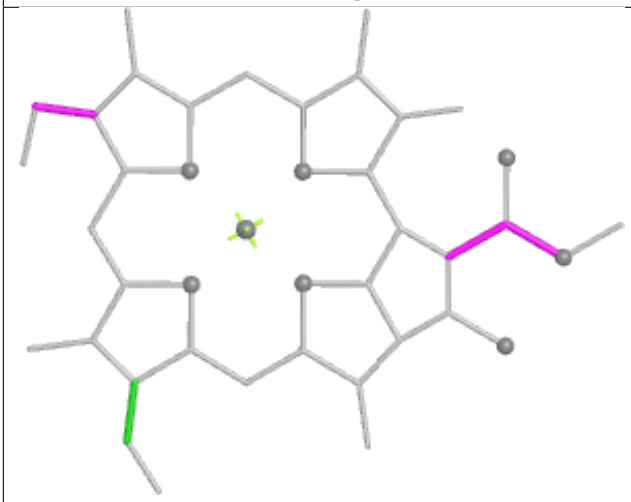
Ligand CLA 3 309



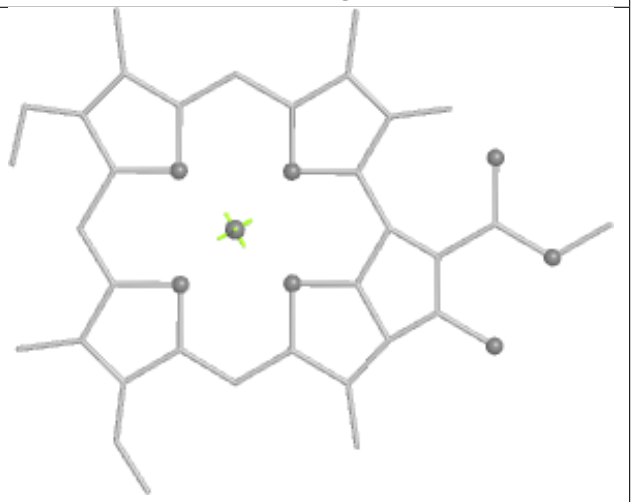
Bond lengths



Bond angles

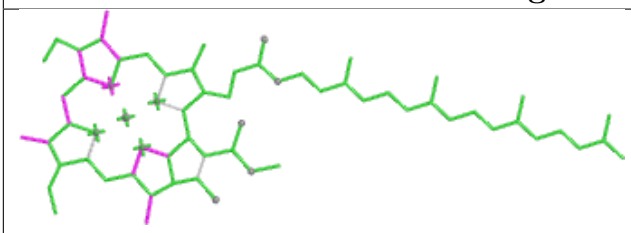


Torsions



Rings

Ligand CLA a 307



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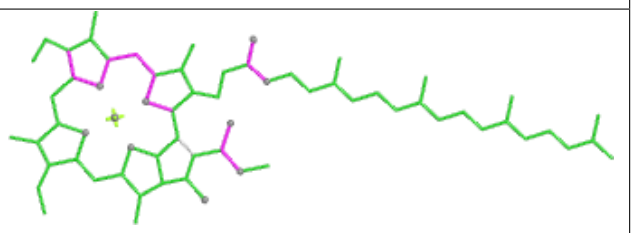
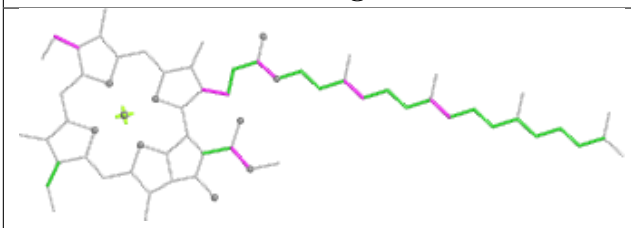
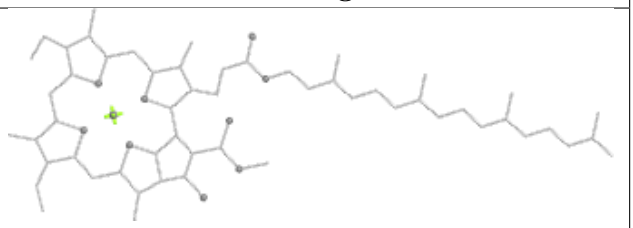


Bond angles

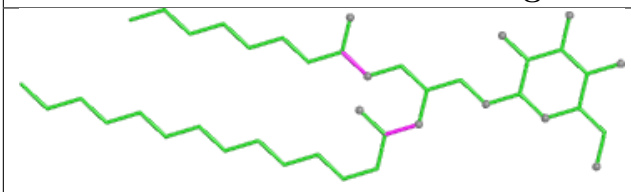


Torsions

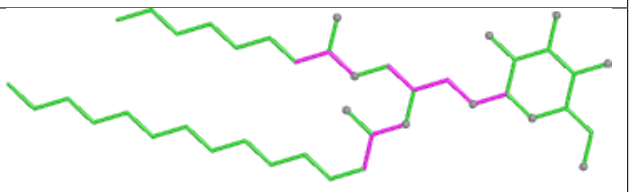


Rings

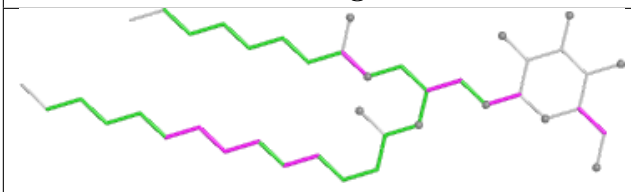
Ligand LMG 2 301



Bond lengths



Bond angles



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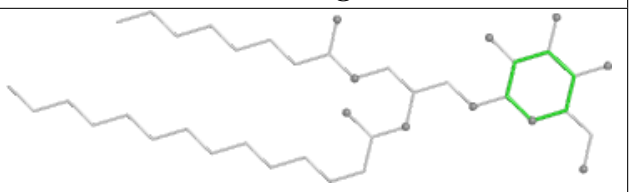
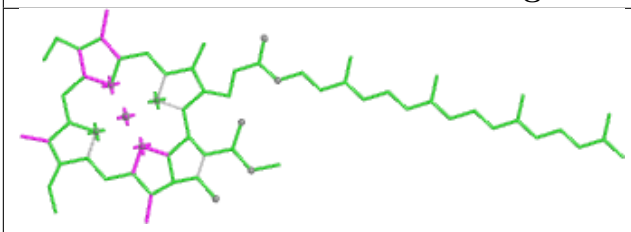
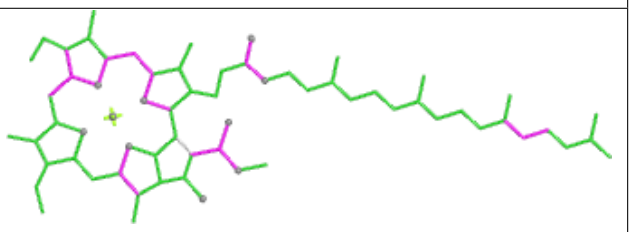


Rings

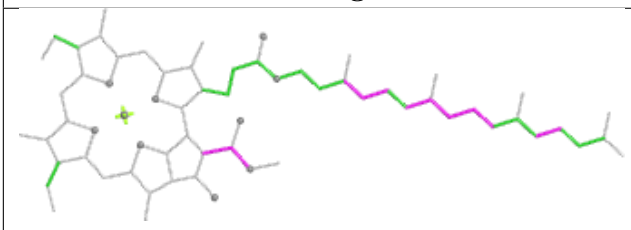
Ligand CLA A 830



Bond lengths



Bond angles



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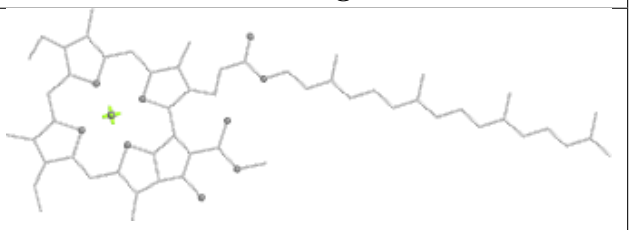
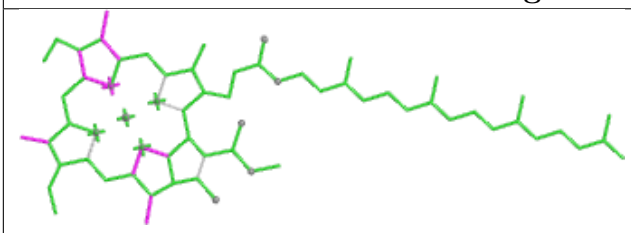


Rings

Ligand CLA A 818



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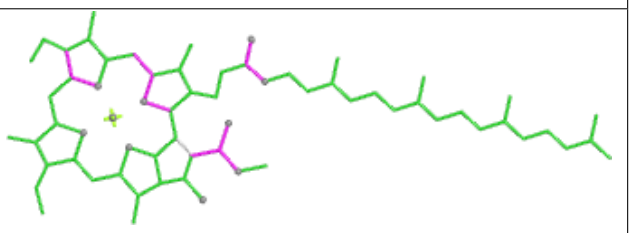
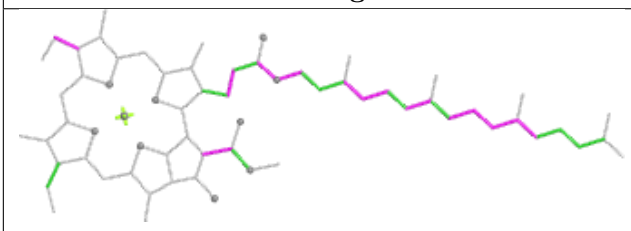
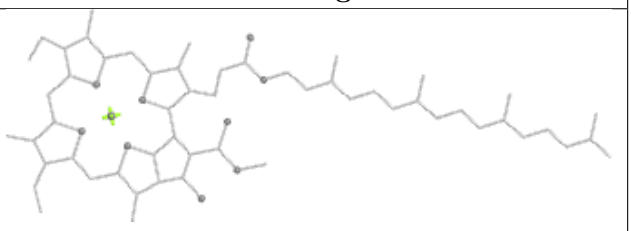


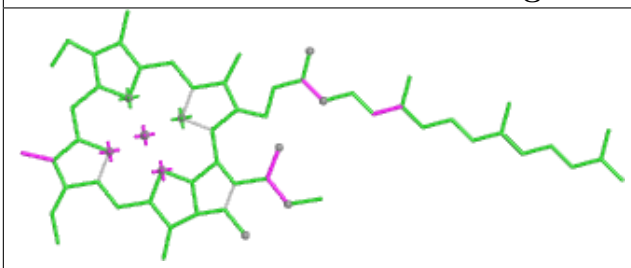
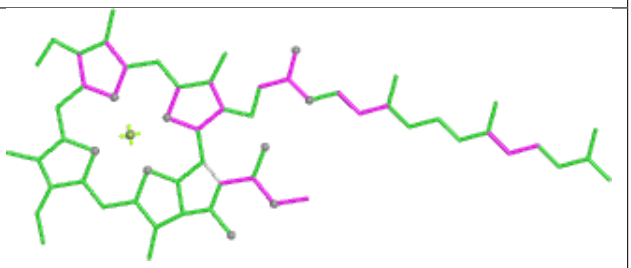
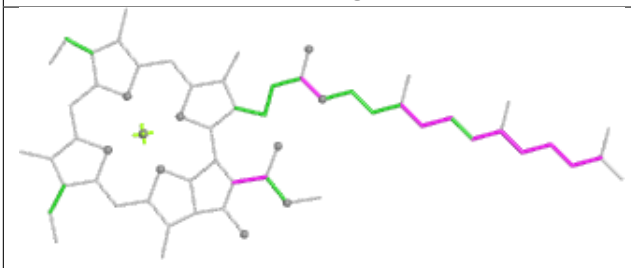
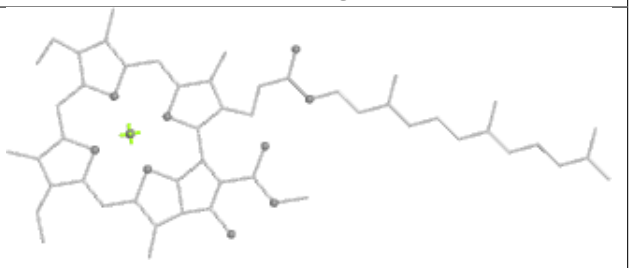
Bond angles

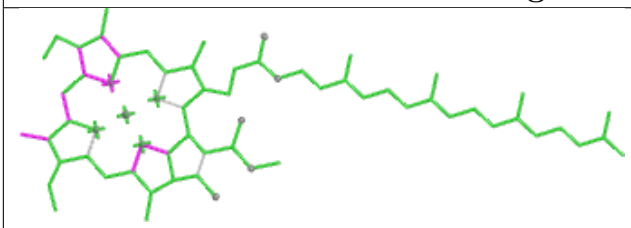
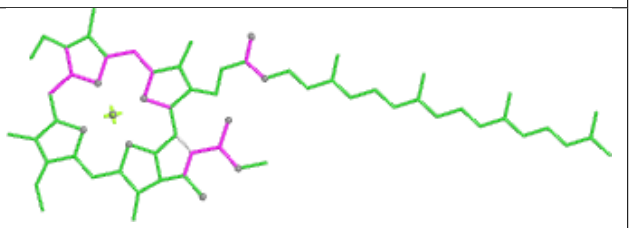
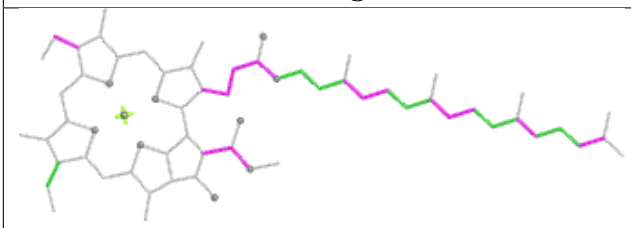
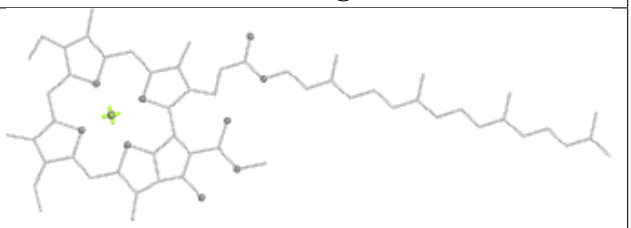


Torsions

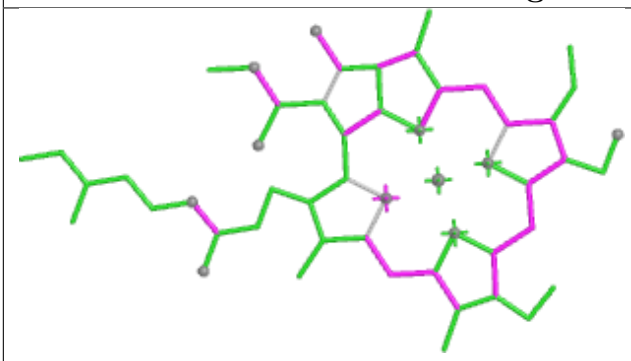


Rings

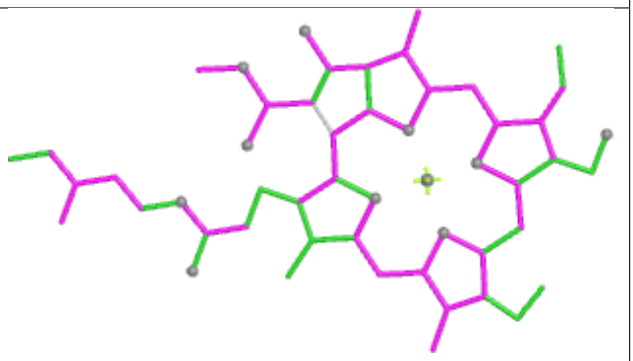
Ligand CLA R 612	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA S 314	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

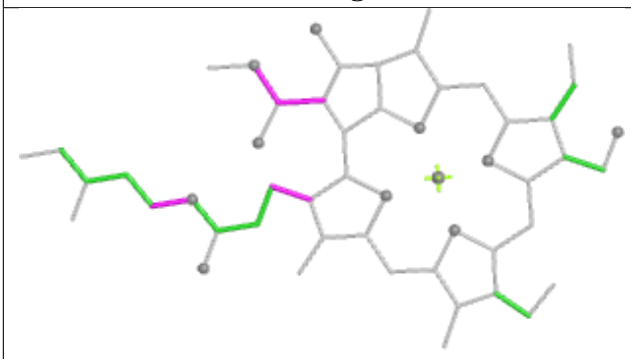
Ligand CHL S 309



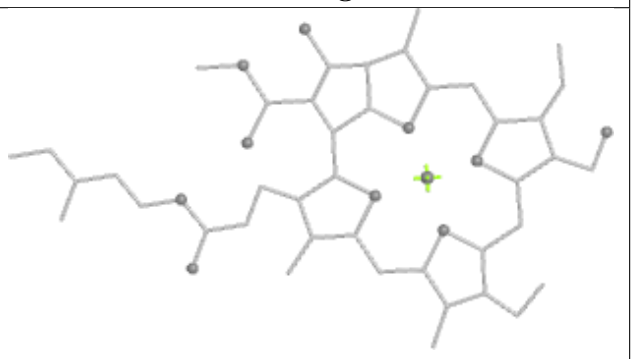
Bond lengths



Bond angles

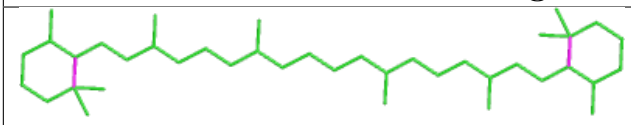


Torsions

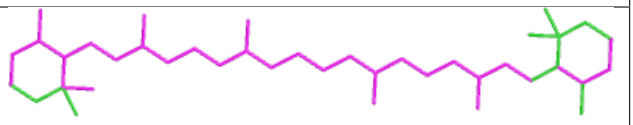


Rings

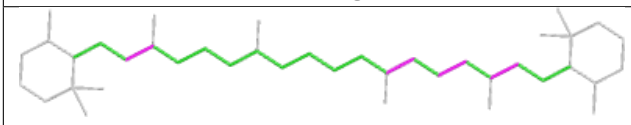
Ligand BCR I 201



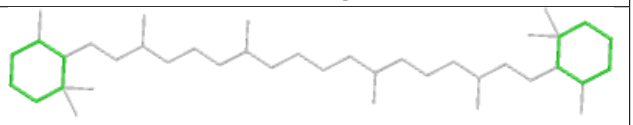
Bond lengths



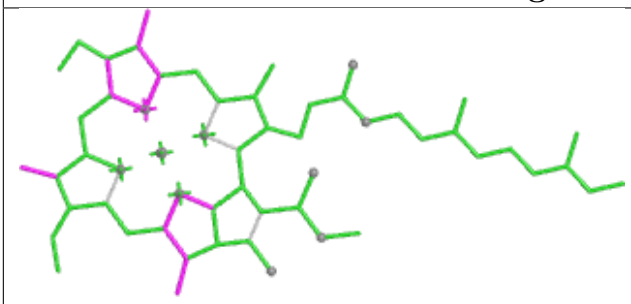
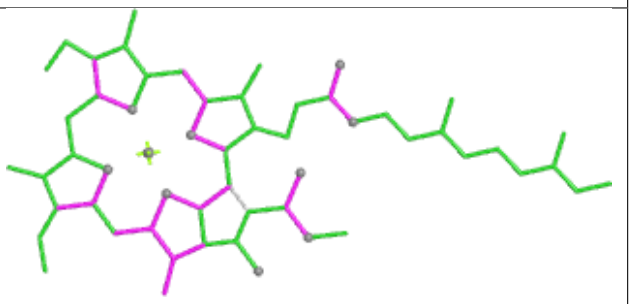
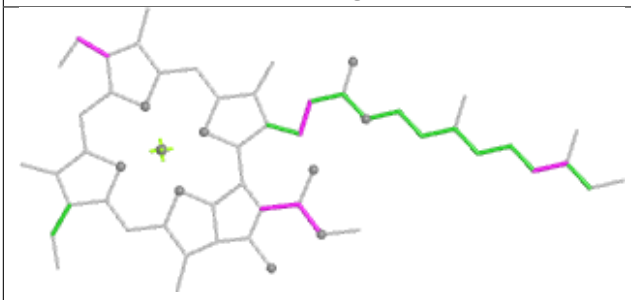
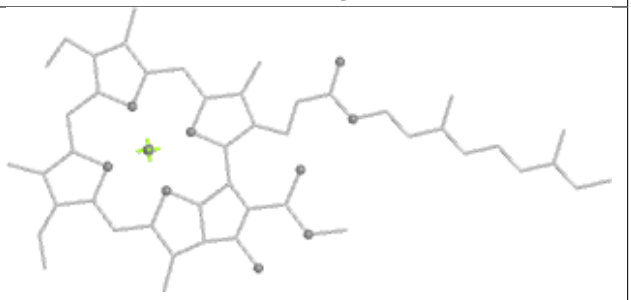
Bond angles

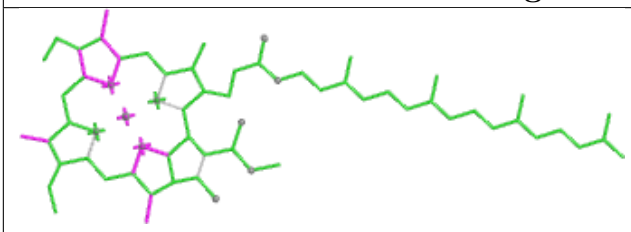
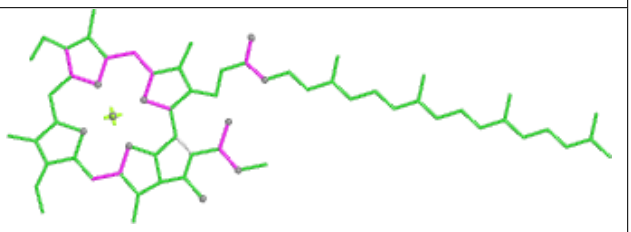
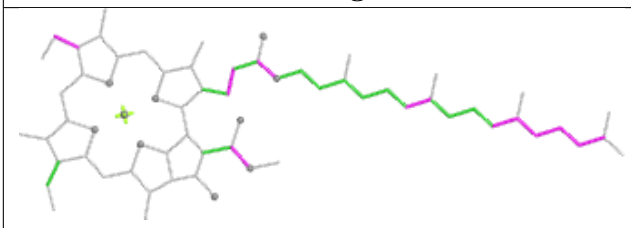
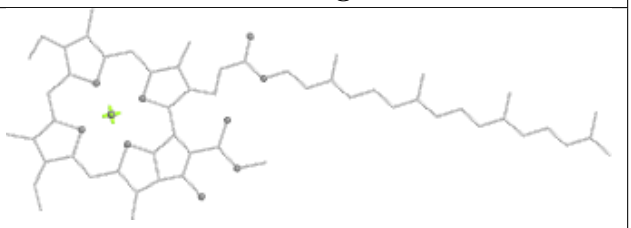


Torsions

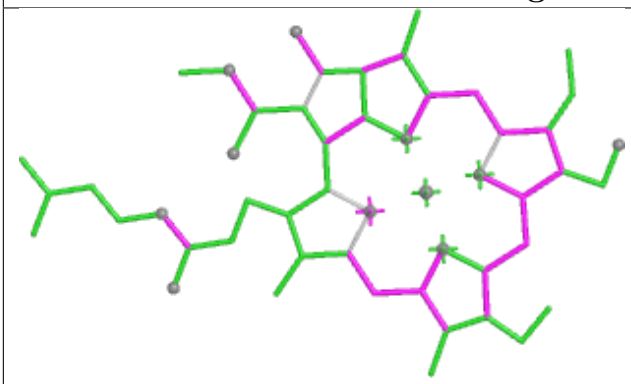


Rings

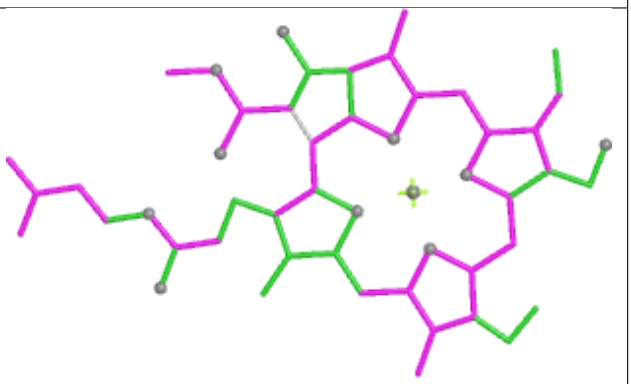
Ligand CLA 5 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

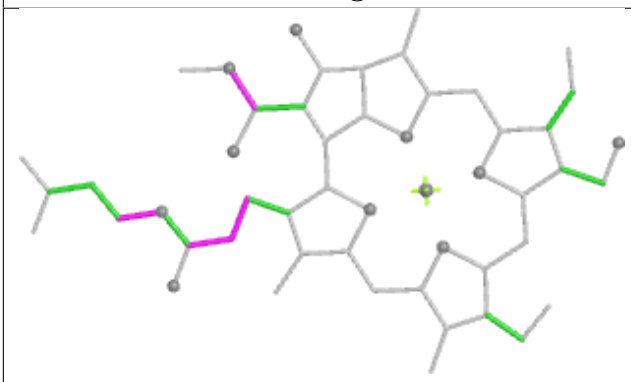
Ligand CHL 4 305



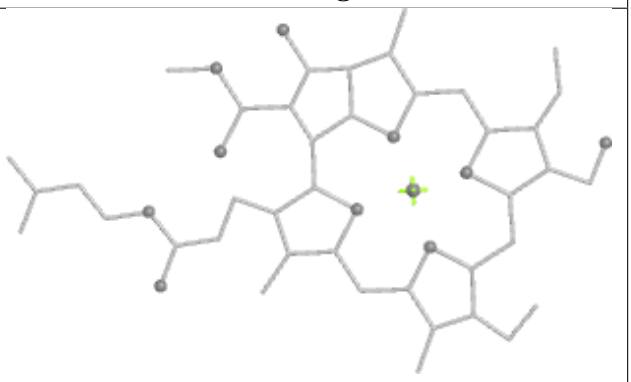
Bond lengths



Bond angles

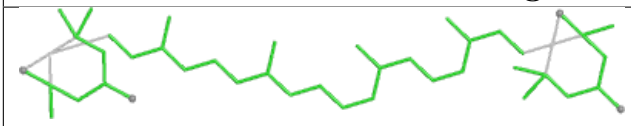


Torsions

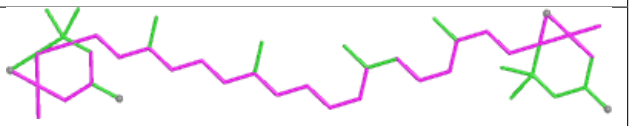


Rings

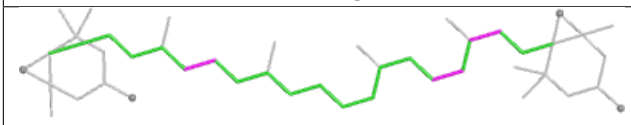
Ligand XAT P 616



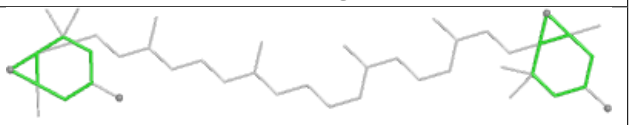
Bond lengths



Bond angles

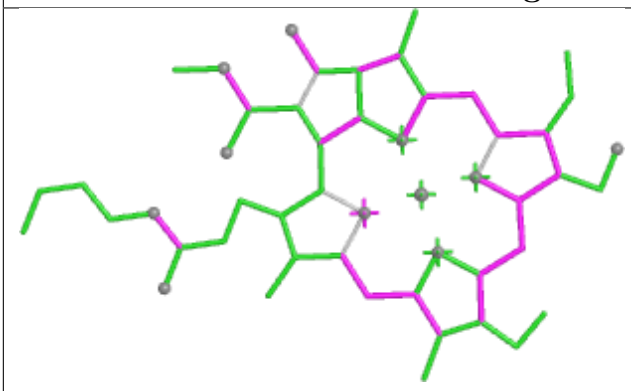


Torsions



Rings

Ligand CHL R 606



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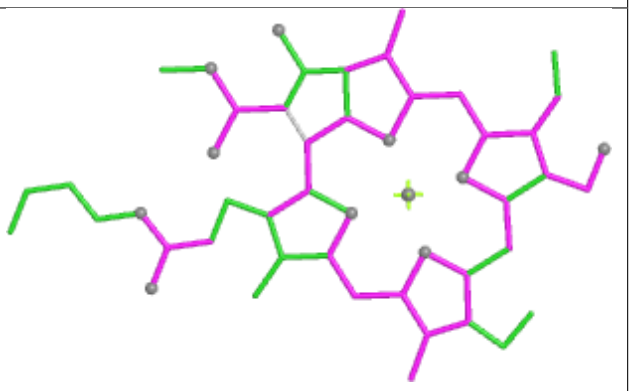

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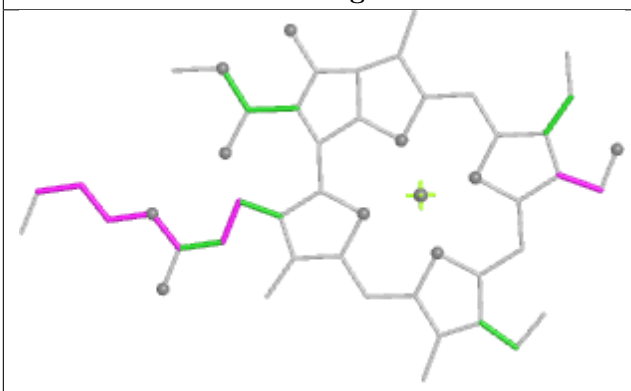

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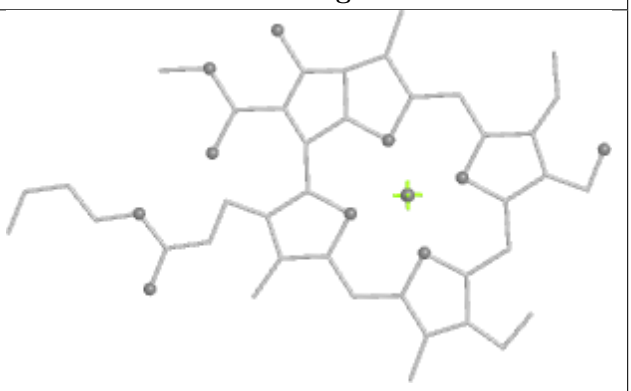
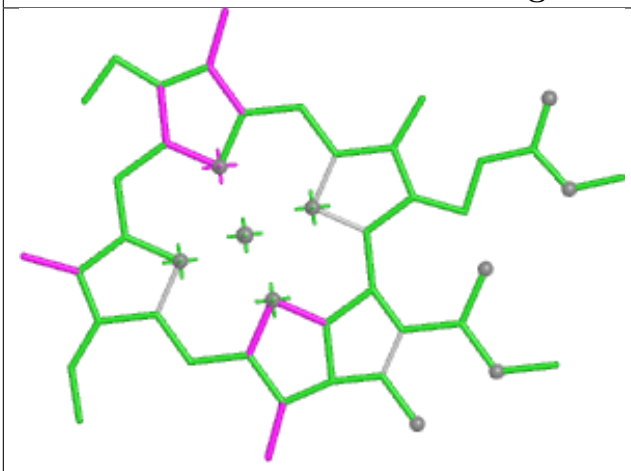


Rings

Ligand CLA a 313



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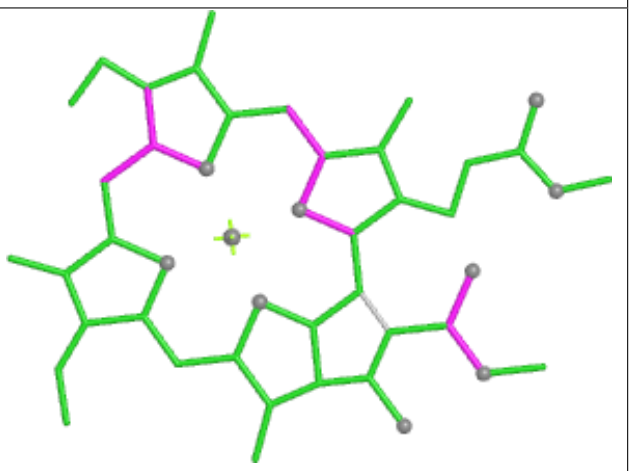
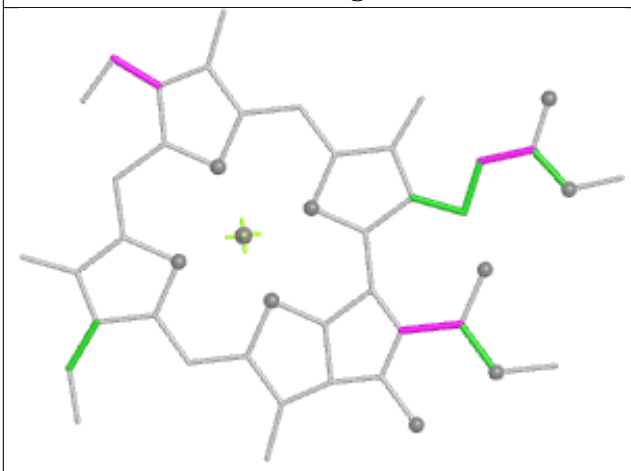


Bond angles



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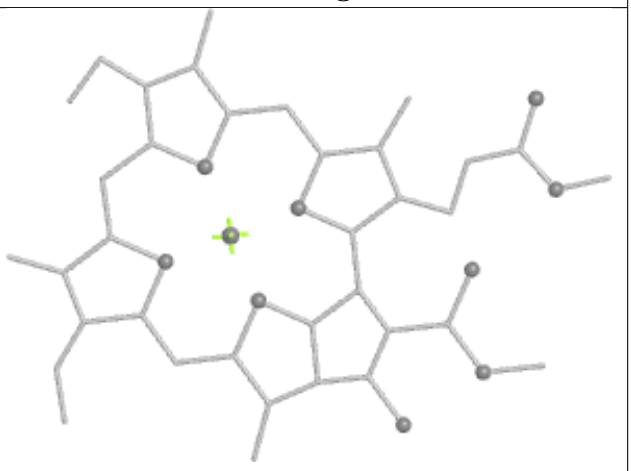
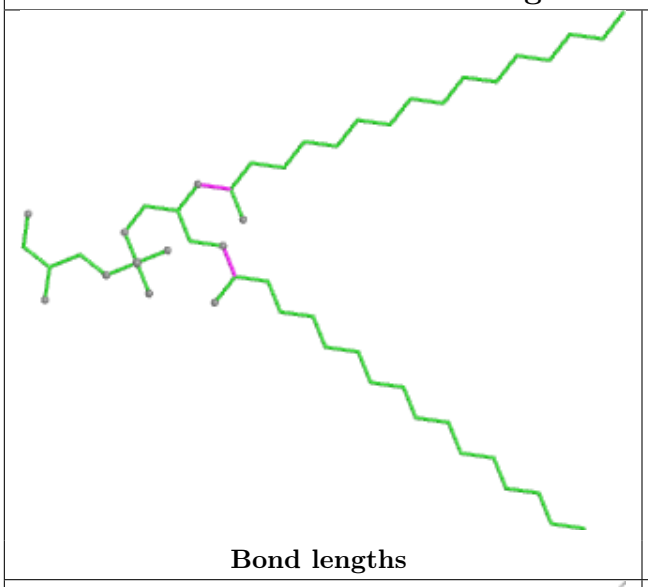


Rings

Ligand LHG P 618



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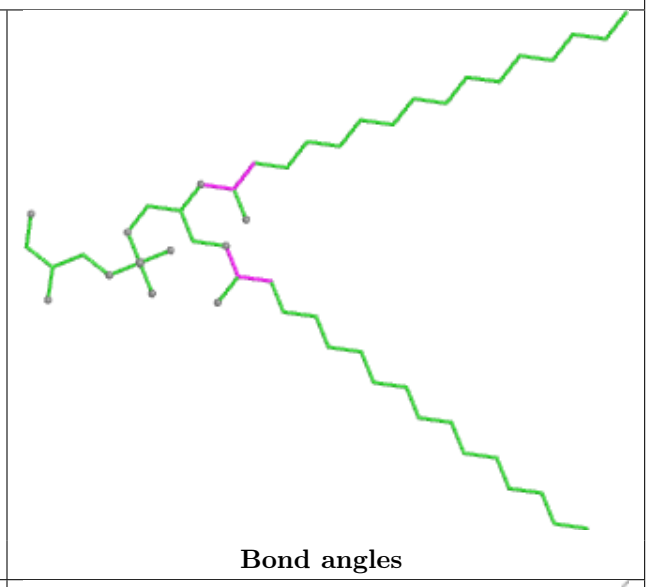
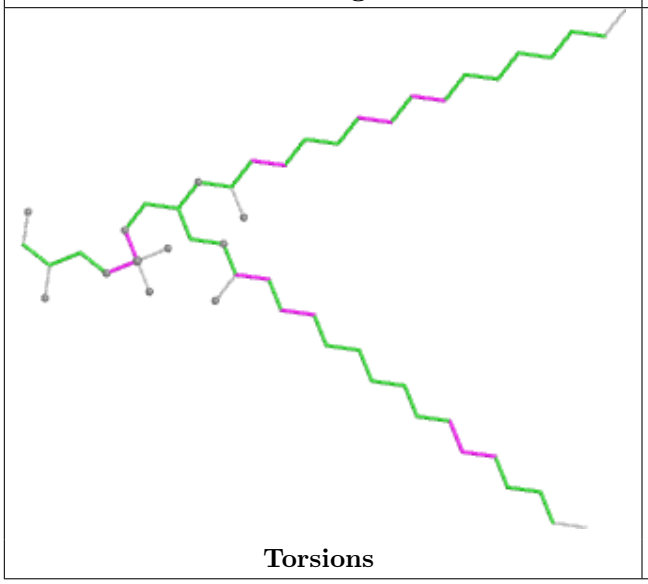


Bond angles



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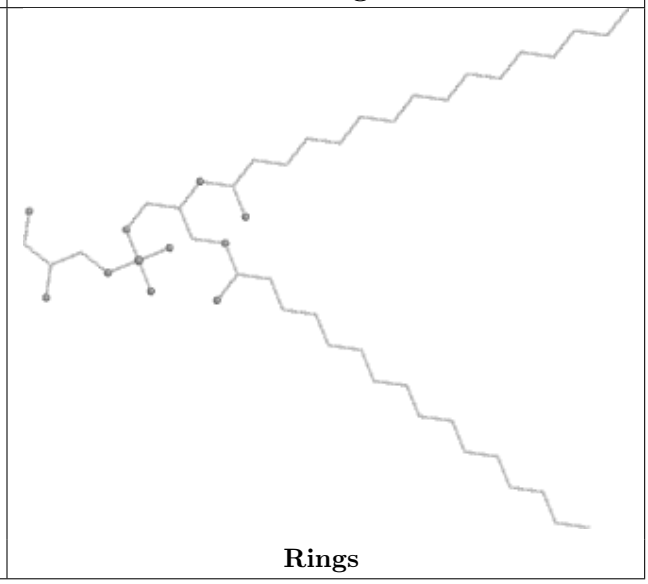
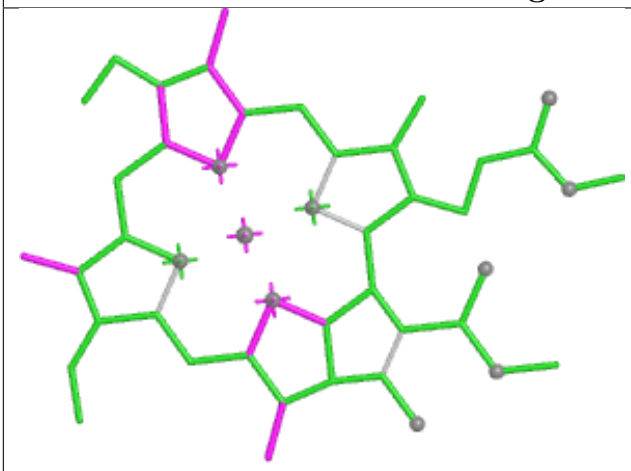
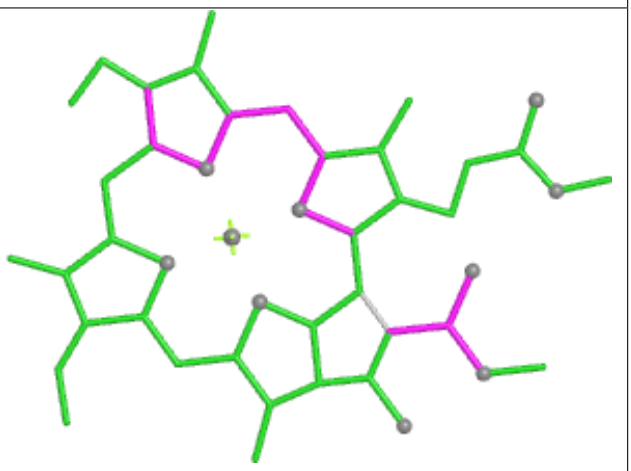


Rings

Ligand CLA 8 311	
	
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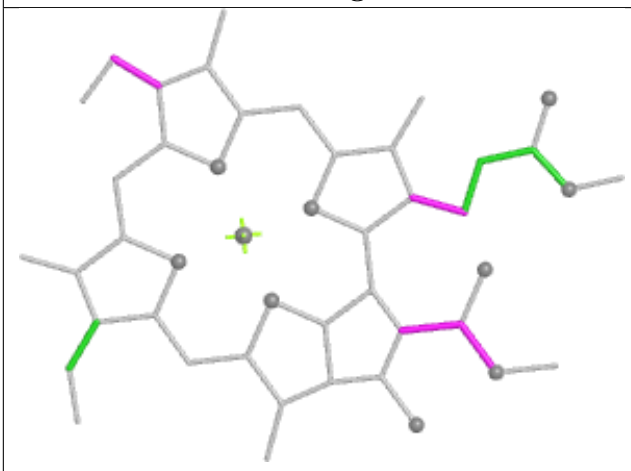
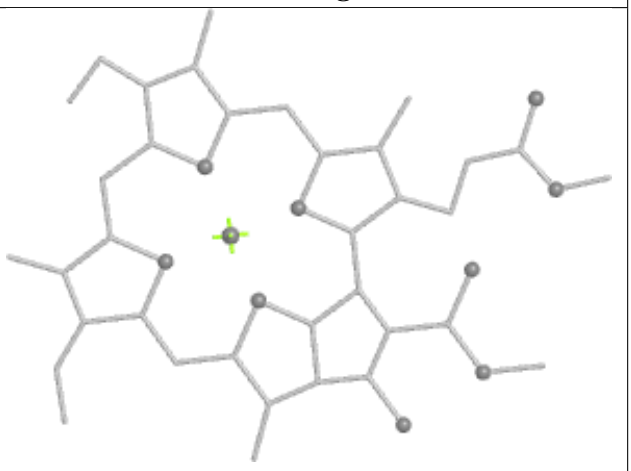
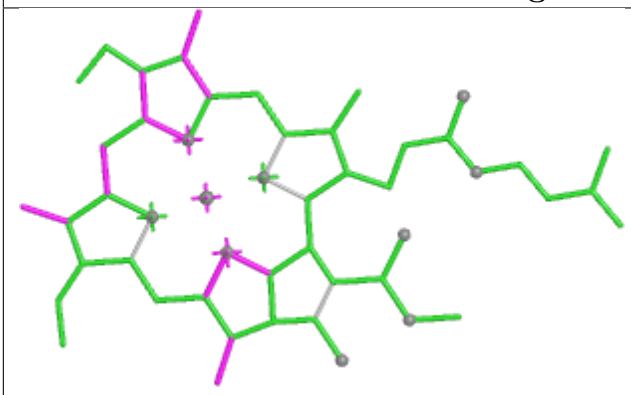
	
Torsions	**Rings**

Ligand CLA 4 303



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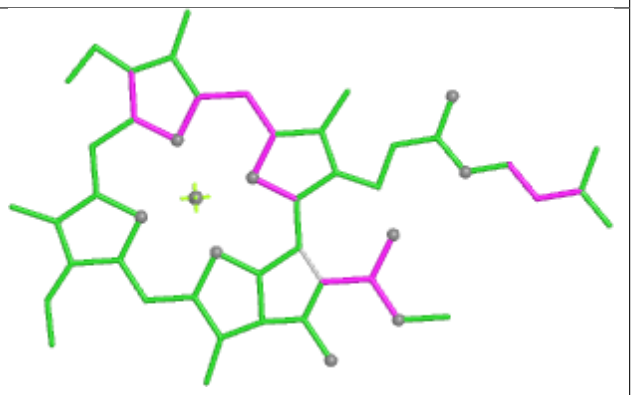
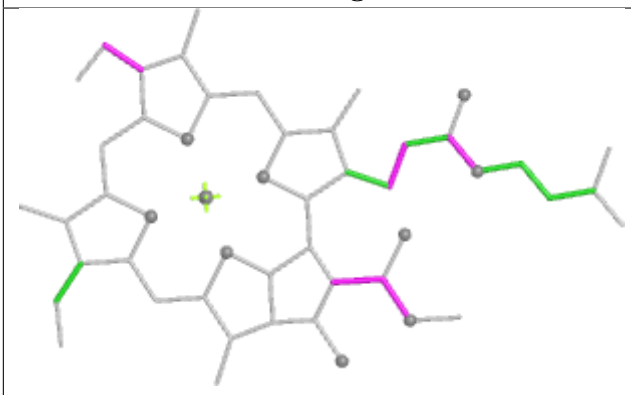


Bond angles



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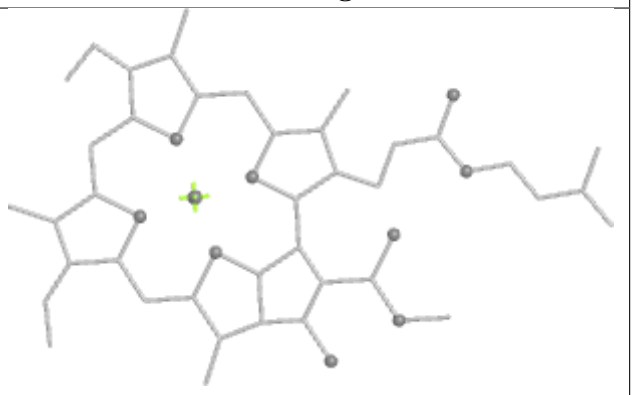
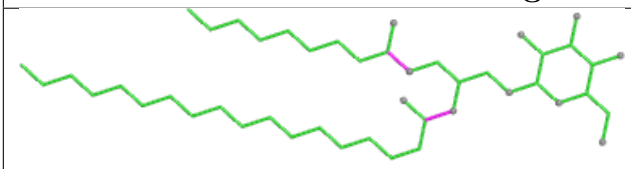


Rings

Ligand LMG 1 619



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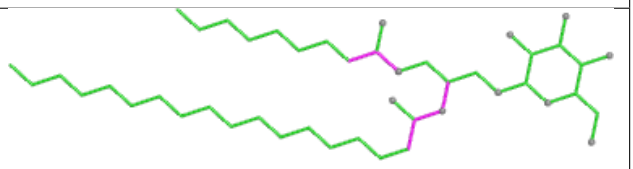
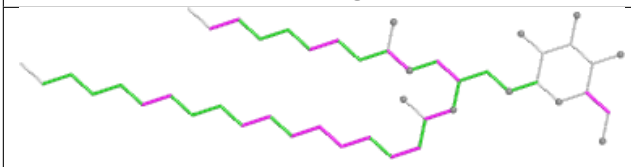


Bond angles



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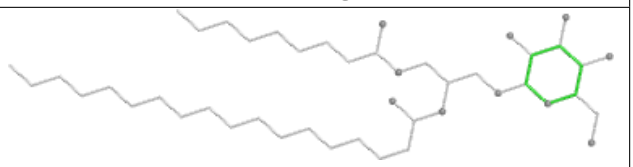
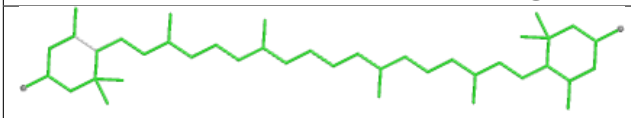


Rings

Ligand LUT S 316



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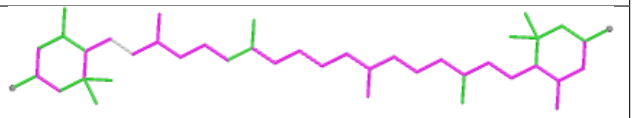

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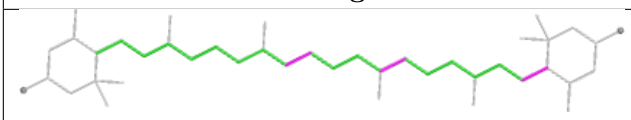

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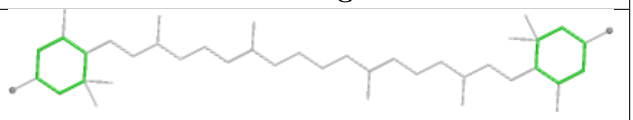
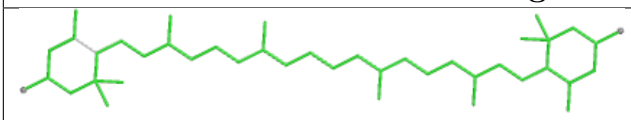
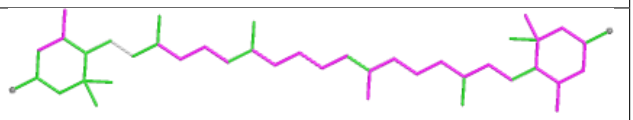


Rings

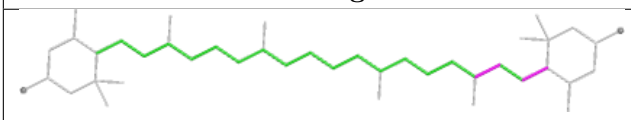
Ligand LUT a 315



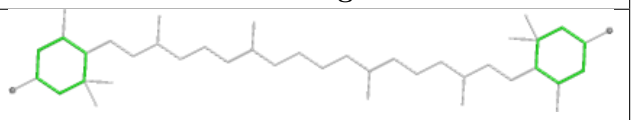
Bond lengths



Bond angles

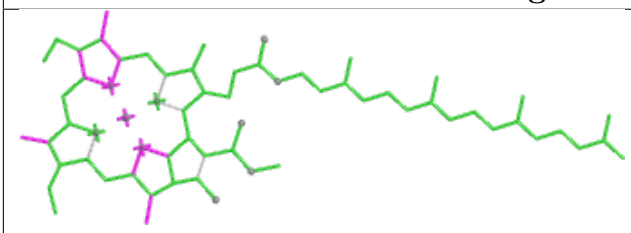


Torsions



Rings

Ligand CLA 3 308



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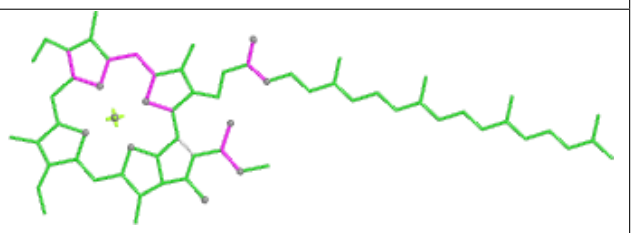
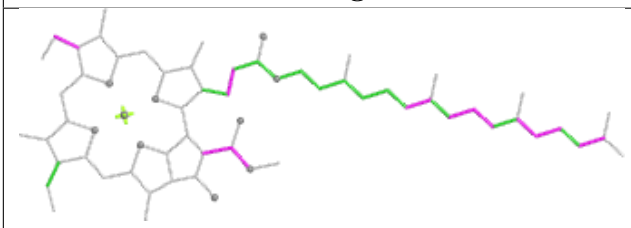


Bond angles



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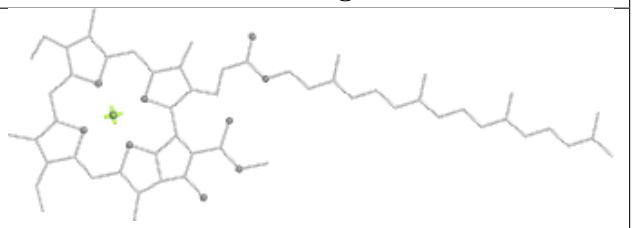
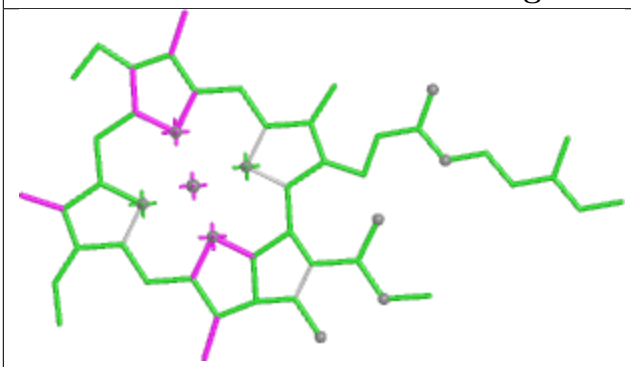


Rings

Ligand CLA A 835



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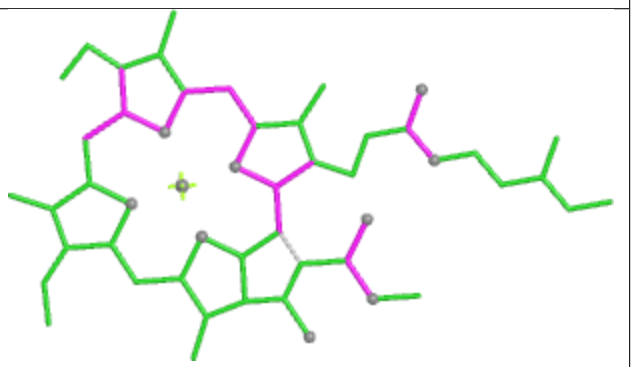
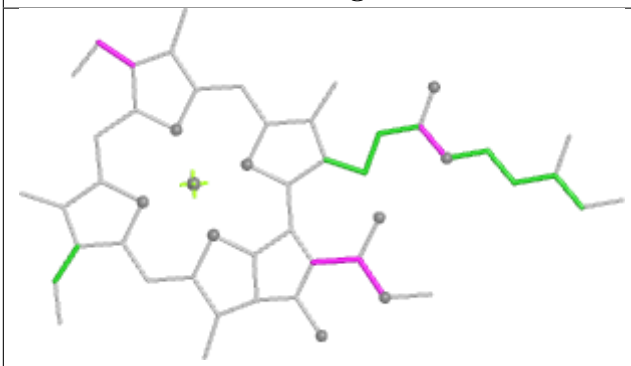


Bond angles



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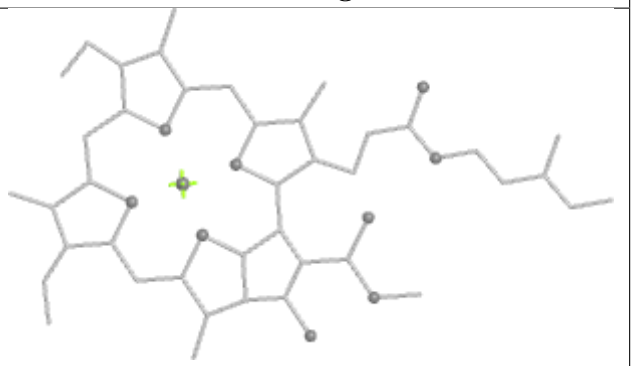
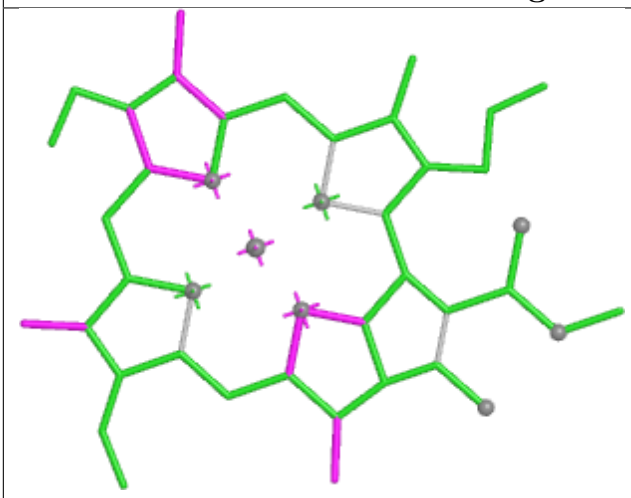


Rings

Ligand CLA 2 308



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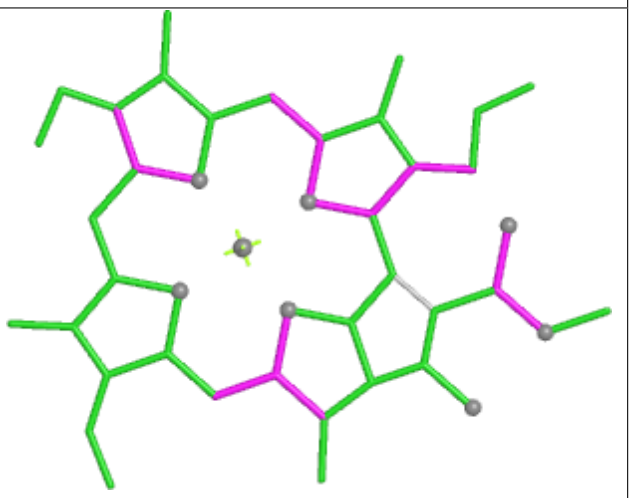
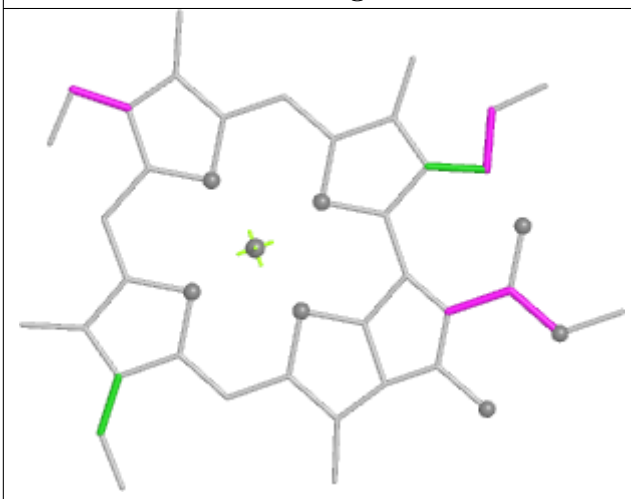


Bond angles



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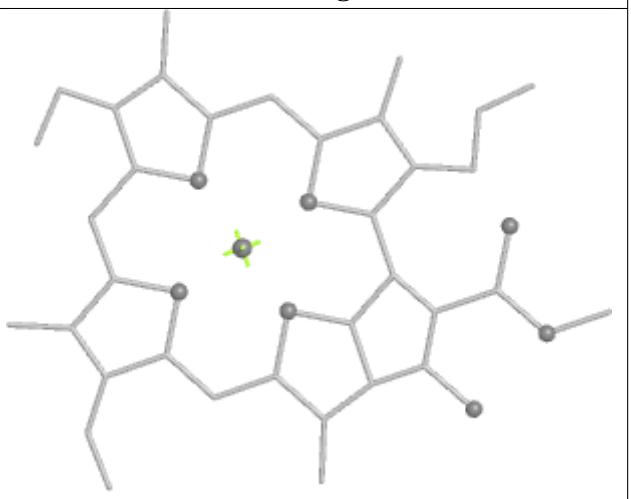
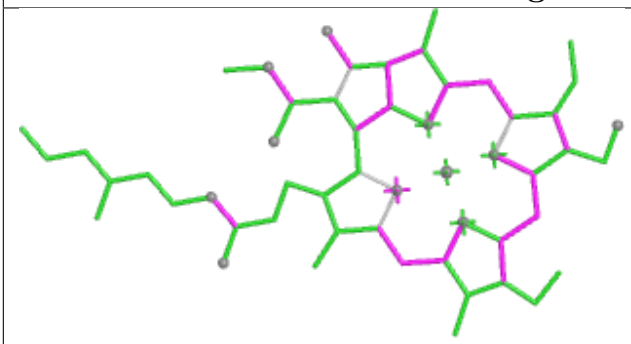


Rings

Ligand CHL 3 306



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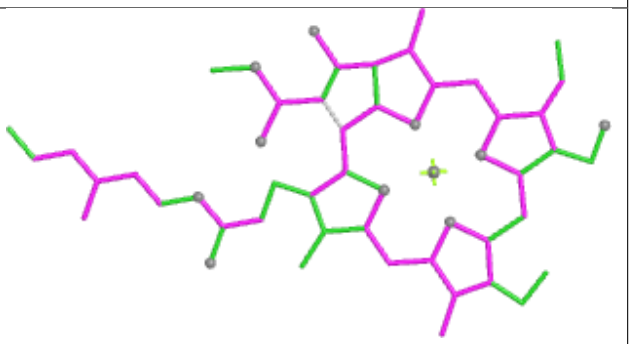
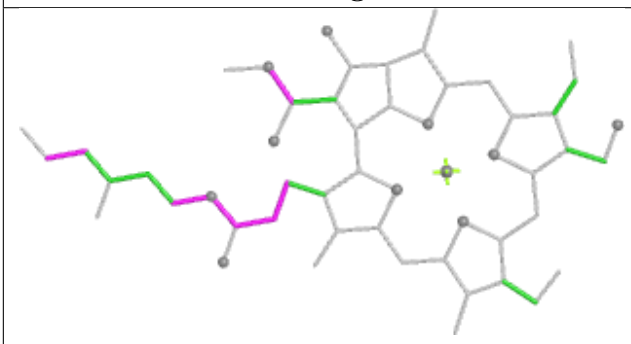
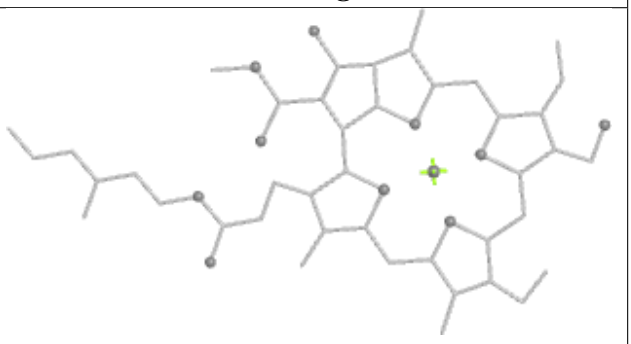


Bond angles

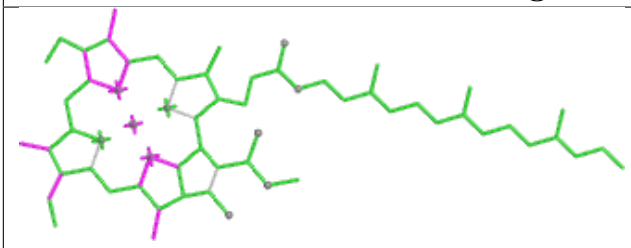


Torsions

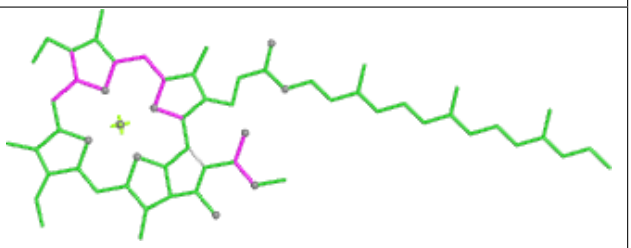


Rings

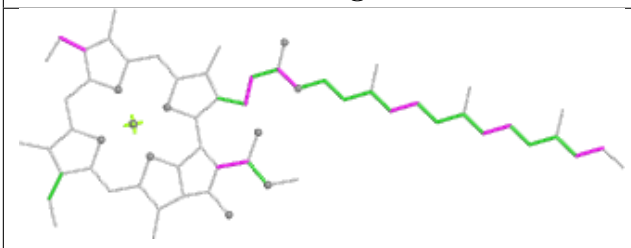
Ligand CLA 8 303



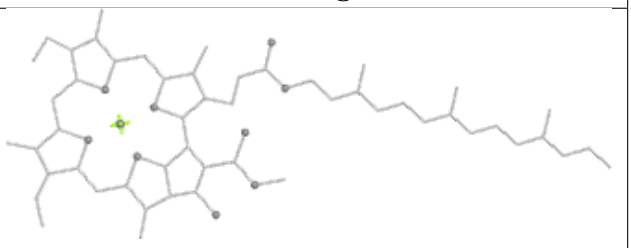
Bond lengths



Bond angles

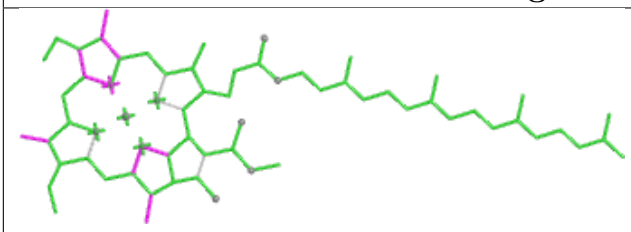


Torsions

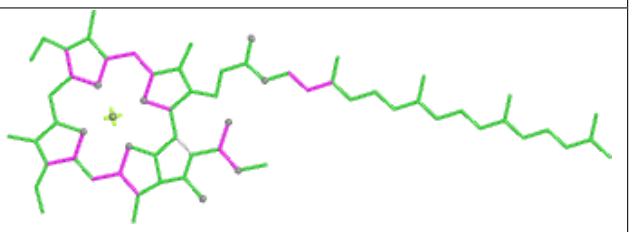


Rings

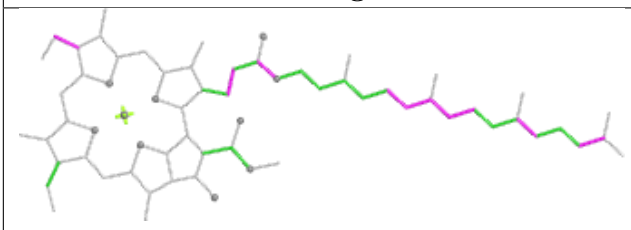
Ligand CLA 2 312



Bond lengths



Bond angles



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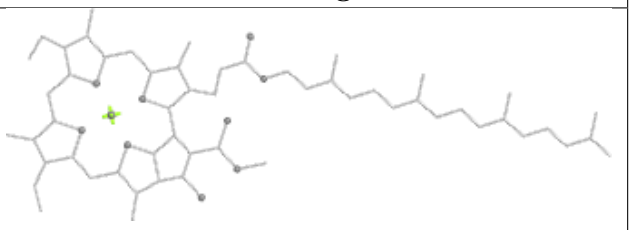
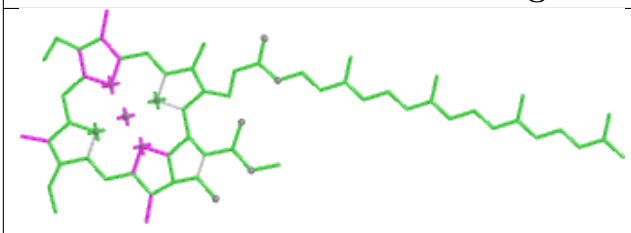


Rings

Ligand CLA 7 301



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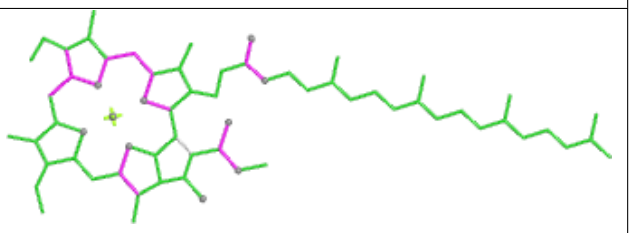
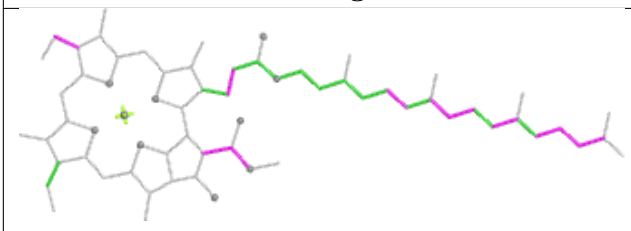


Bond angles



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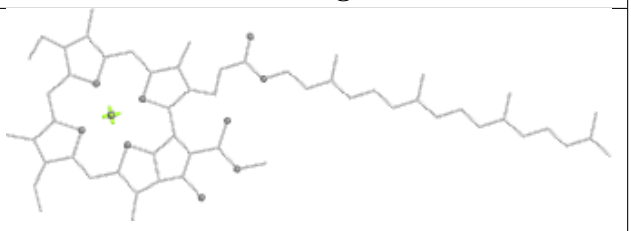
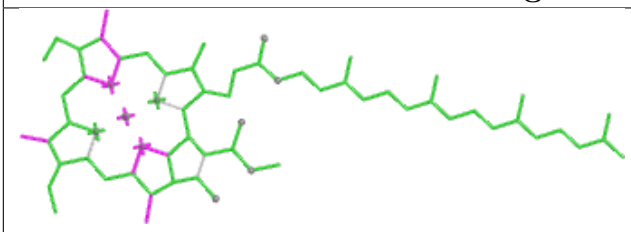


Rings

Ligand CLA B 825



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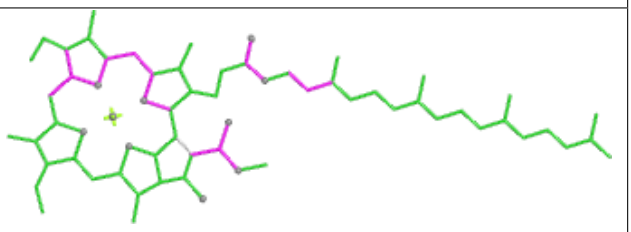
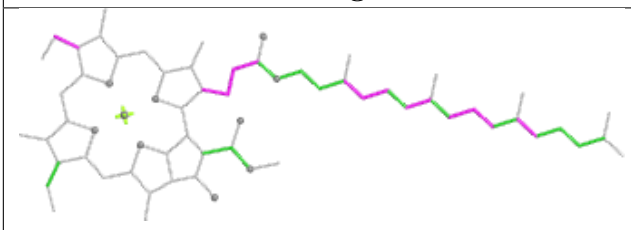


Bond angles



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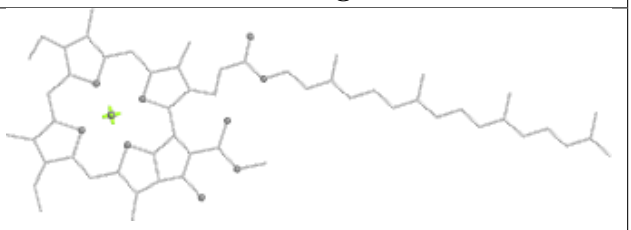
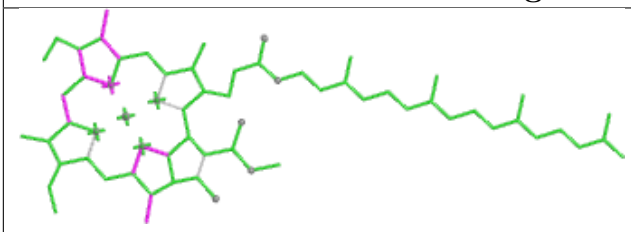


Rings

Ligand CLA T 608



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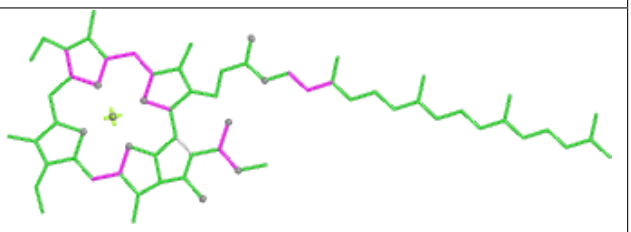
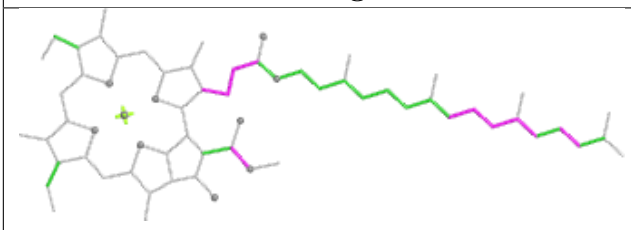


Bond angles



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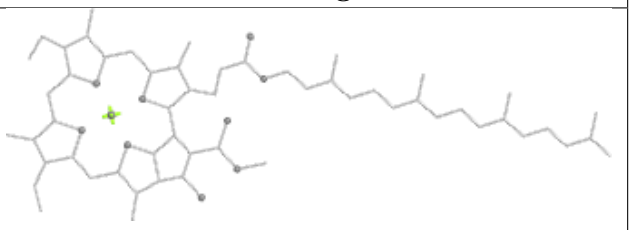
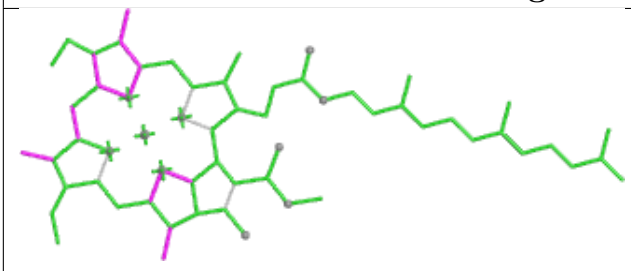


Rings

Ligand CLA a 308



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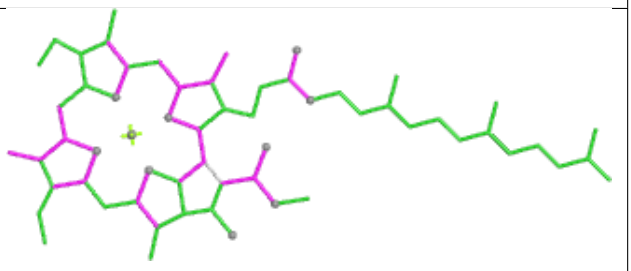
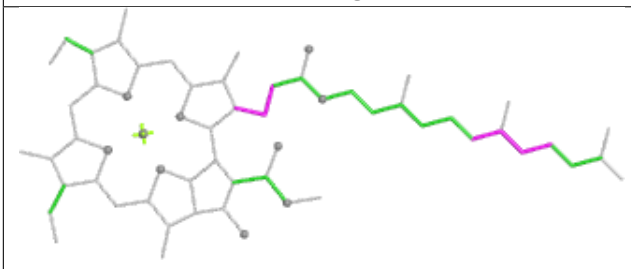


Bond angles



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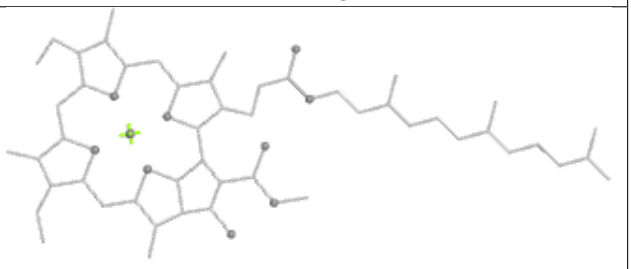
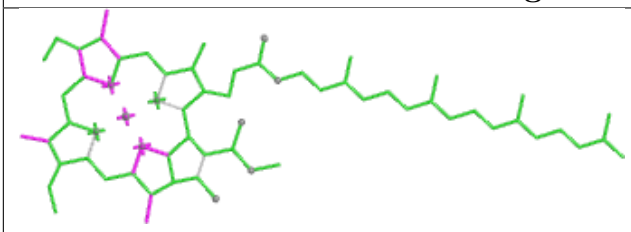


Rings

Ligand CLA B 837



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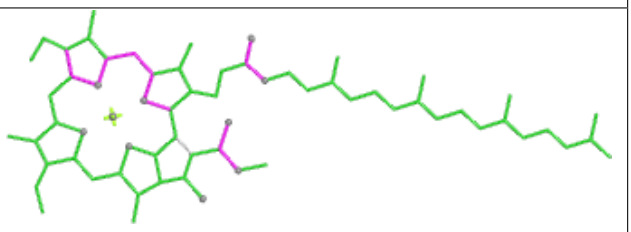
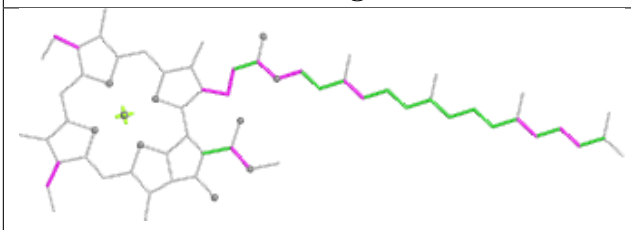


Bond angles



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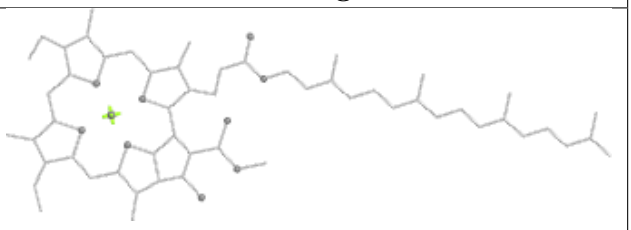
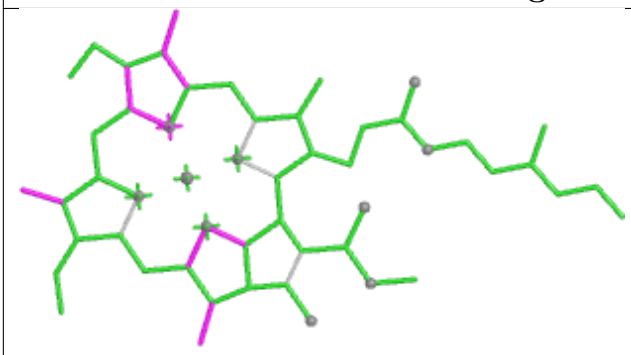
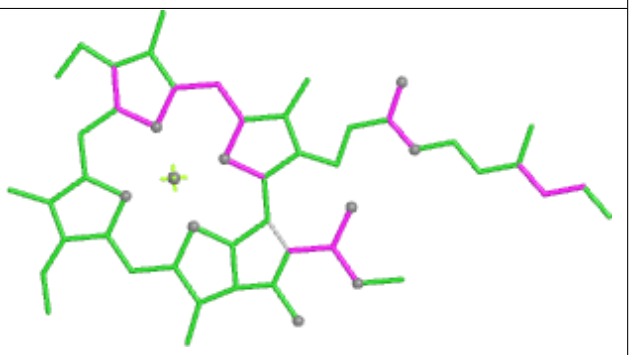


Rings

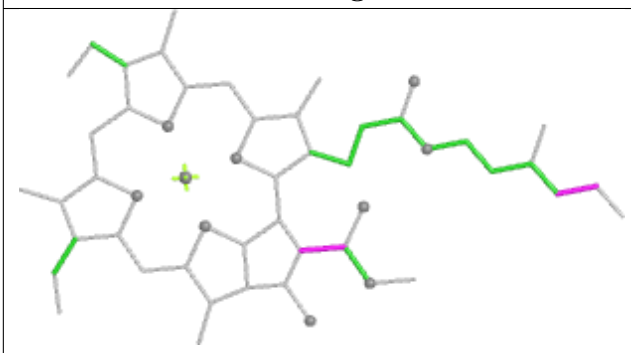
Ligand CLA 1 605



Bond lengths



Bond angles



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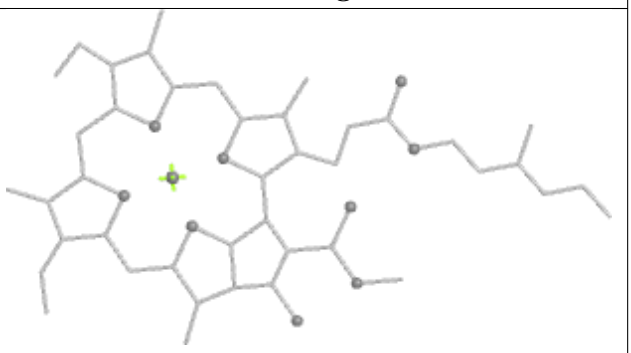
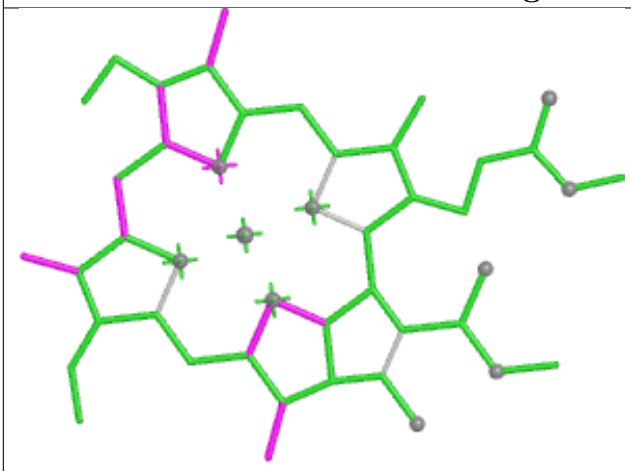
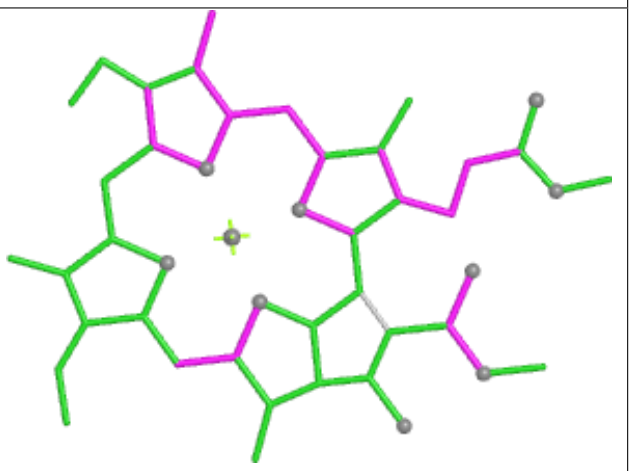


Rings

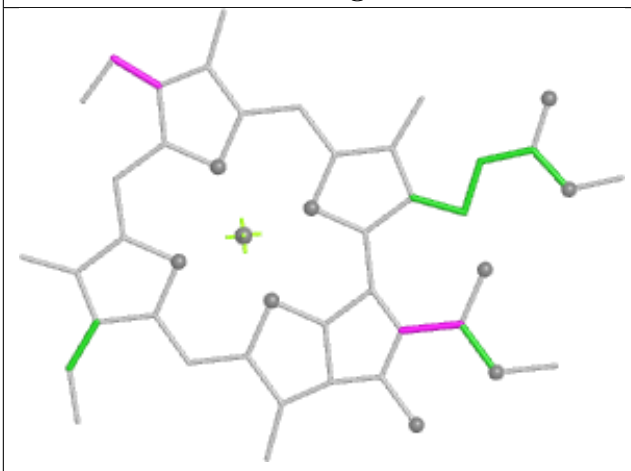
Ligand CLA G 202



Bond lengths



Bond angles



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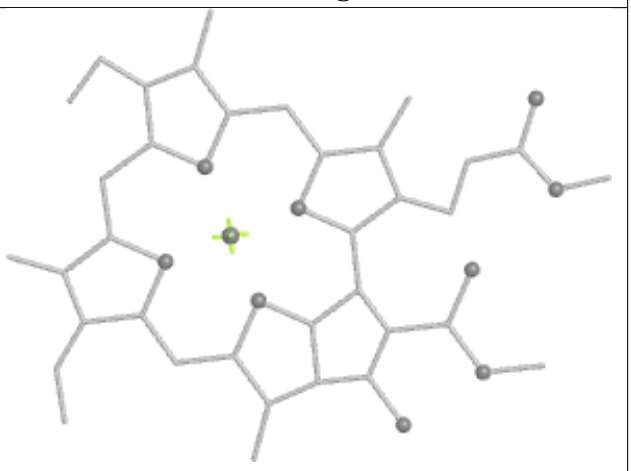
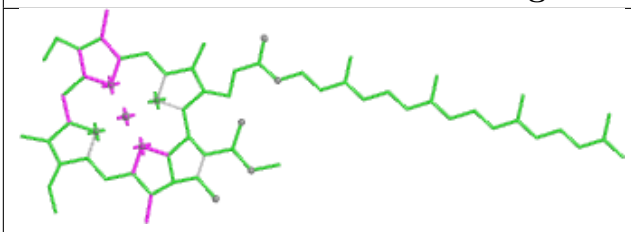


Rings

Ligand CLA 5 324



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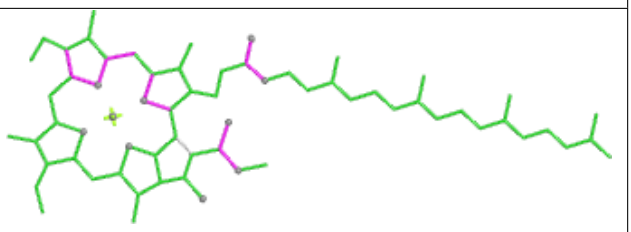
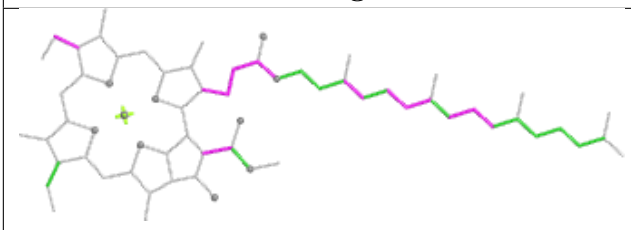


Bond angles



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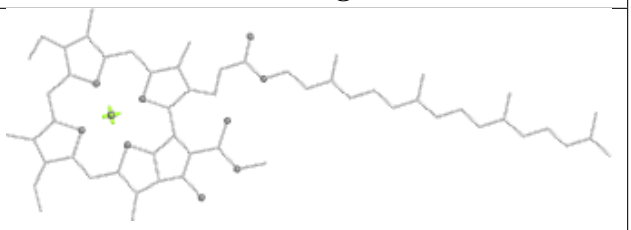
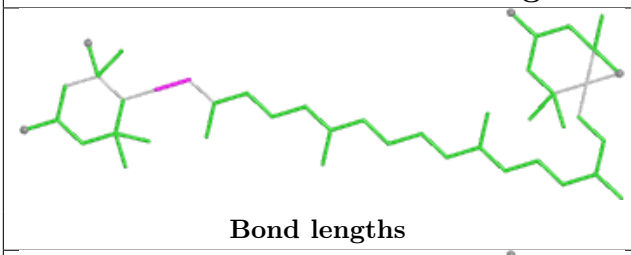


Rings

Ligand NEX T 616



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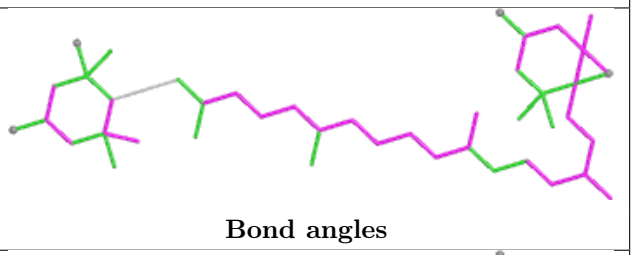
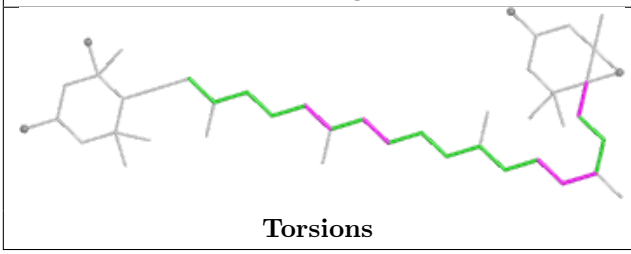


Bond angles



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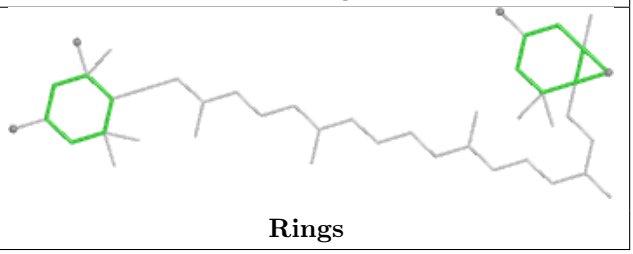
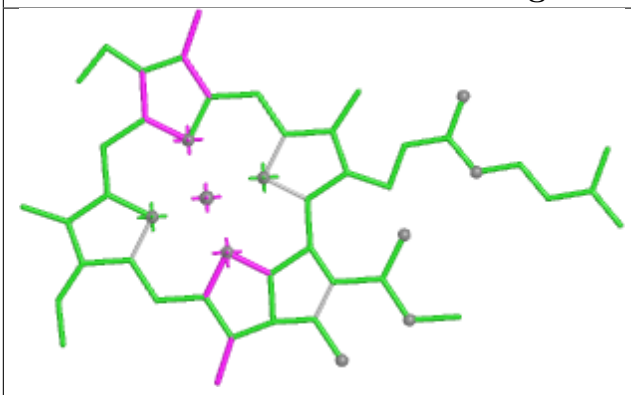


Rings

Ligand CLA 2 307



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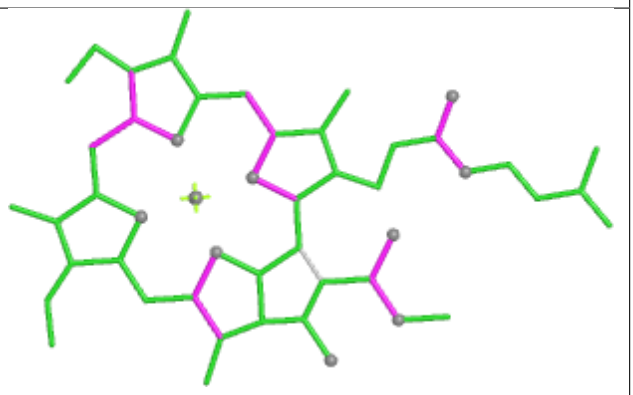
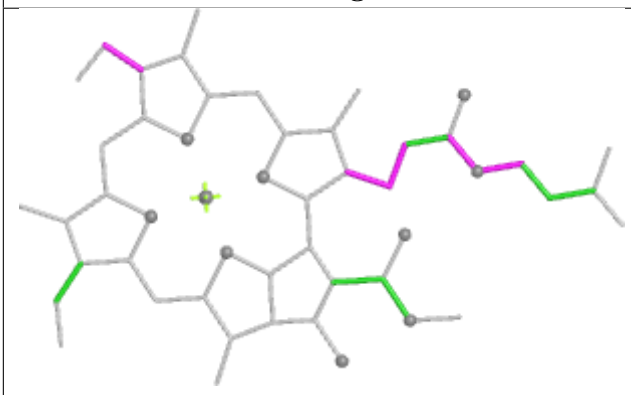


Bond angles



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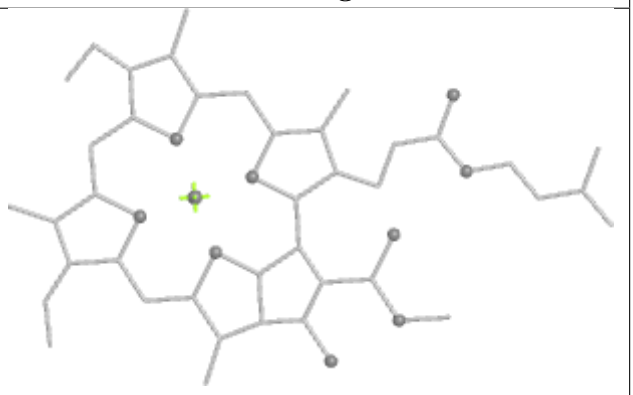
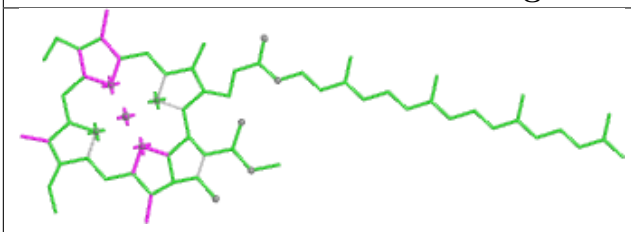


Rings

Ligand CLA A 829



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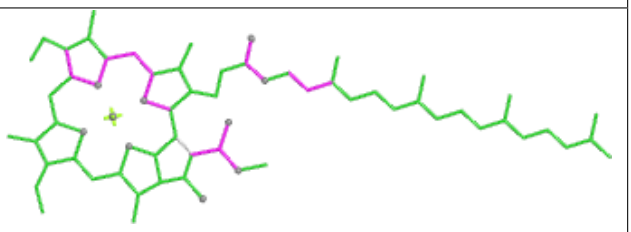
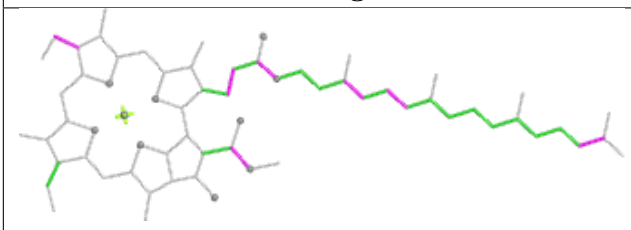
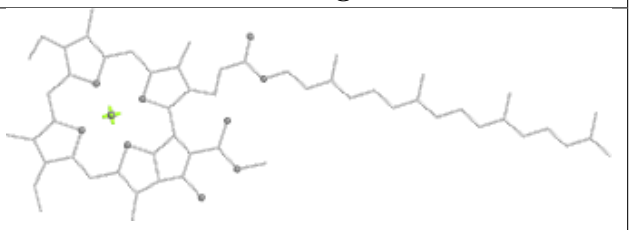


Bond angles

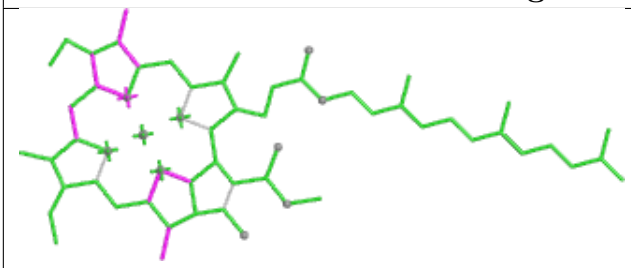


Torsions

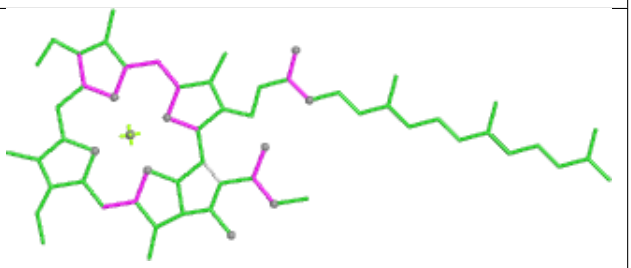


Rings

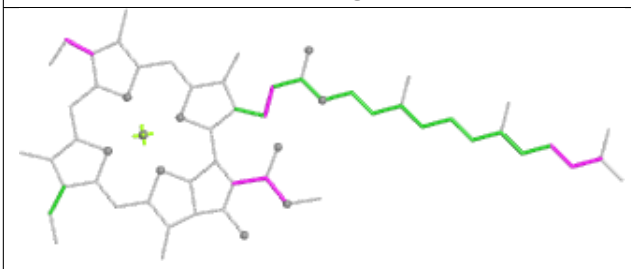
Ligand CLA S 311



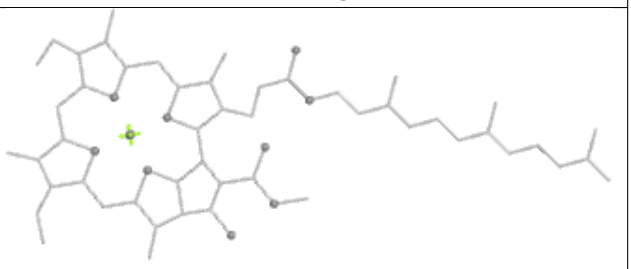
Bond lengths



Bond angles



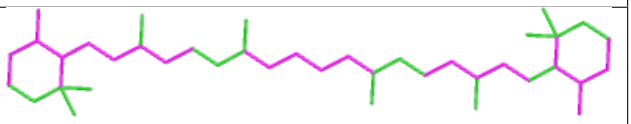
Torsions



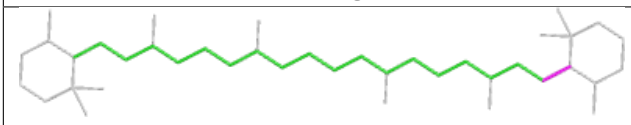
Rings

Ligand BCR L 208

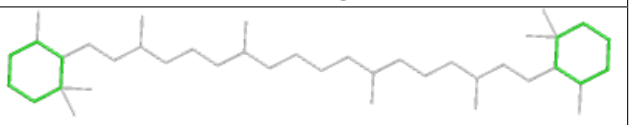
Bond lengths



Bond angles

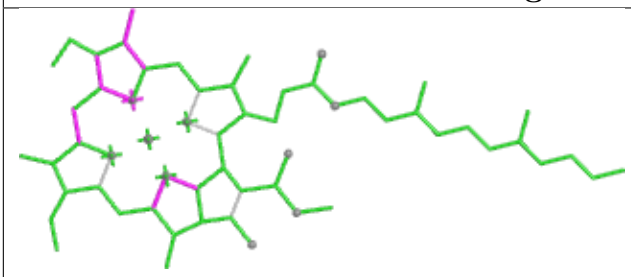


Torsions

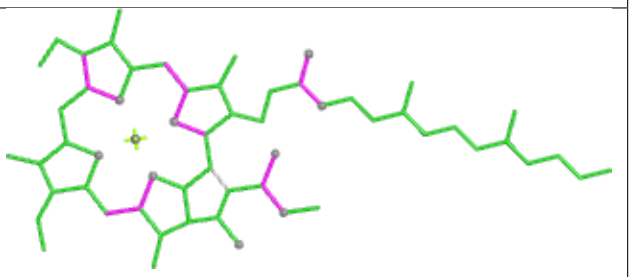


Rings

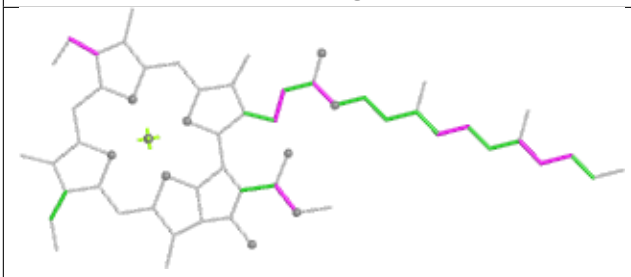
Ligand CLA P 613



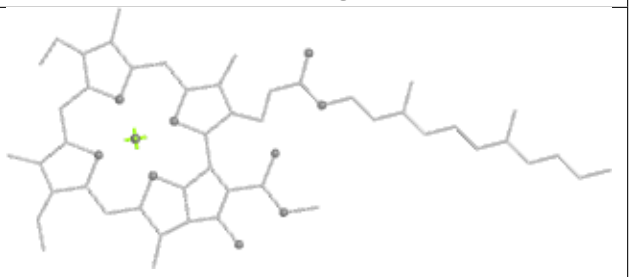
Bond lengths



Bond angles

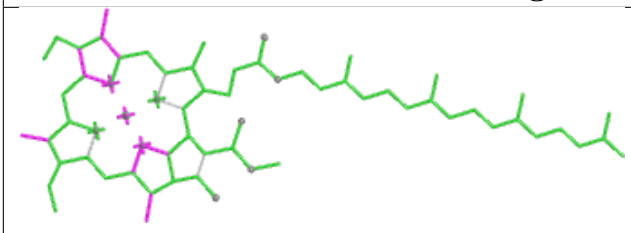


Torsions

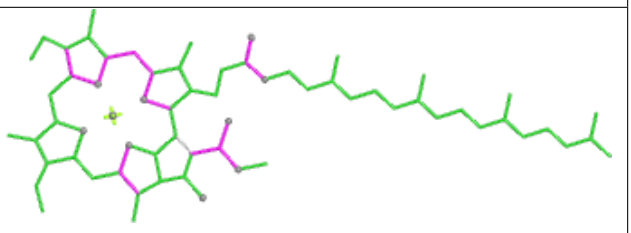


Rings

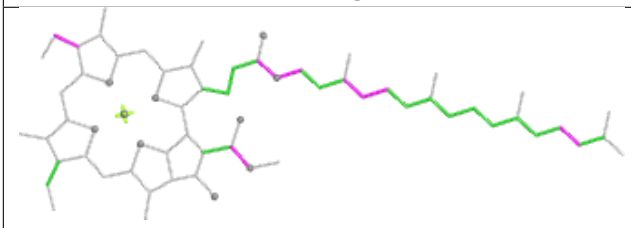
Ligand CLA 1 613



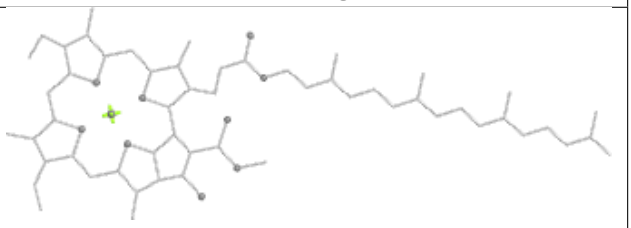
Bond lengths



Bond angles

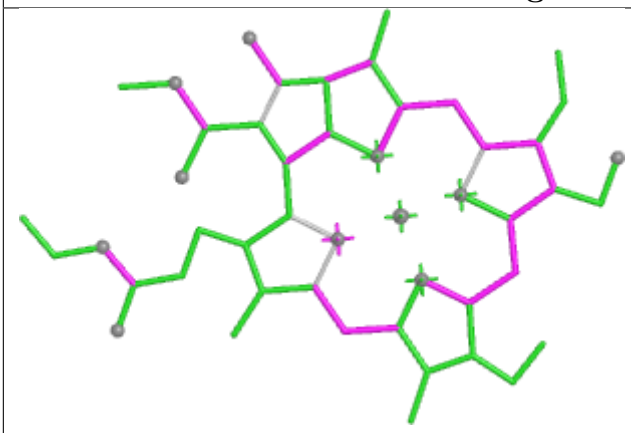


Torsions

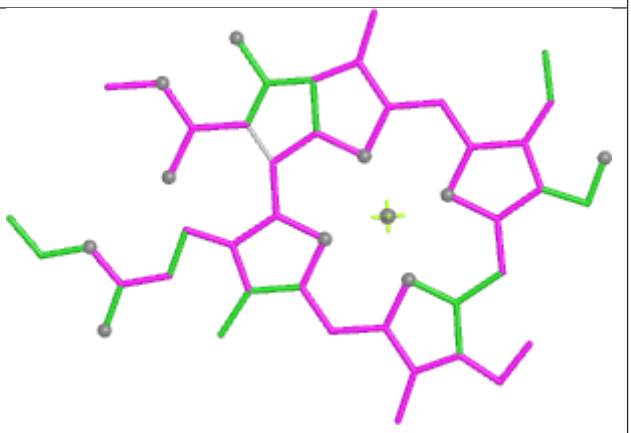


Rings

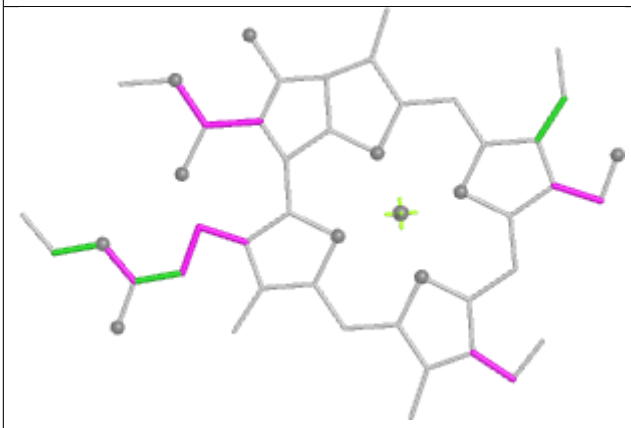
Ligand CHL S 306



Bond lengths



Bond angles



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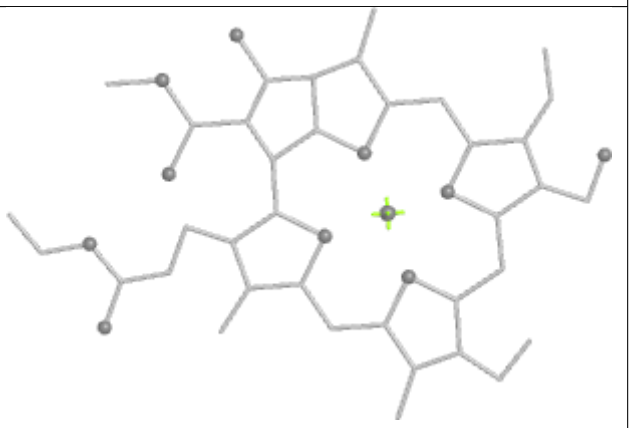
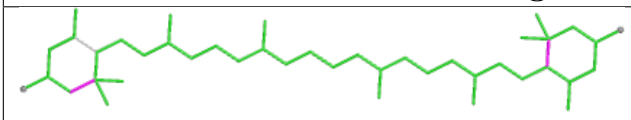


Rings

Ligand LUT 7 315



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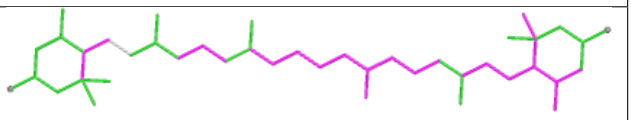
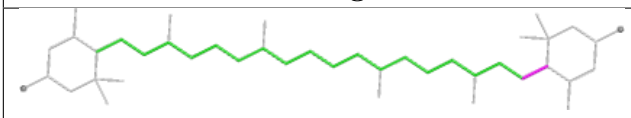


Bond angles



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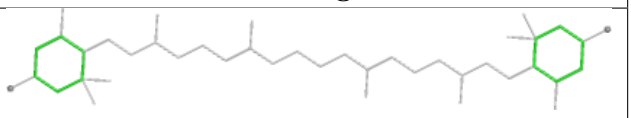
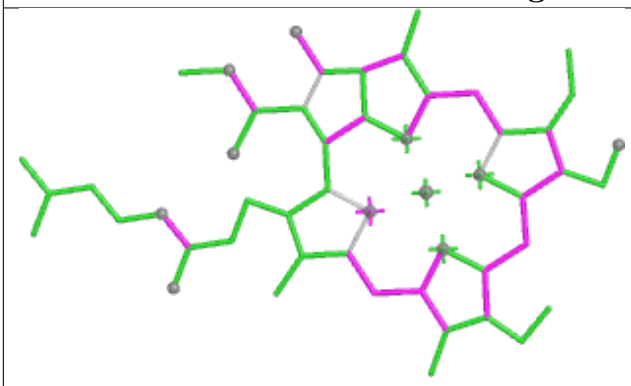
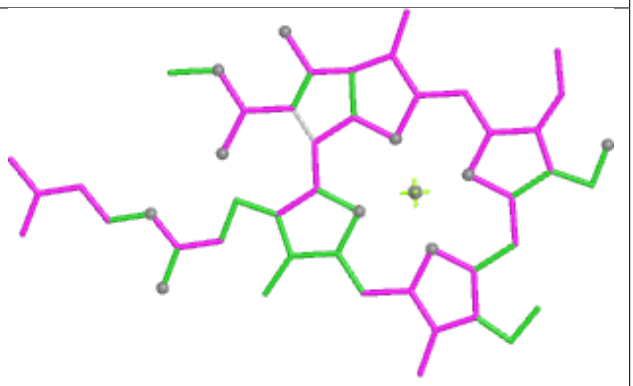


Rings

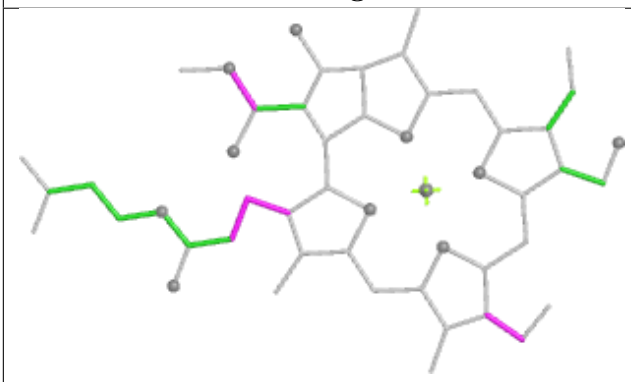
Ligand CHL 4 306



Bond lengths



Bond angles



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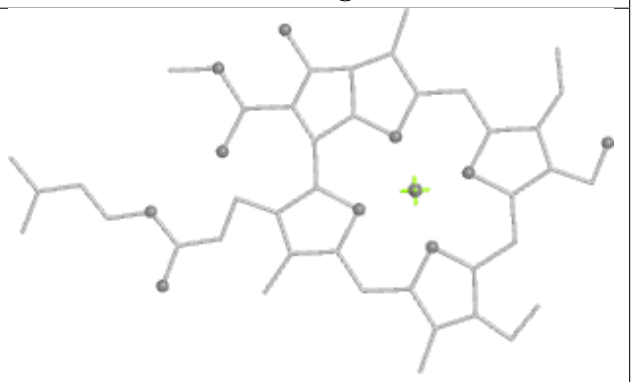
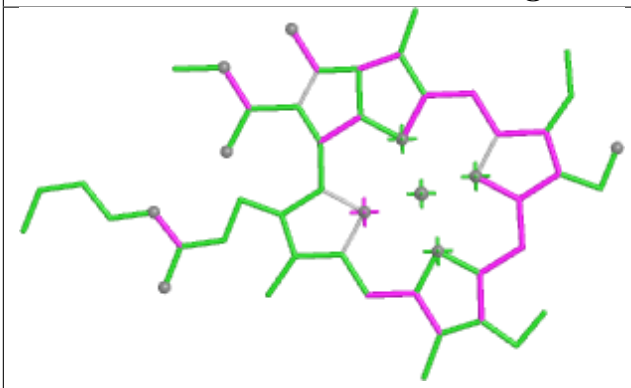


Rings

Ligand CHL T 601



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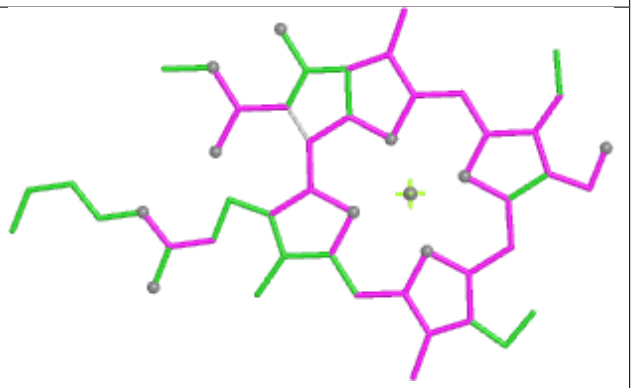
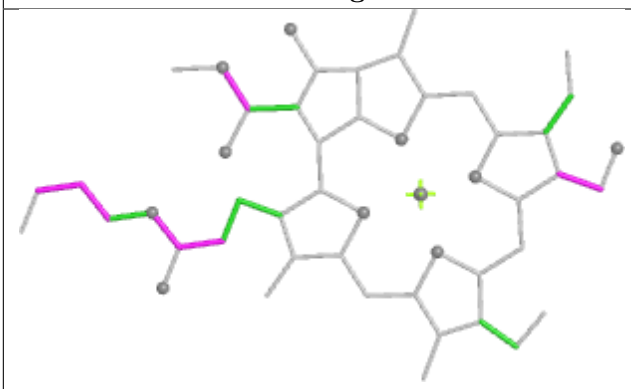
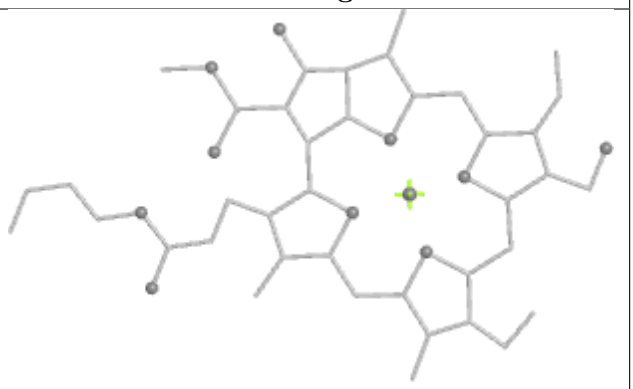


Bond angles

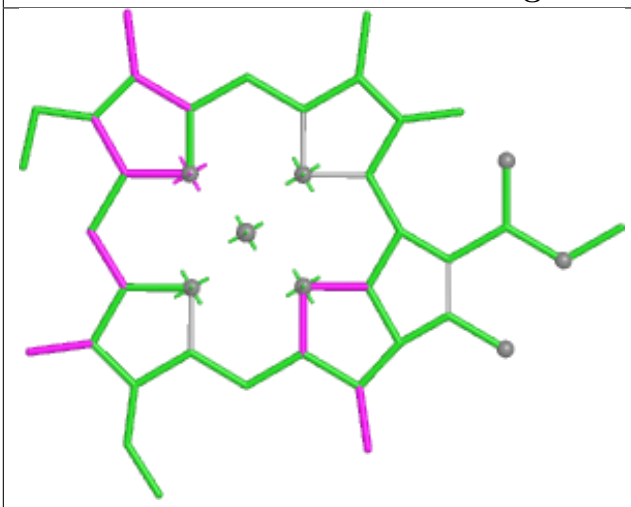


Torsions



Rings

Ligand CLA O 201



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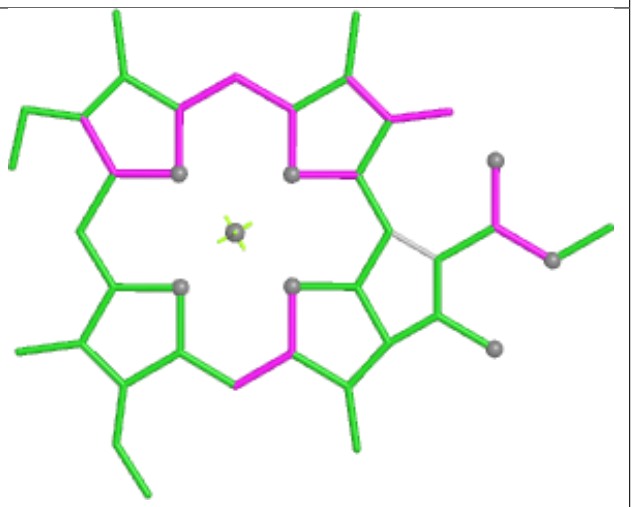
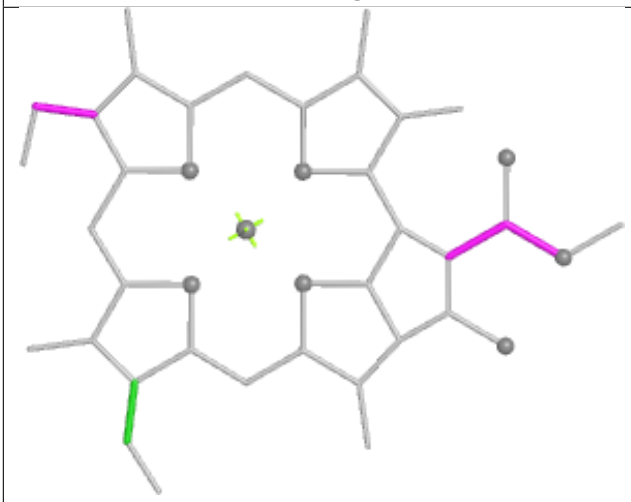


Bond angles



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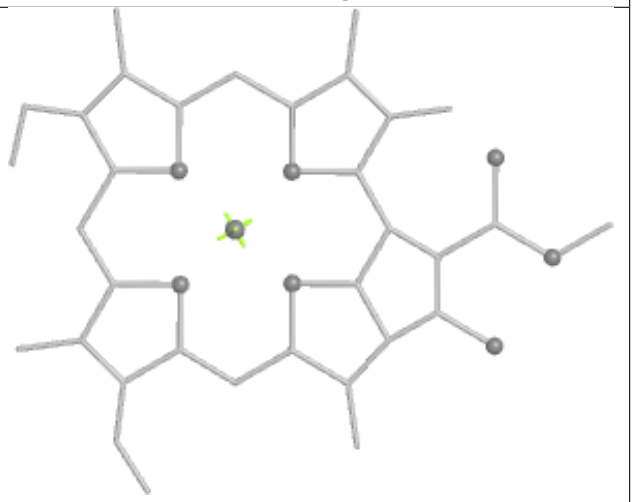
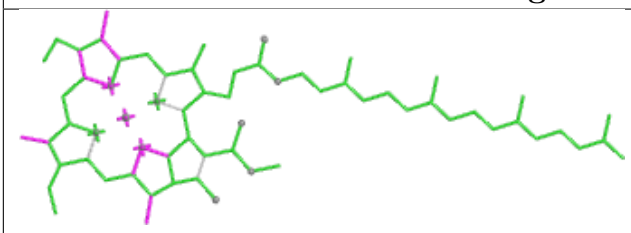


Rings

Ligand CLA 2 304



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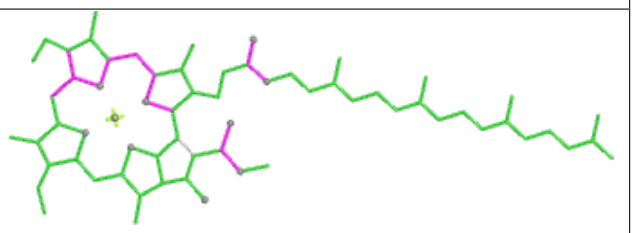
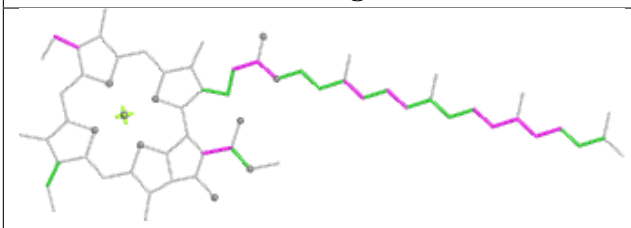
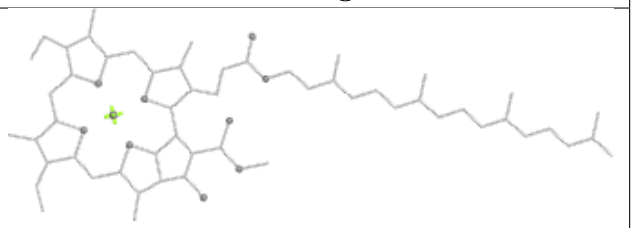


Bond angles

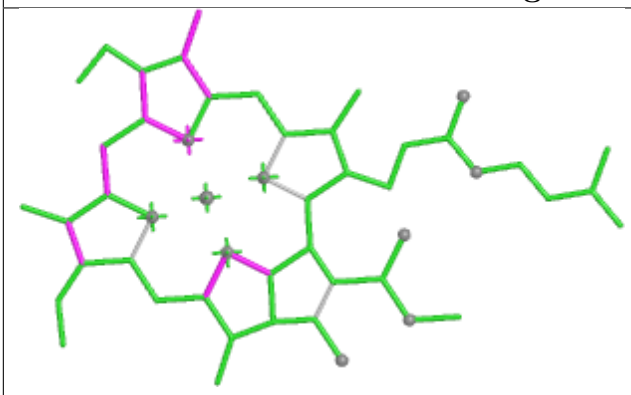


Torsions



Rings

Ligand CLA R 604



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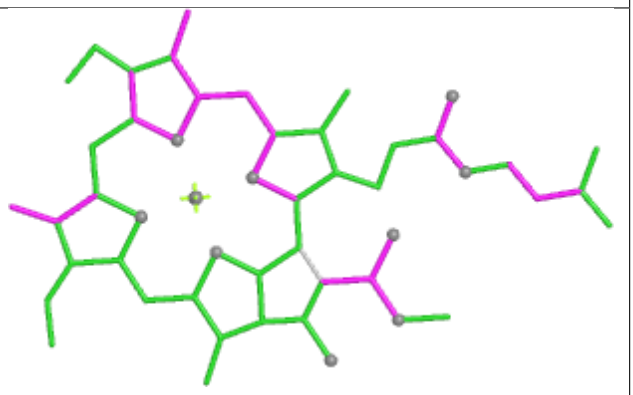
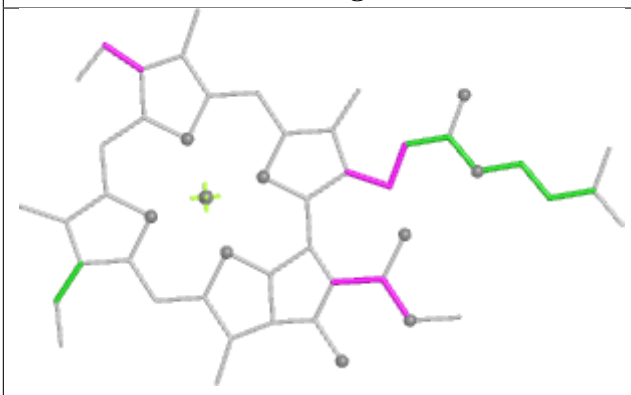


Bond angles



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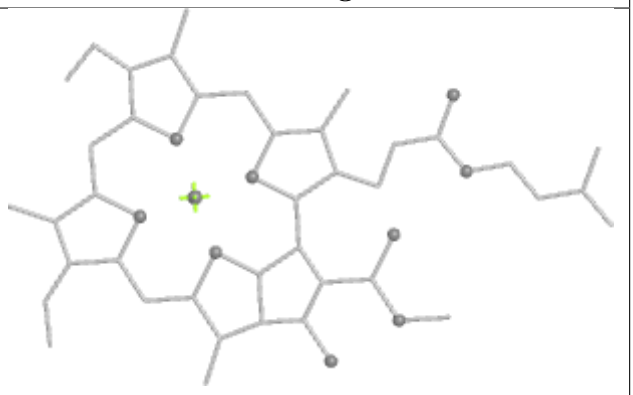
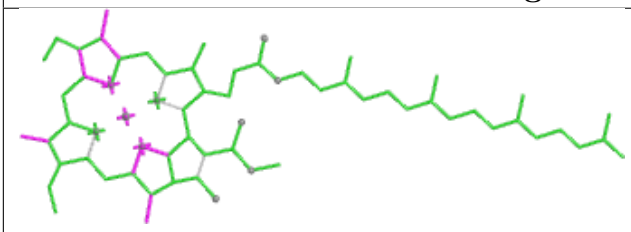


Rings

Ligand CLA B 801



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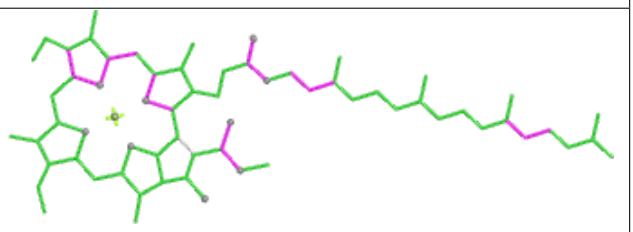
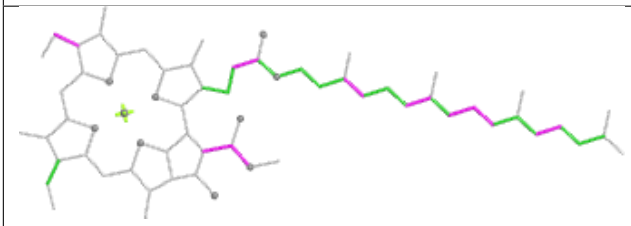
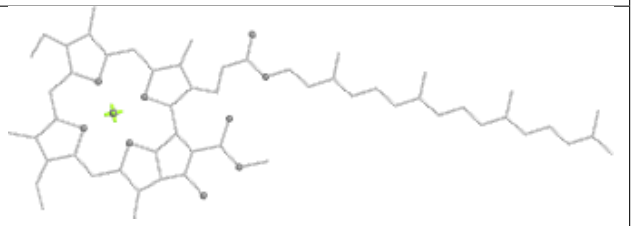


Bond angles

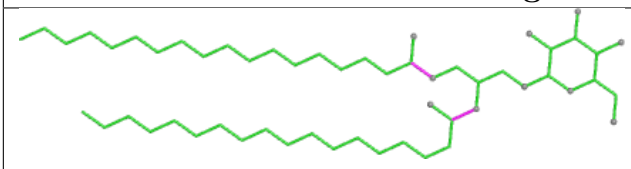


Torsions

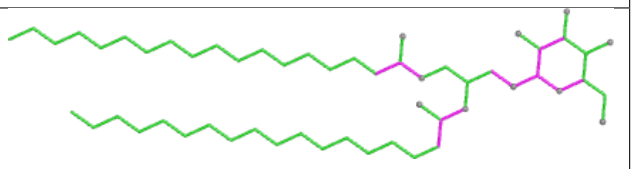


Rings

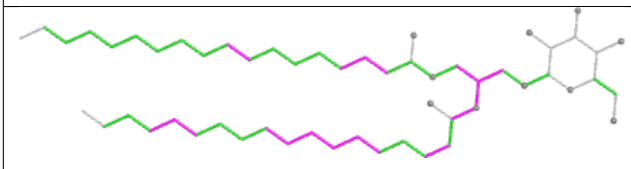
Ligand LMG J 107



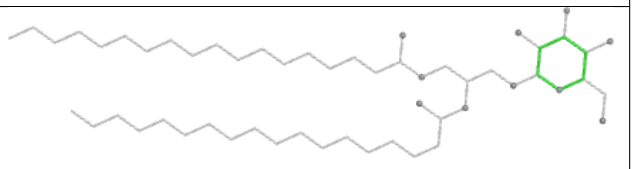
Bond lengths



Bond angles

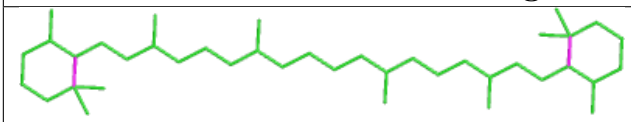


Torsions

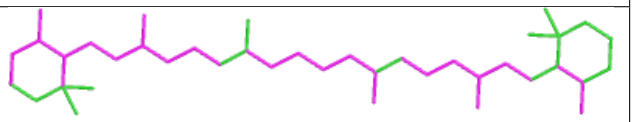


Rings

Ligand BCR B 842

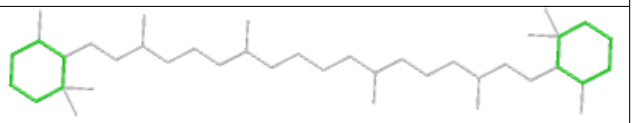


Bond lengths



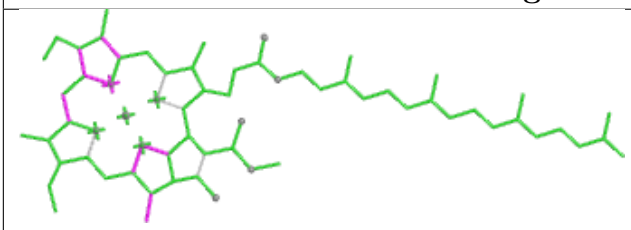
Bond angles

Torsions



Rings

Ligand CLA U 312



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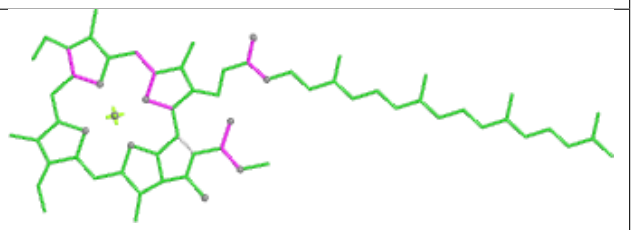
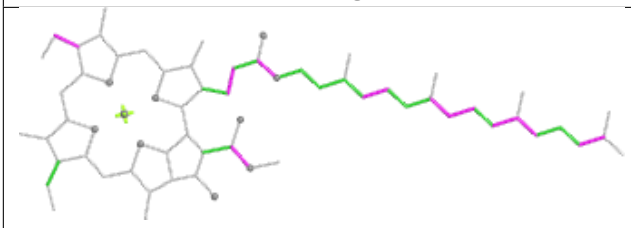
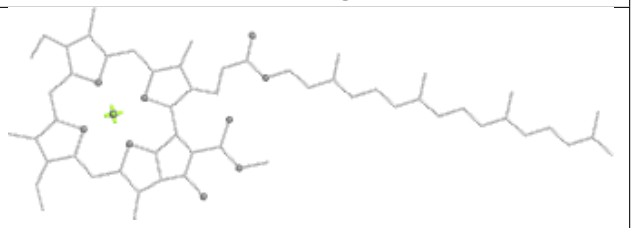


Bond angles

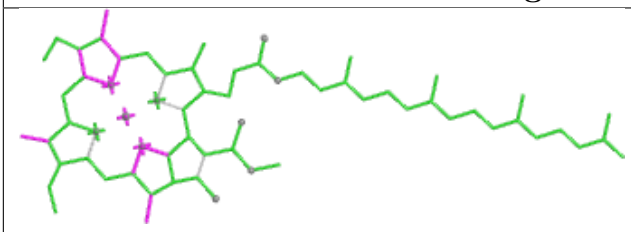


Torsions

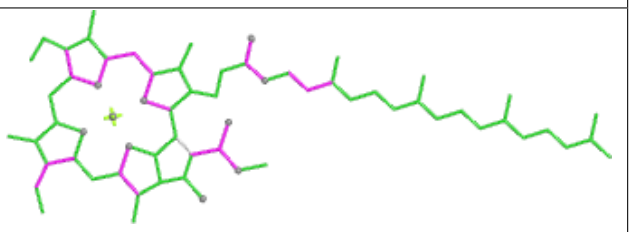


Rings

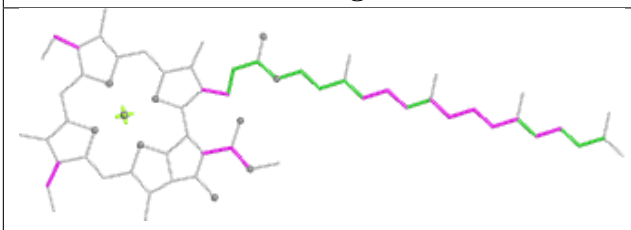
Ligand CLA B 824



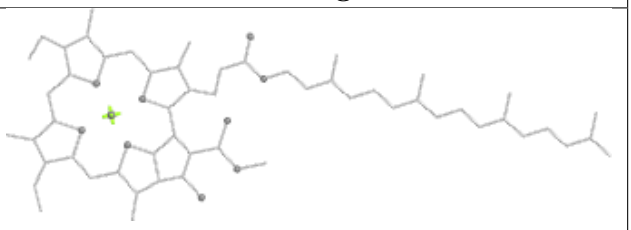
Bond lengths



Bond angles

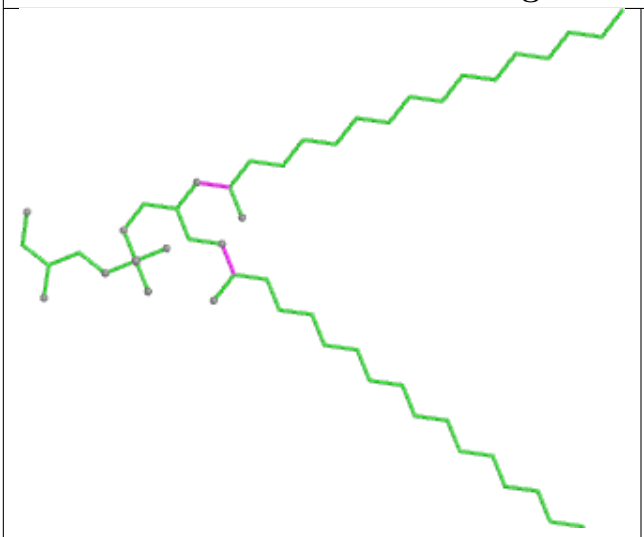


Torsions



Rings

Ligand LHG Q 617



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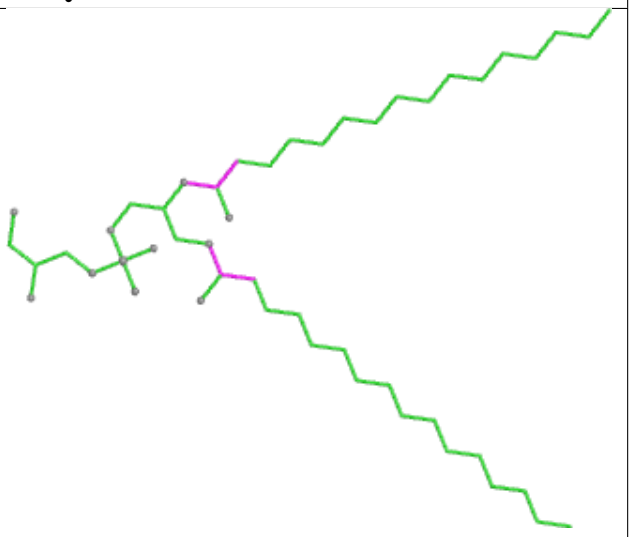
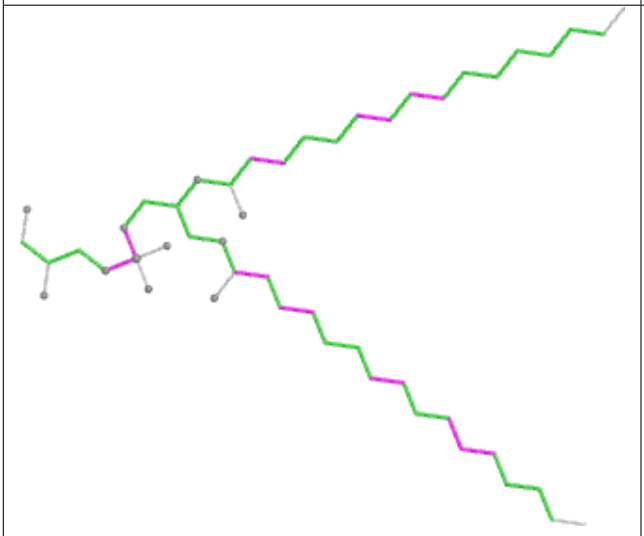


Bond angles



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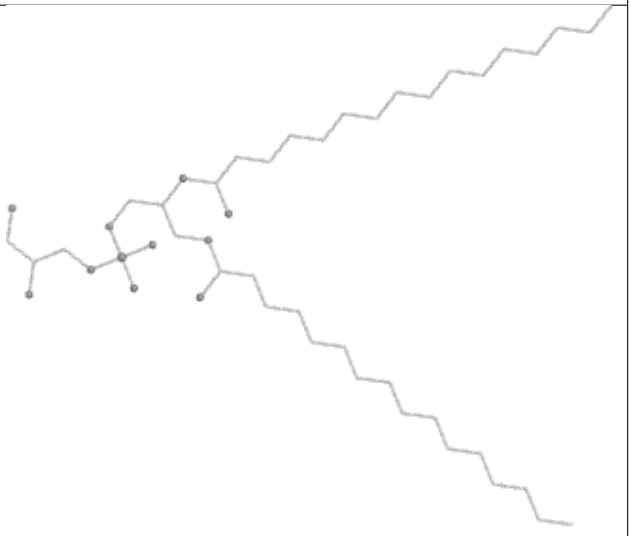
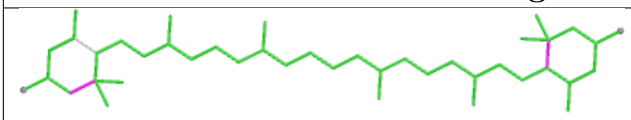


Rings

Ligand LUT 1 616



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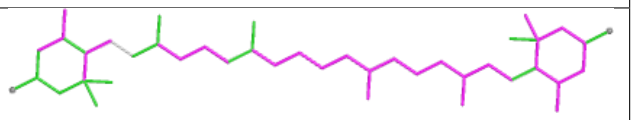
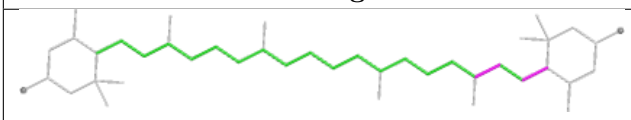
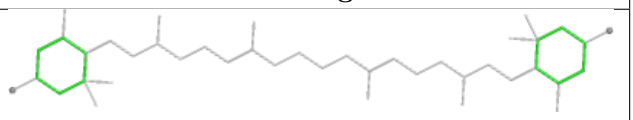


Bond angles

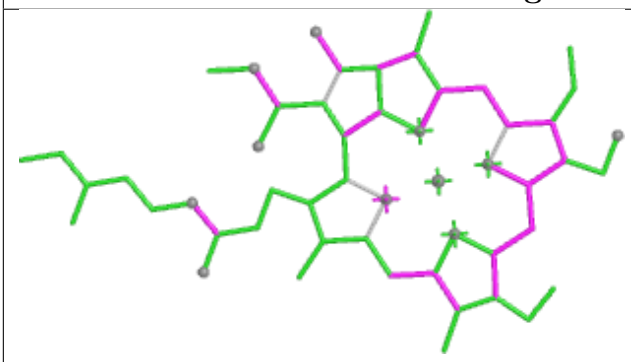


Torsions



Rings

Ligand CHL P 607



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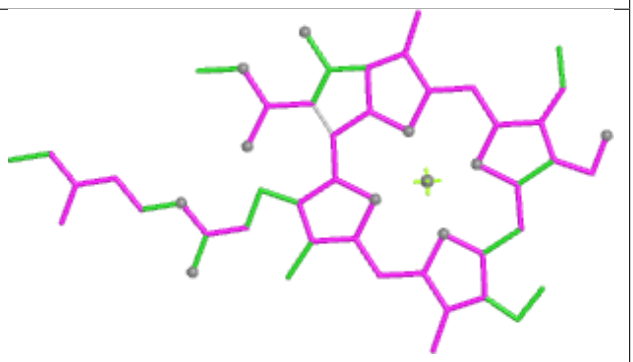
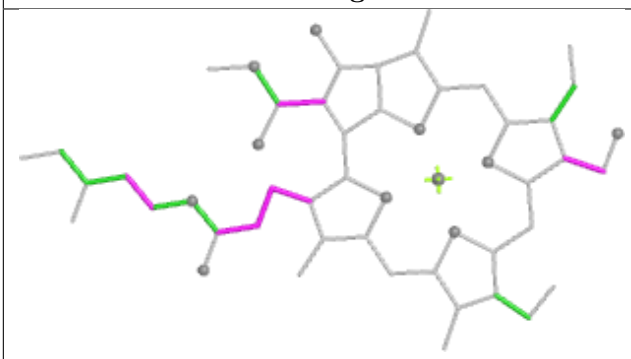
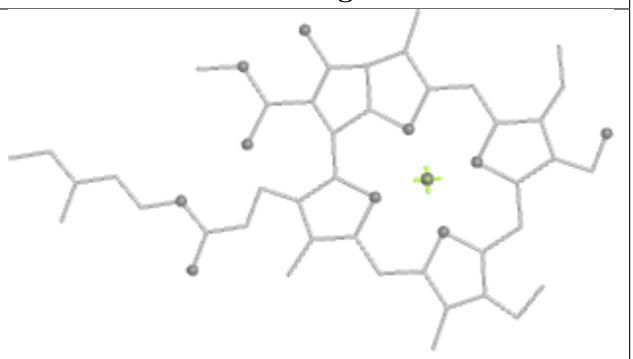


Bond angles



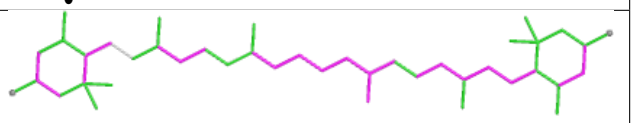
Torsions



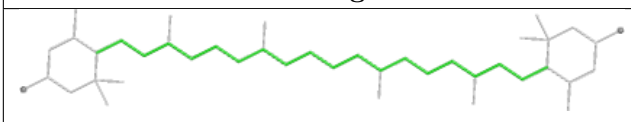
Rings

Ligand LUT Q 614

Bond lengths



Bond angles



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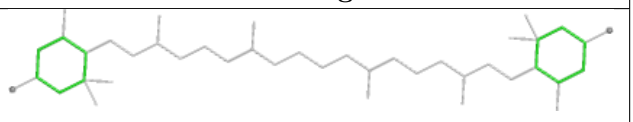
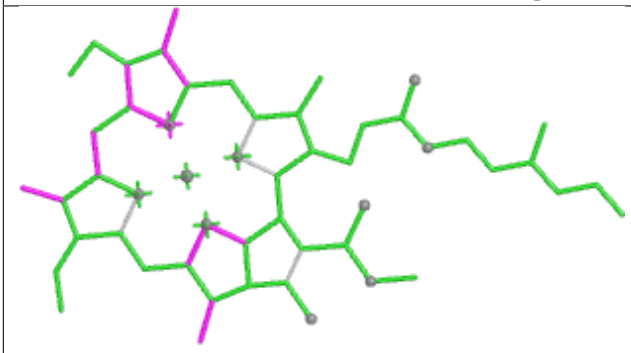


Rings

Ligand CLA 5 312



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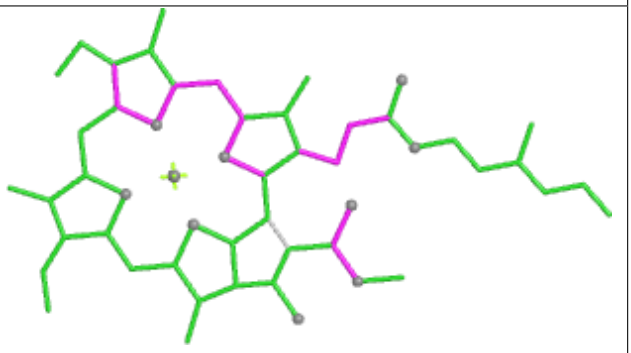
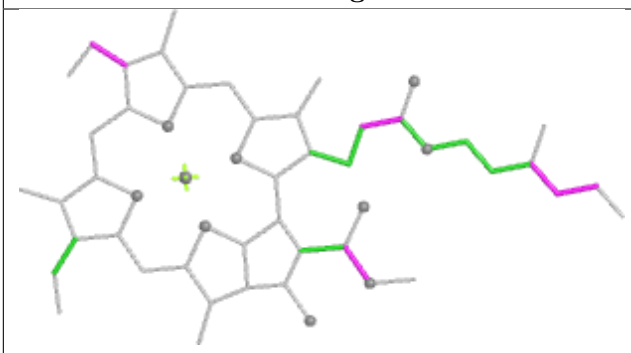


Bond angles



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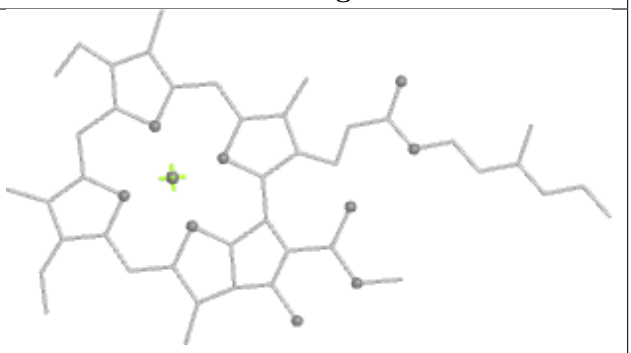
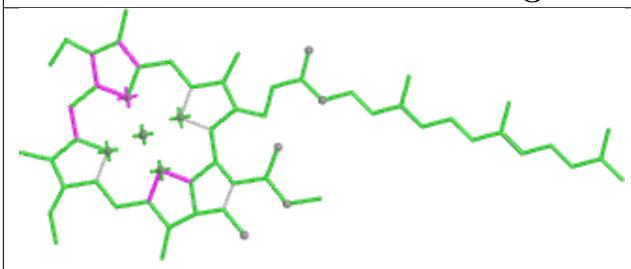
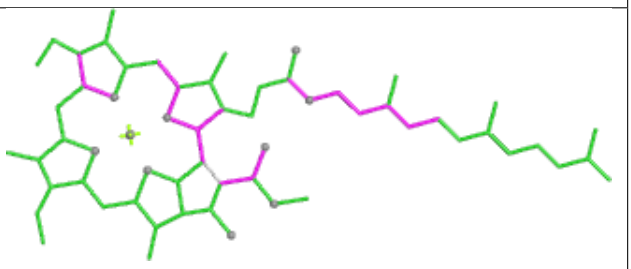


Rings

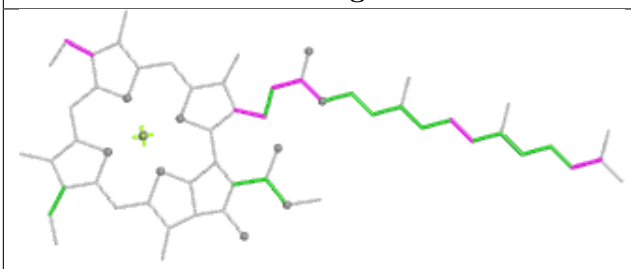
Ligand CLA R 611



Bond lengths



Bond angles



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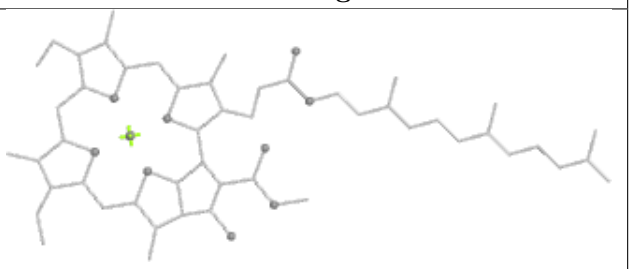
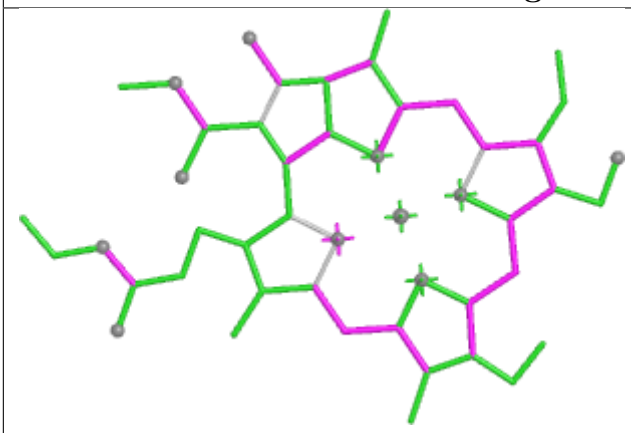


Rings

Ligand CHL T 604



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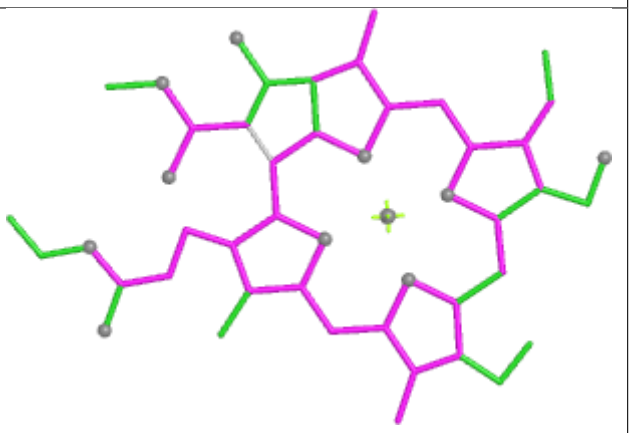

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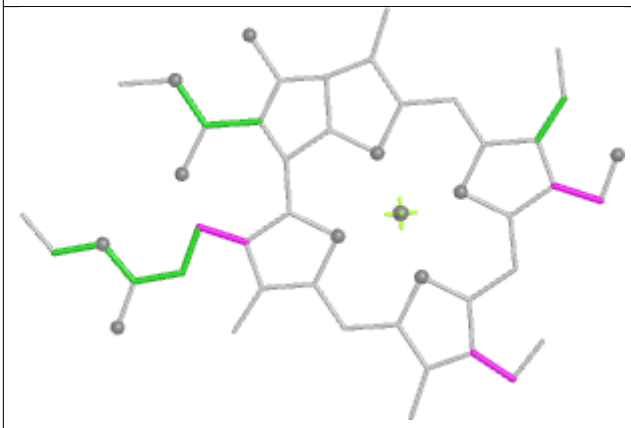

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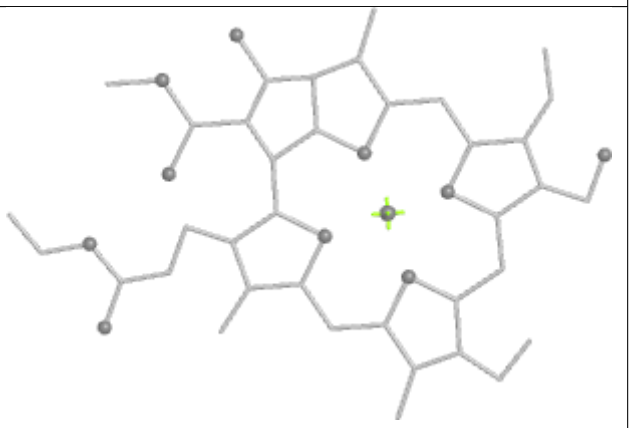
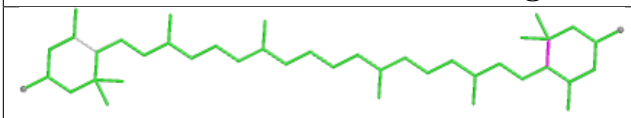
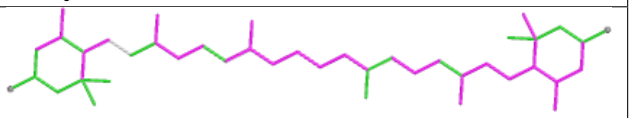


Rings

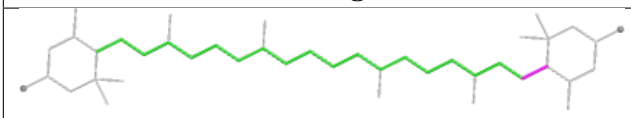
Ligand LUT Q 615



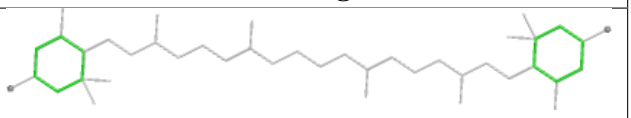
Bond lengths



Bond angles

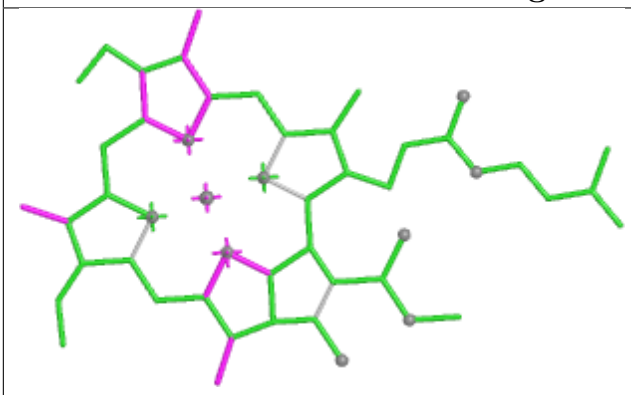


Torsions



Rings

Ligand CLA 6 609



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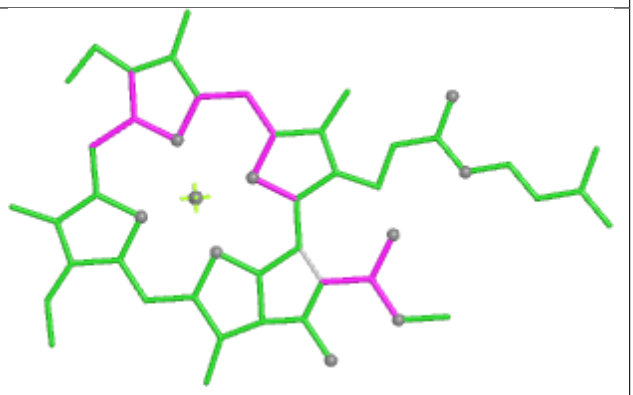
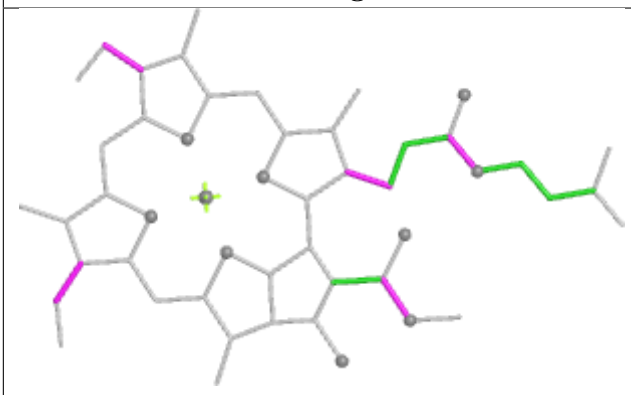


Bond angles



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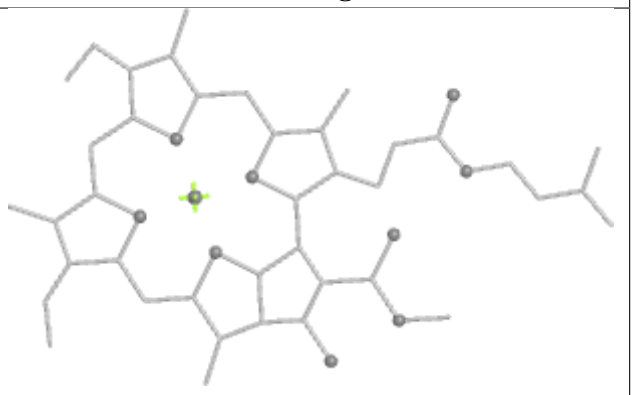
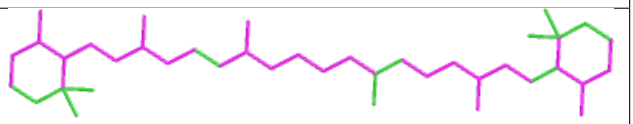


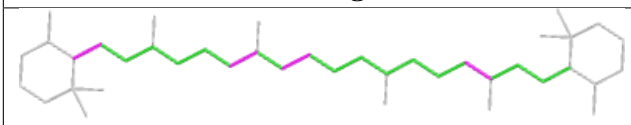
Rings

Ligand BCR 4 321

Bond lengths



Bond angles



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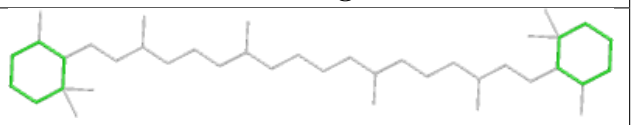
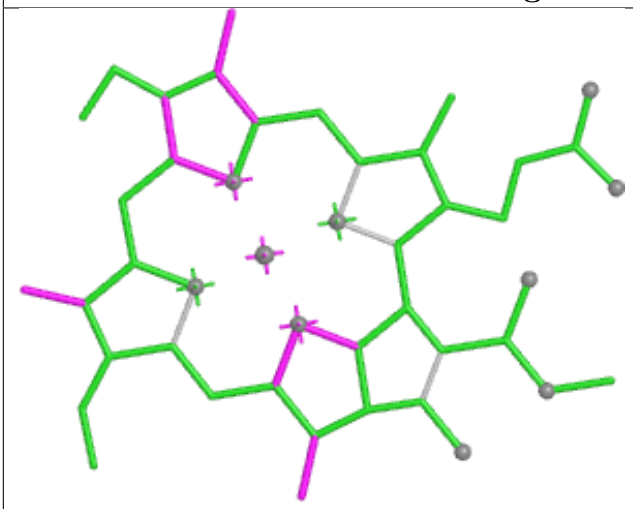


Rings

Ligand CLA A 834



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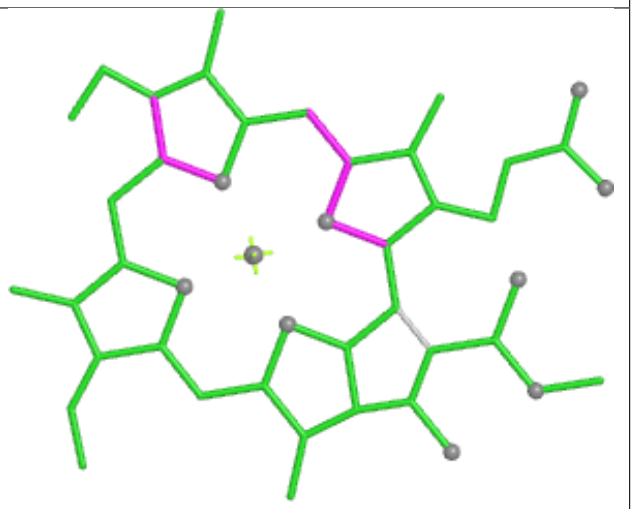
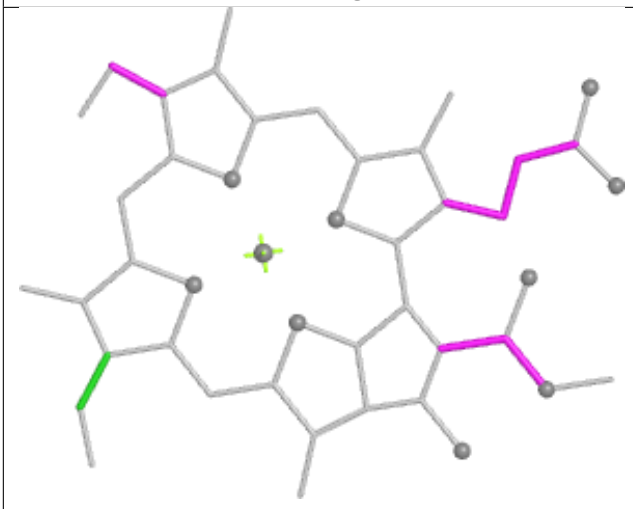


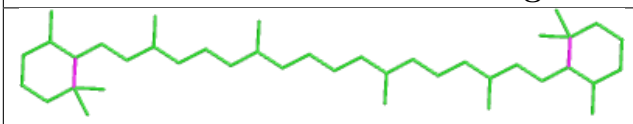
Bond angles



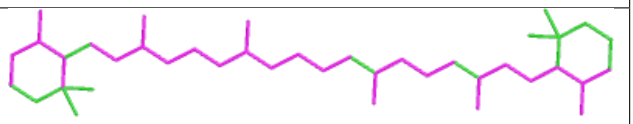
Torsions

Rings

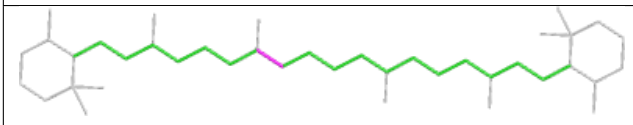
Ligand BCR F 803



Bond lengths



Bond angles



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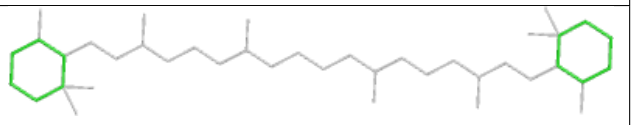
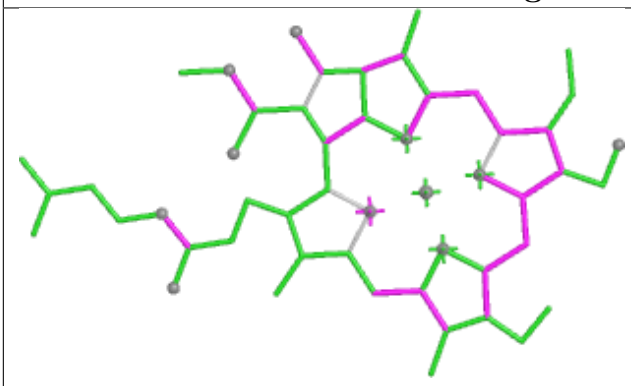


Rings

Ligand CHL P 601



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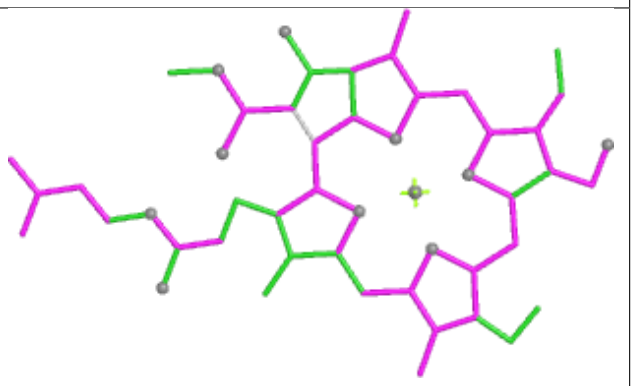
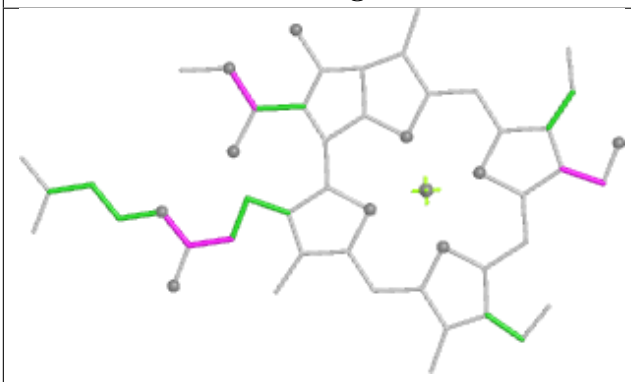


Bond angles



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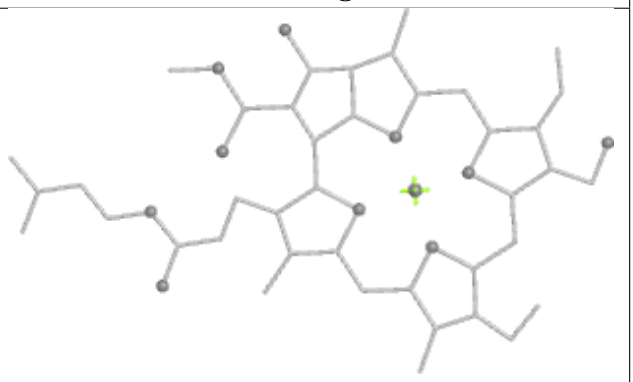
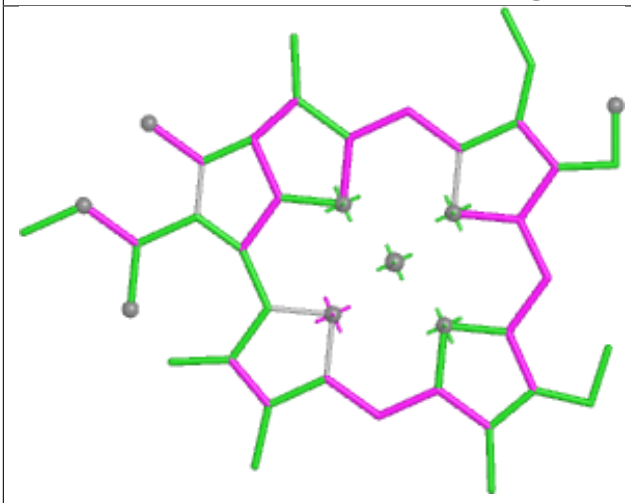


Rings

Ligand CHL 9 306



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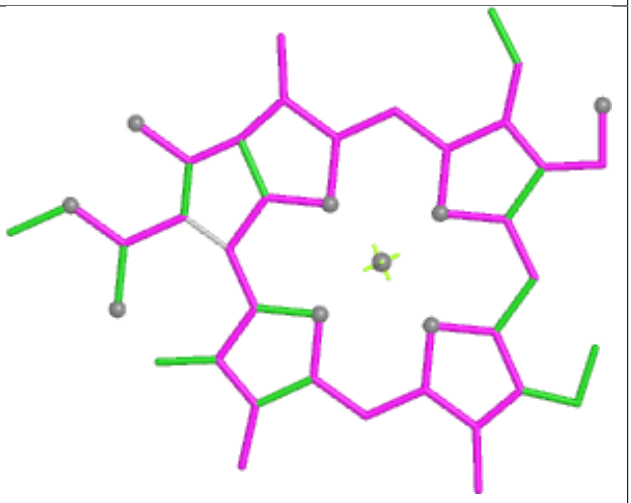
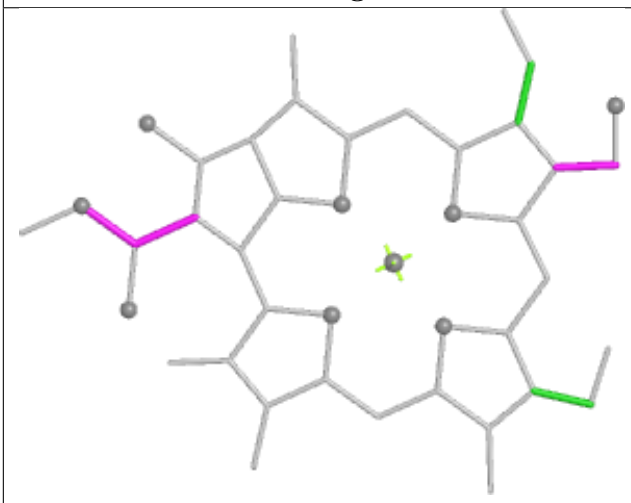
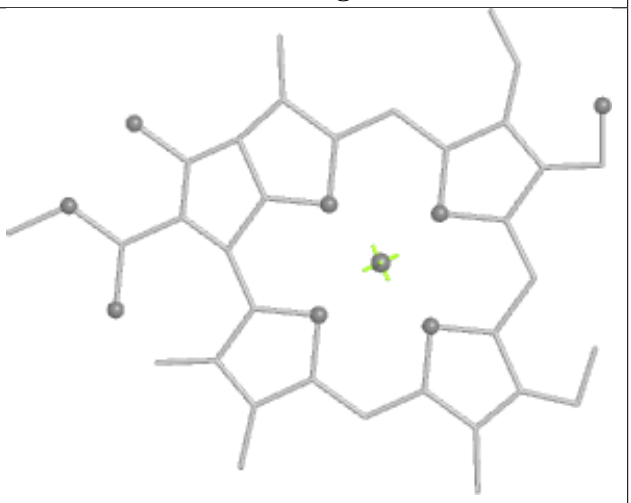


Bond angles

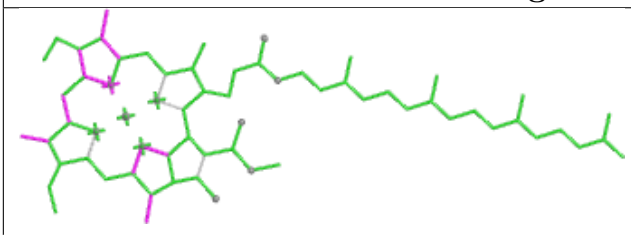


Torsions



Rings

Ligand CLA a 301



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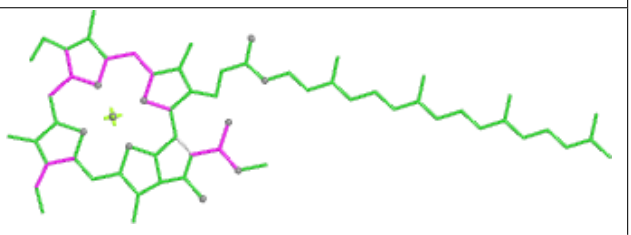
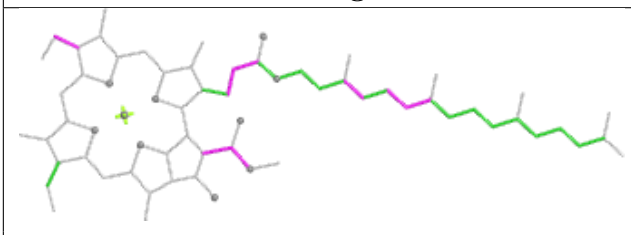


Bond angles



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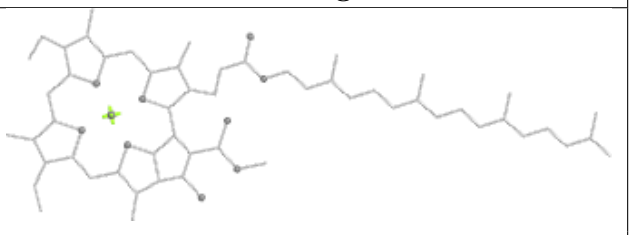
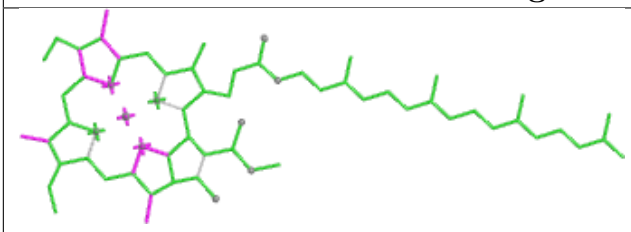


Rings

Ligand CLA 8 313



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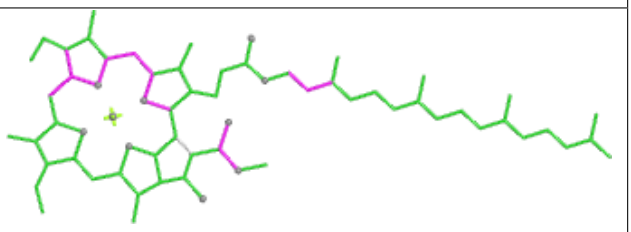
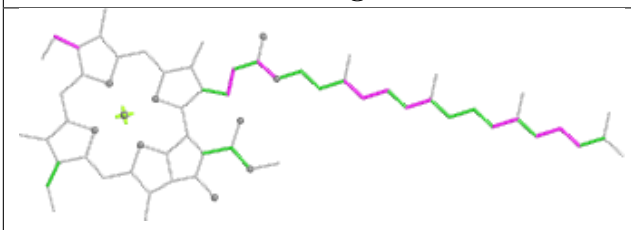


Bond angles



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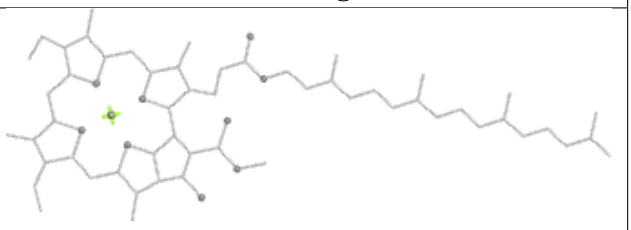
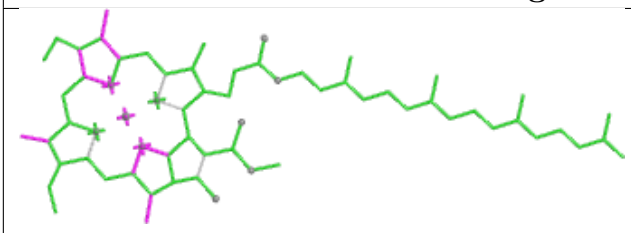


Rings

Ligand CLA 8 302



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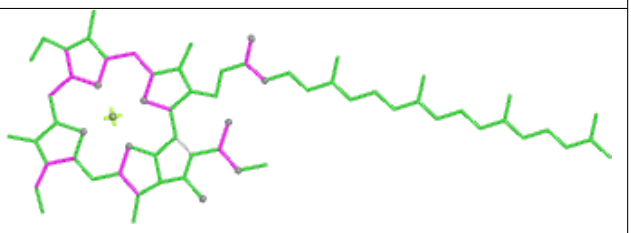
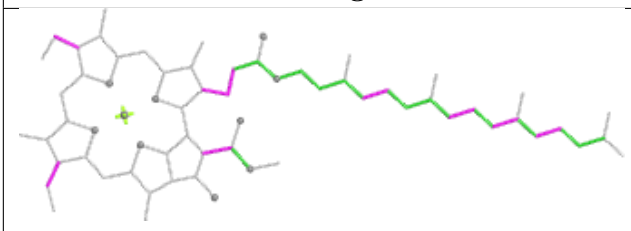


Bond angles



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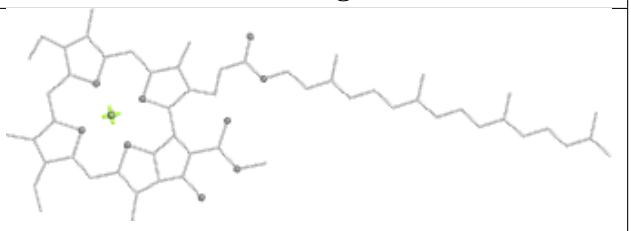
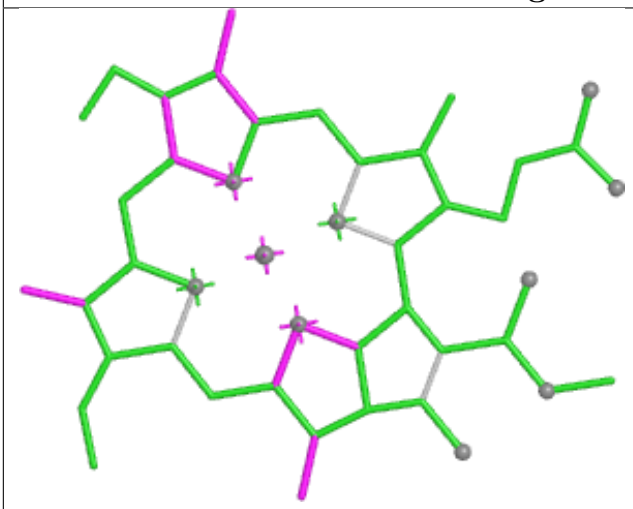


Rings

Ligand CLA 6 614



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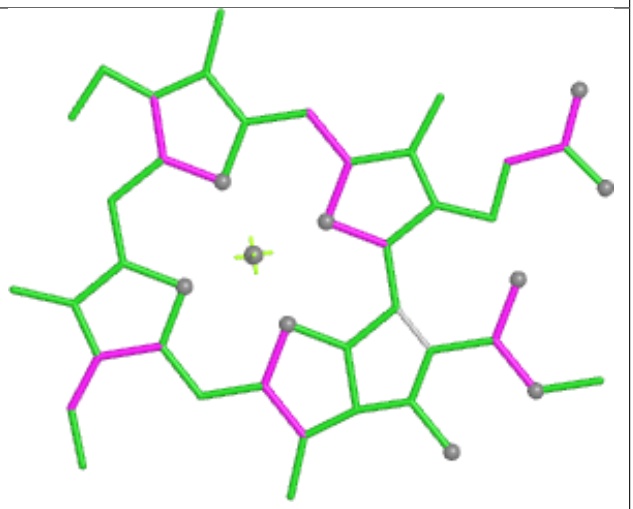
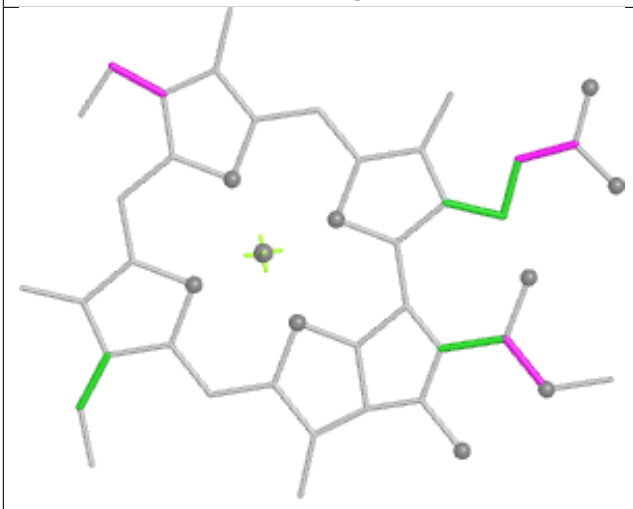


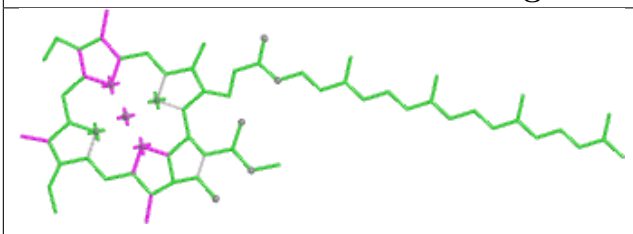
Bond angles



Torsions

Rings

Ligand CLA A 832



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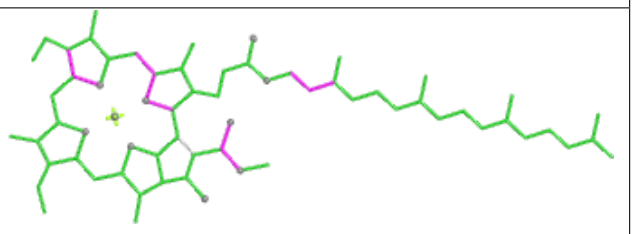

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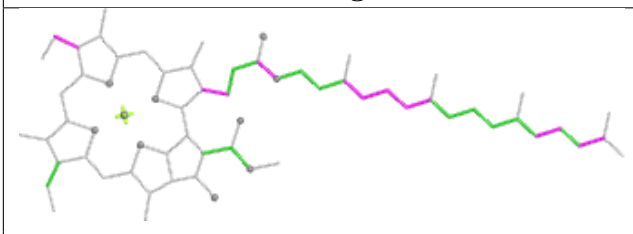

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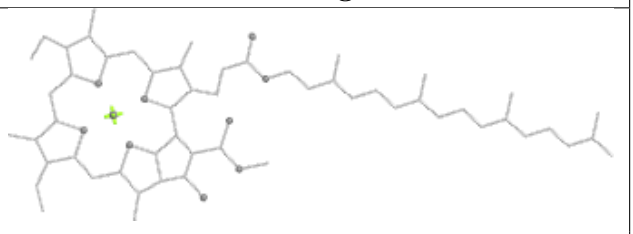
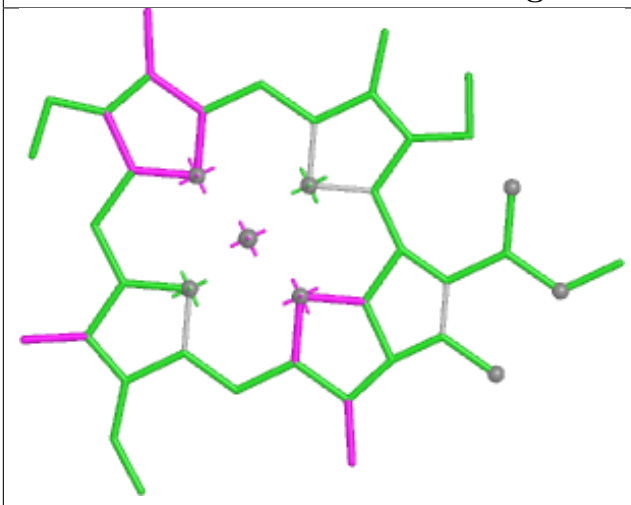


Rings

Ligand CLA L 206



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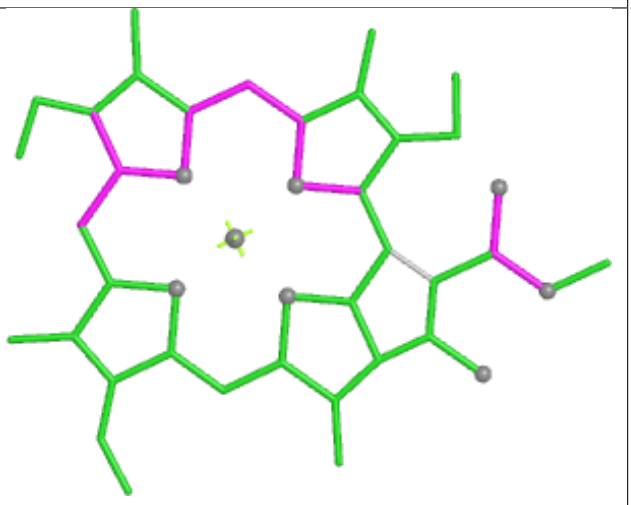
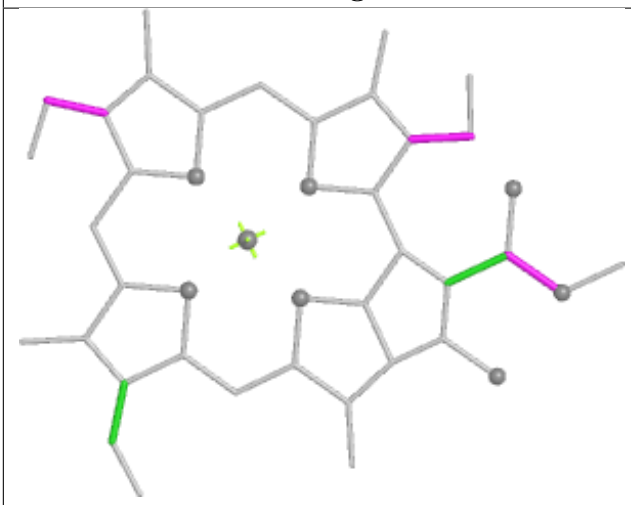


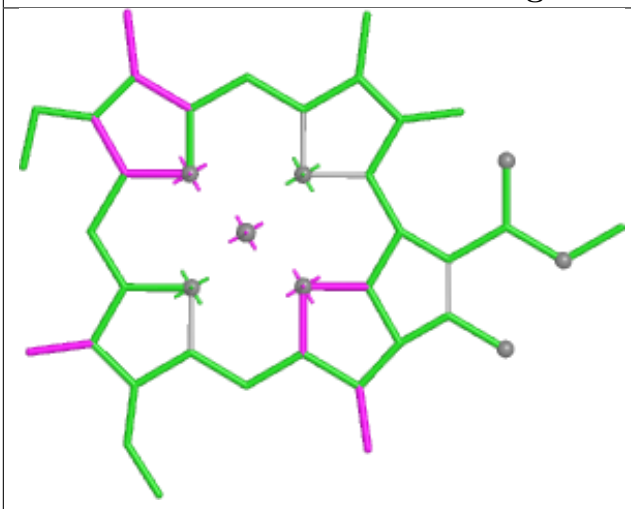
Bond angles



Torsions

Rings

Ligand CLA L 209



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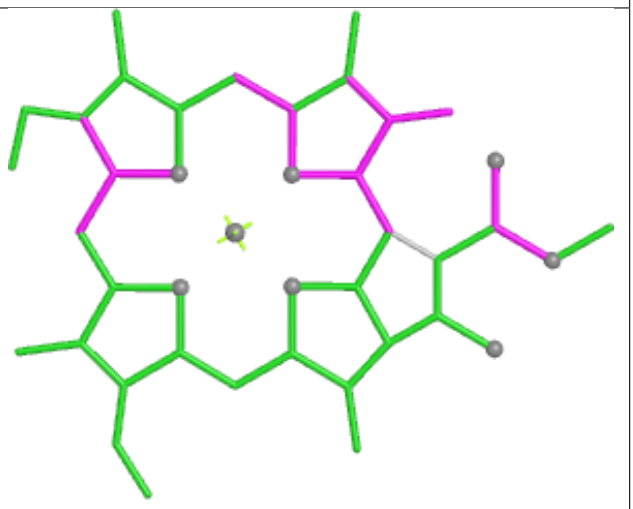

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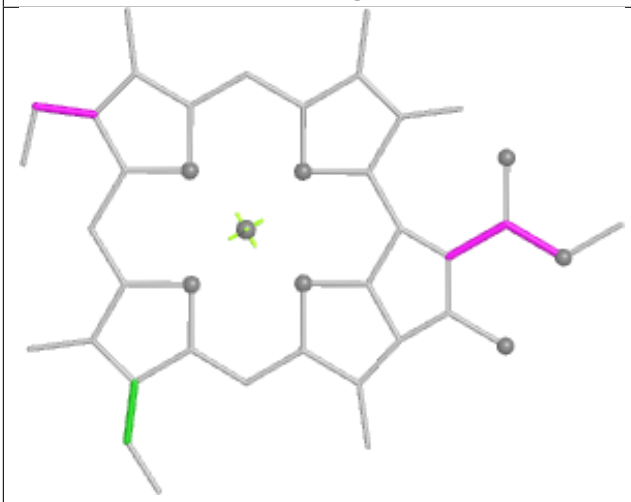

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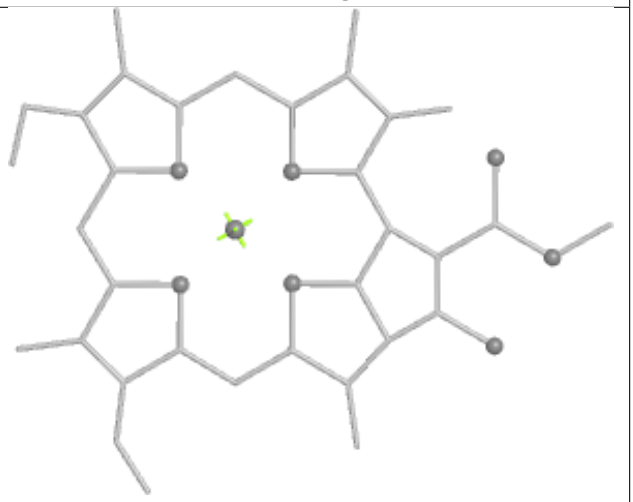
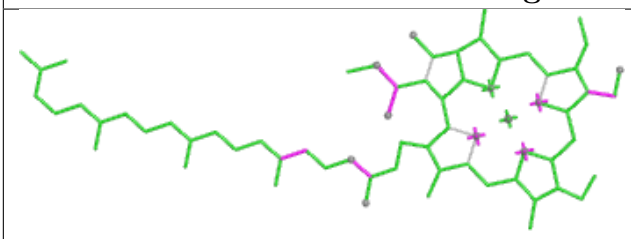


Rings

Ligand CHL Q 608



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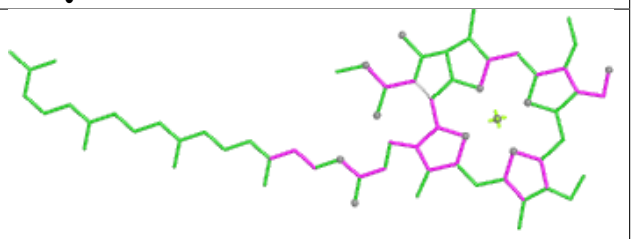
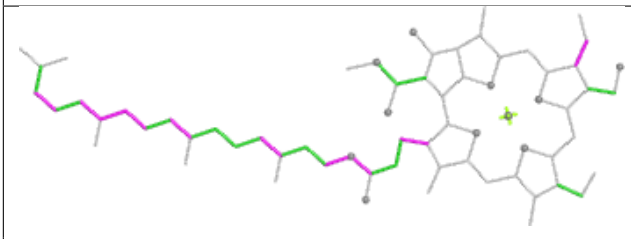


Bond angles



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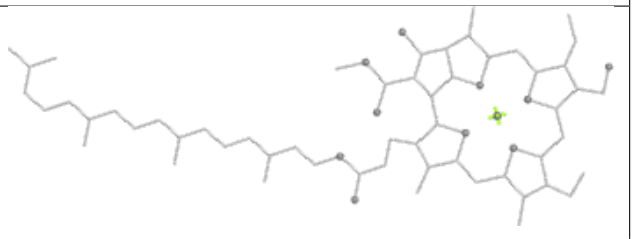
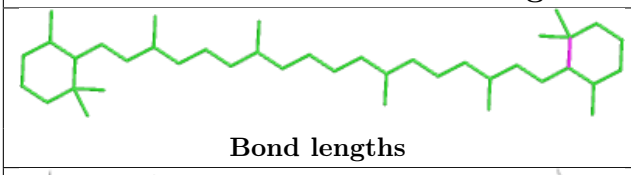


Rings

Ligand BCR 3 319



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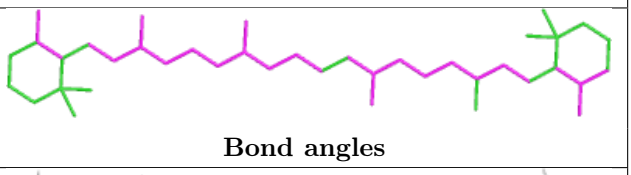
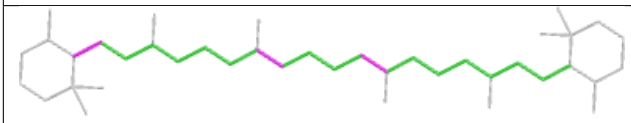


Bond angles



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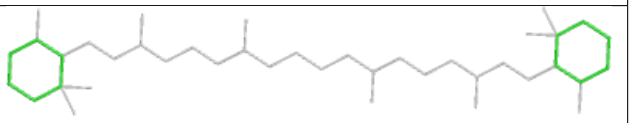
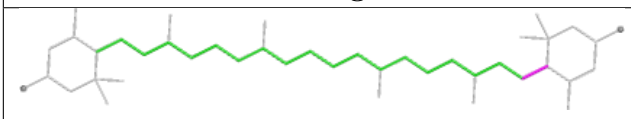


Rings

Ligand LUT a 314

Bond lengths

Bond angles



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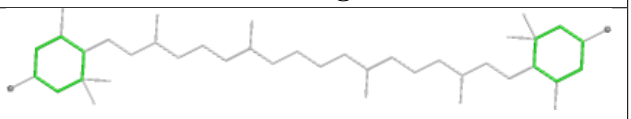
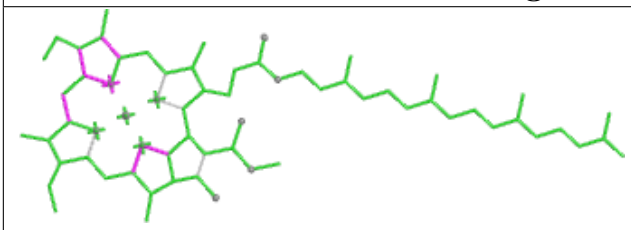


Rings

Ligand CLA P 602



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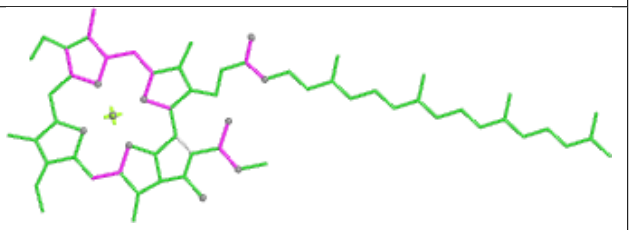
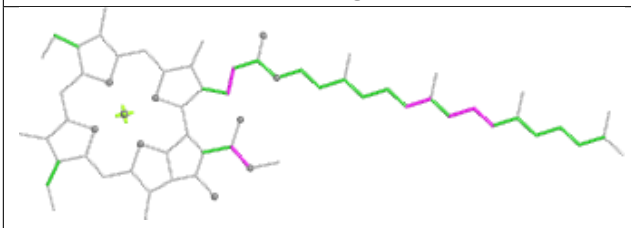


Bond angles



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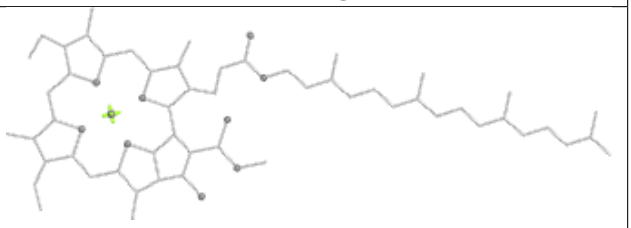
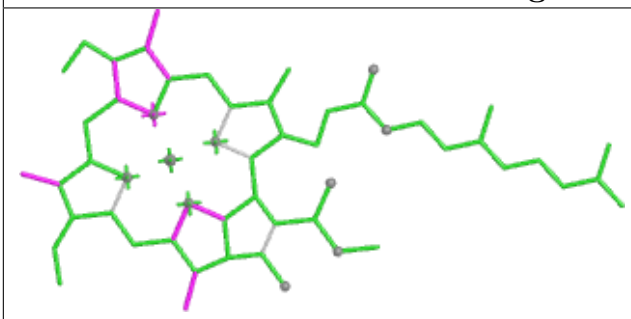


Rings

Ligand CLA 6 611



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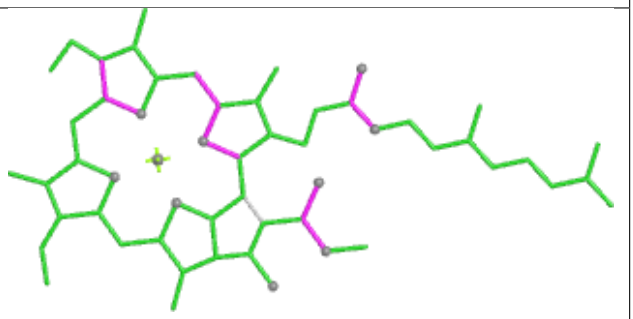
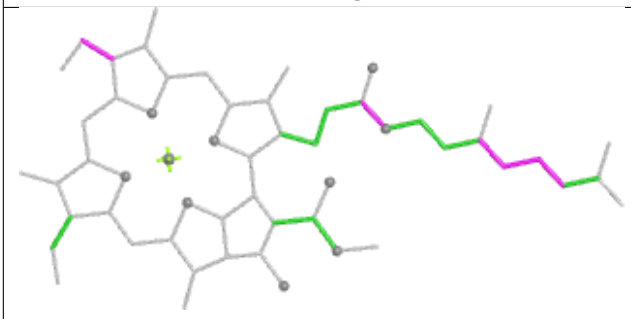


Bond angles



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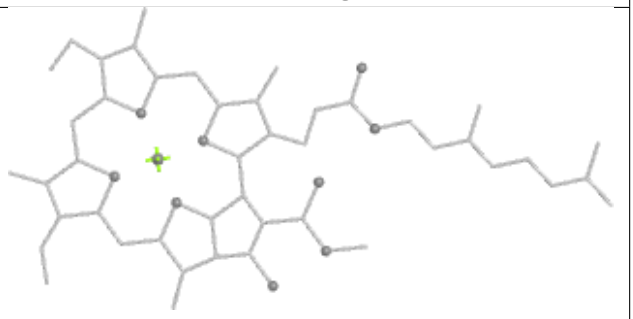
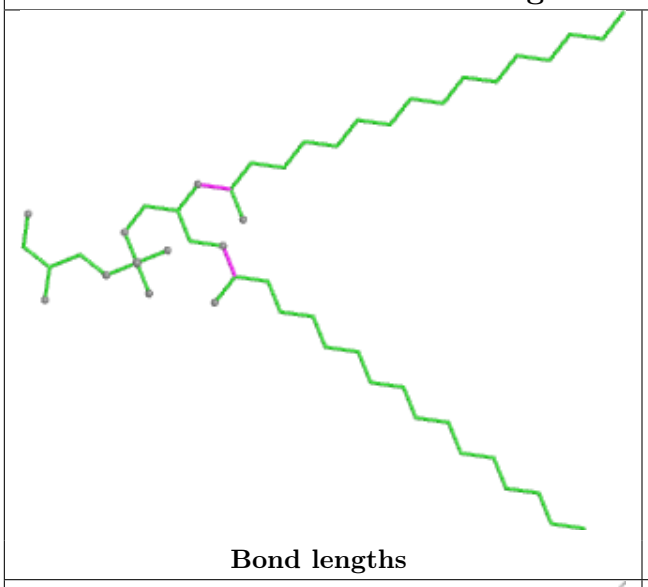


Rings

Ligand LHG S 319



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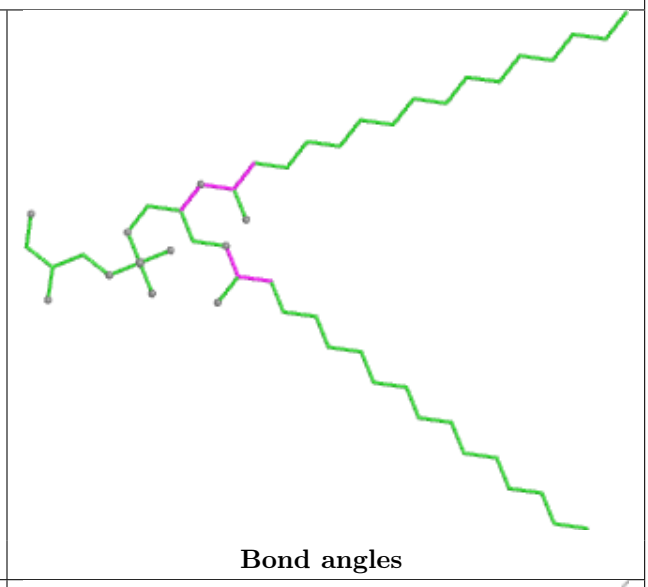
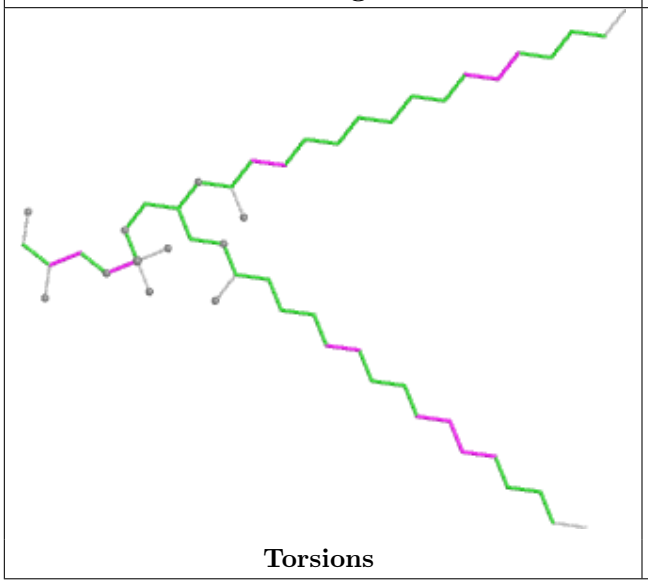


Bond angles



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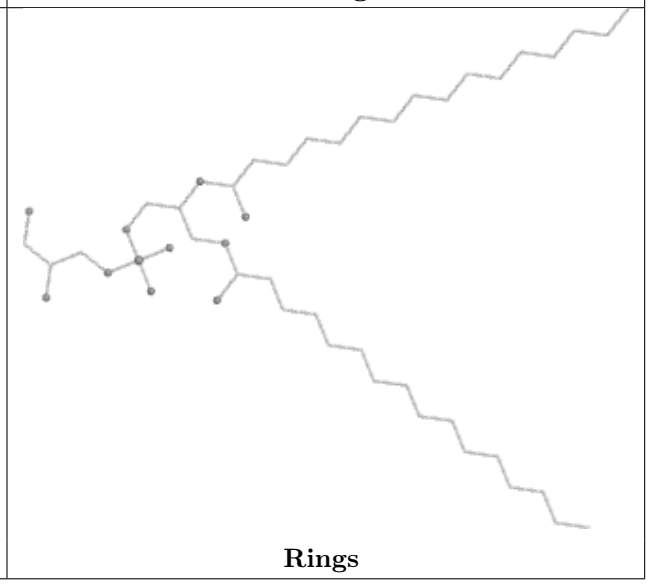
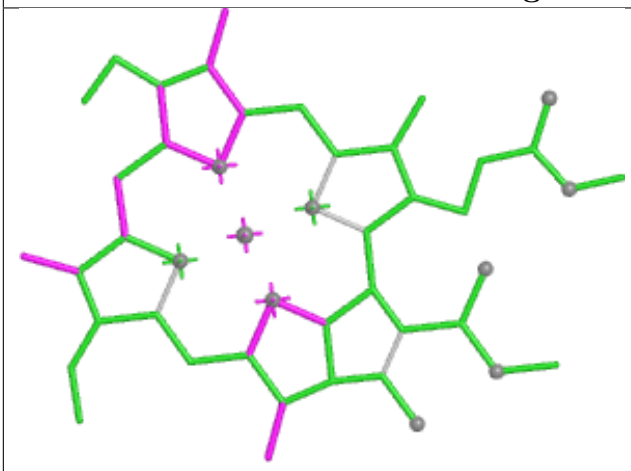
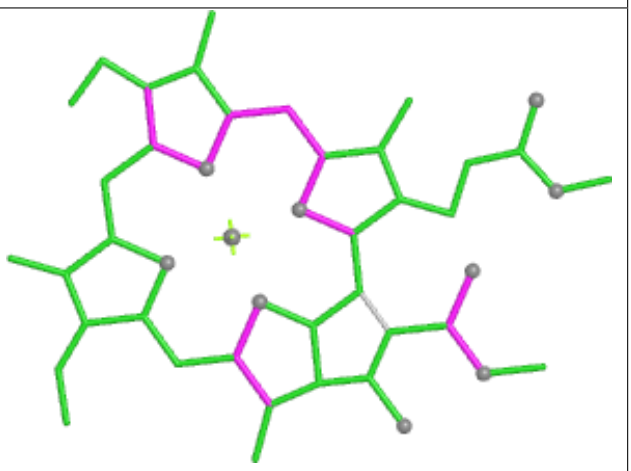


Rings

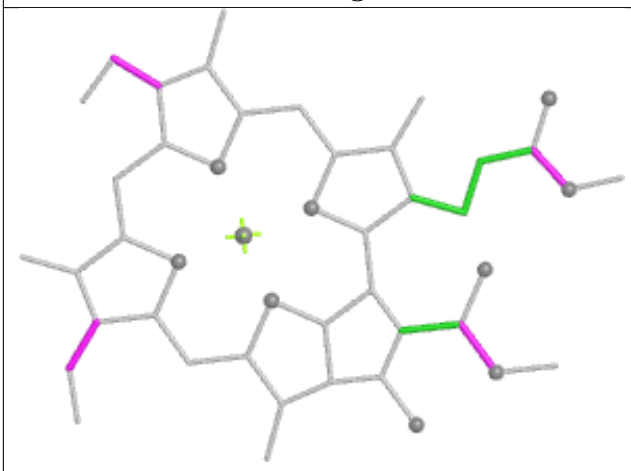
Ligand CLA K 203



Bond lengths



Bond angles



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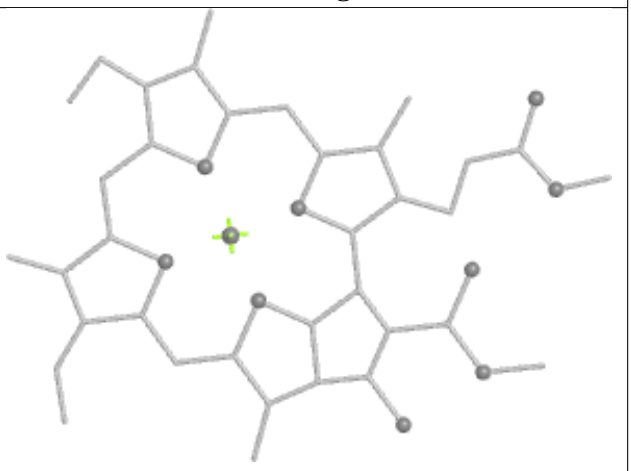
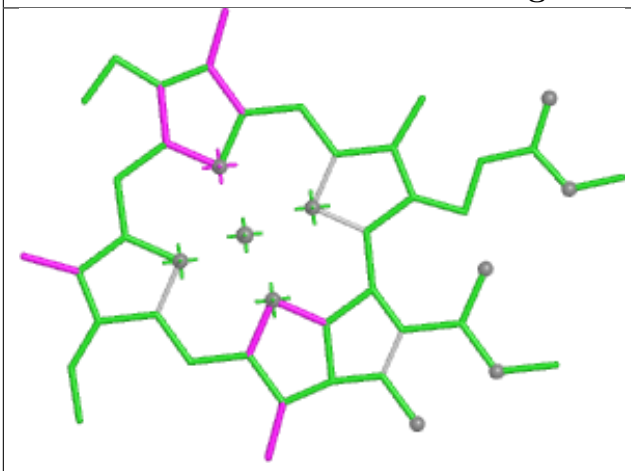
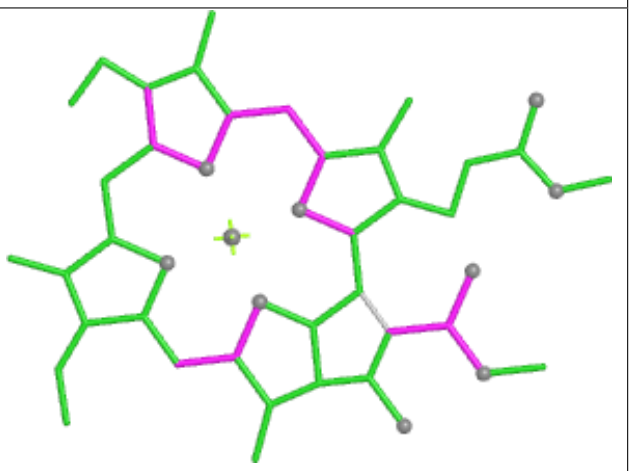


Rings

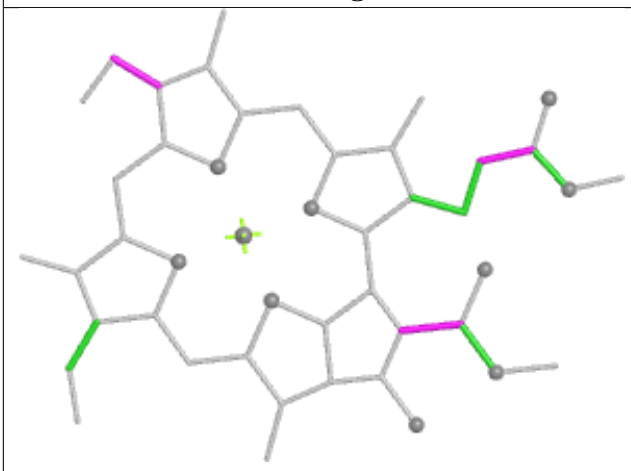
Ligand CLA 6 616



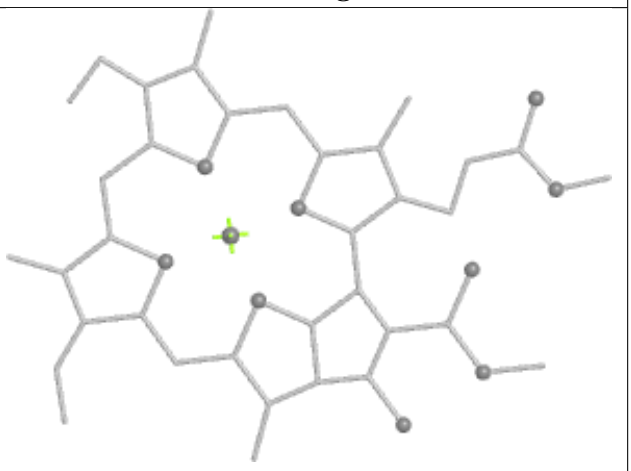
Bond lengths



Bond angles

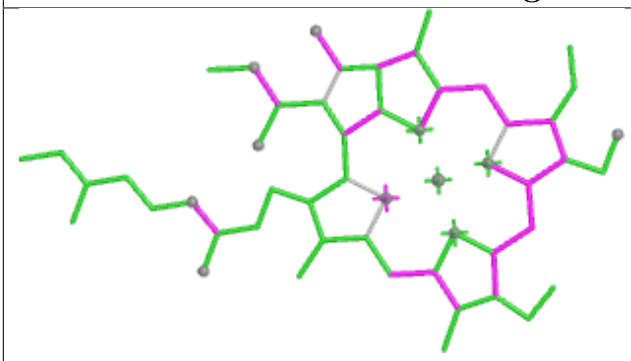


Torsions



Rings

Ligand CHL R 607



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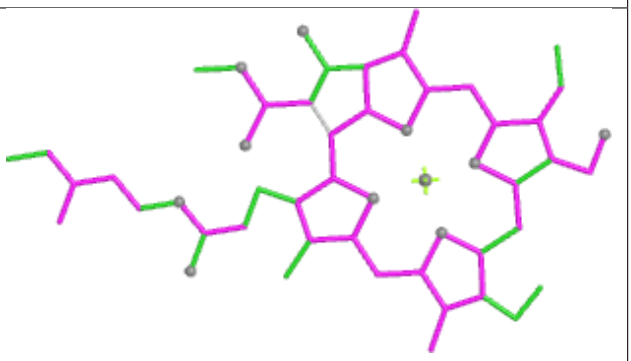
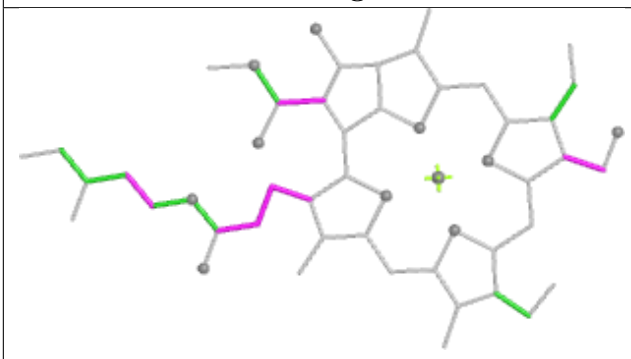


Bond angles



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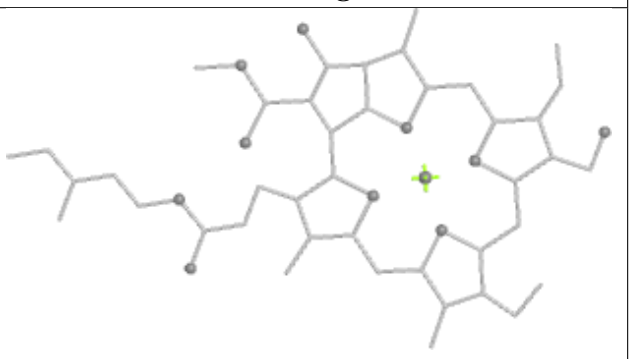
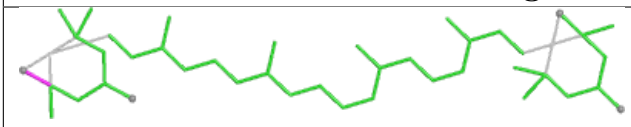


Rings

Ligand XAT Q 616



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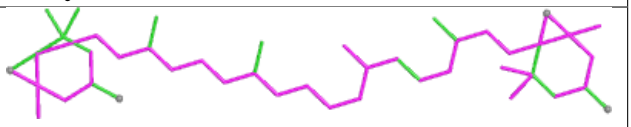
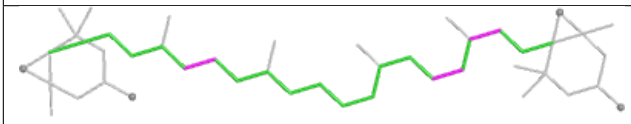
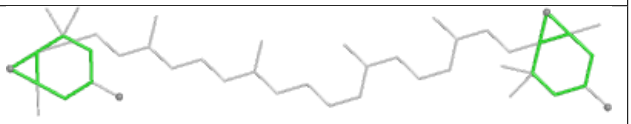


Bond angles

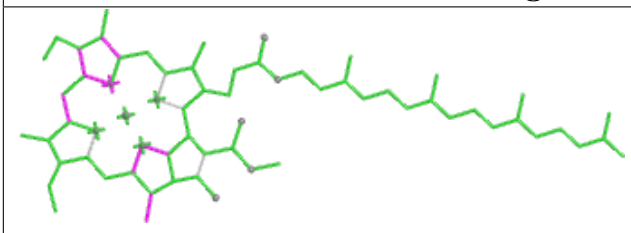


Torsions

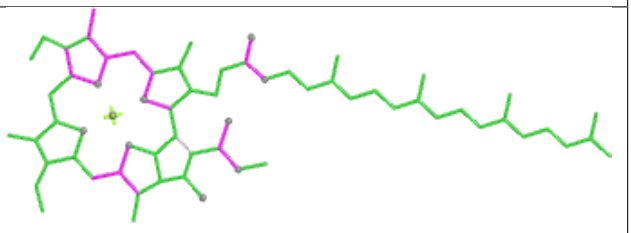


Rings

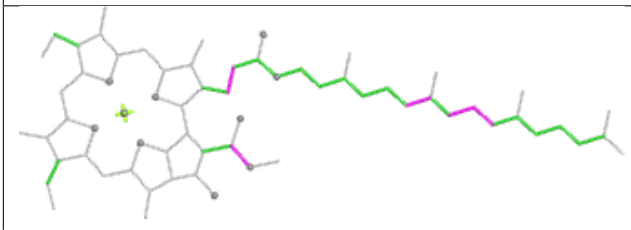
Ligand CLA T 602



Bond lengths



Bond angles



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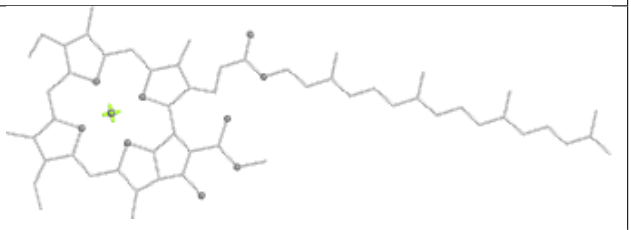
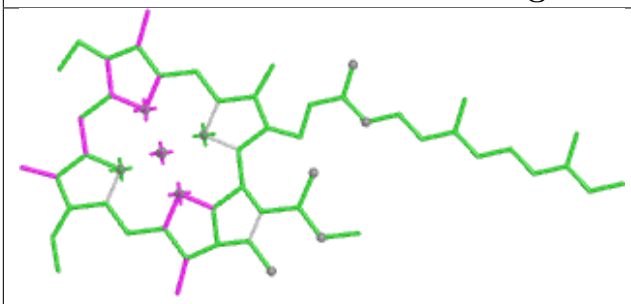
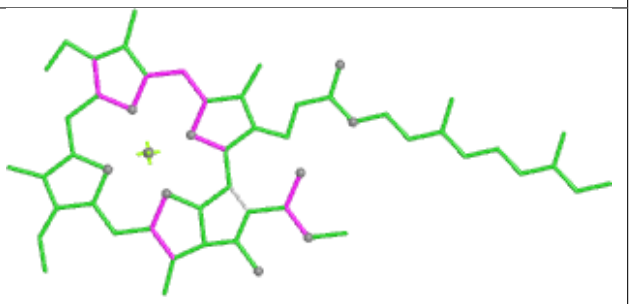
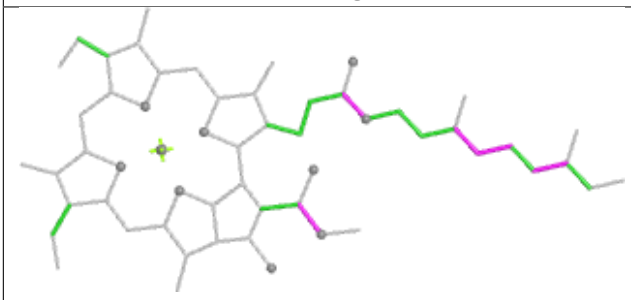
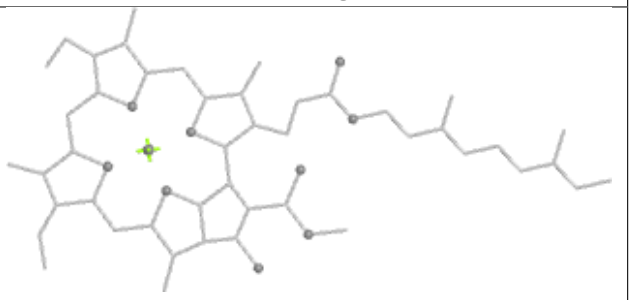
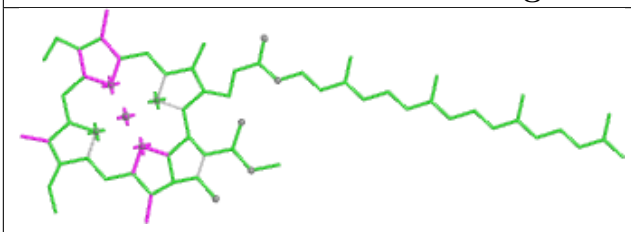
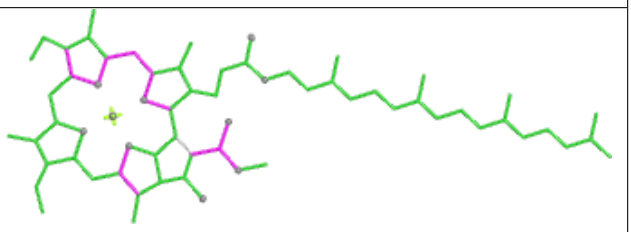
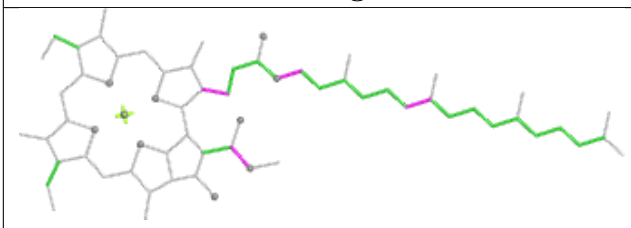
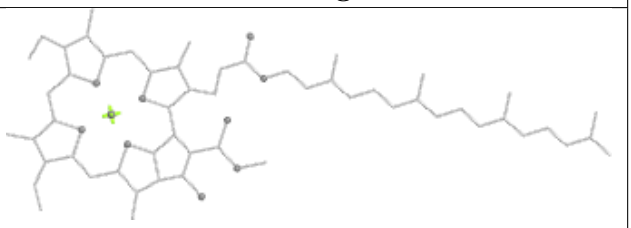
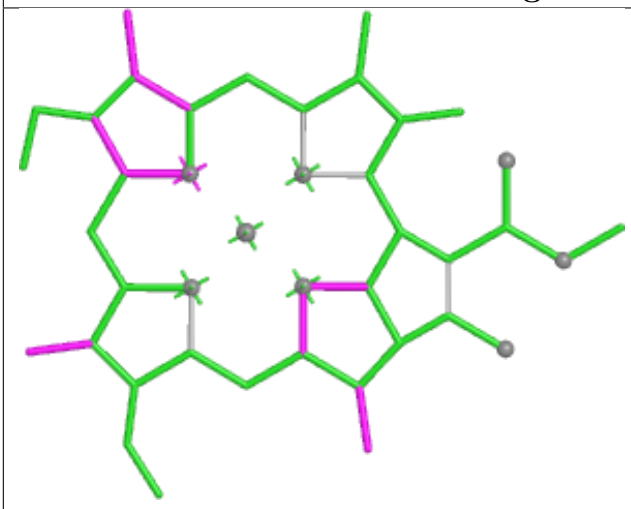


Rings

Ligand CLA 7 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 202



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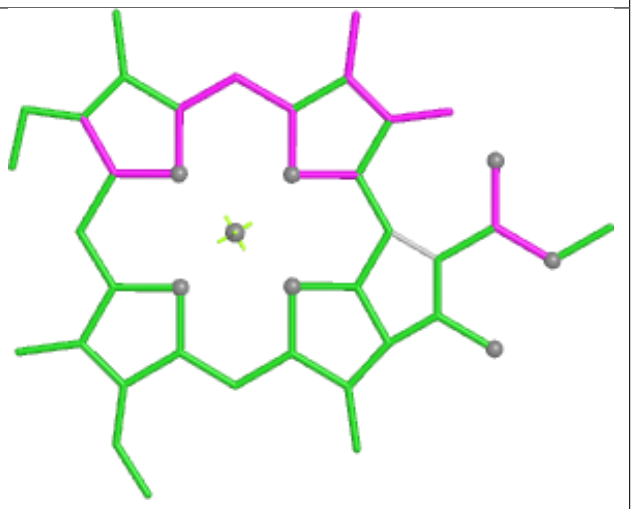
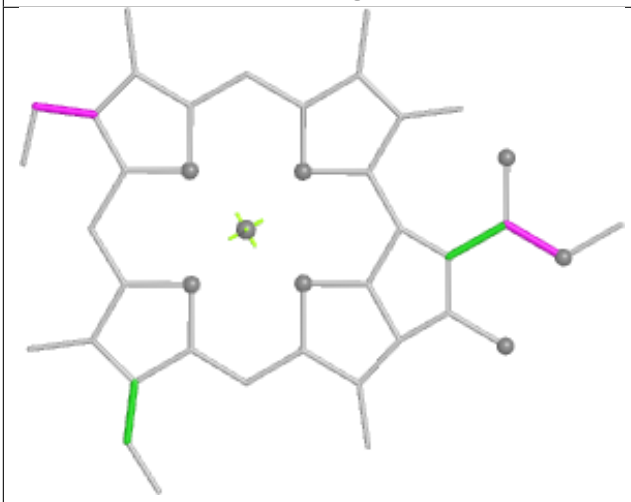
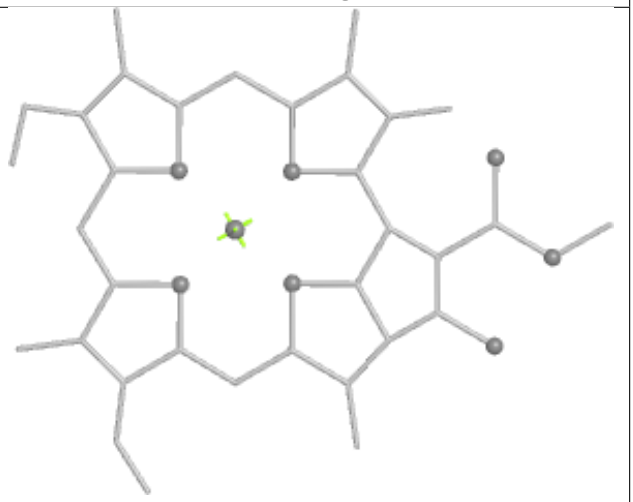


Bond angles

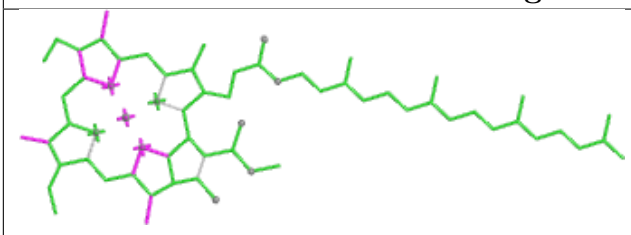


Torsions



Rings

Ligand CLA B 811



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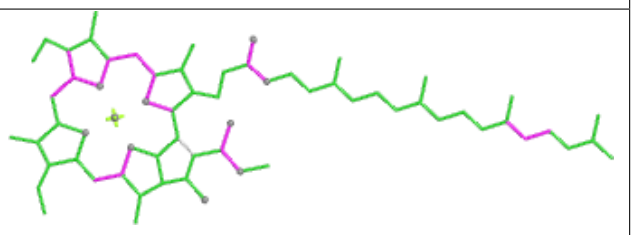

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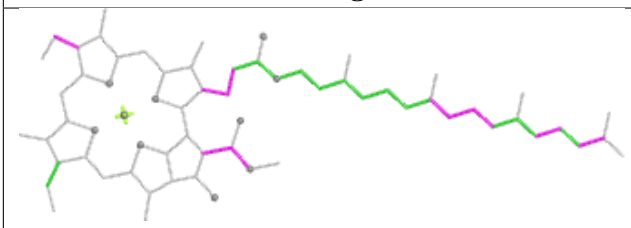

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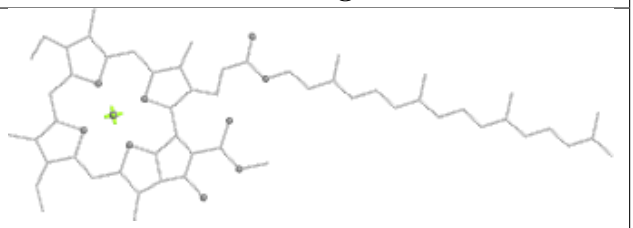
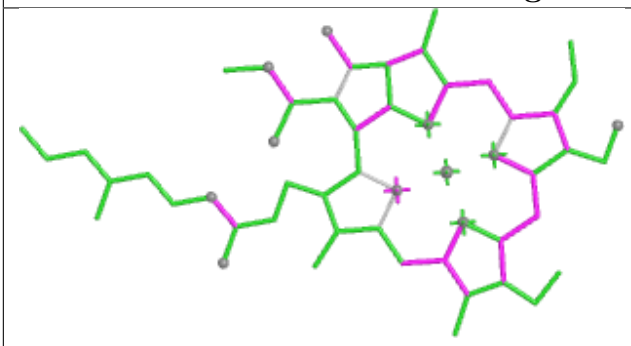


Rings

Ligand CHL P 622



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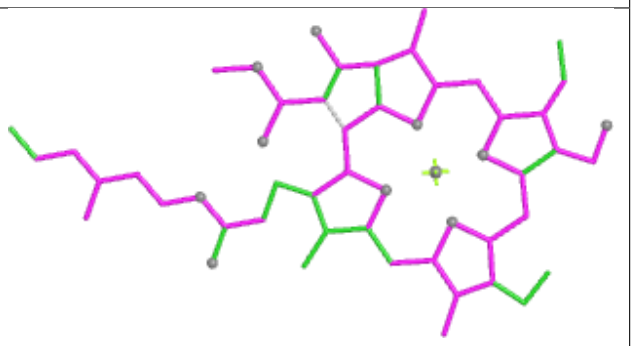
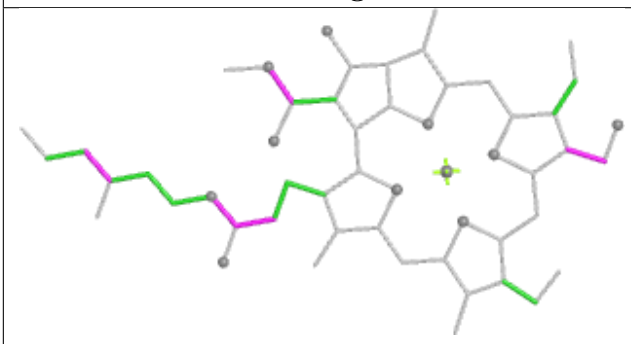


Bond angles



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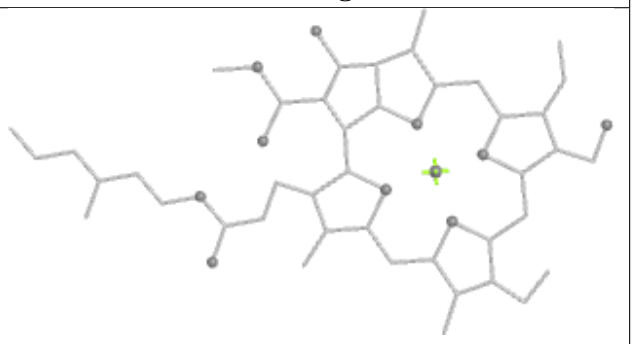
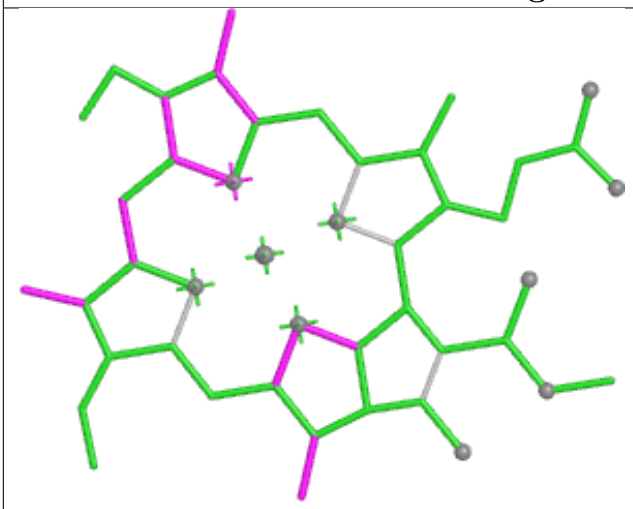


Rings

Ligand CLA 9 311



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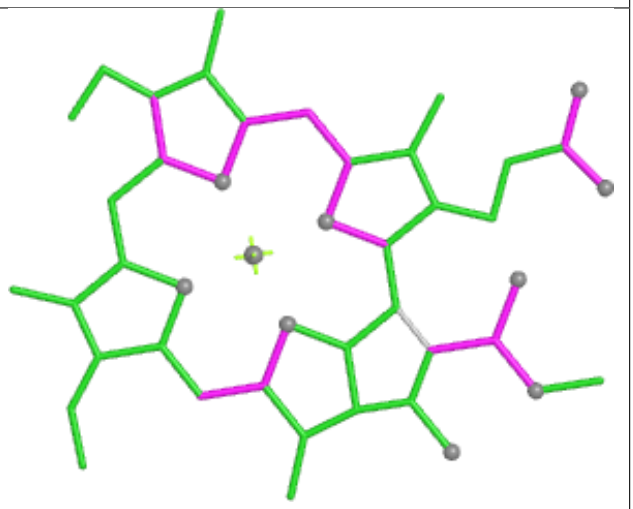
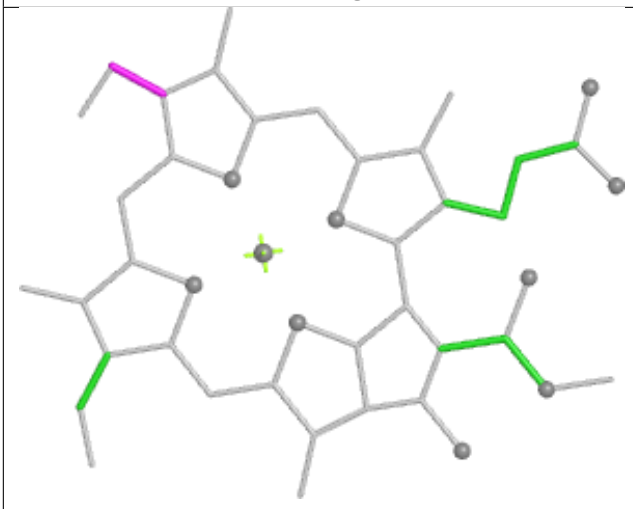


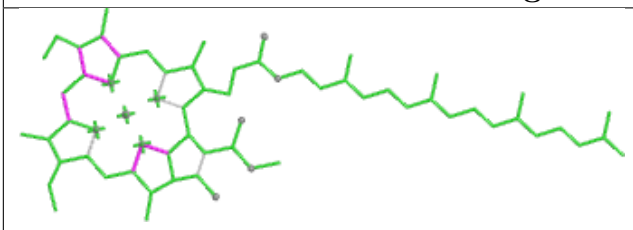
Bond angles



Torsions

Rings

Ligand CLA R 603



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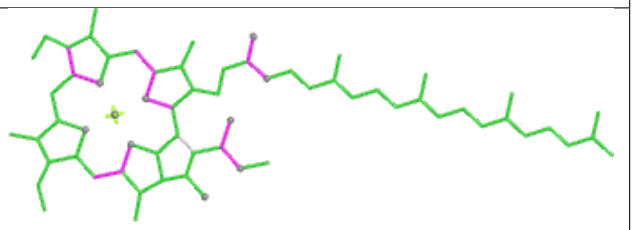
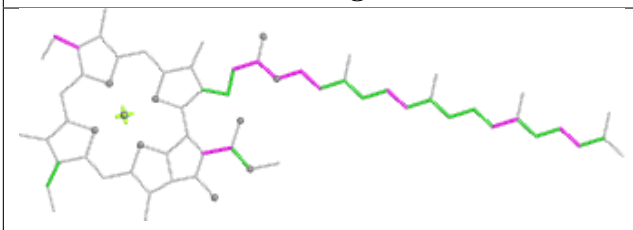
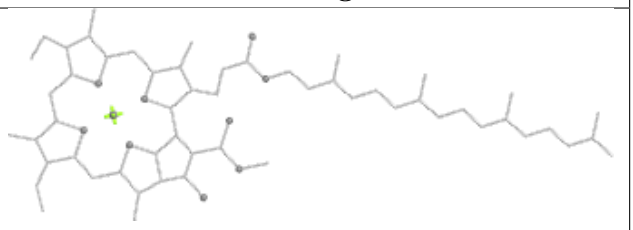


Bond angles

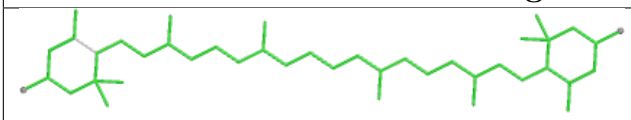


Torsions



Rings

Ligand LUT P 614



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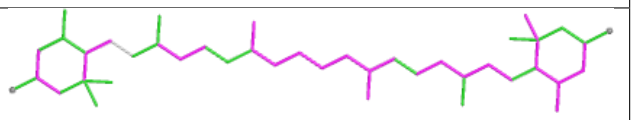
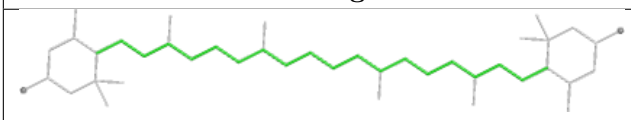


Bond angles



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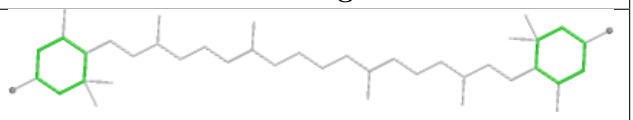
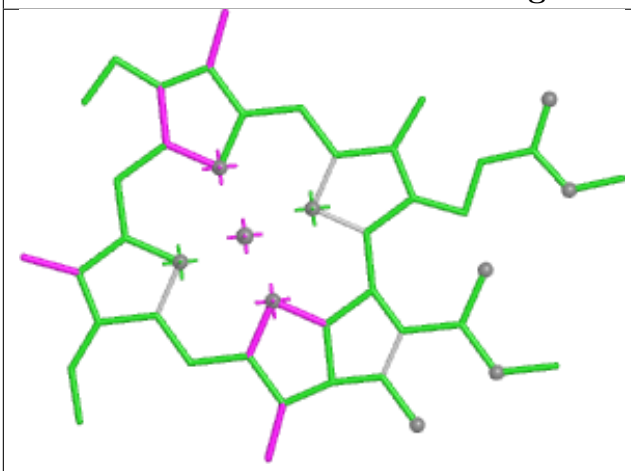


Rings

Ligand CLA 9 304



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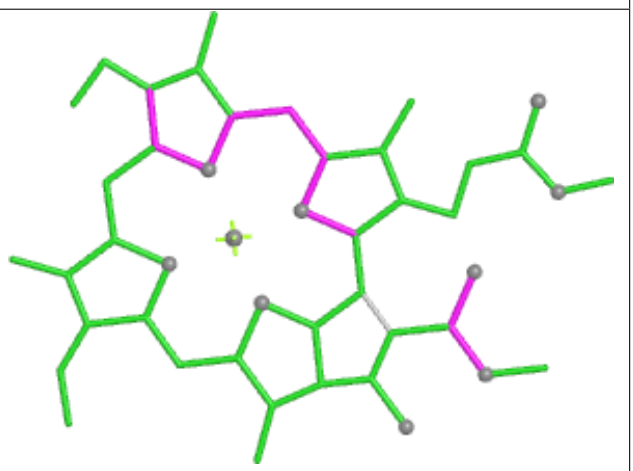
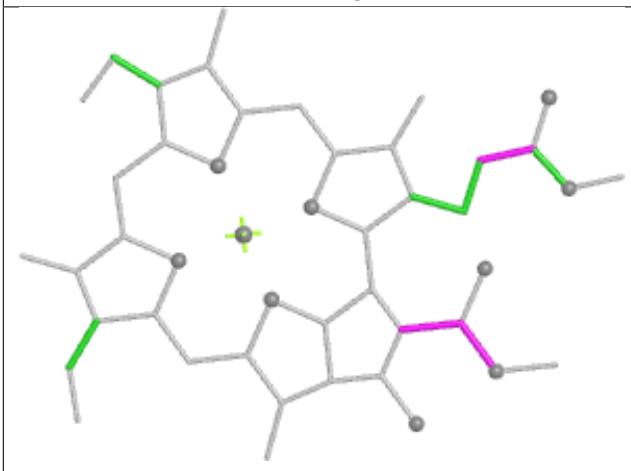
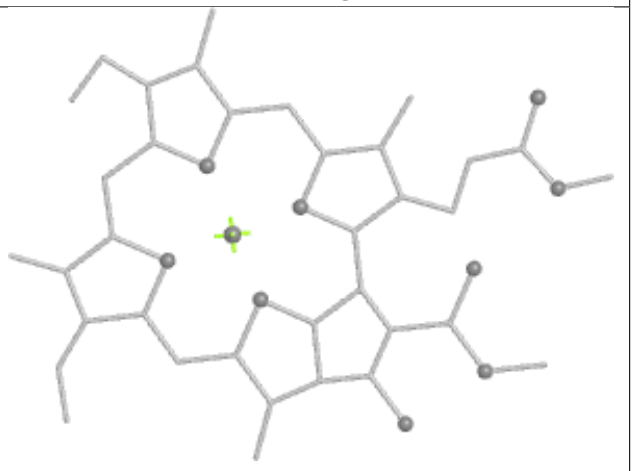


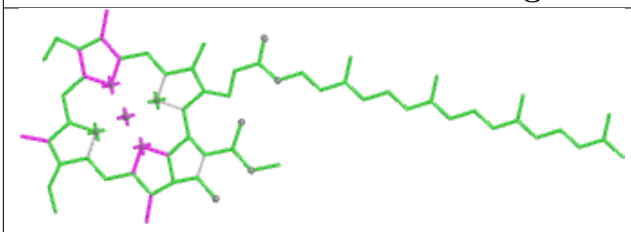
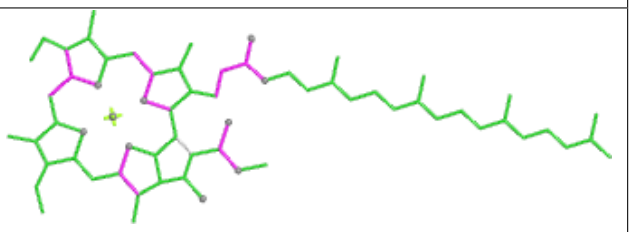
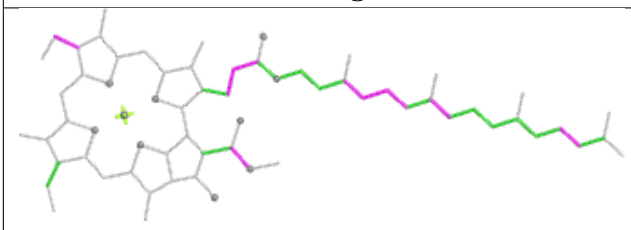
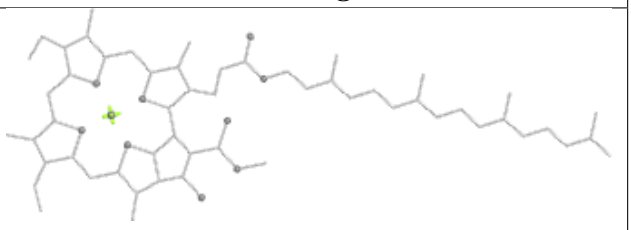
Bond angles

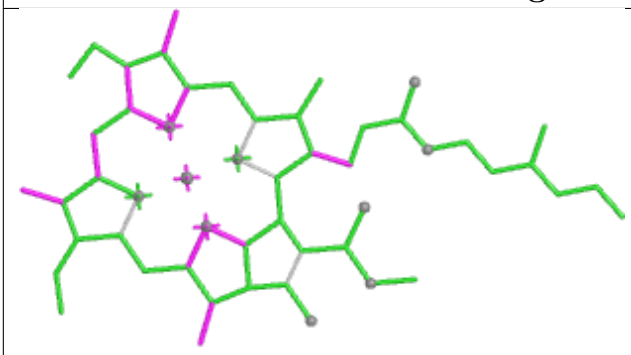
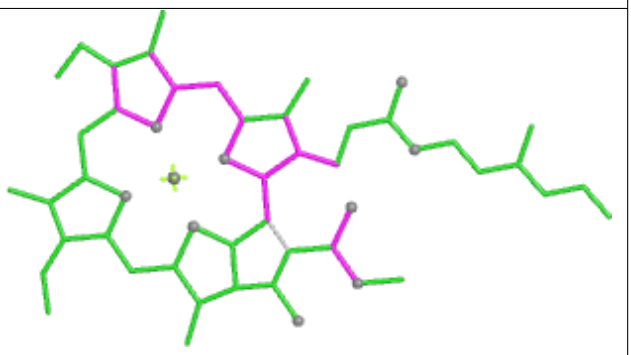
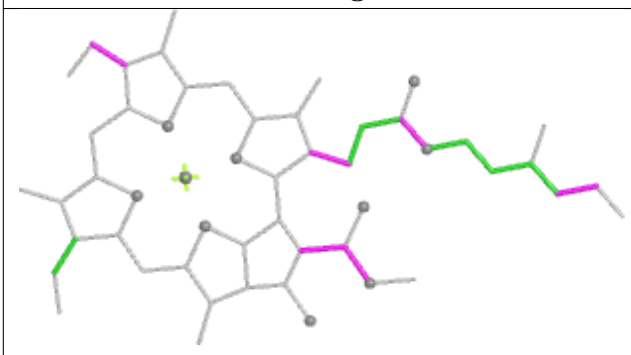
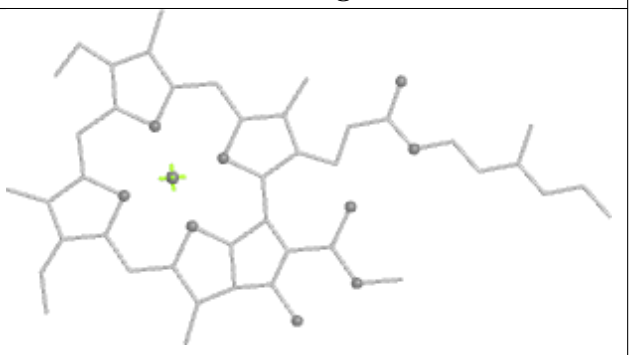


Torsions

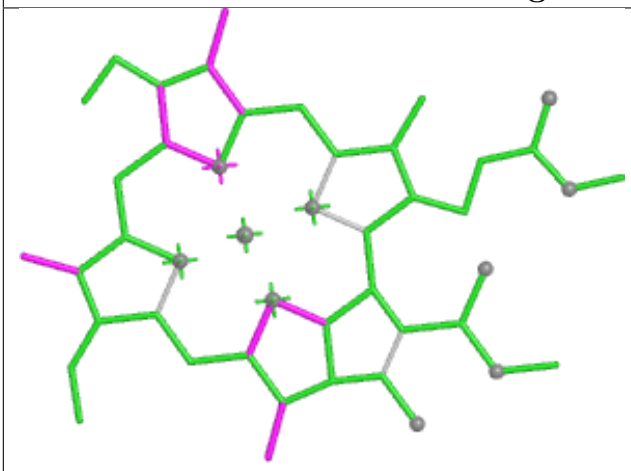


Rings

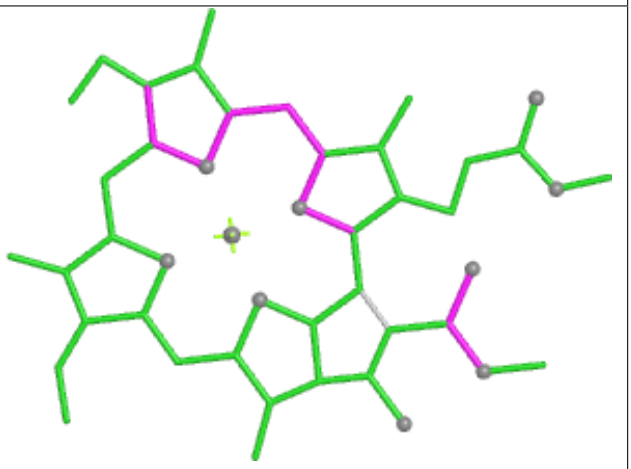
Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

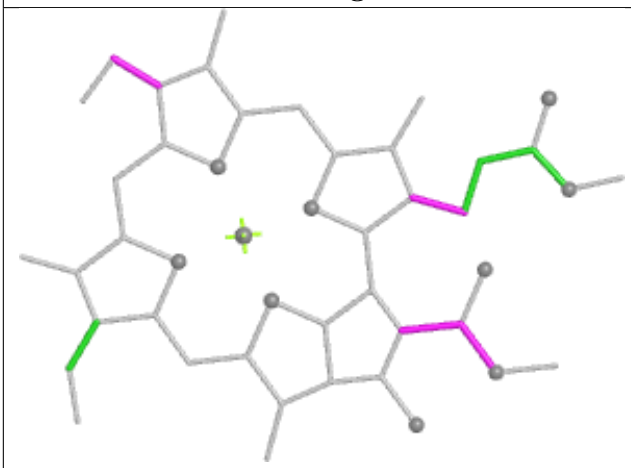
Ligand CLA 5 315



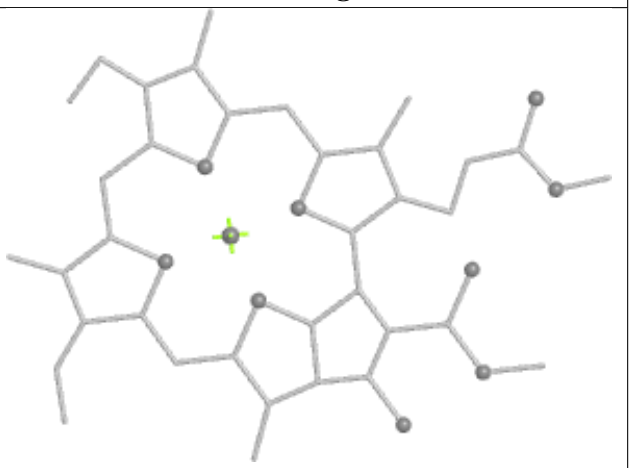
Bond lengths



Bond angles

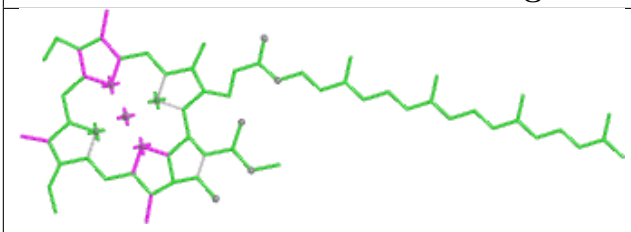


Torsions



Rings

Ligand CLA B 823



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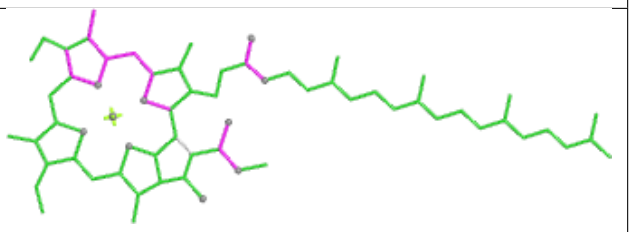
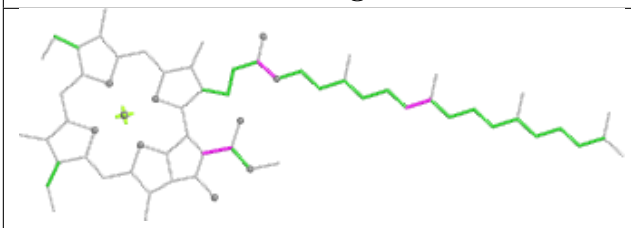


Bond angles



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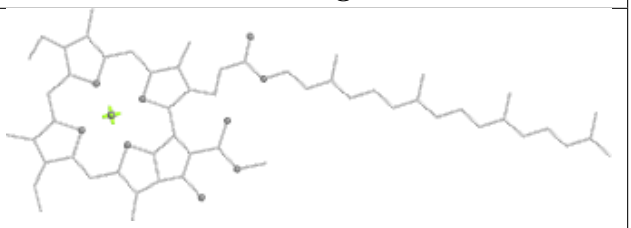
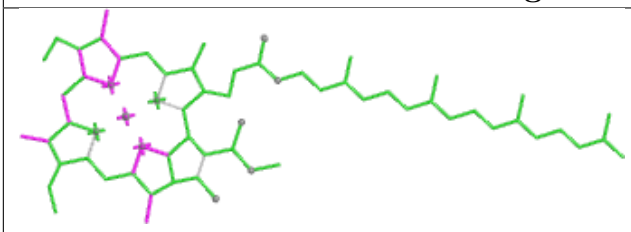


Rings

Ligand CLA B 830



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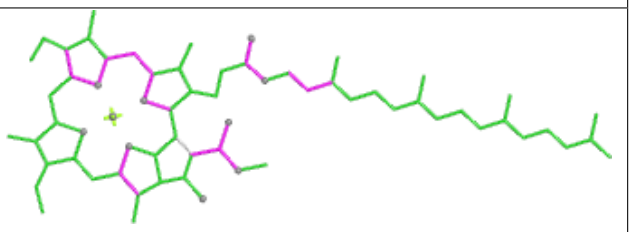

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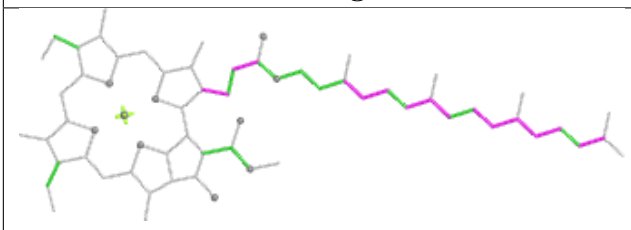

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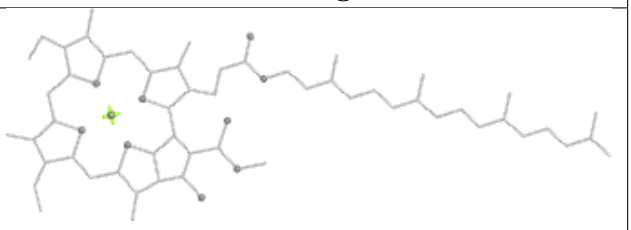
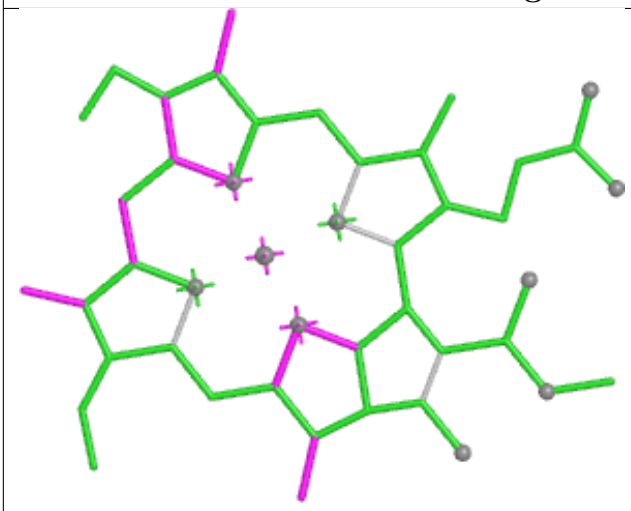


Rings

Ligand CLA B 803



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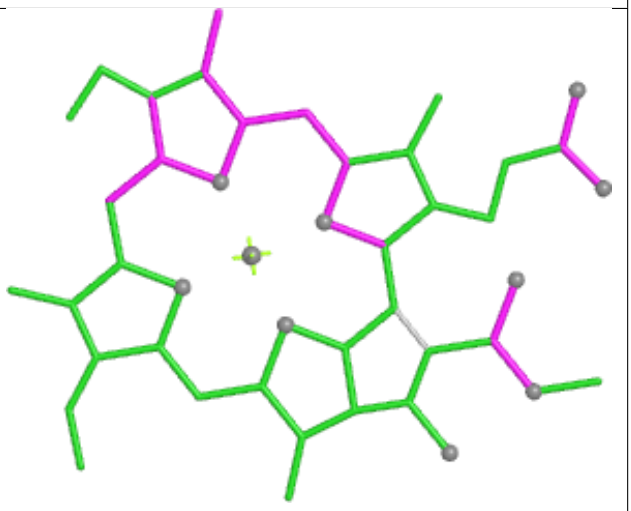

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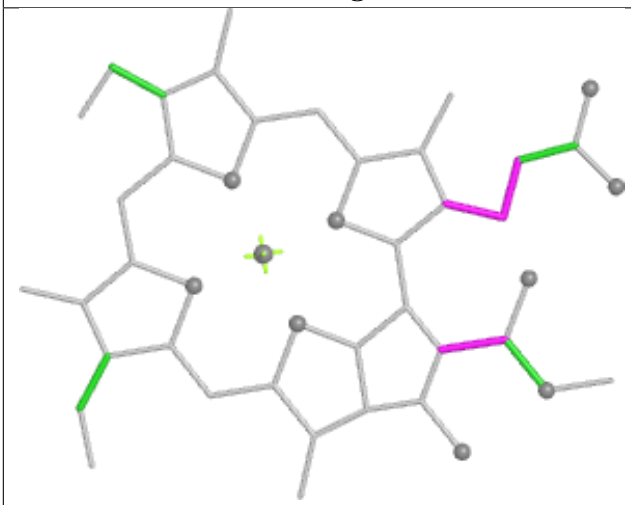

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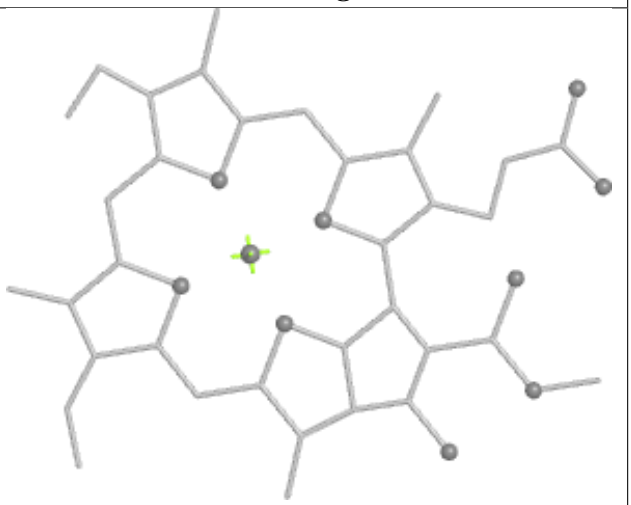
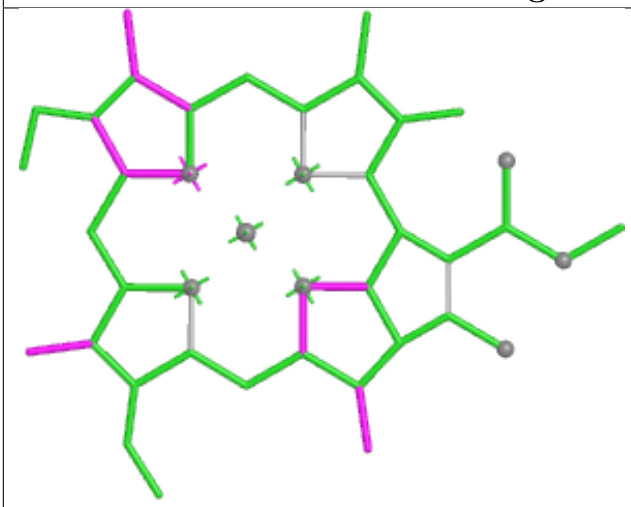


Rings

Ligand CLA 4 313



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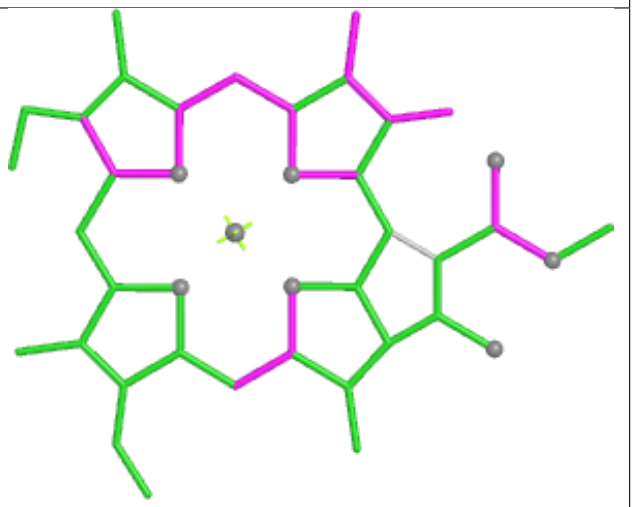

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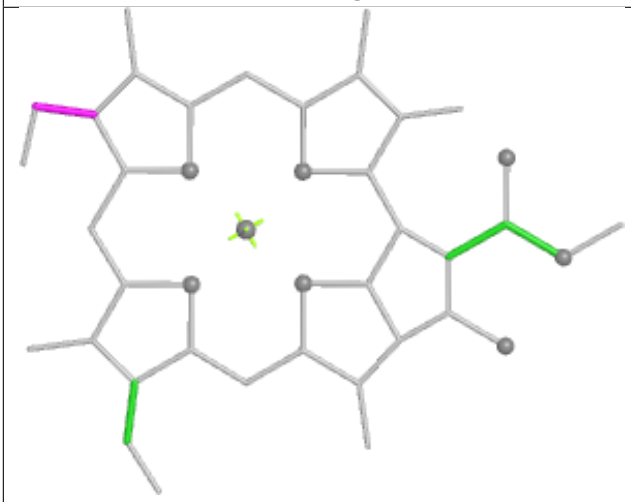

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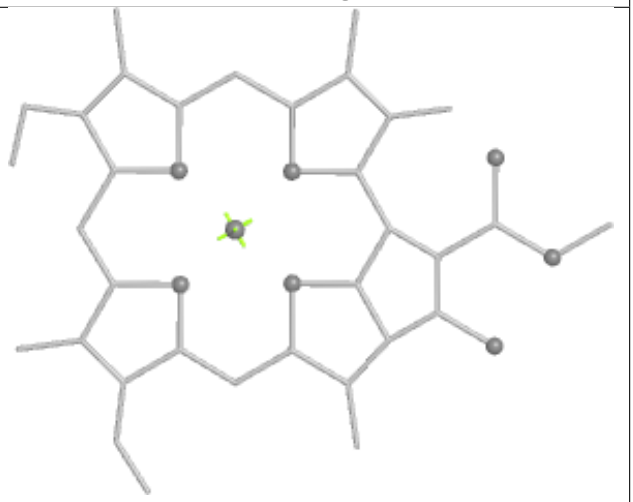
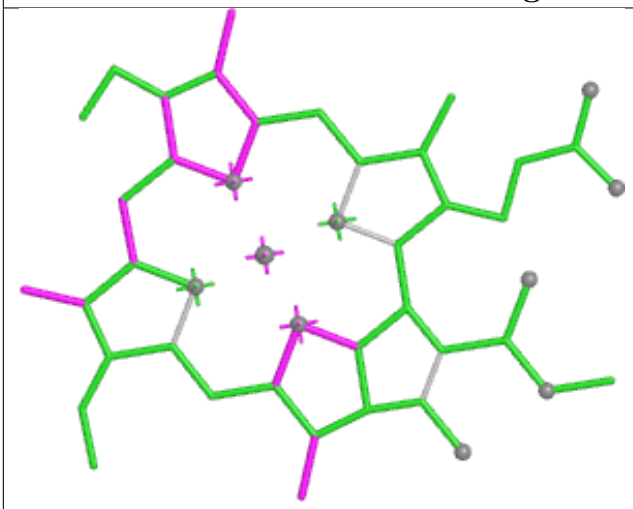


Rings

Ligand CLA K 202



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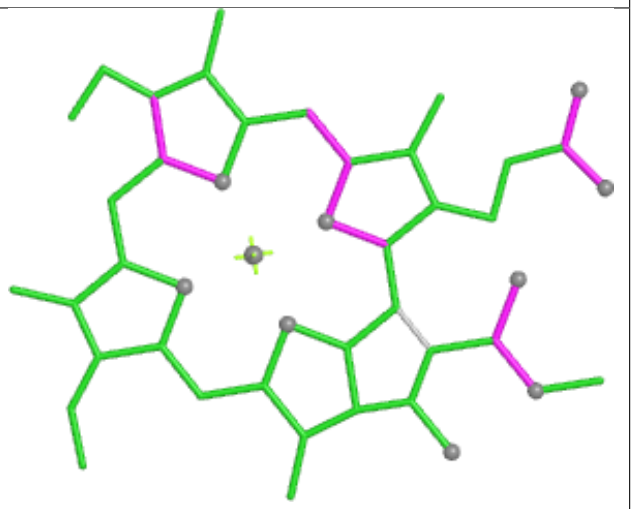

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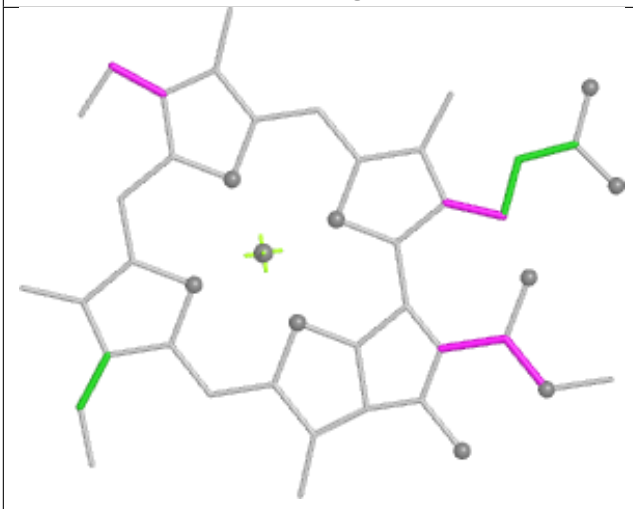
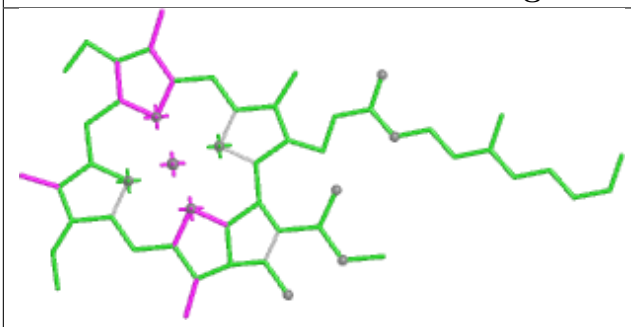


Torsions

Rings

Ligand CLA A 813



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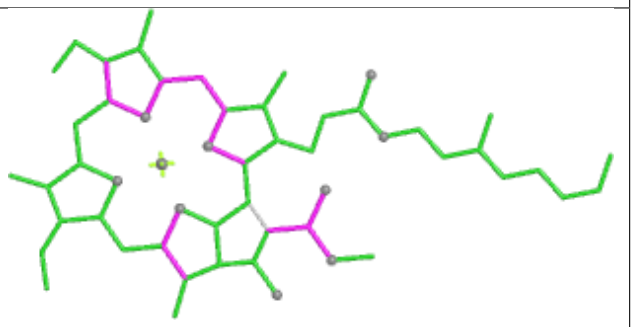

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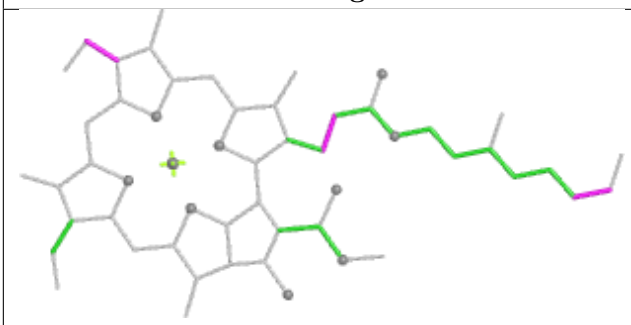

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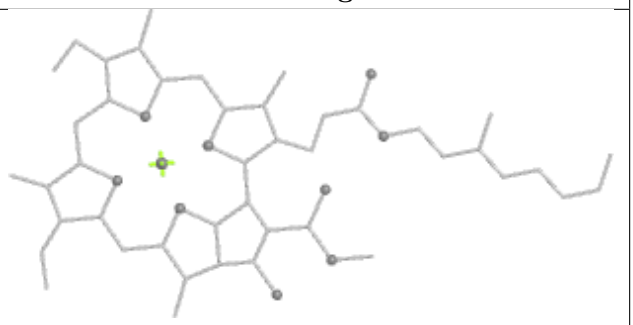
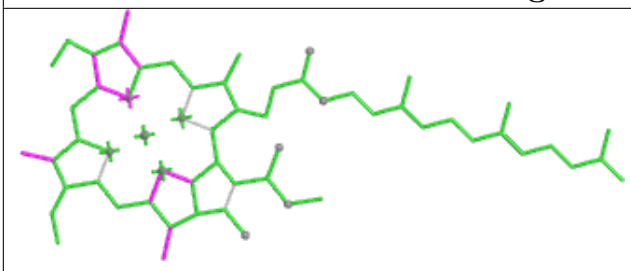


Rings

Ligand CLA 6 610



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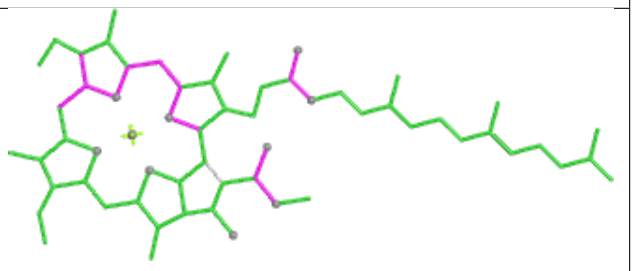

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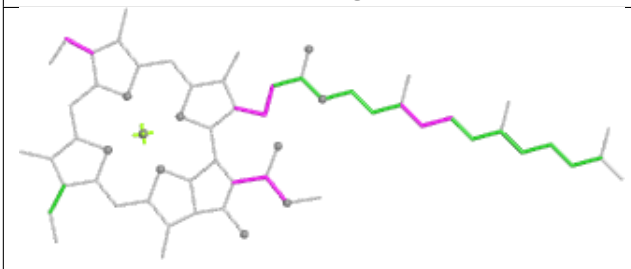

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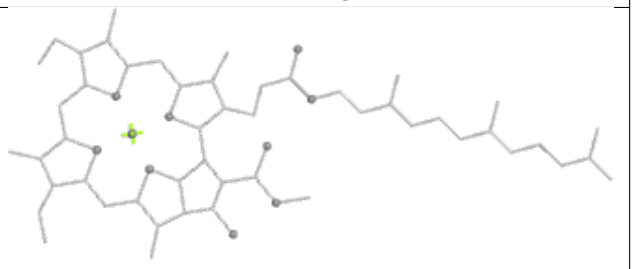
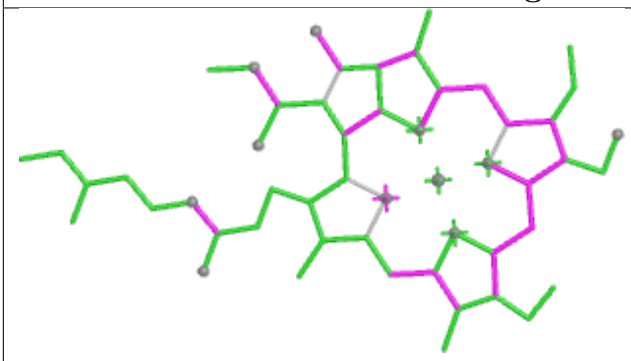


Rings

Ligand CHL T 607



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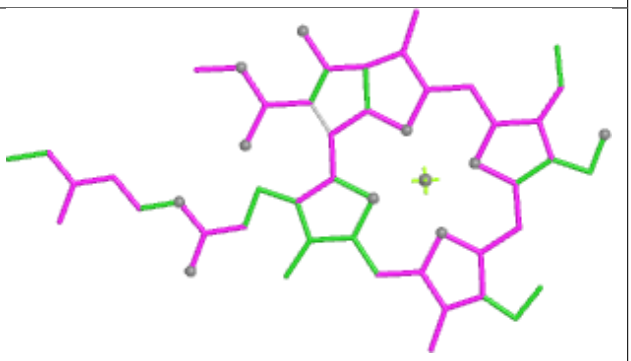

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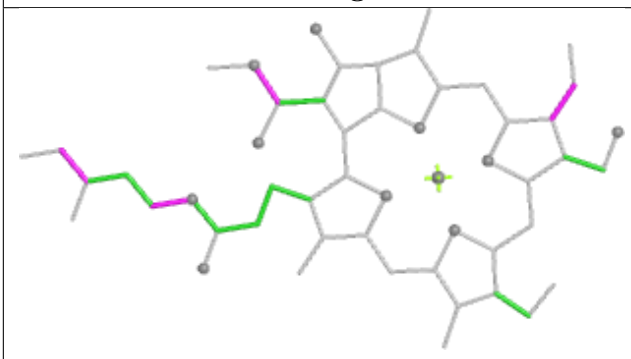

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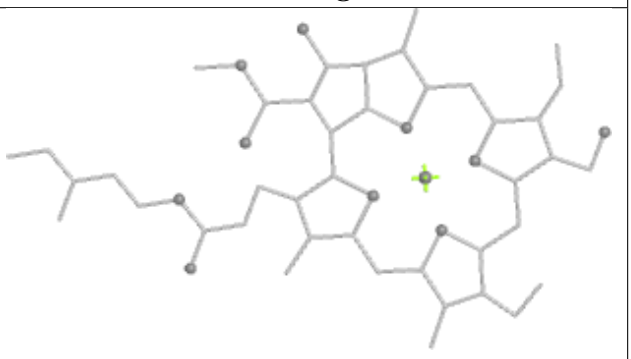
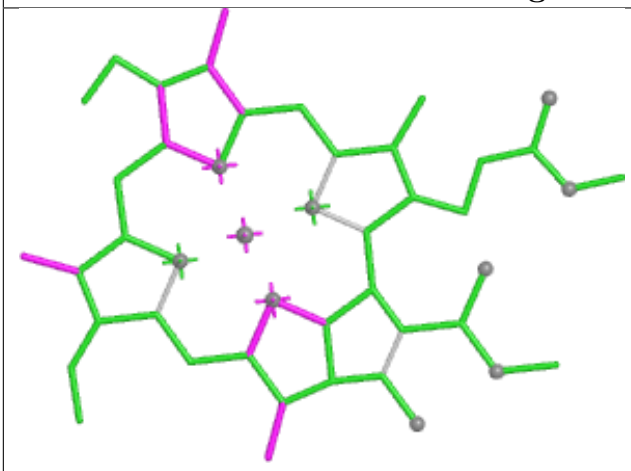


Rings

Ligand CLA 2 314



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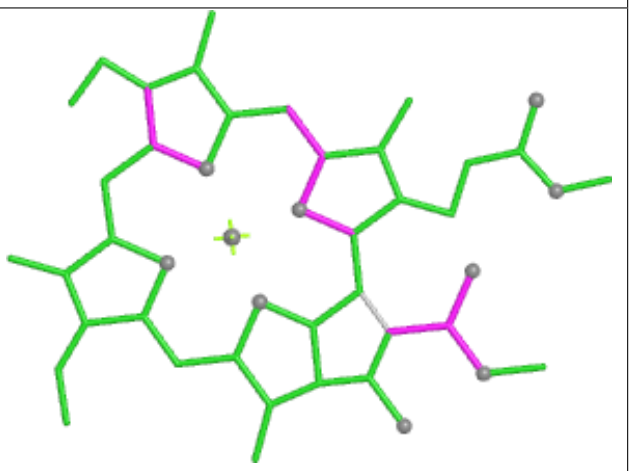

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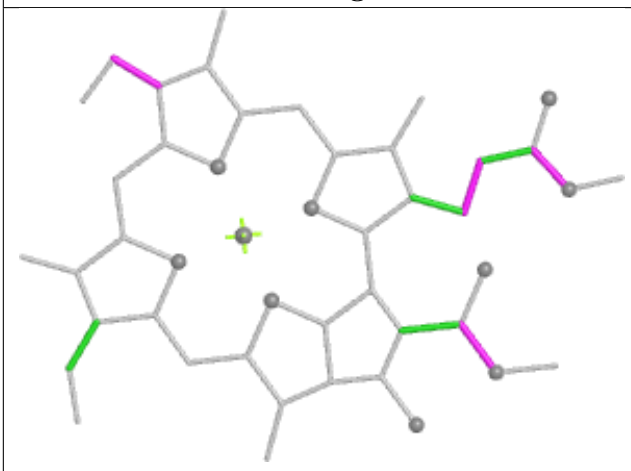

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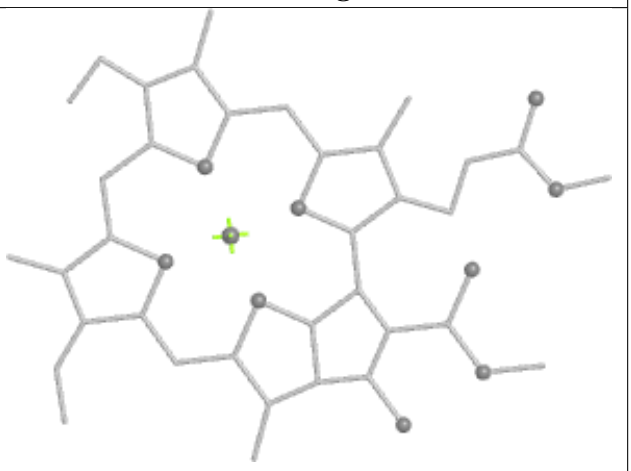
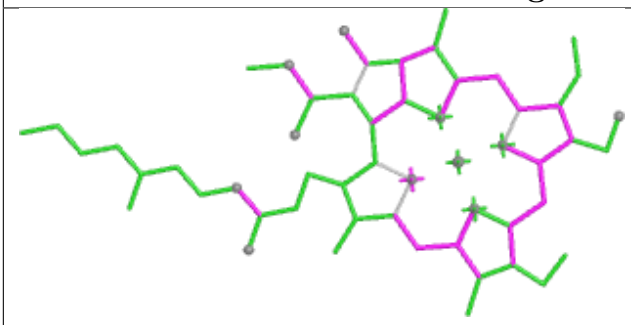


Rings

Ligand CHL 7 305



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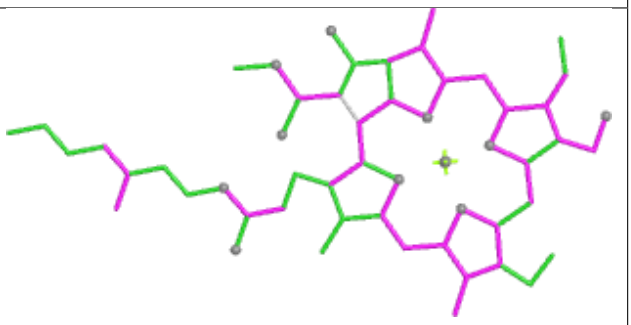

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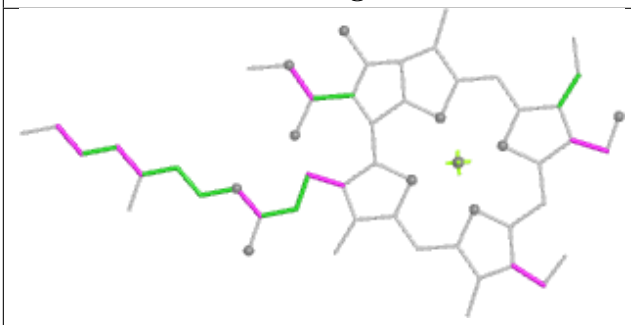

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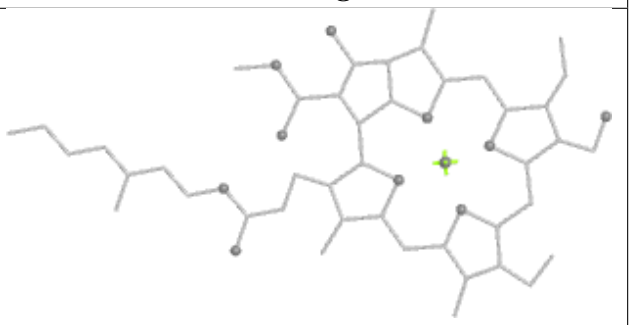
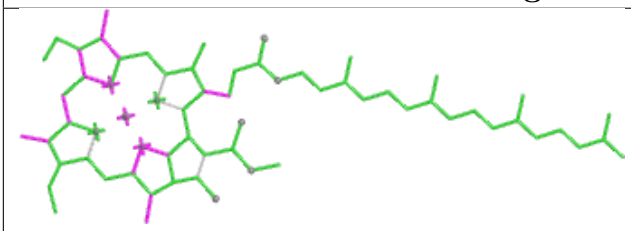


Rings

Ligand CLA A 802



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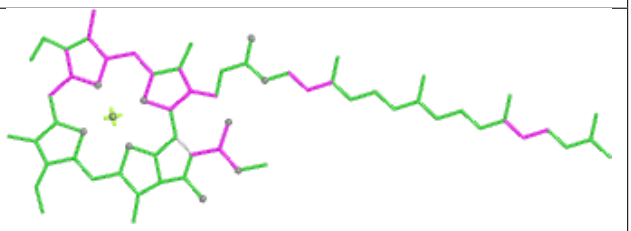

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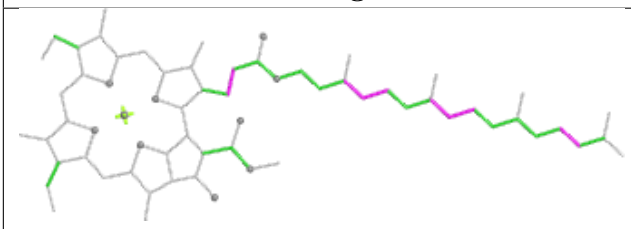

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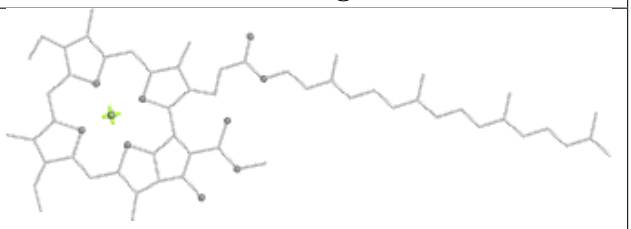
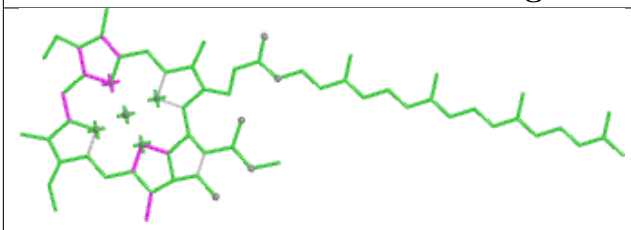
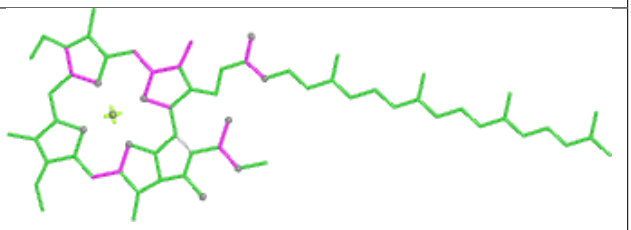
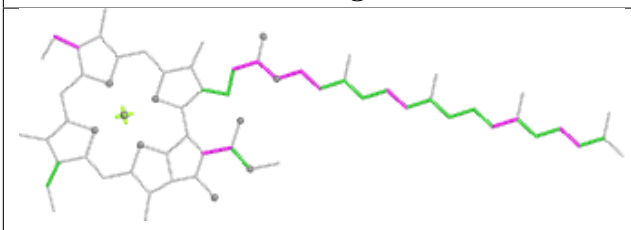
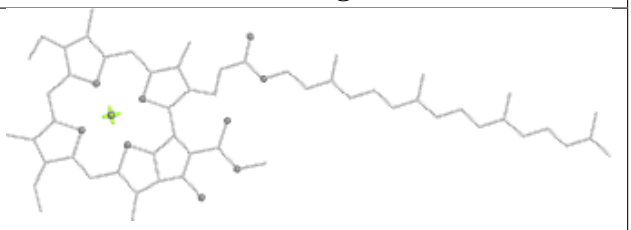
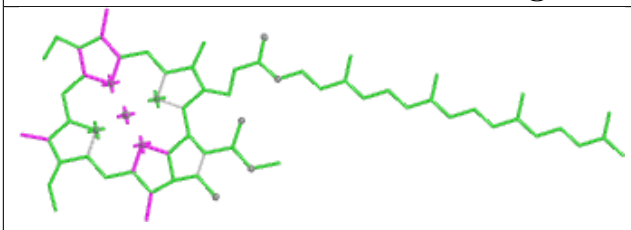
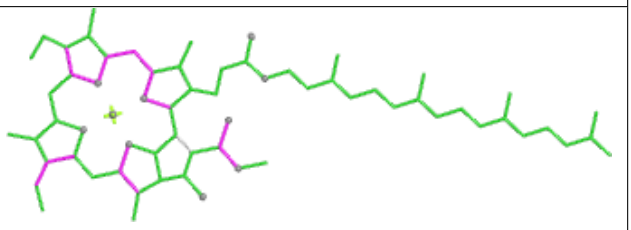


Rings

Ligand CLA P 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 303	
	
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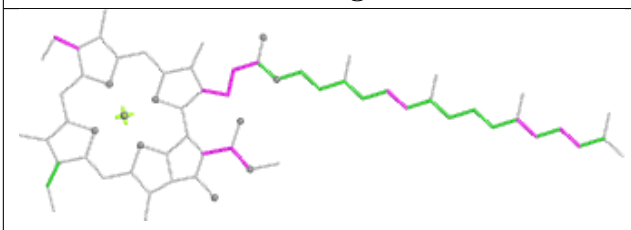
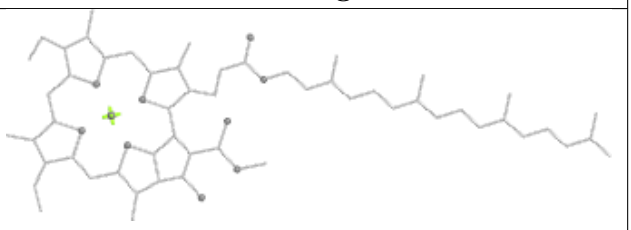
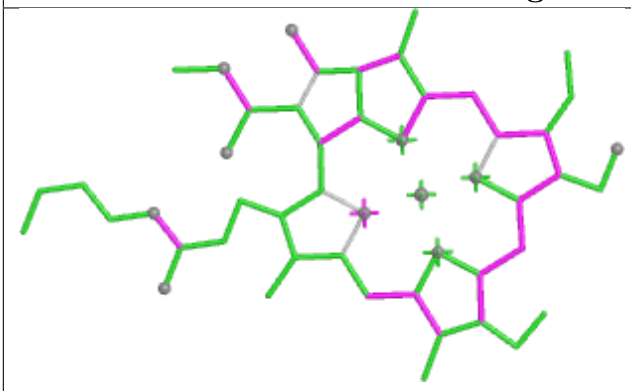
	
Torsions	Rings

Ligand CHL S 307



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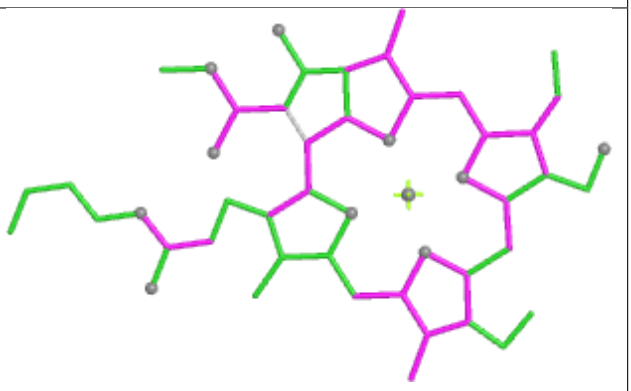
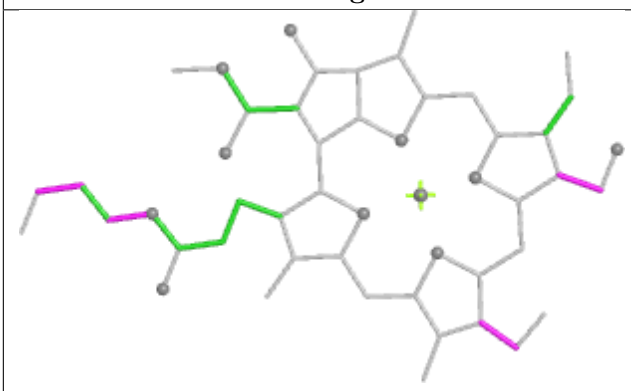
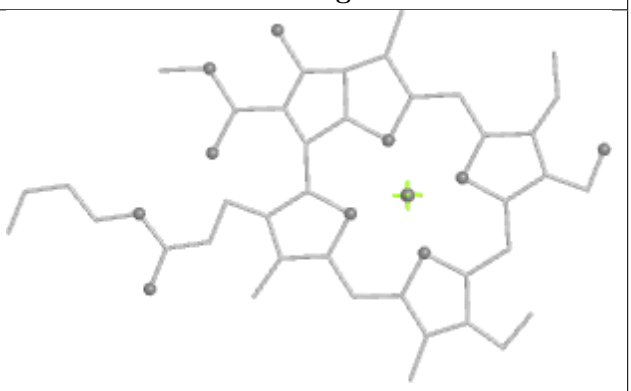


Bond angles

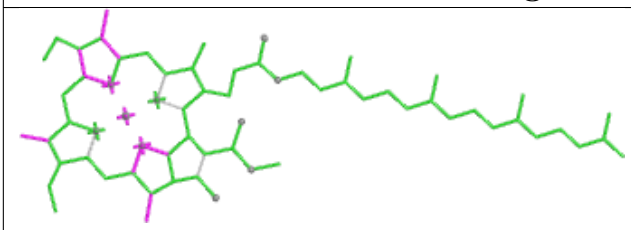


Torsions



Rings

Ligand CLA A 839



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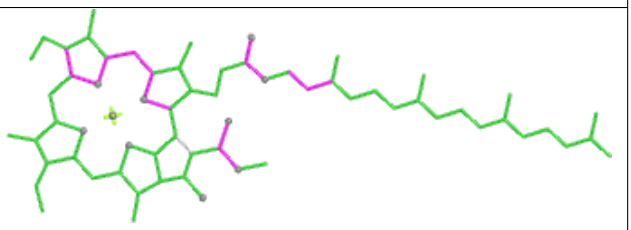
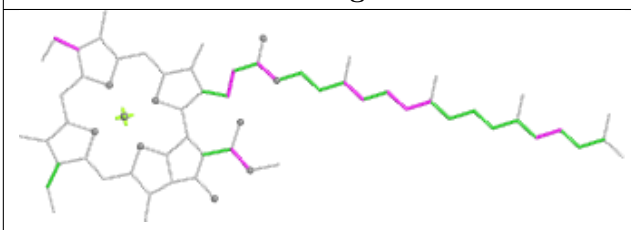
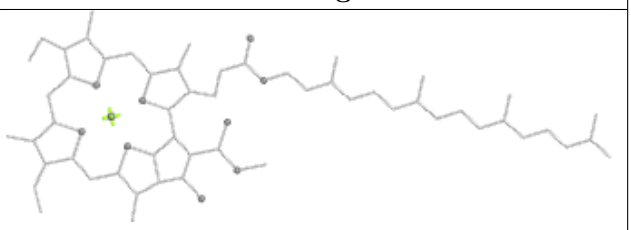


Bond angles

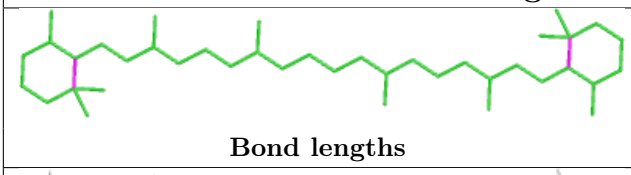


Torsions



Rings

Ligand BCR F 801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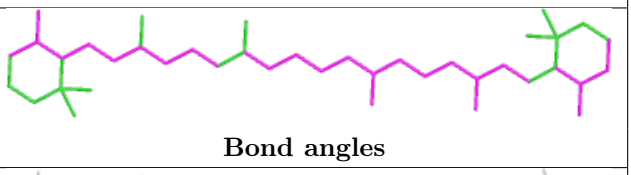
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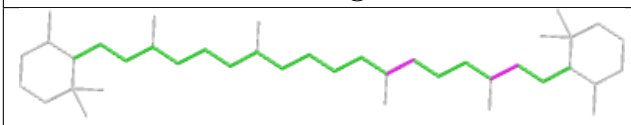
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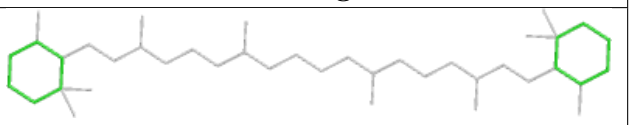
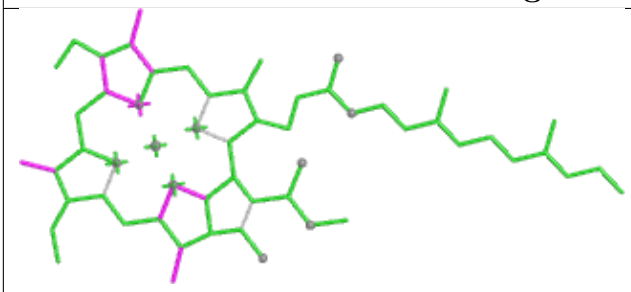

Rings

Ligand CLA A 817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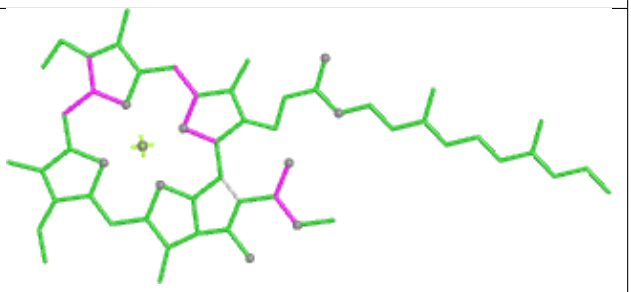
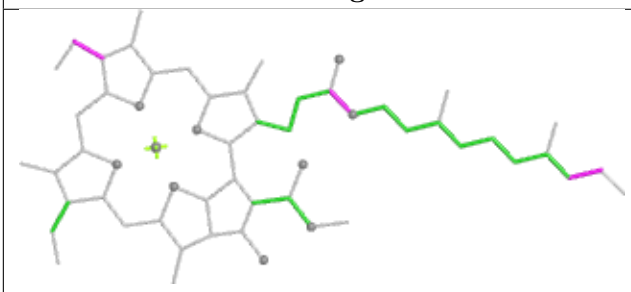

Bond angles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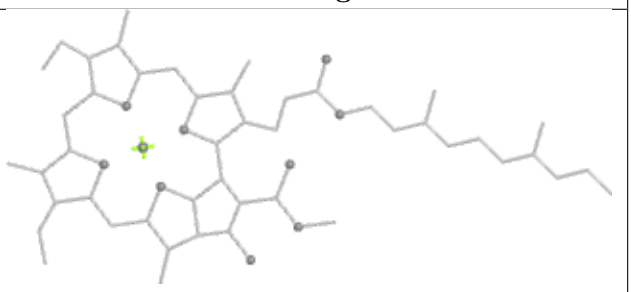
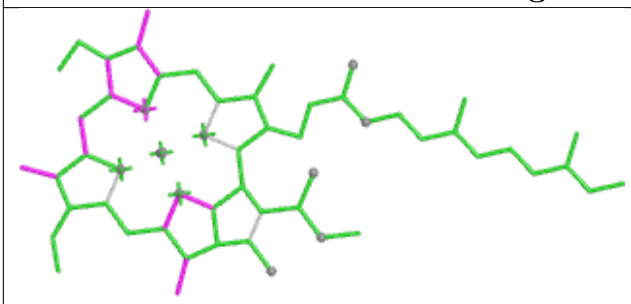

Rings

Ligand CLA 6 613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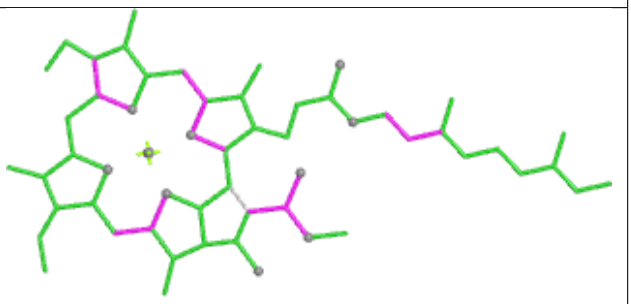
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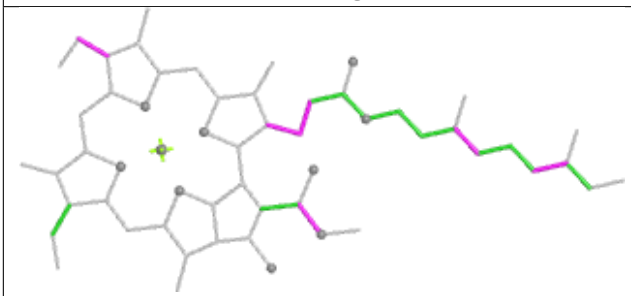
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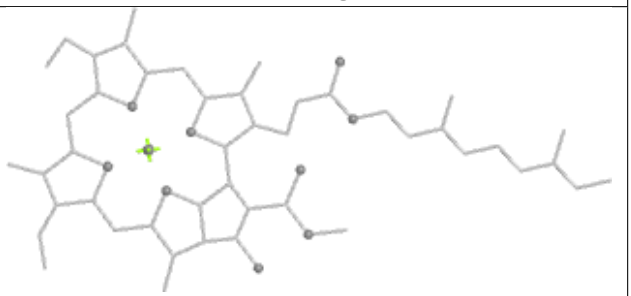
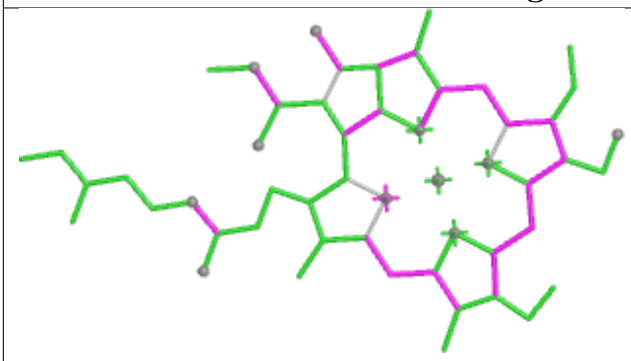

Rings

Ligand CHL S 308



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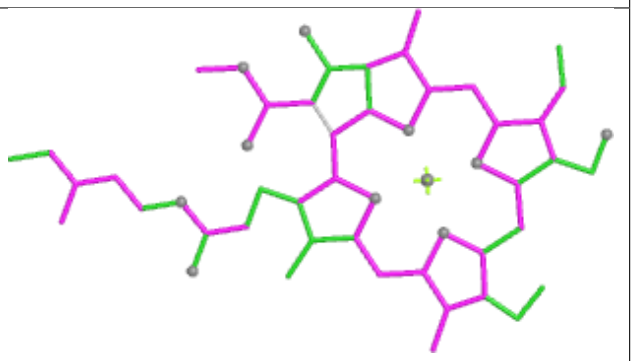

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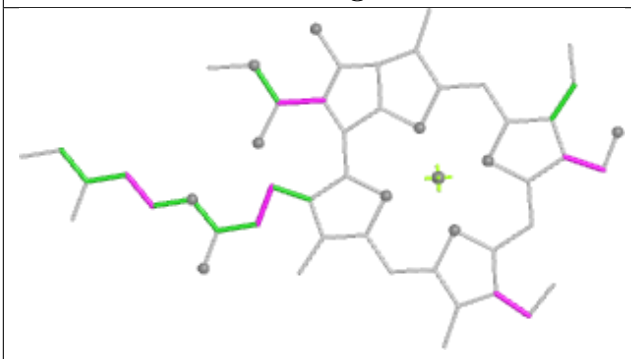

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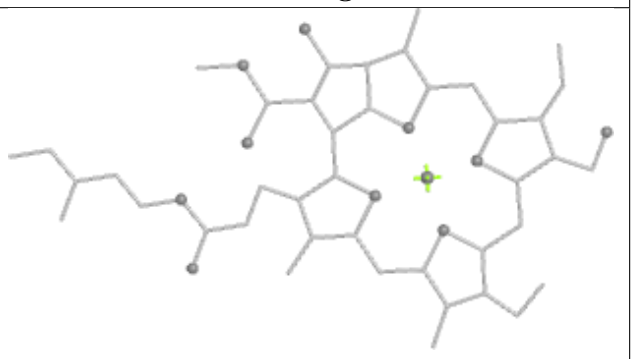
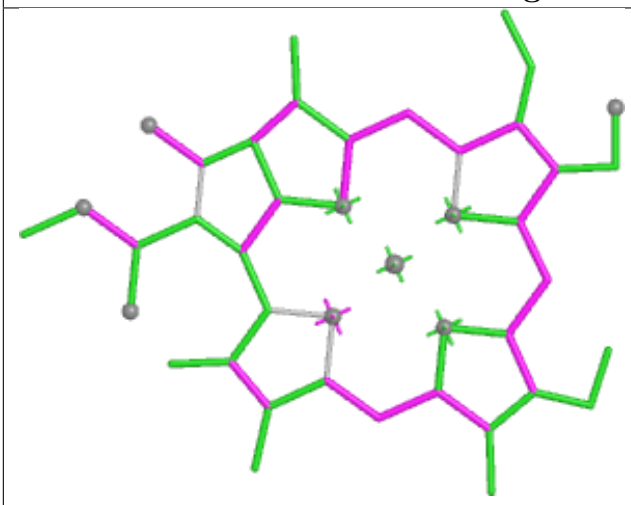


Rings

Ligand CHL Q 605



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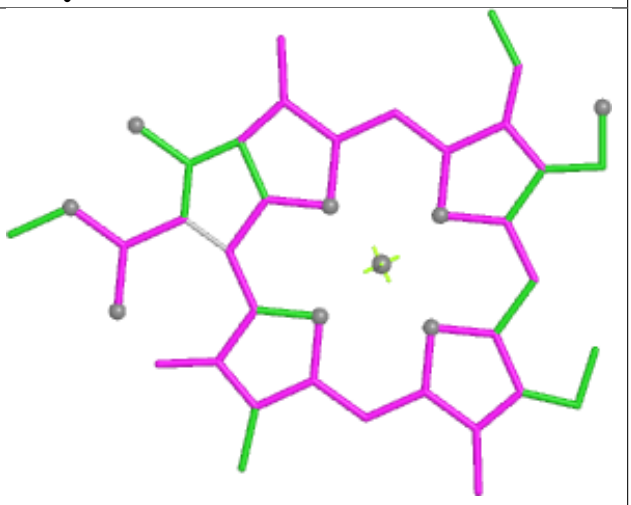
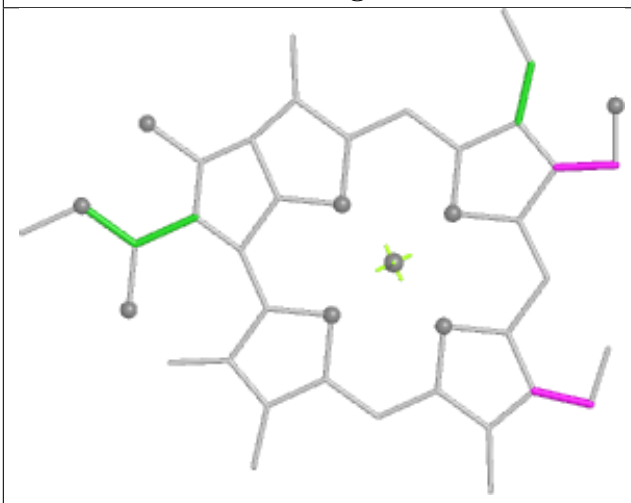


Bond angles



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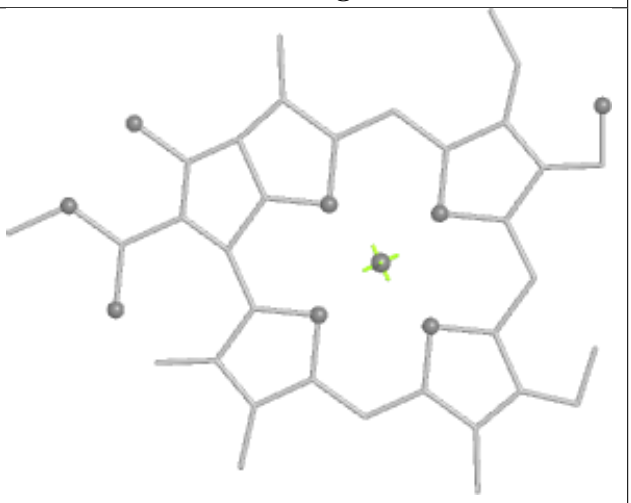
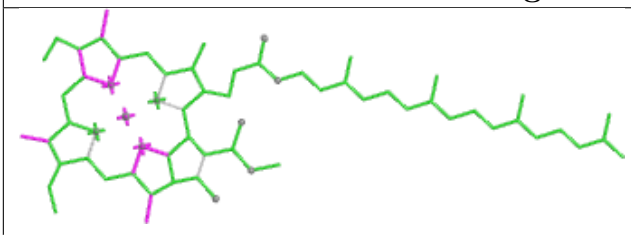


Rings

Ligand CLA A 819



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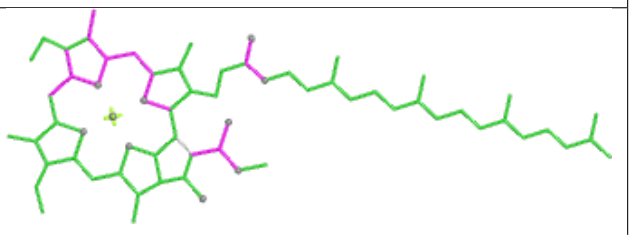
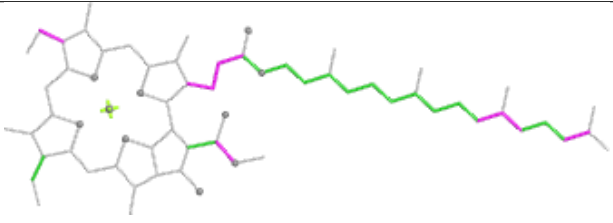


Bond angles



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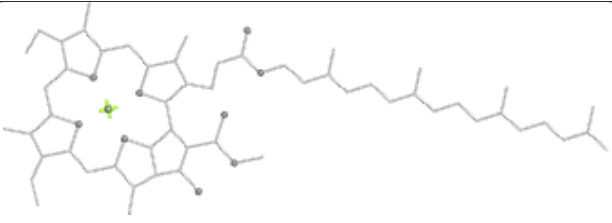
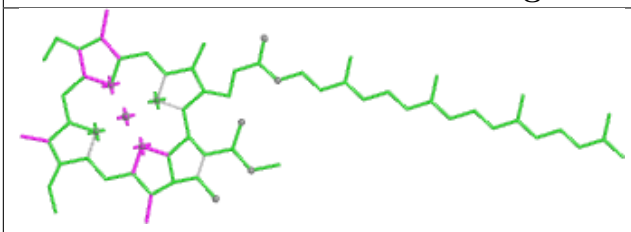
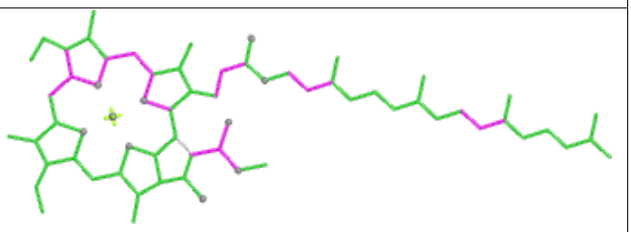
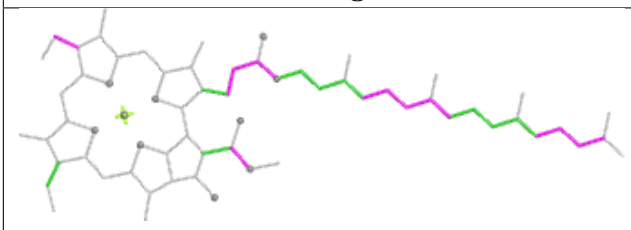
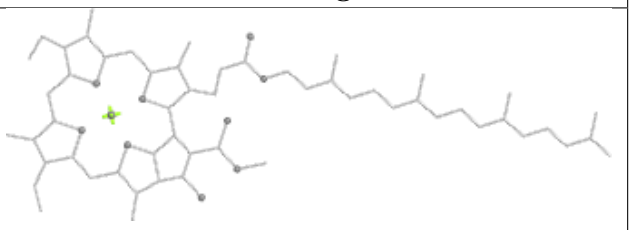


Rings

Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

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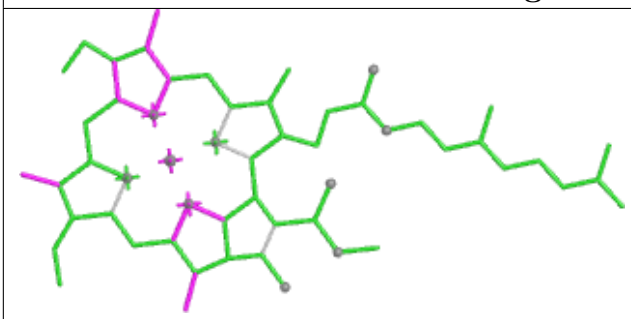
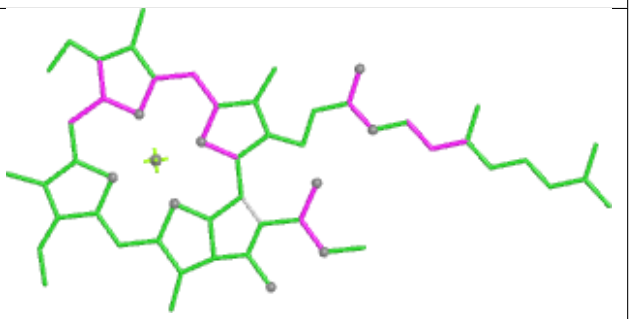
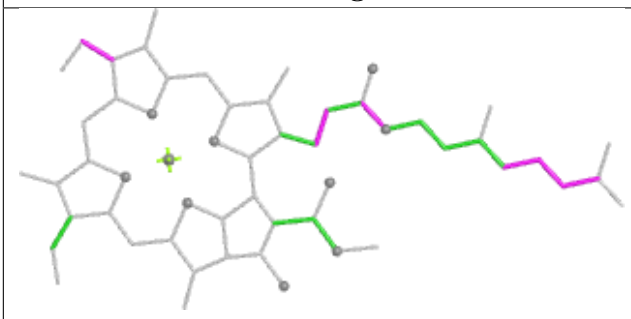
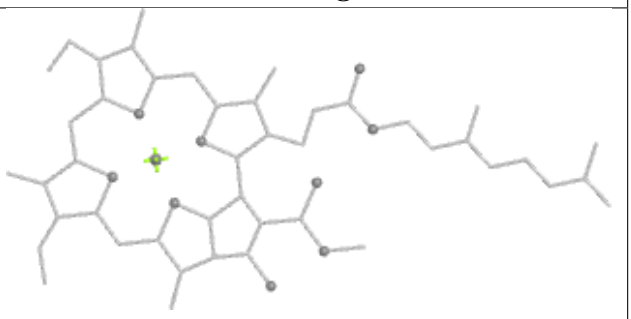
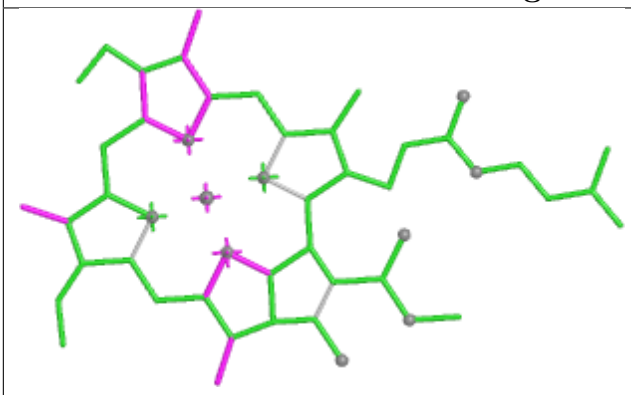
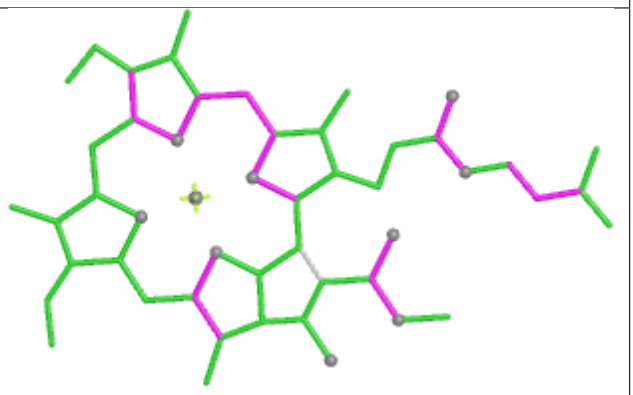
 Bond lengths	 Bond angles
 Torsions	 Rings

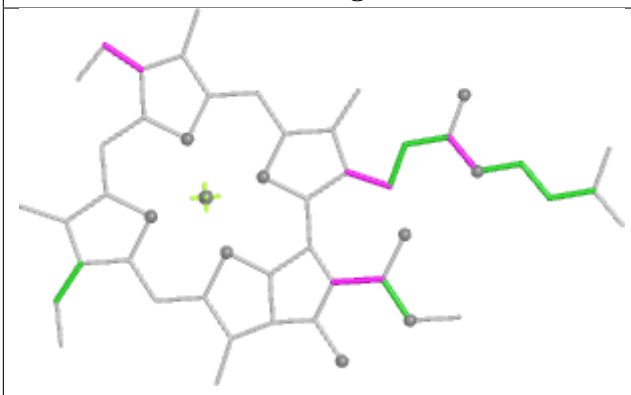
Ligand CLA A 831



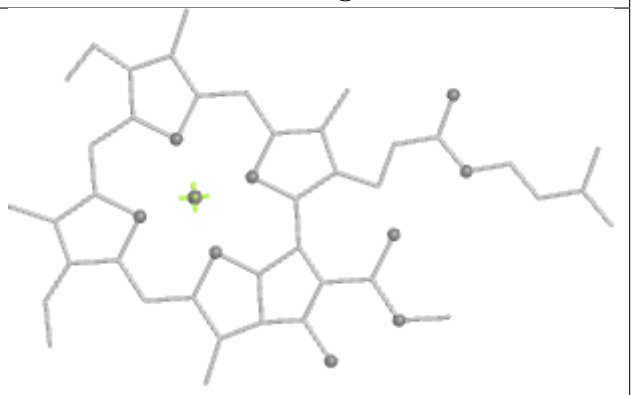
Bond lengths



Bond angles

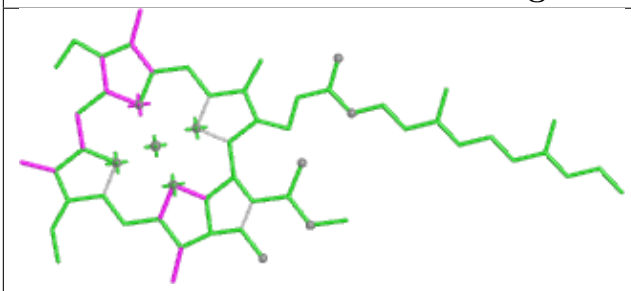


Torsions

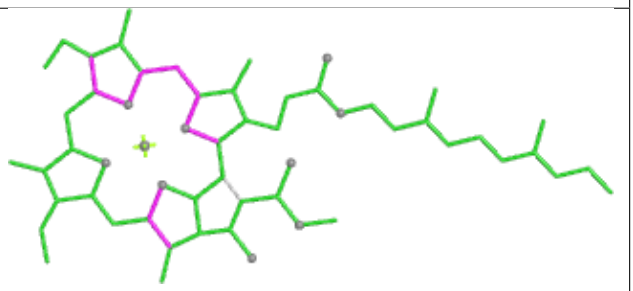


Rings

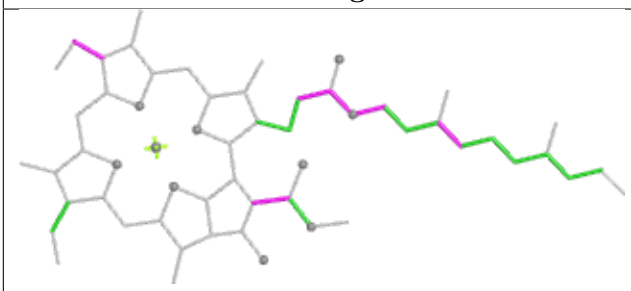
Ligand CLA a 302



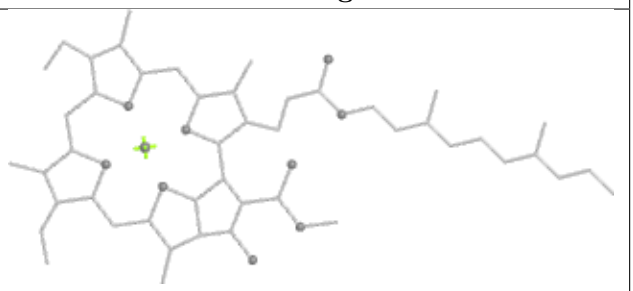
Bond lengths



Bond angles

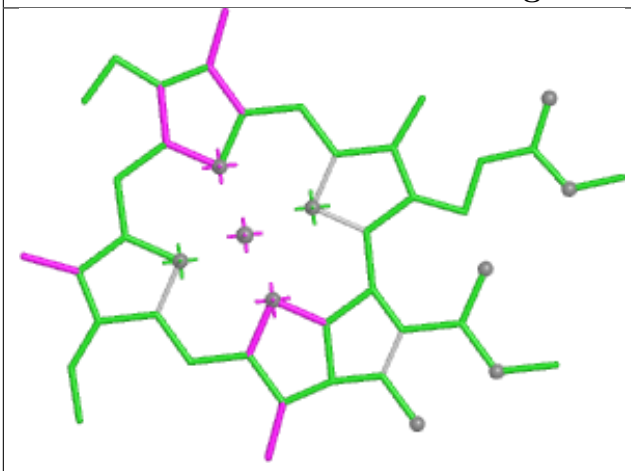


Torsions

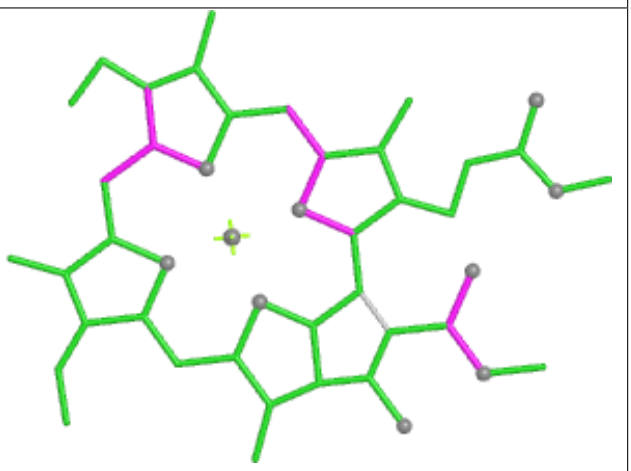


Rings

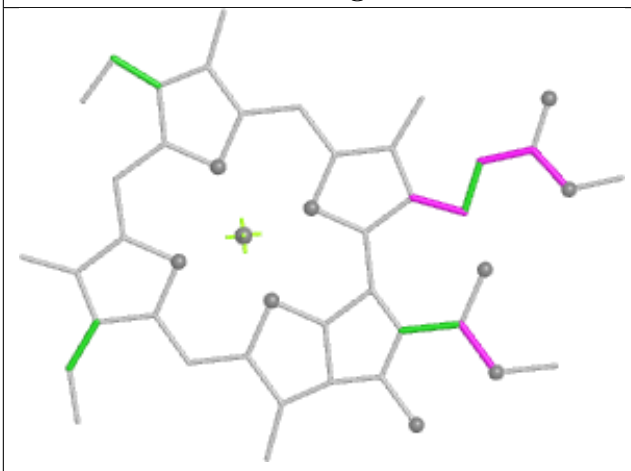
Ligand CLA H 201



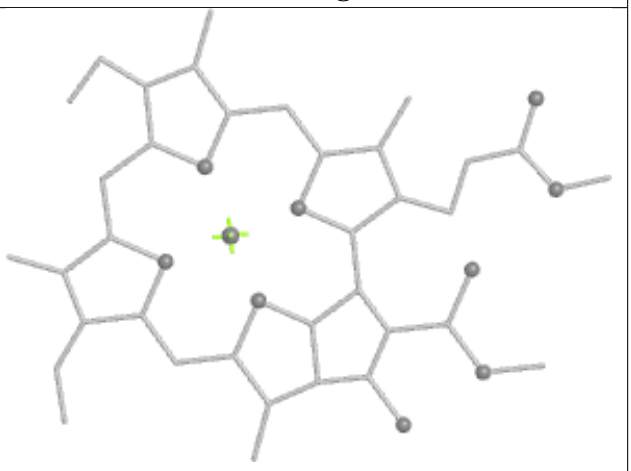
Bond lengths



Bond angles

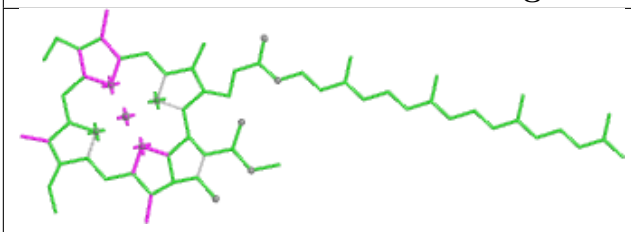


Torsions

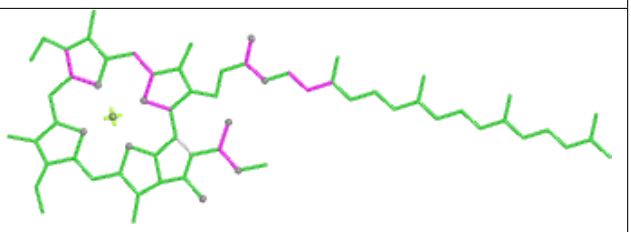


Rings

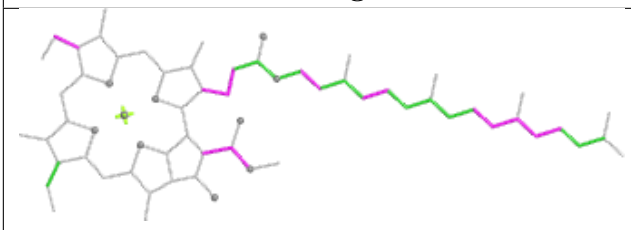
Ligand CLA A 851



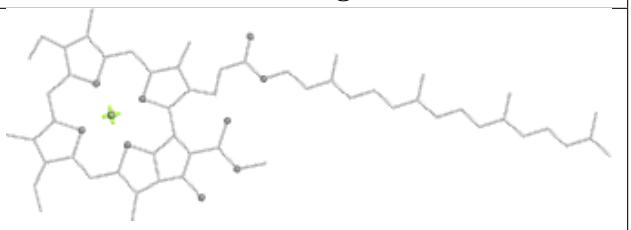
Bond lengths



Bond angles

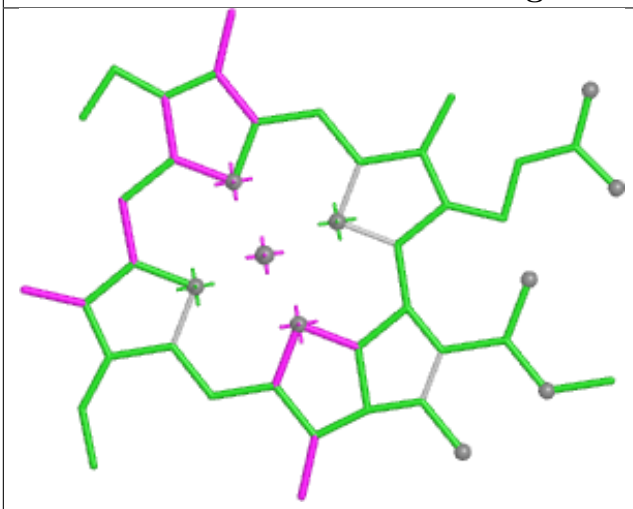


Torsions



Rings

Ligand CLA F 802



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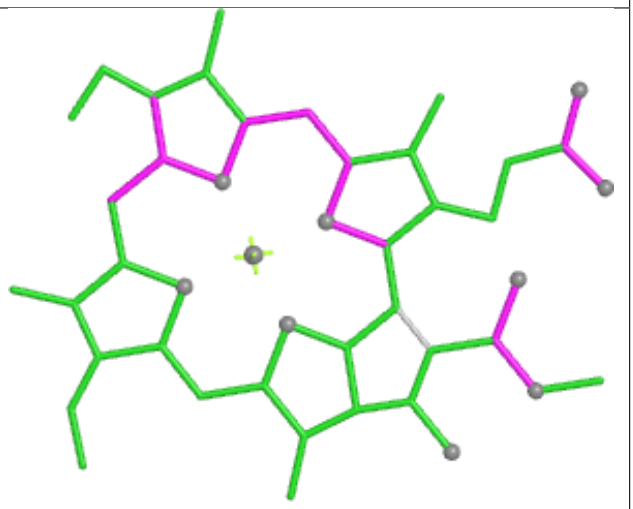
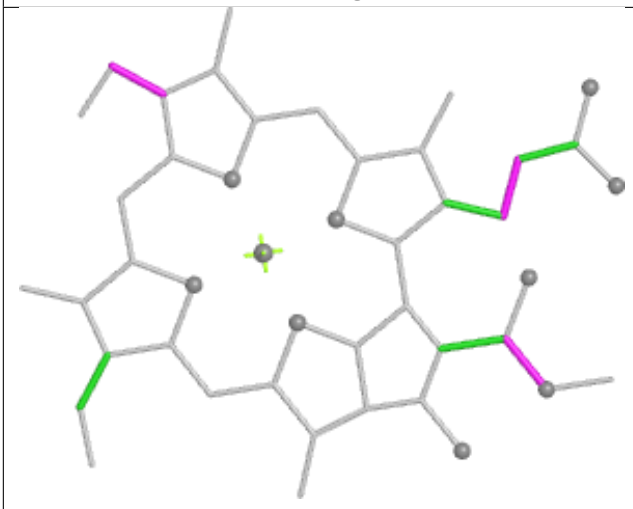


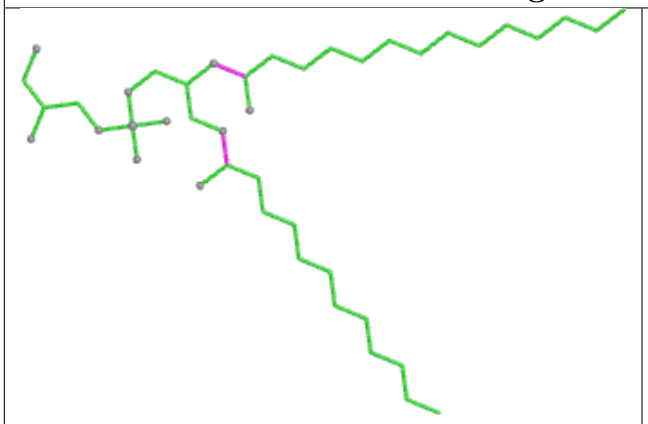
Bond angles



Torsions

Rings

Ligand LHG a 317



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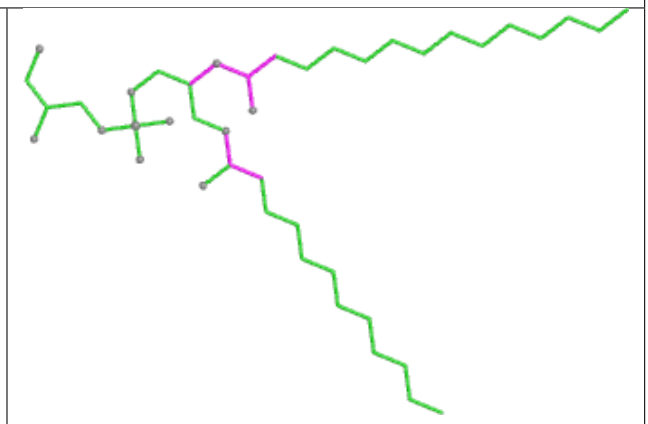
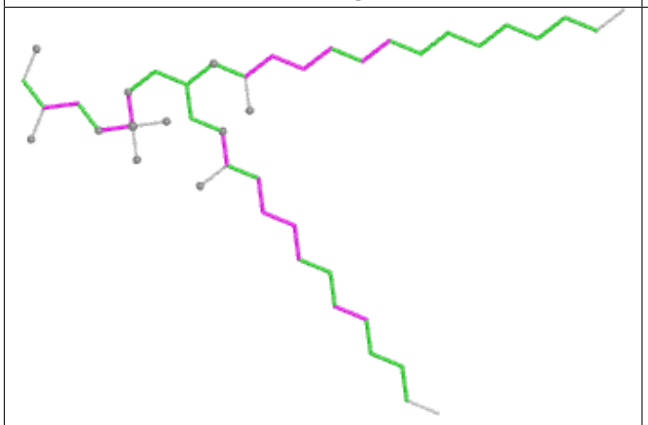
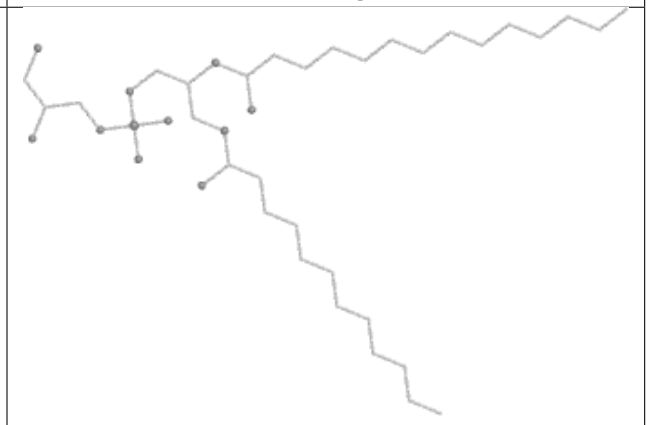


Bond angles

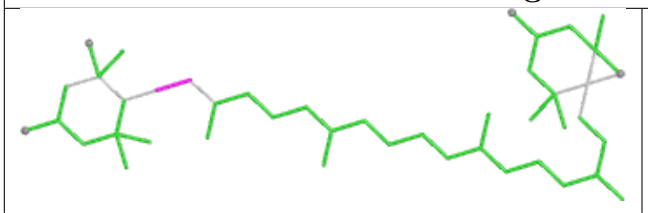


Torsions



Rings

Ligand NEX P 617



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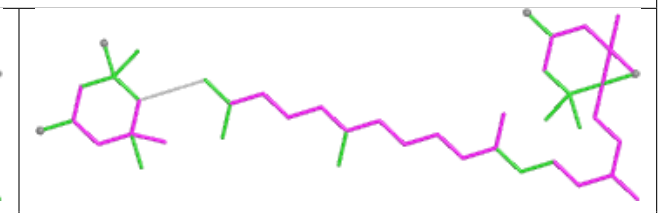
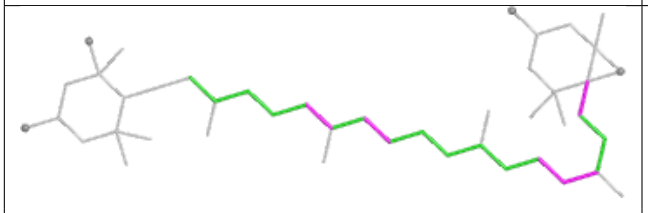


Bond angles



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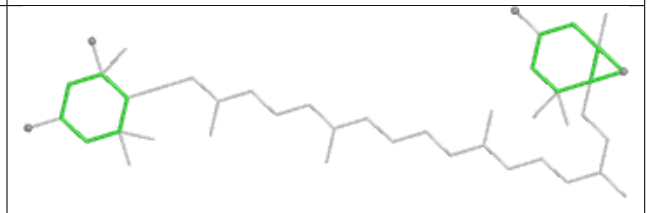
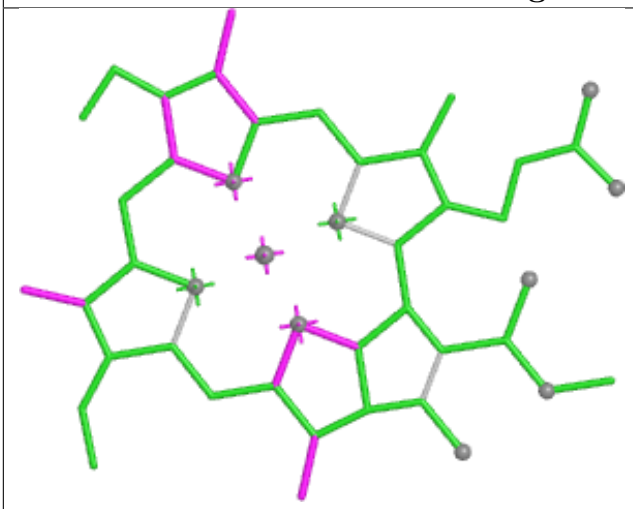


Rings

Ligand CLA 5 314



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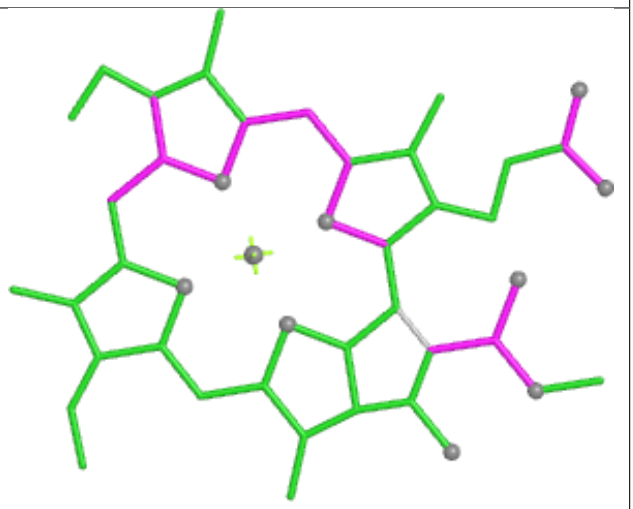
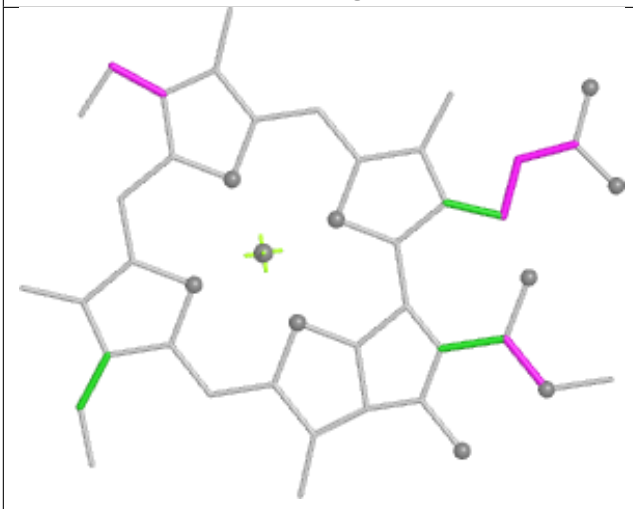


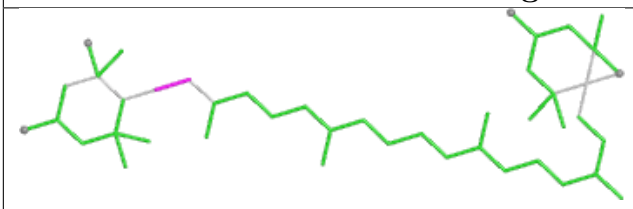
Bond angles



Torsions

Rings

Ligand NEX U 316



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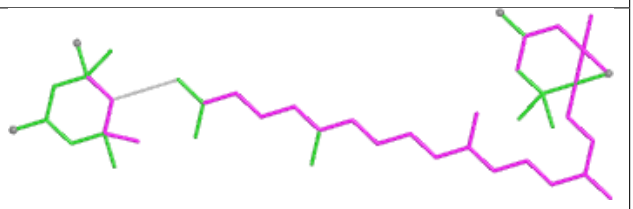
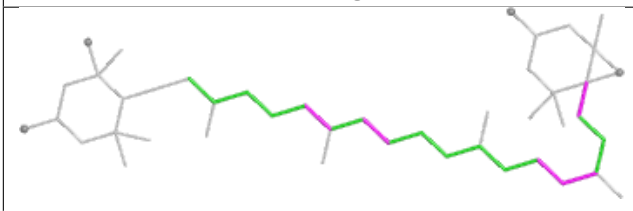


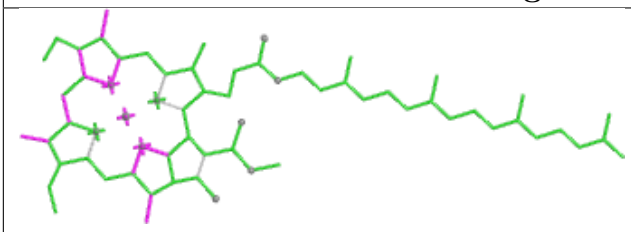
Bond angles



Torsions

Rings

Ligand CLA A 827



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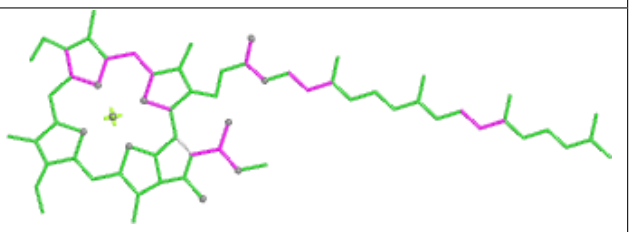
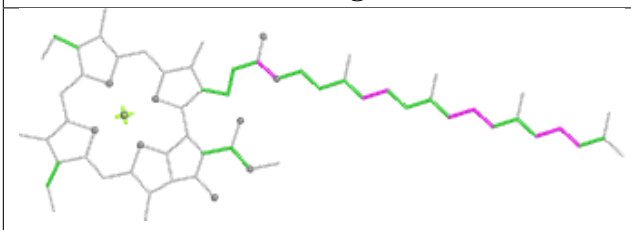
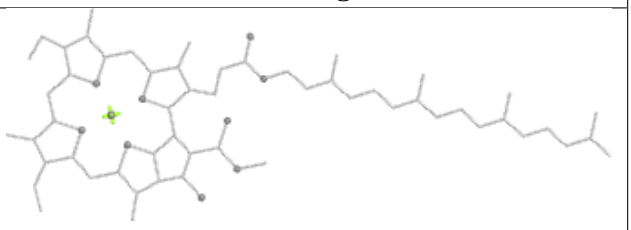


Bond angles

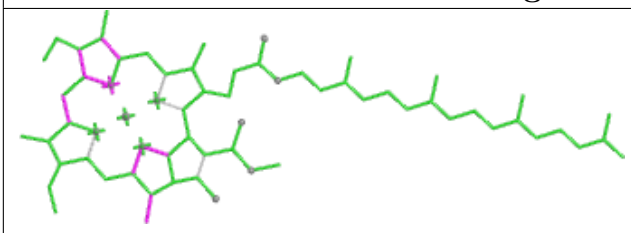


Torsions

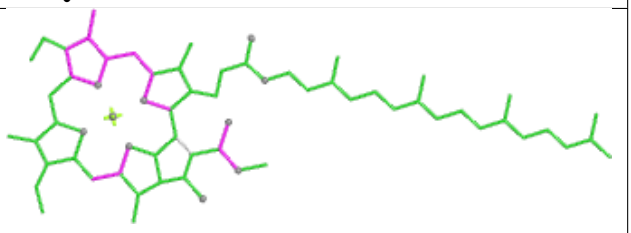


Rings

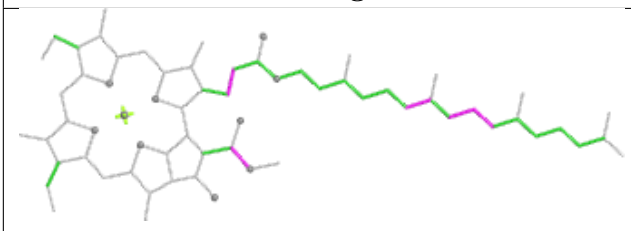
Ligand CLA Q 602



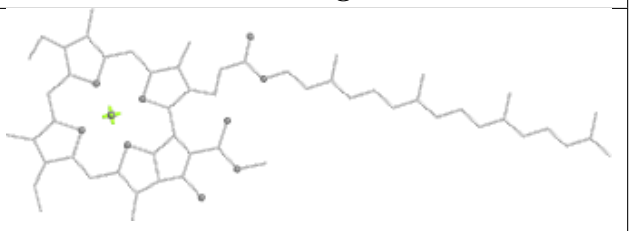
Bond lengths



Bond angles

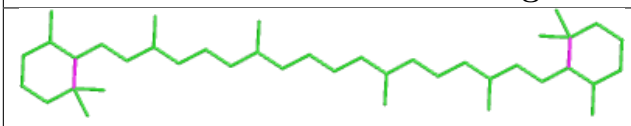


Torsions



Rings

Ligand BCR A 846



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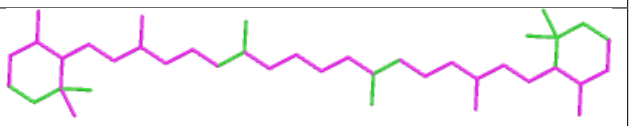
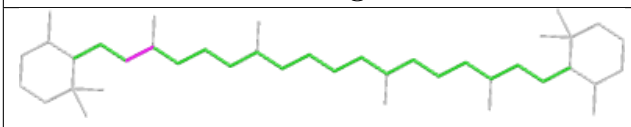


Bond angles



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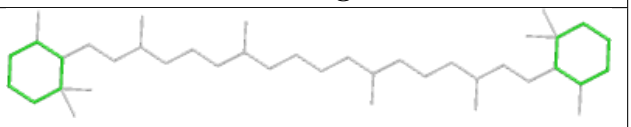
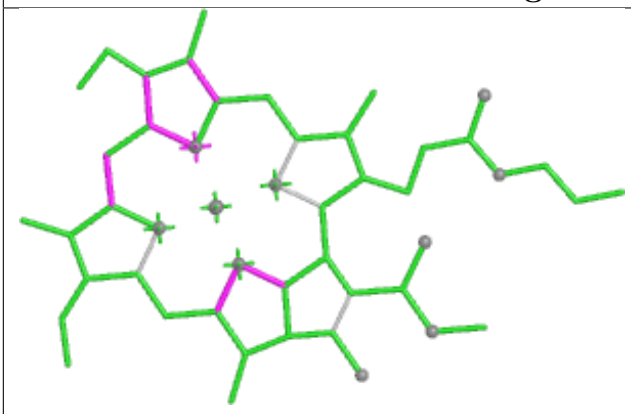


Rings

Ligand CLA T 612



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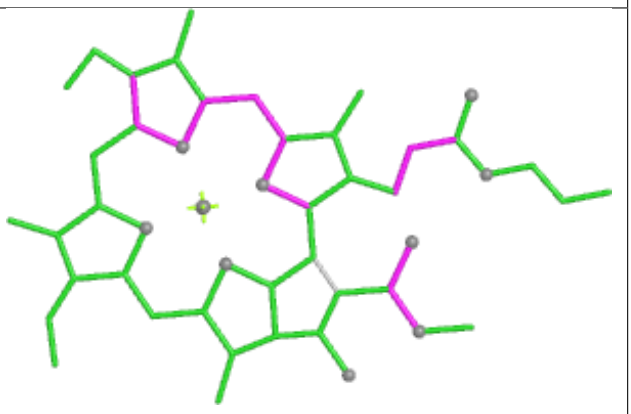
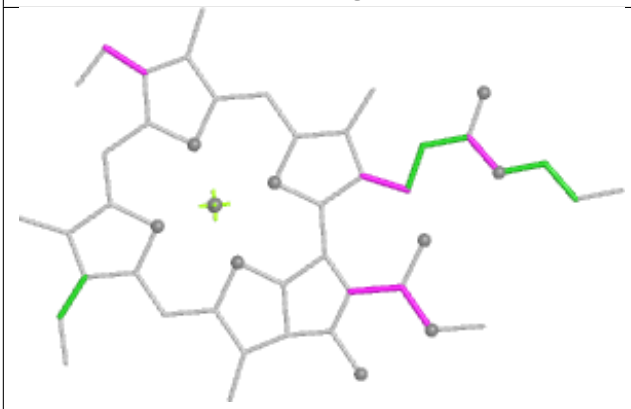


Bond angles



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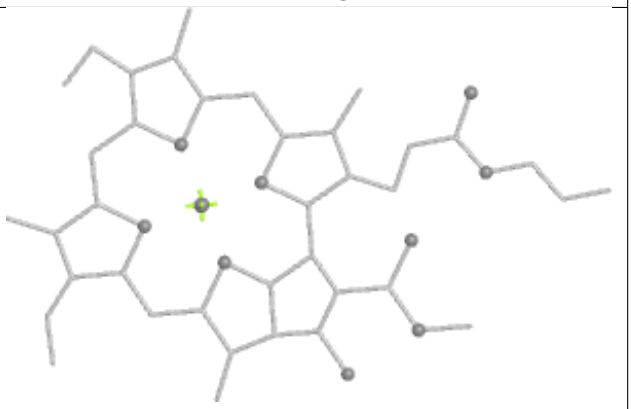
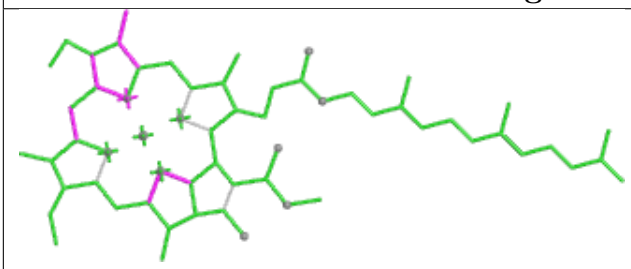


Rings

Ligand CLA T 609



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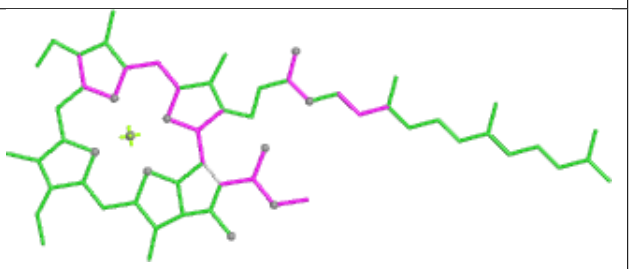
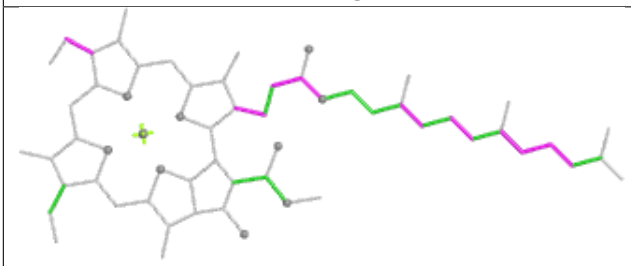
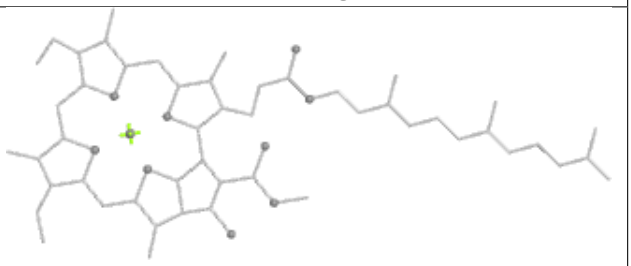


Bond angles

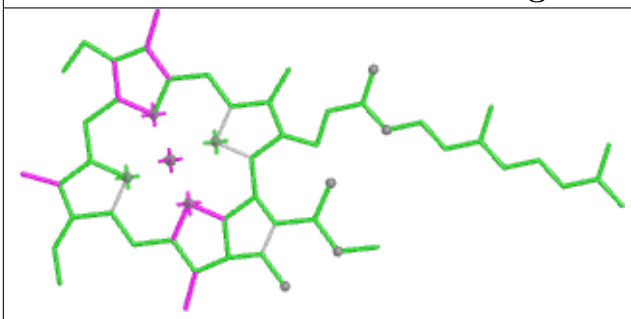


Torsions



Rings

Ligand CLA 5 311



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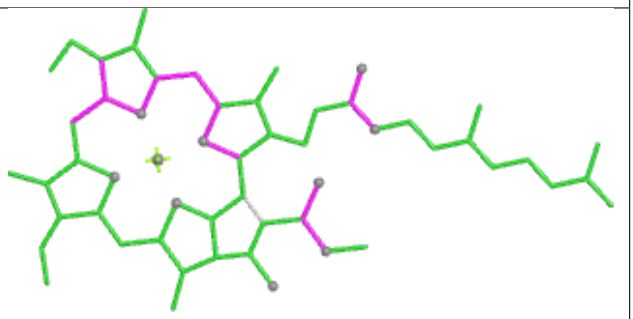
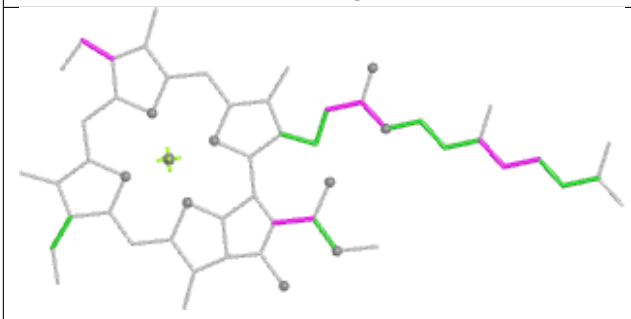


Bond angles



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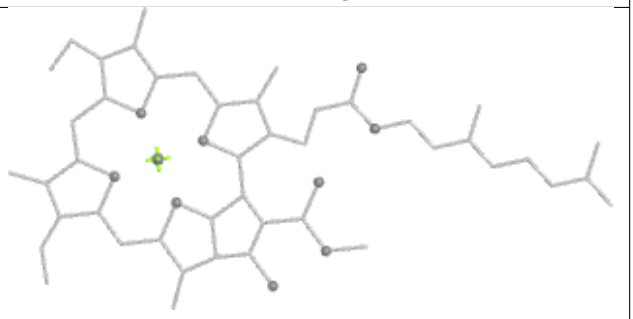
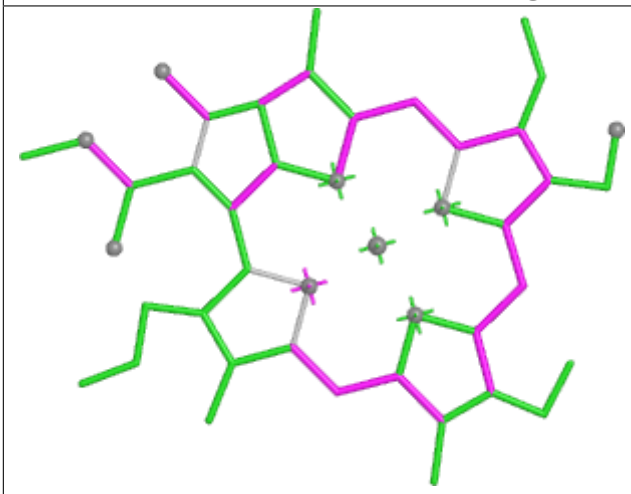


Rings

Ligand CHL T 606



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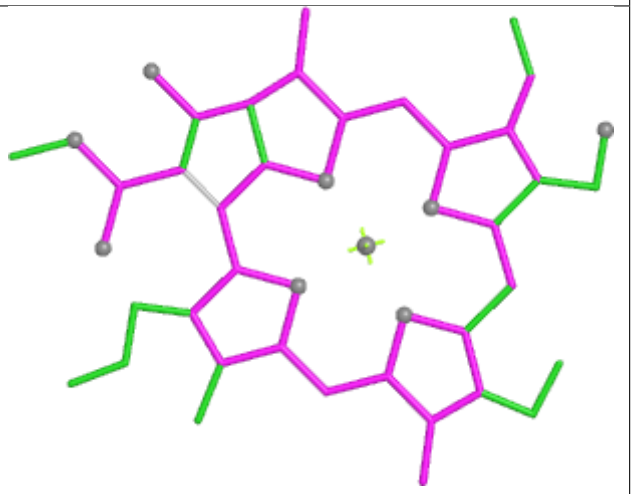
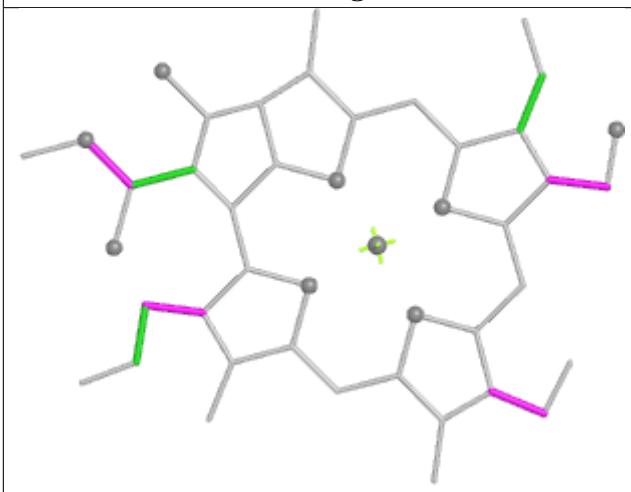


Bond angles



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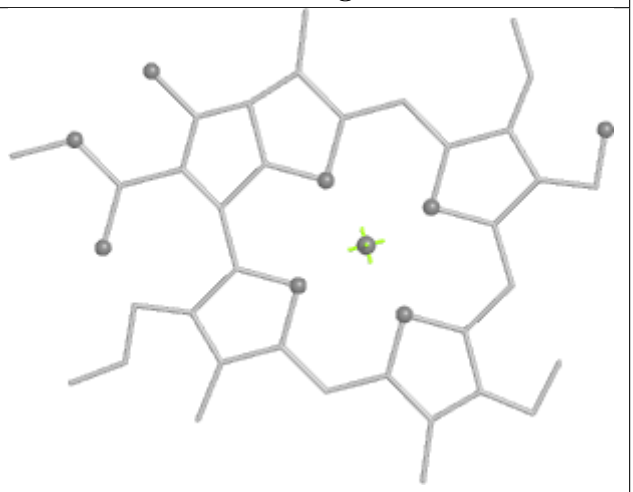
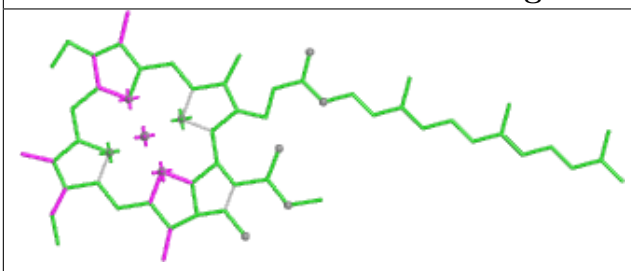
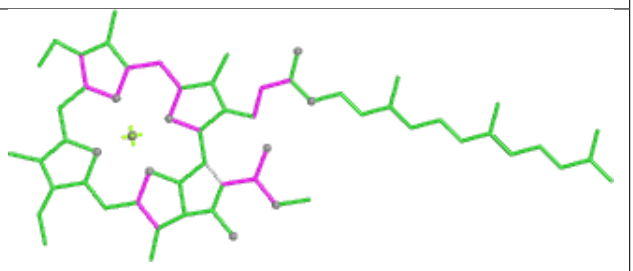


Rings

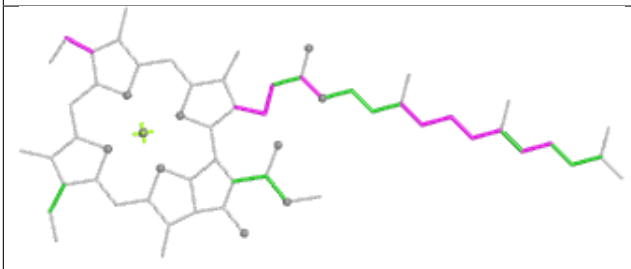
Ligand CLA B 816



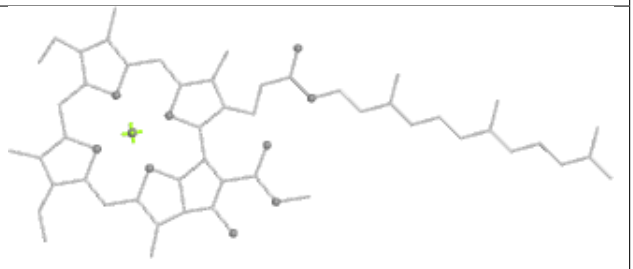
Bond lengths



Bond angles

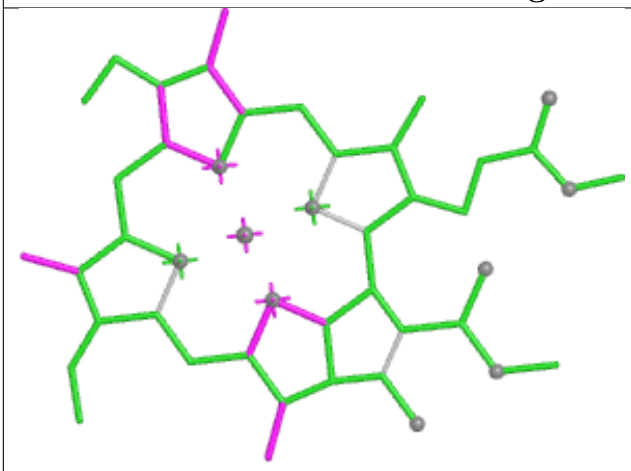


Torsions



Rings

Ligand CLA 3 310



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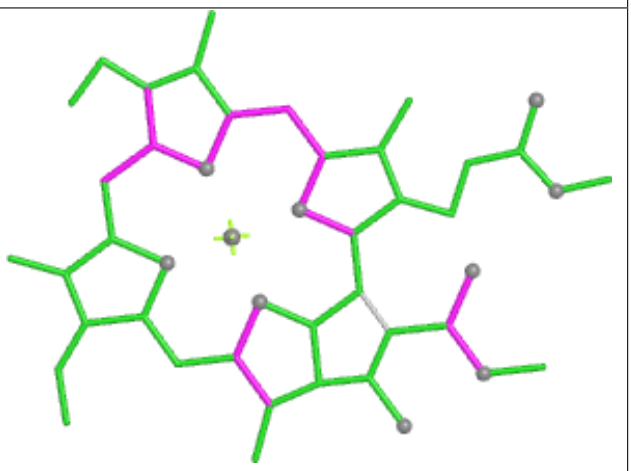

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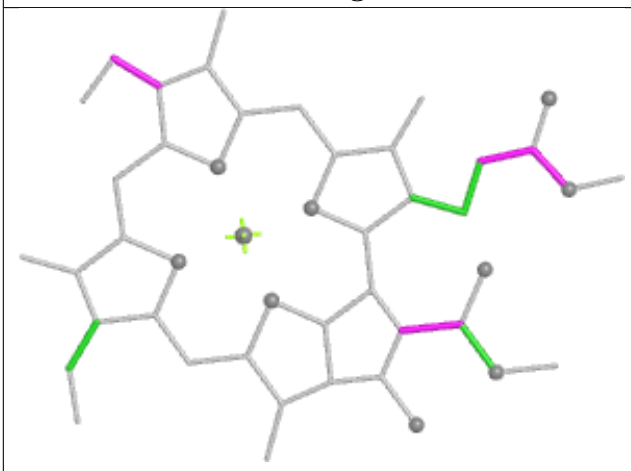

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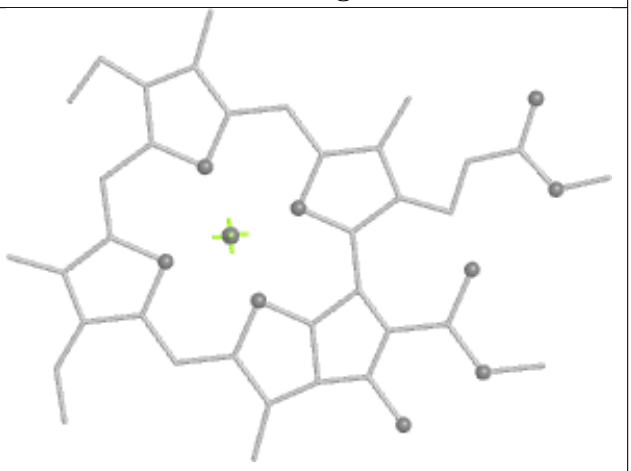
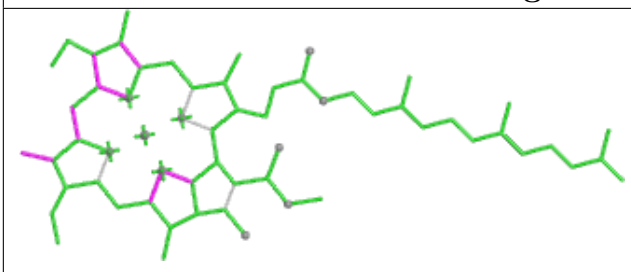


Rings

Ligand CLA Q 612



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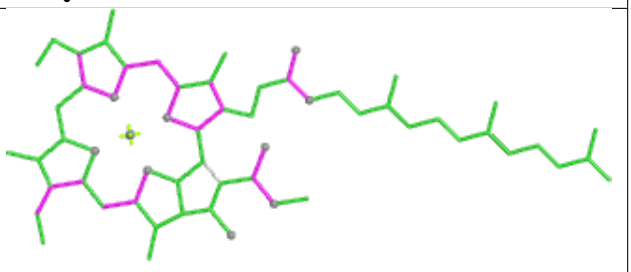

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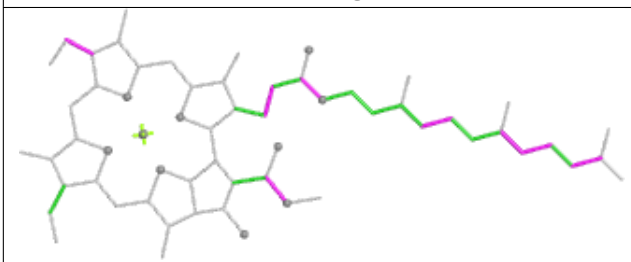

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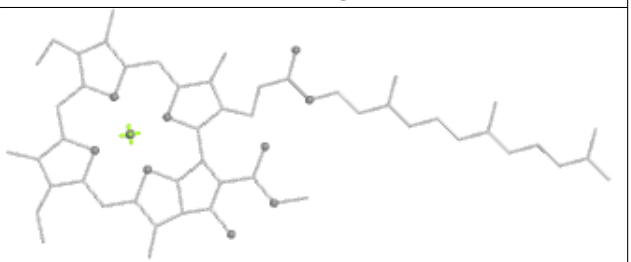
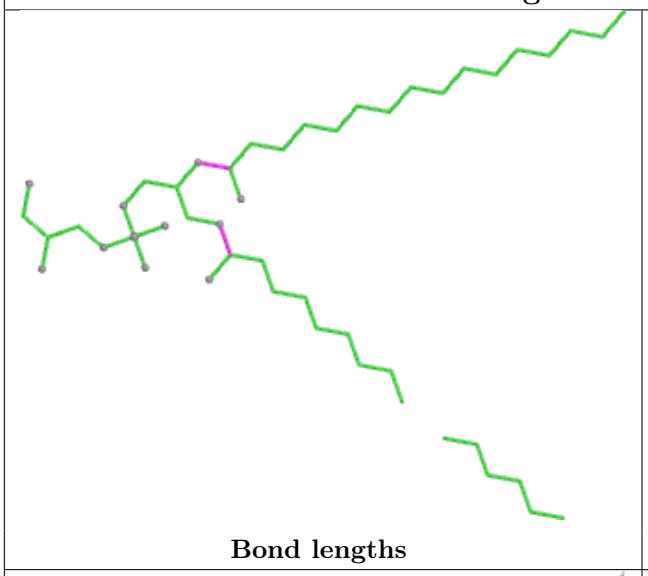


Rings

Ligand LHG A 852



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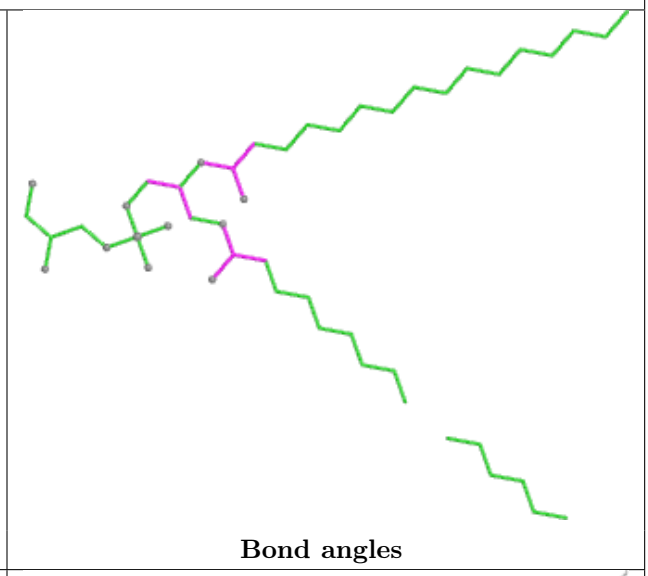
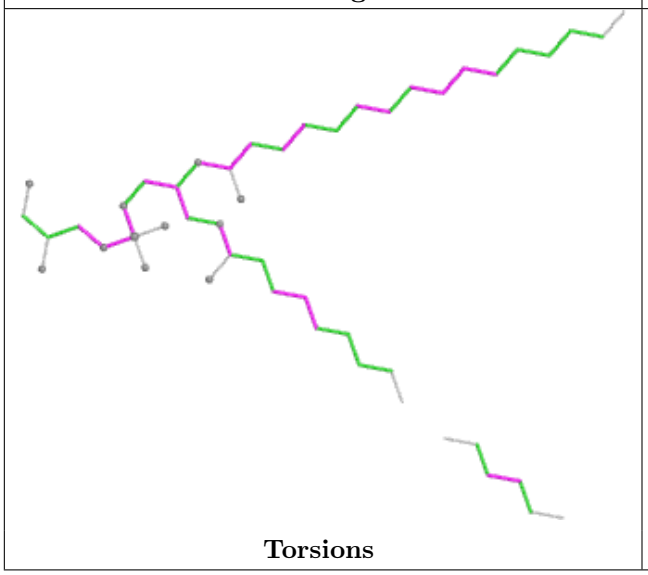


Bond angles



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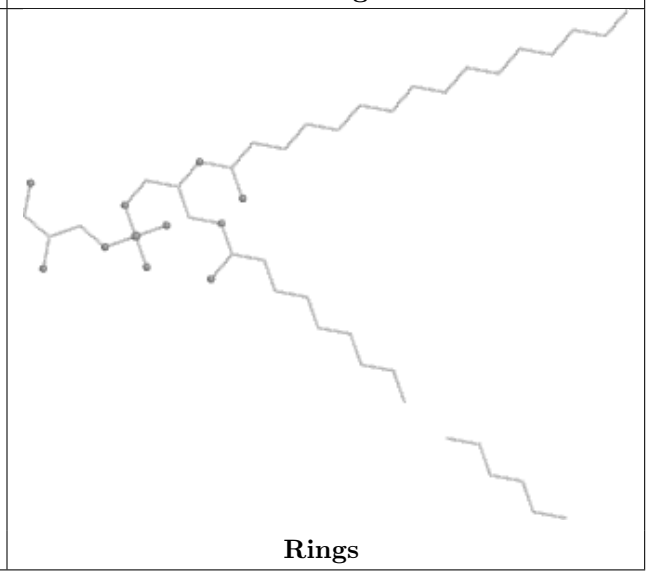
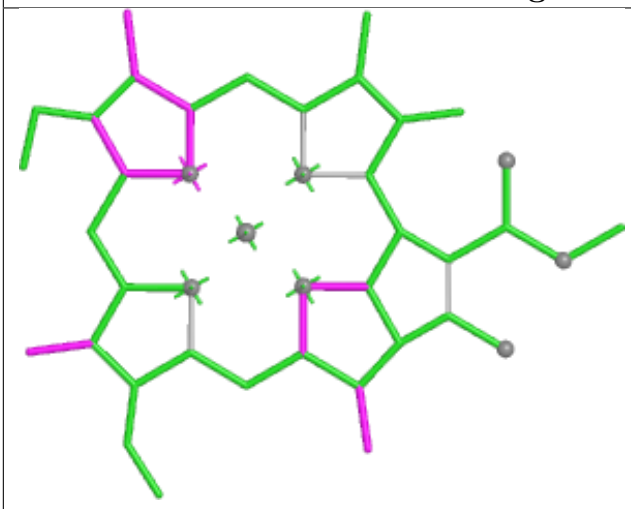


Rings

Ligand CLA 2 306



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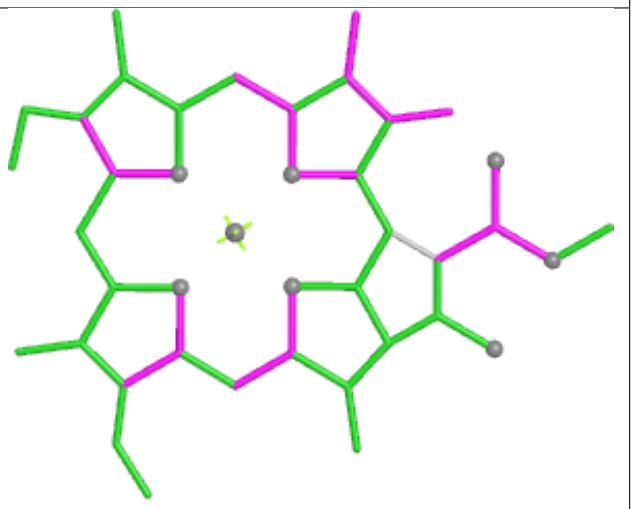
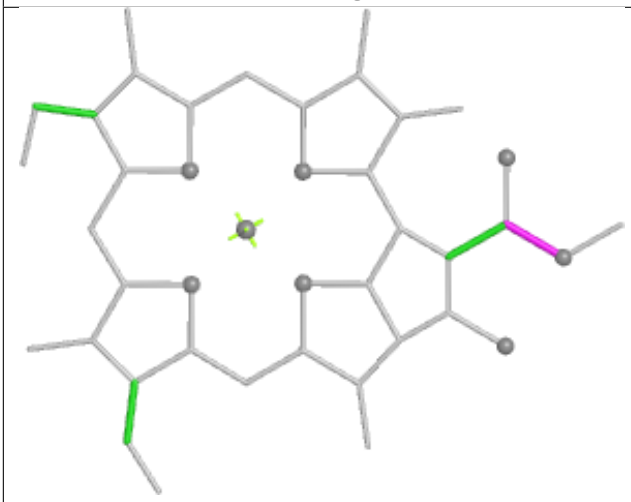


Bond angles



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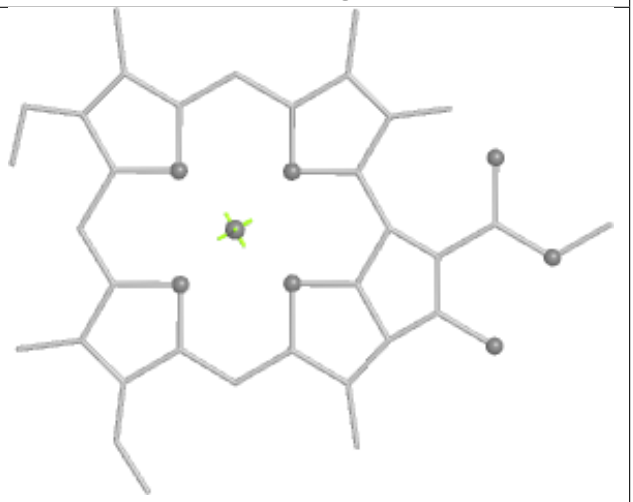

Rings

Ligand BCR A 848

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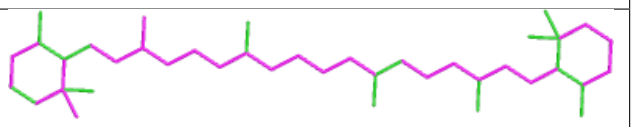
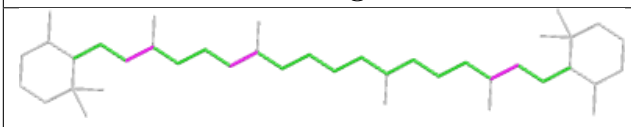


Bond angles



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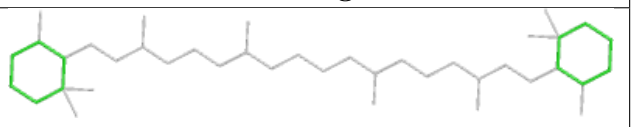
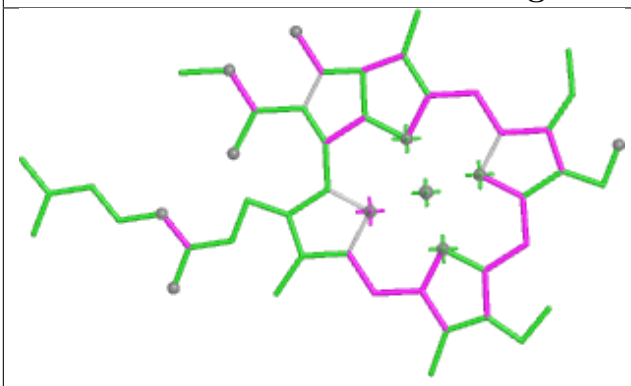


Rings

Ligand CHL 9 307



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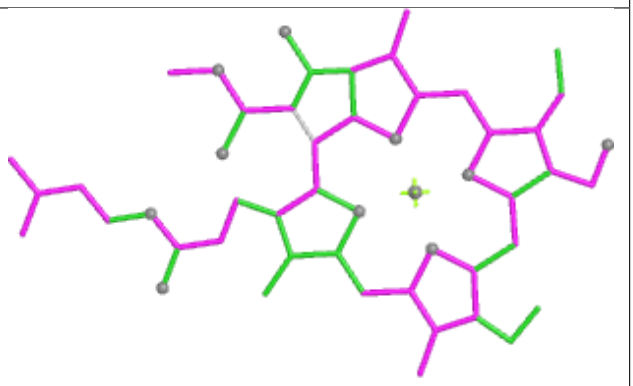
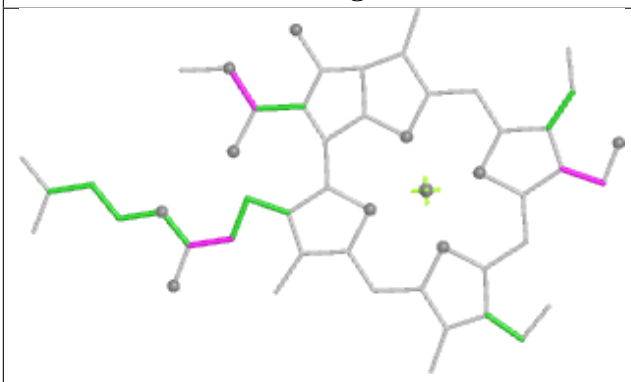


Bond angles



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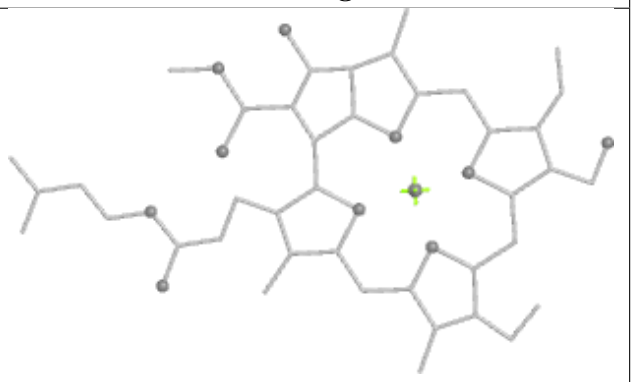
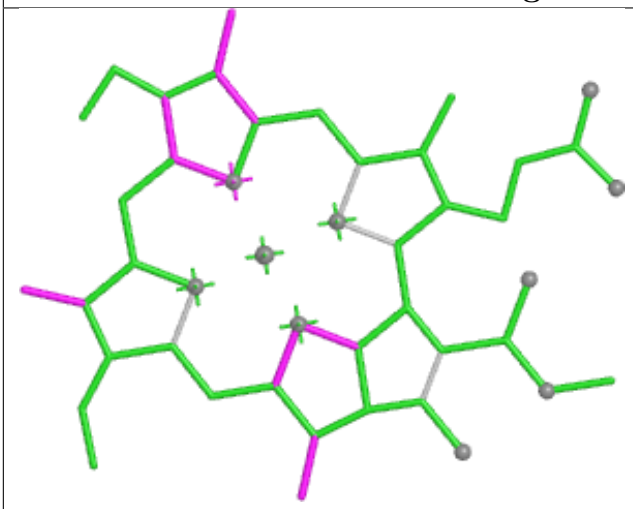


Rings

Ligand CLA K 205



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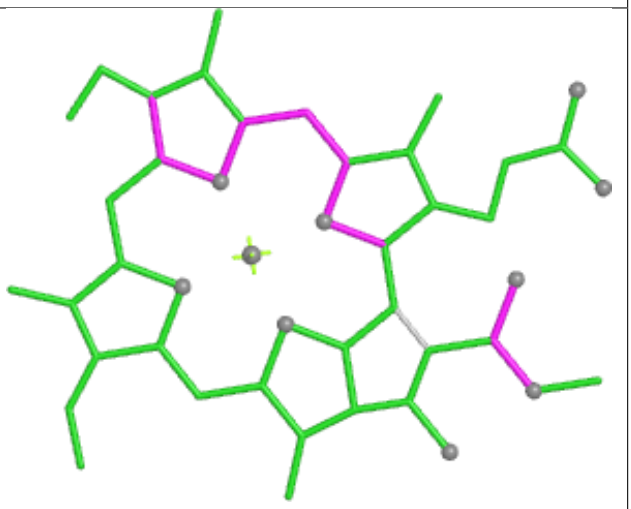
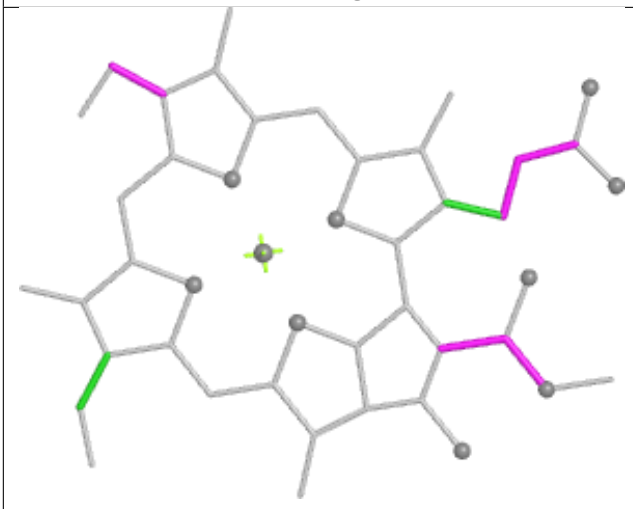


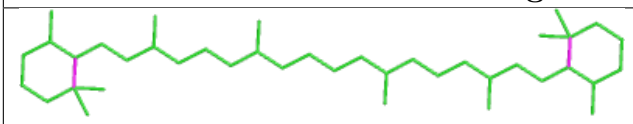
Bond angles



Torsions

Rings

Ligand BCR 5 323



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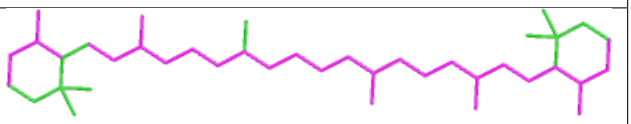
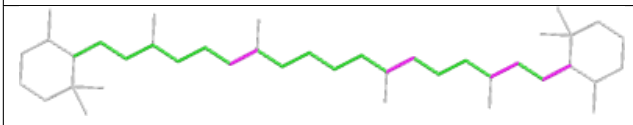
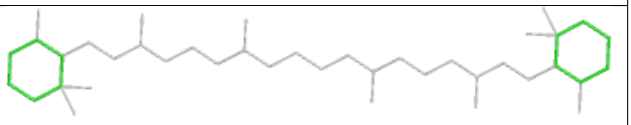


Bond angles

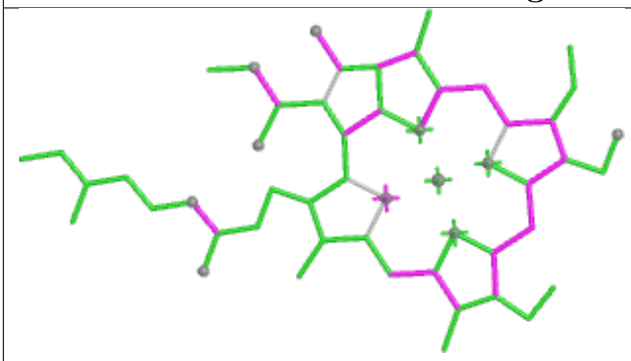


Torsions



Rings

Ligand CHL S 310



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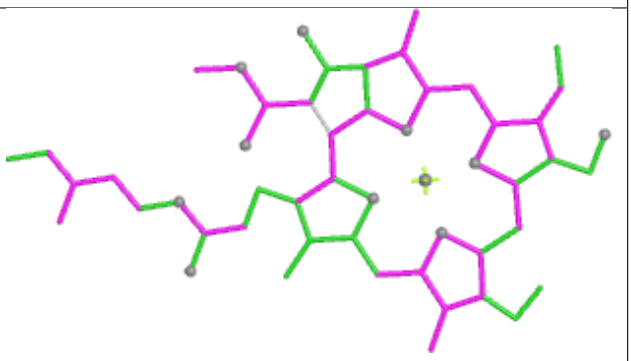
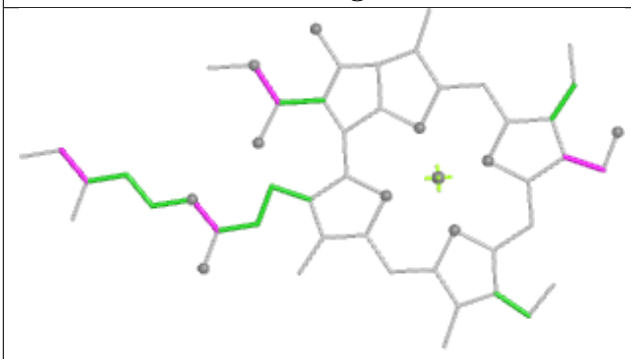
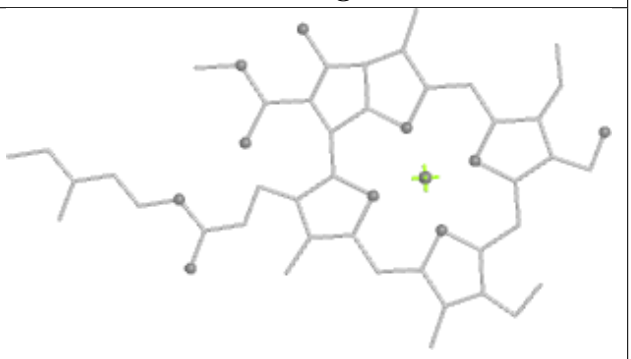


Bond angles

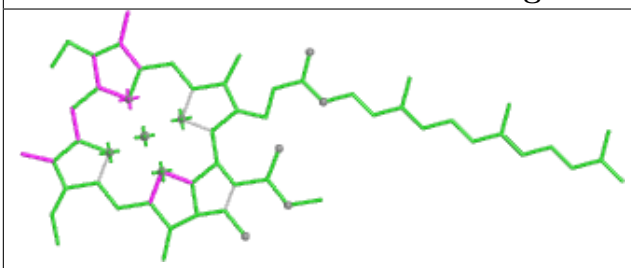


Torsions



Rings

Ligand CLA Q 611



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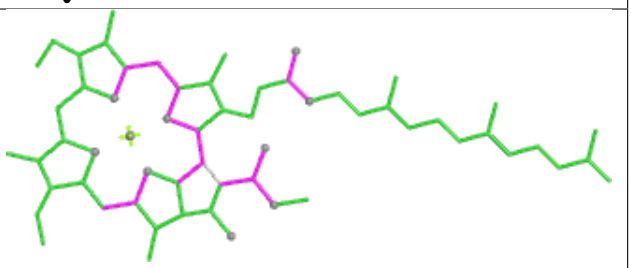
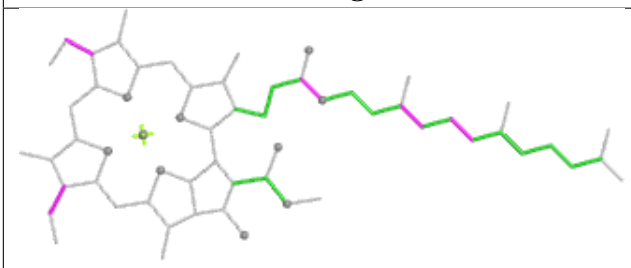


Bond angles



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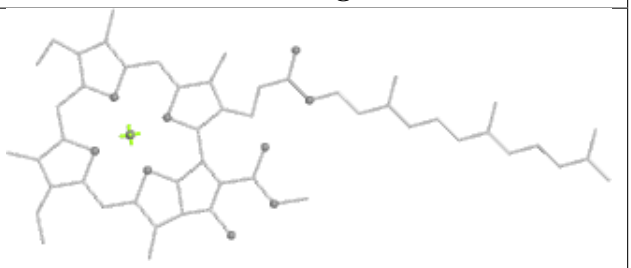
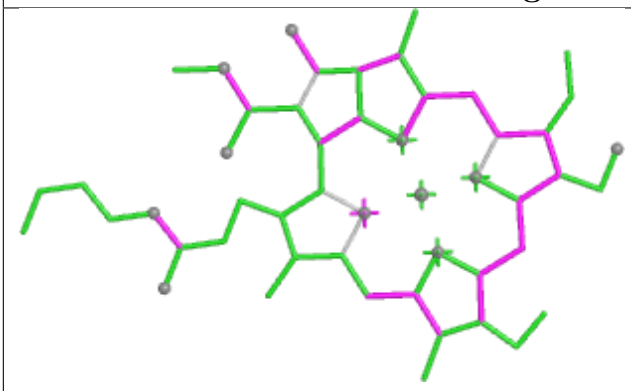


Rings

Ligand CHL Q 606



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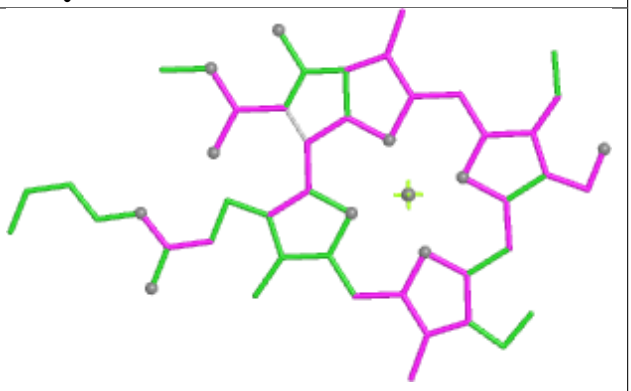
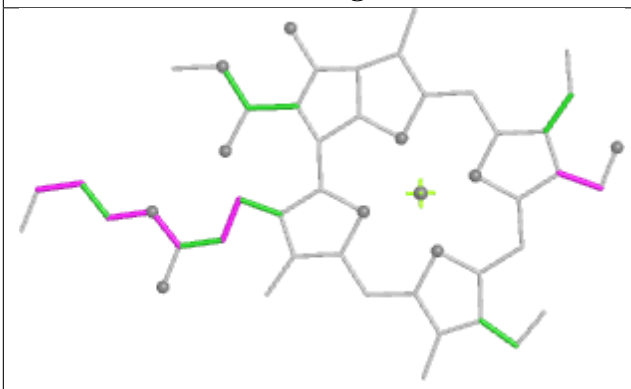


Bond angles



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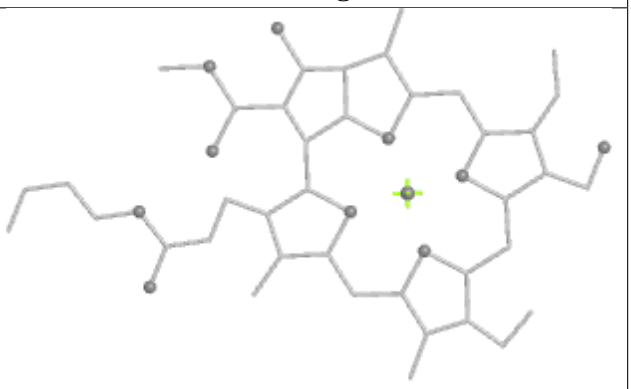
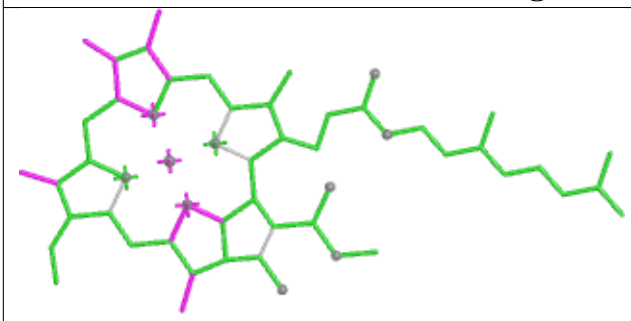


Rings

Ligand CLA 9 301



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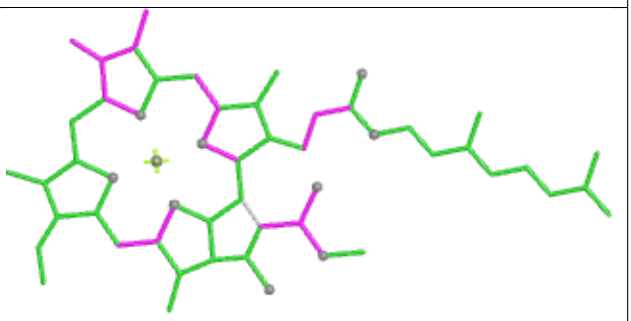
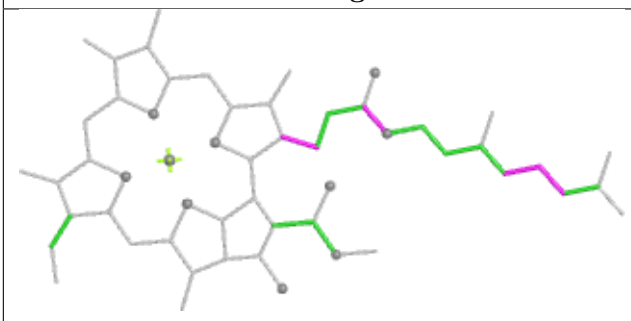


Bond angles



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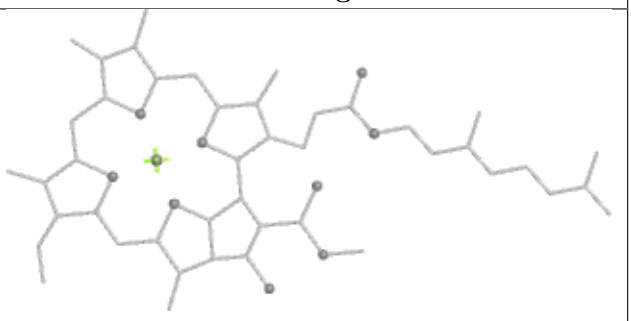
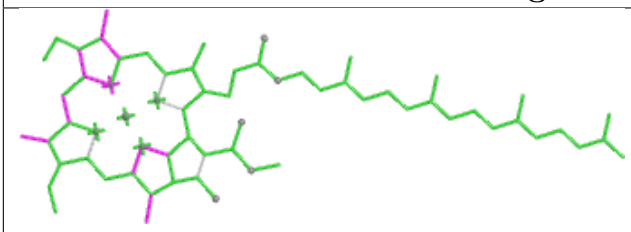


Rings

Ligand CLA a 309



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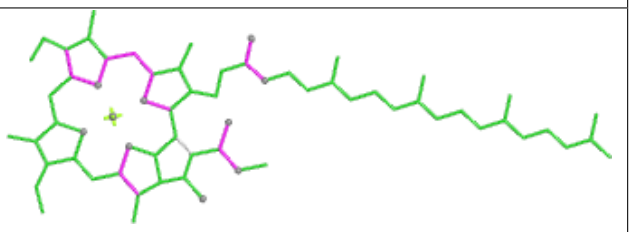
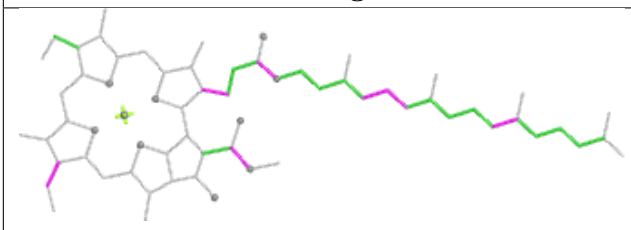


Bond angles



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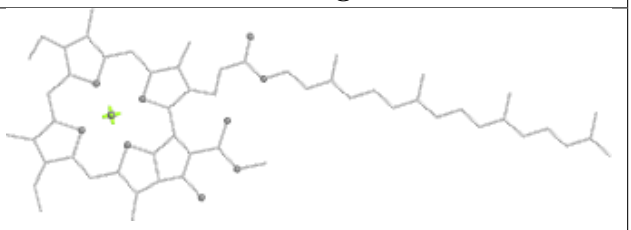
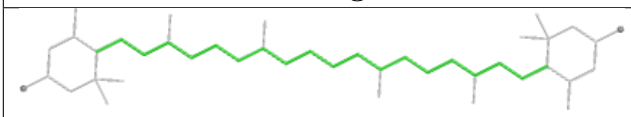


Rings

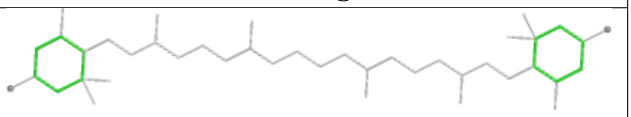
Ligand LUT T 613

Bond lengths

Bond angles

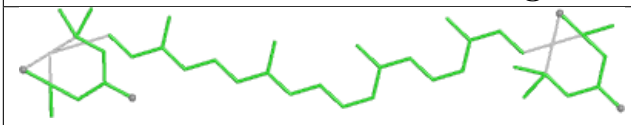


Torsions

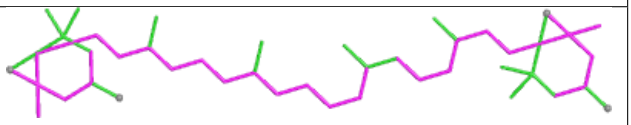


Rings

Ligand XAT P 620

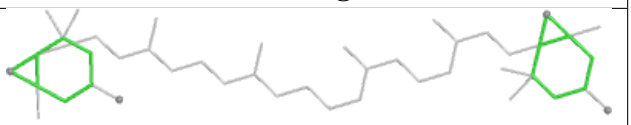


Bond lengths

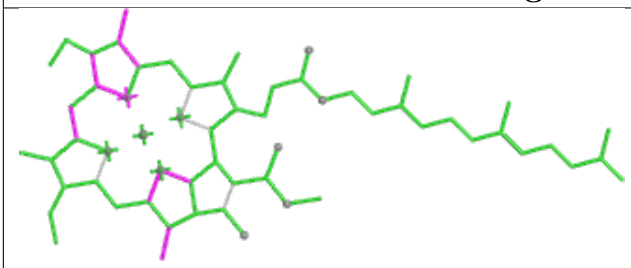
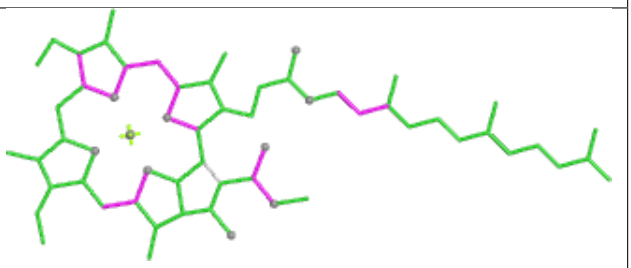
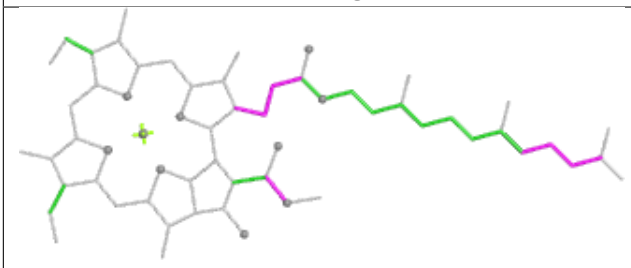
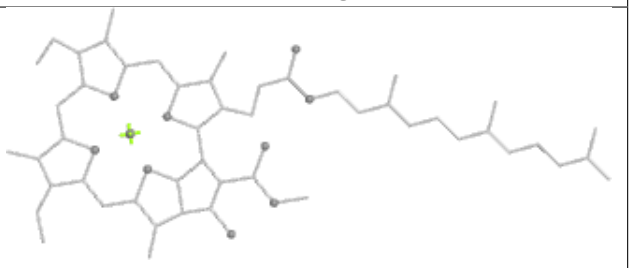


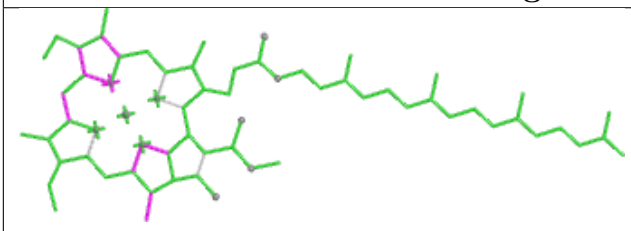
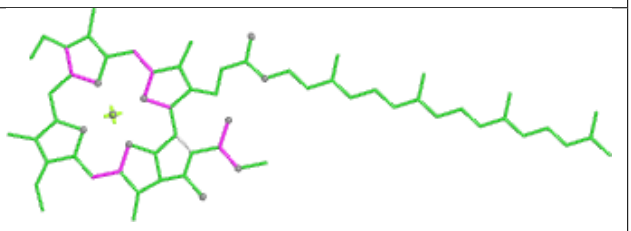
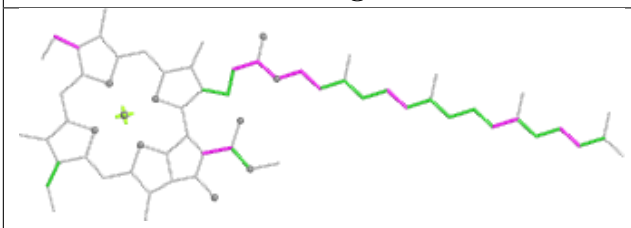
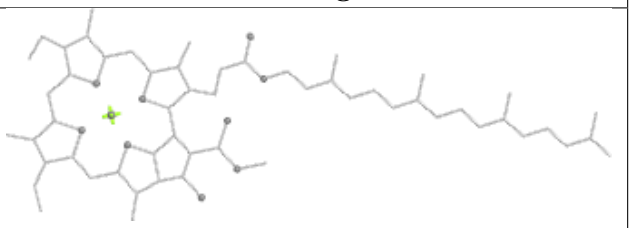
Bond angles

Torsions

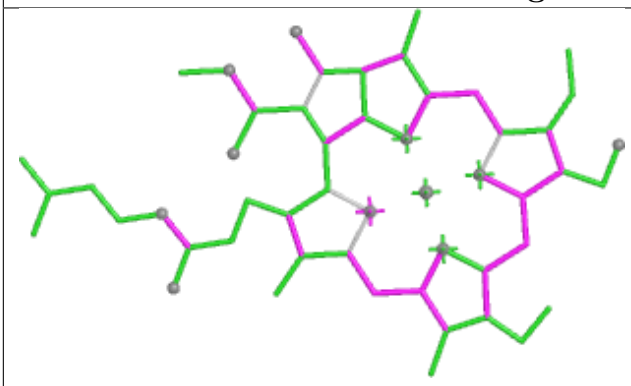


Rings

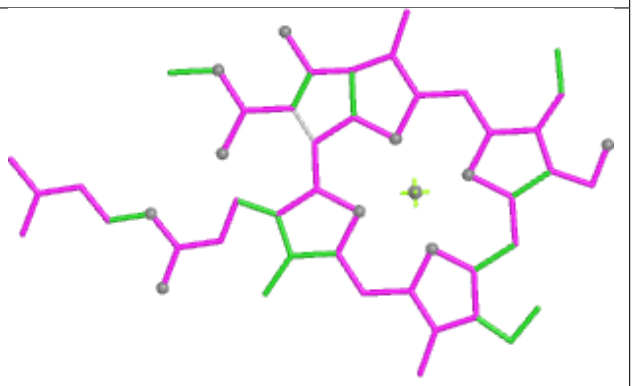
Ligand CLA P 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA U 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

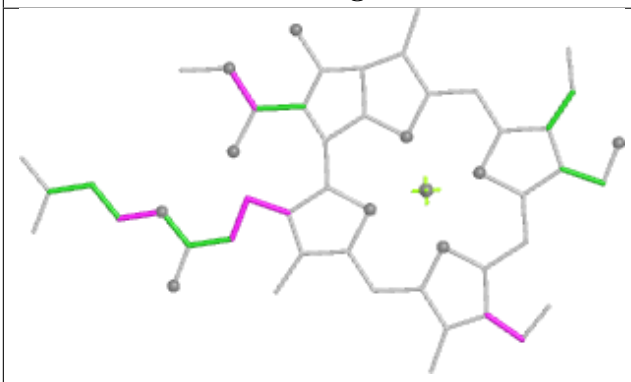
Ligand CHL 5 308



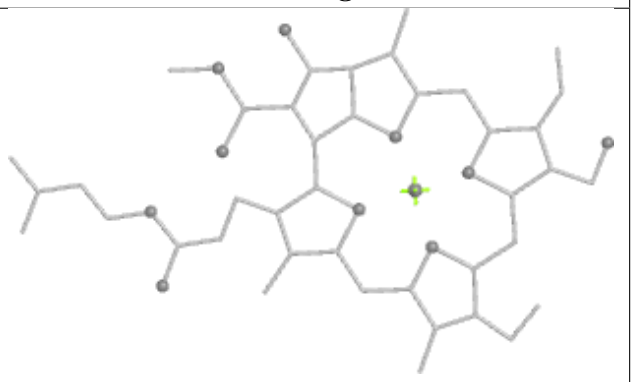
Bond lengths



Bond angles

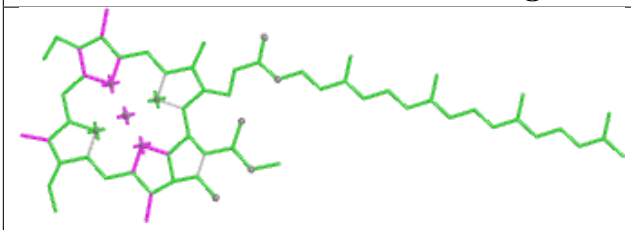


Torsions



Rings

Ligand CLA A 801



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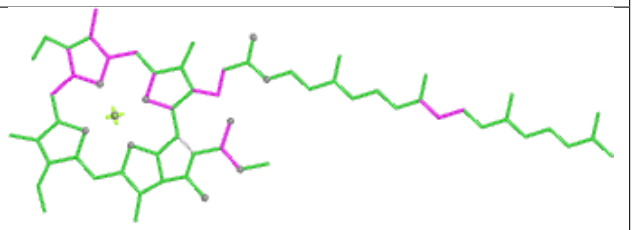
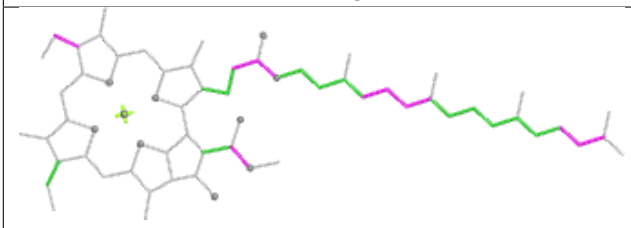


Bond angles



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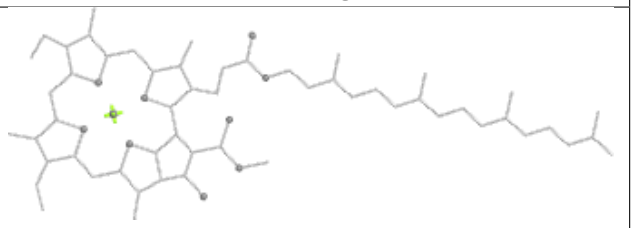
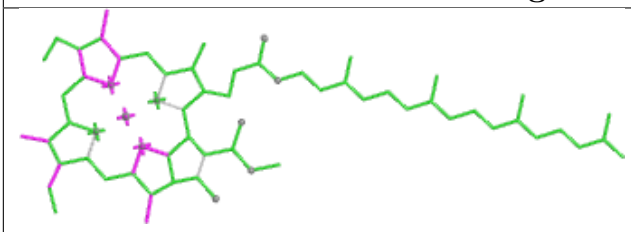


Rings

Ligand CLA 5 303



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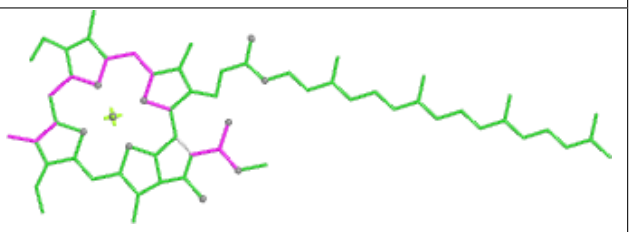
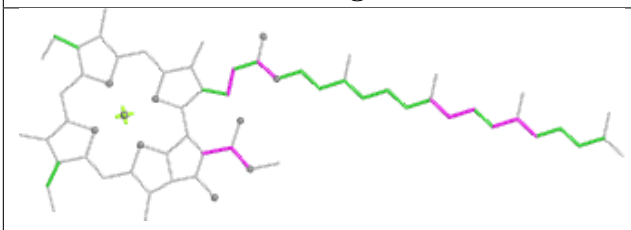


Bond angles



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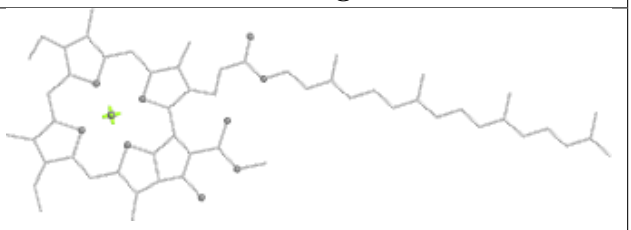
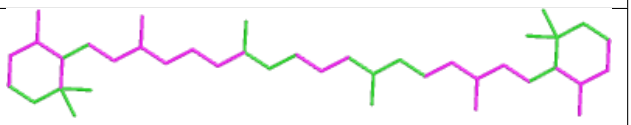


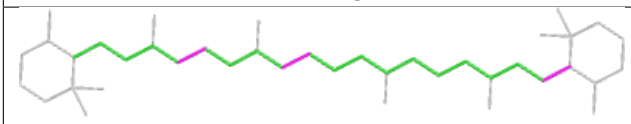
Rings

Ligand BCR O 205

Bond lengths



Bond angles



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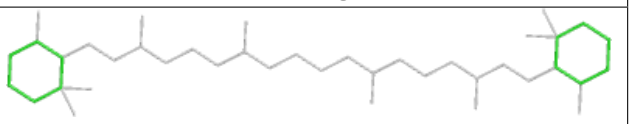
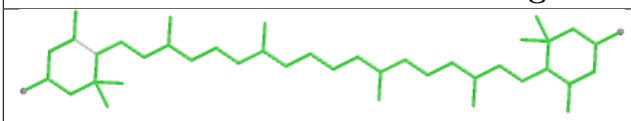


Rings

Ligand LUT a 316



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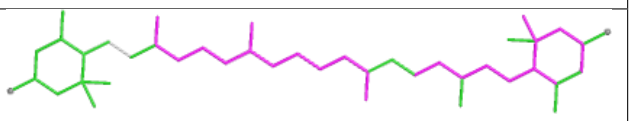
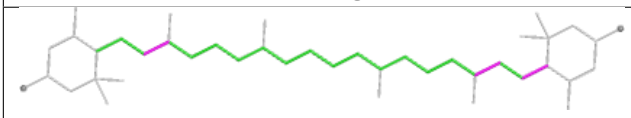
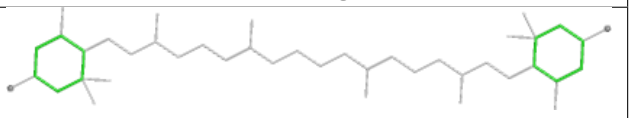


Bond angles

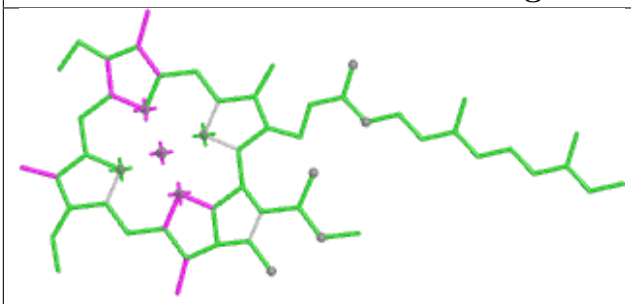


Torsions



Rings

Ligand CLA B 818



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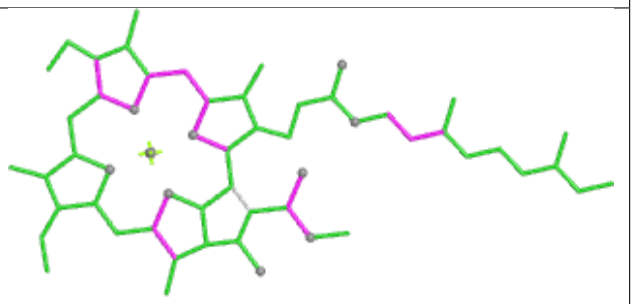
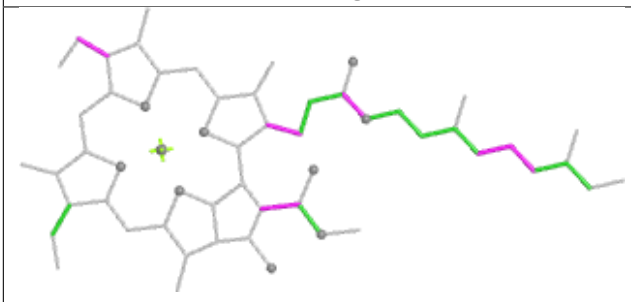


Bond angles



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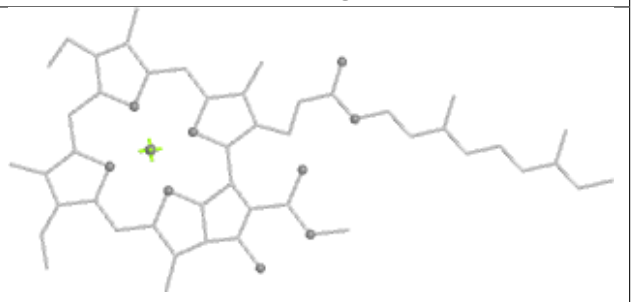
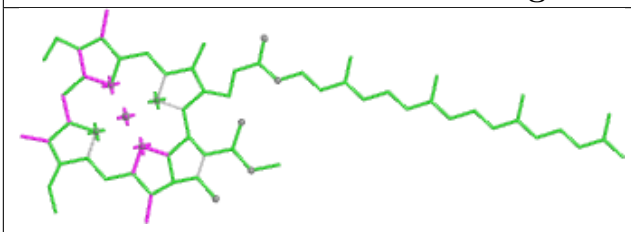
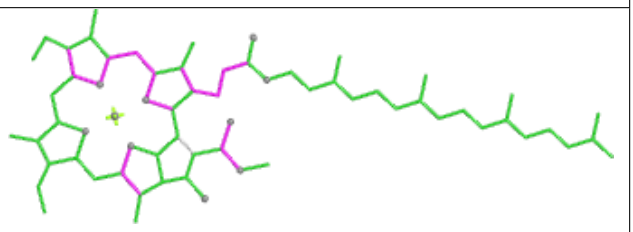


Rings

Ligand CLA 3 302



Bond lengths



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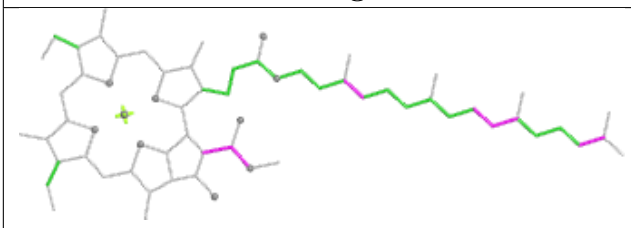

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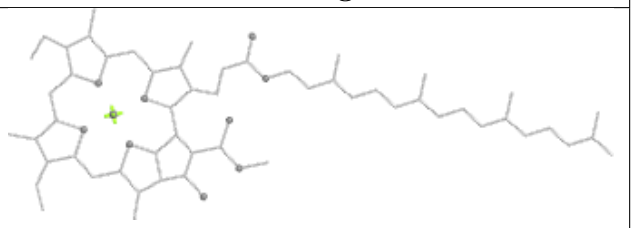
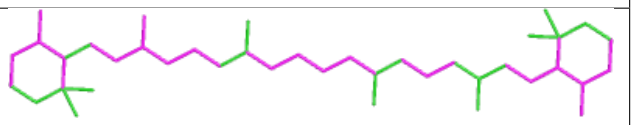


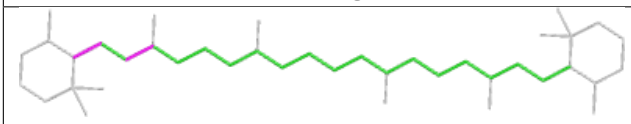
Rings

Ligand BCR B 841

Bond lengths



Bond angles



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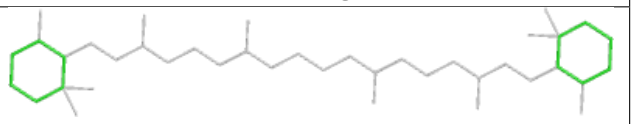
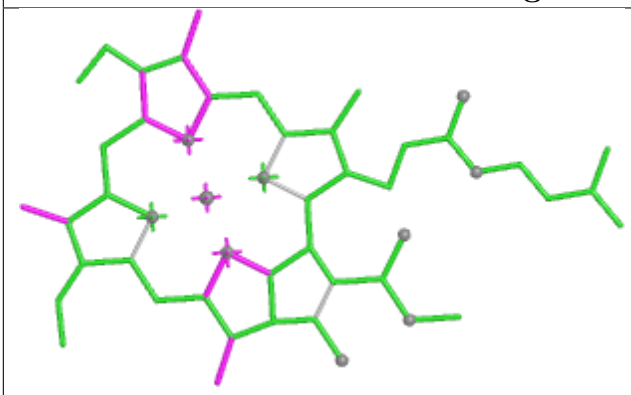


Rings

Ligand CLA A 833



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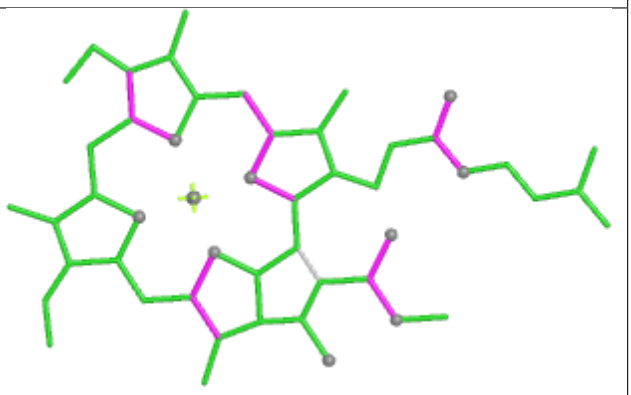
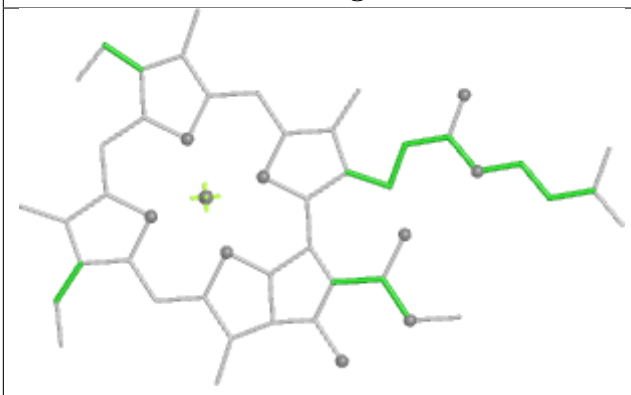


Bond angles



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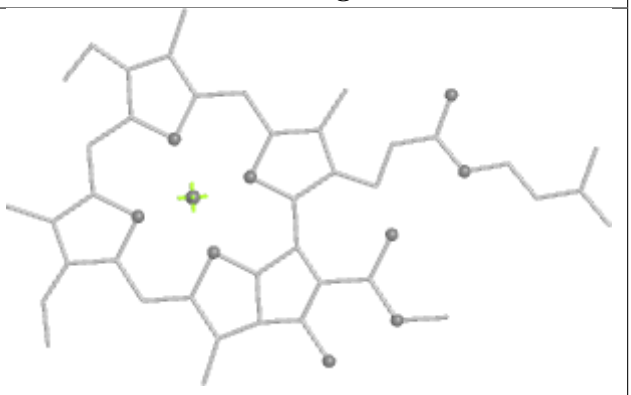
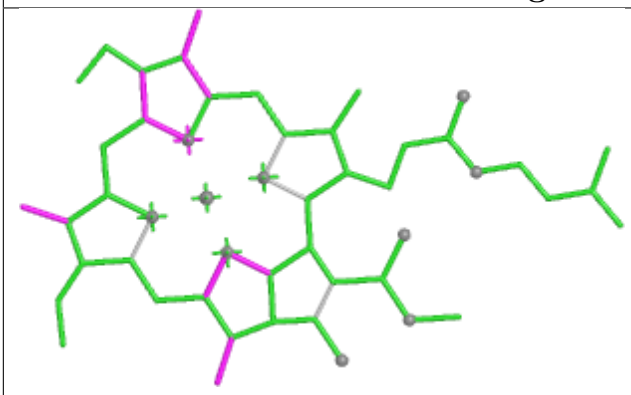


Rings

Ligand CLA 9 308



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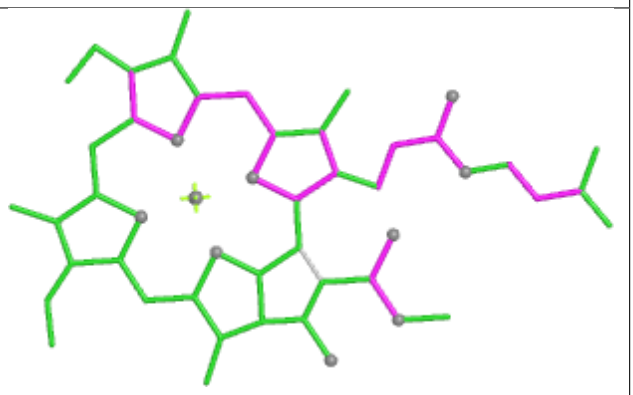
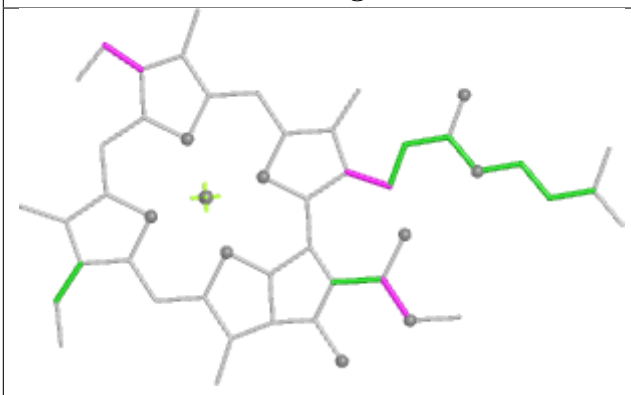


Bond angles



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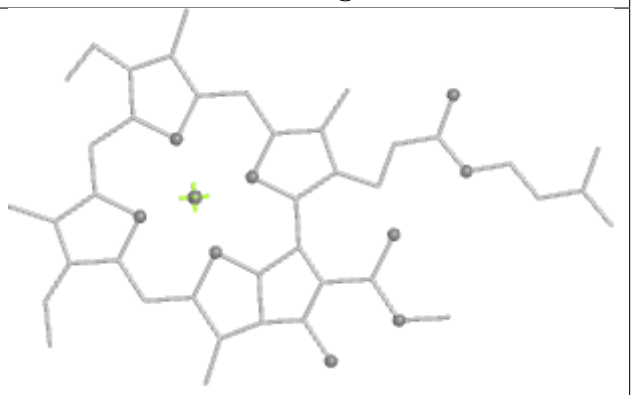
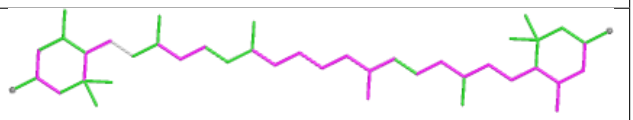


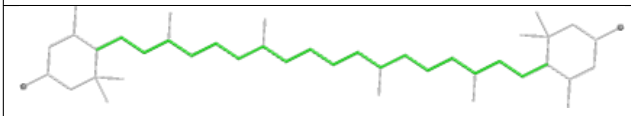
Rings

Ligand LUT U 314

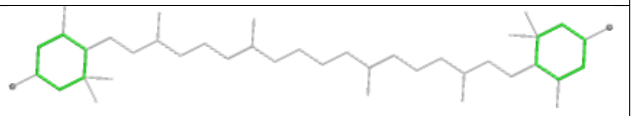
Bond lengths



Bond angles

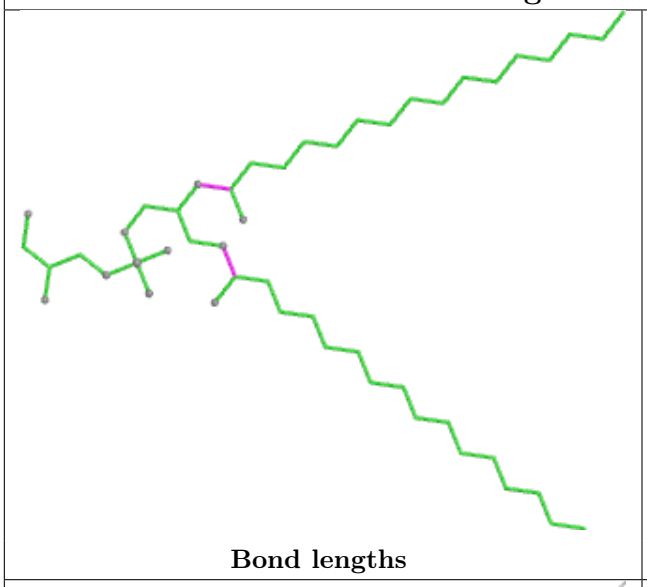


Torsions

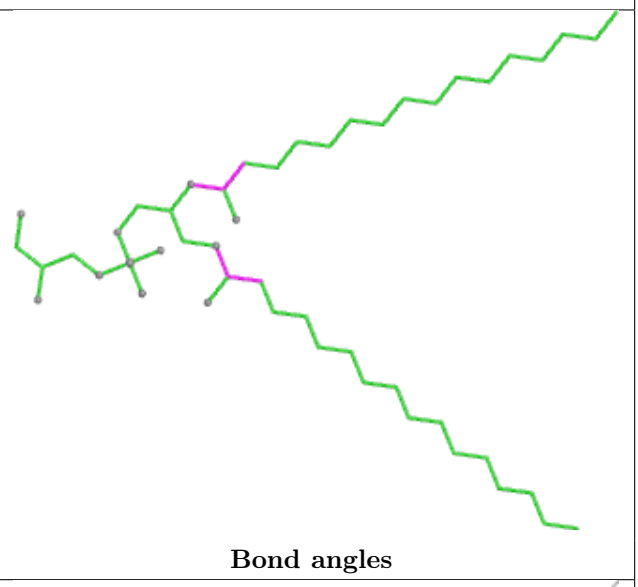


Rings

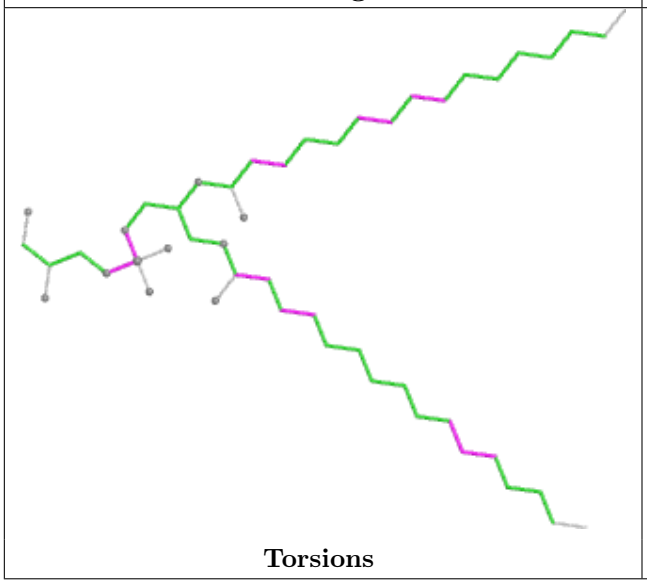
Ligand LHG T 617



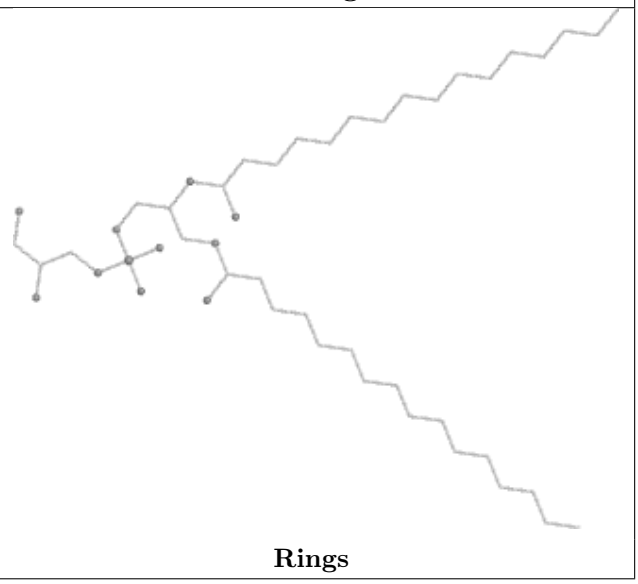
Bond lengths



Bond angles



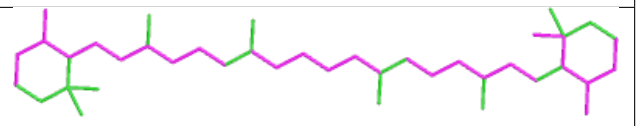
Torsions



Rings

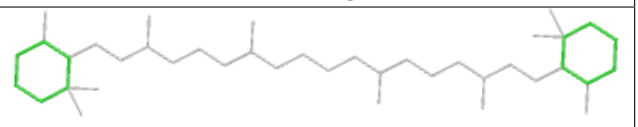
Ligand BCR B 844

Bond lengths



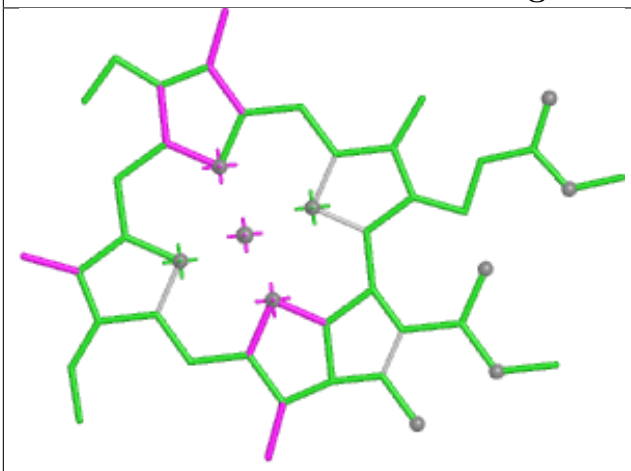
Bond angles

Torsions



Rings

Ligand CLA 7 302



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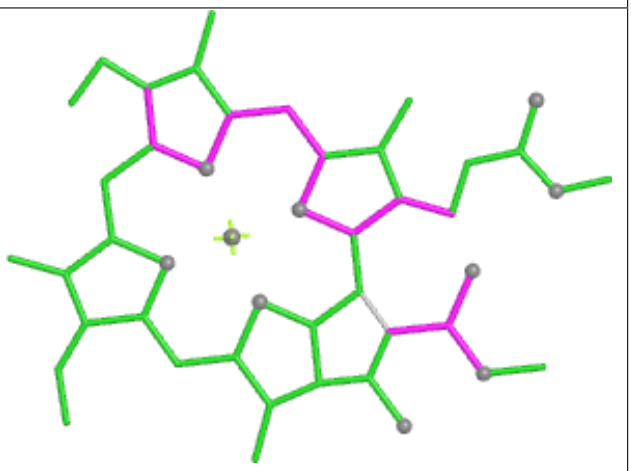
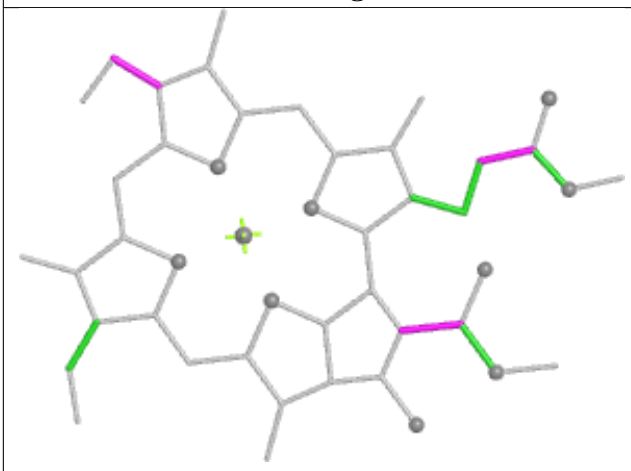
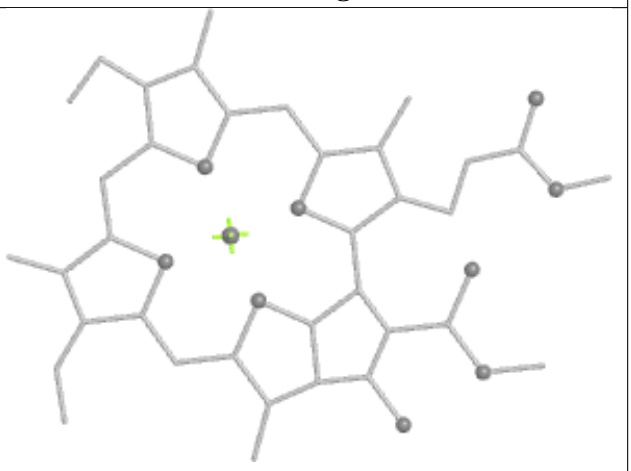


Bond angles

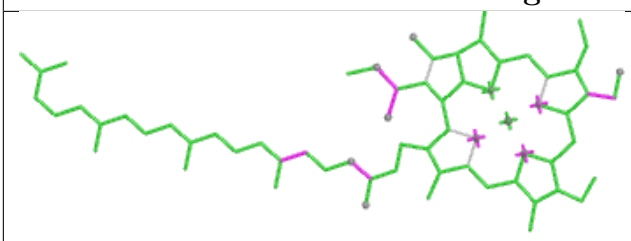


Torsions



Rings

Ligand CHL R 609



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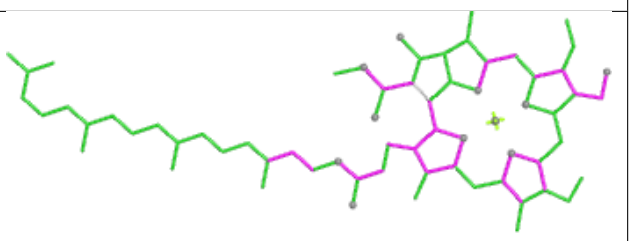
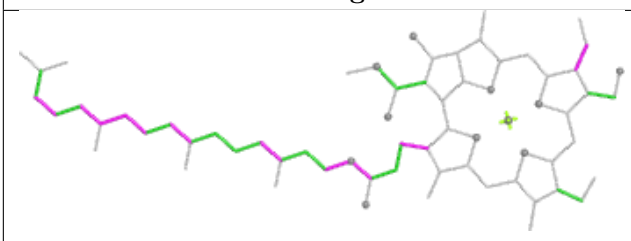


Bond angles



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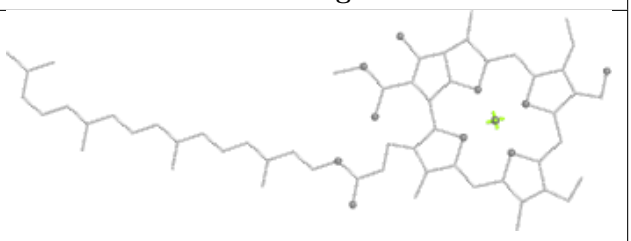
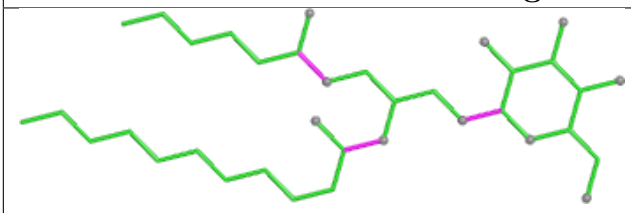


Rings

Ligand LMG 7 319



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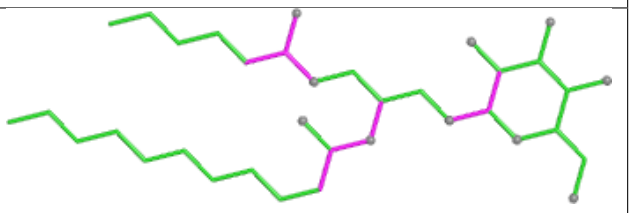

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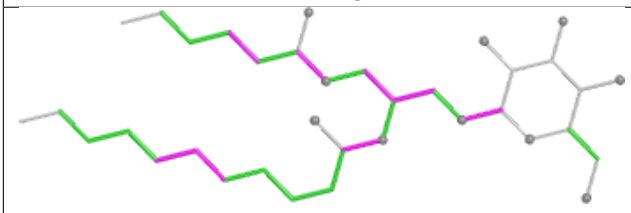

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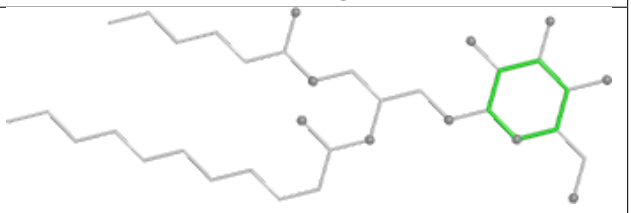
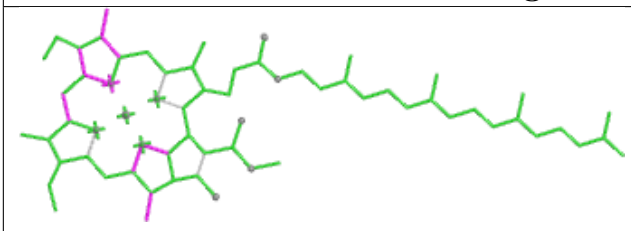


Rings

Ligand CLA U 302



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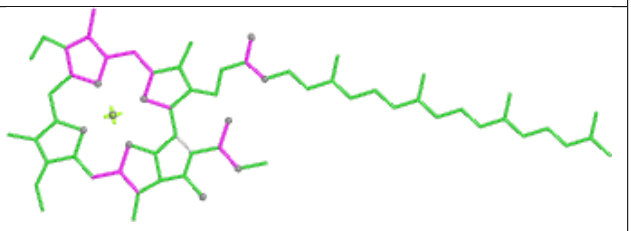
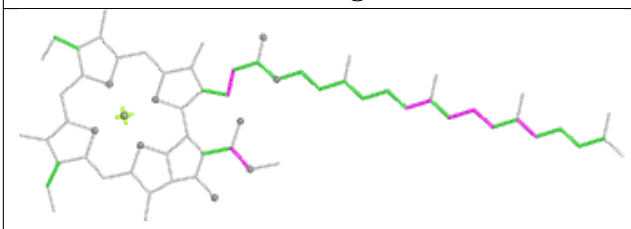


Bond angles



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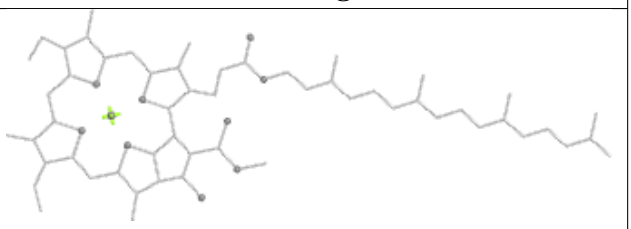
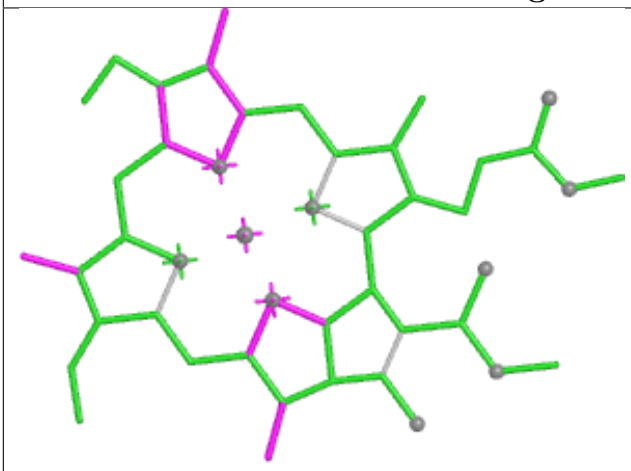


Rings

Ligand CLA 3 313



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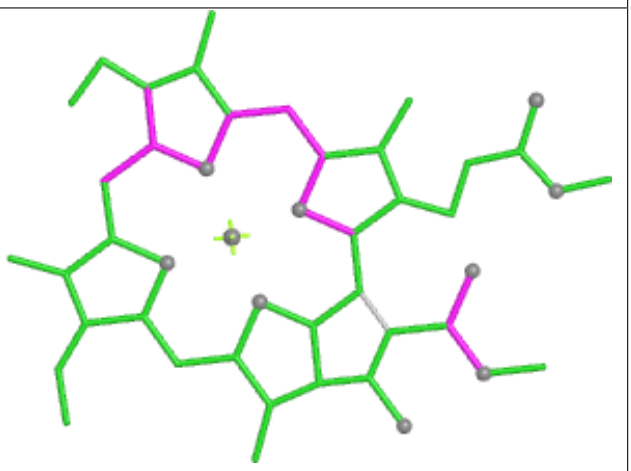
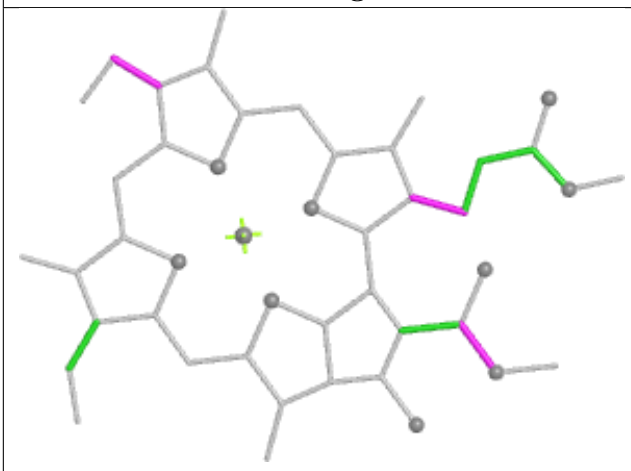


Bond angles



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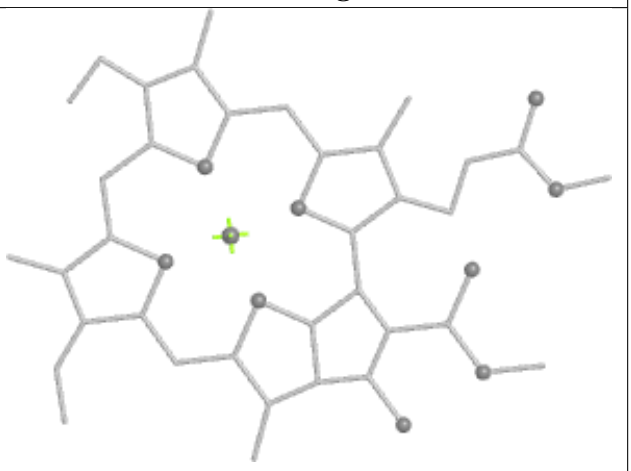
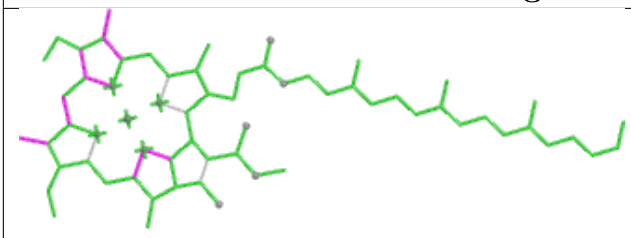


Rings

Ligand CLA R 610



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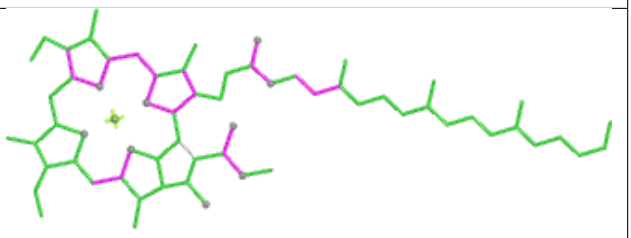
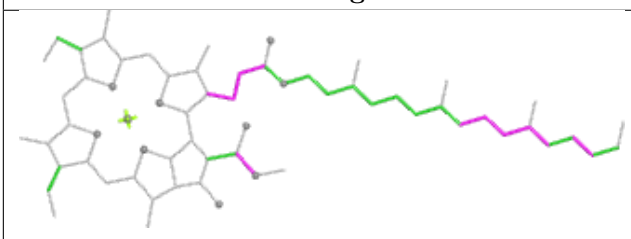


Bond angles



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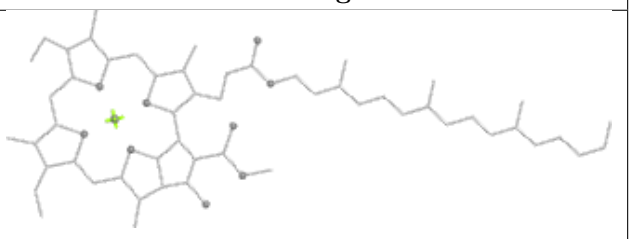
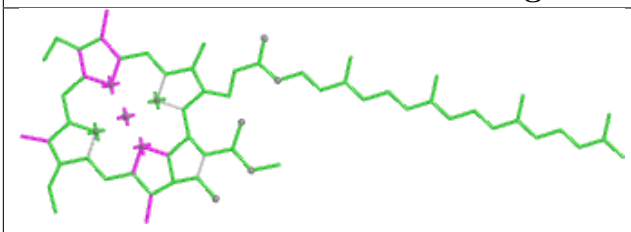


Rings

Ligand CLA B 809



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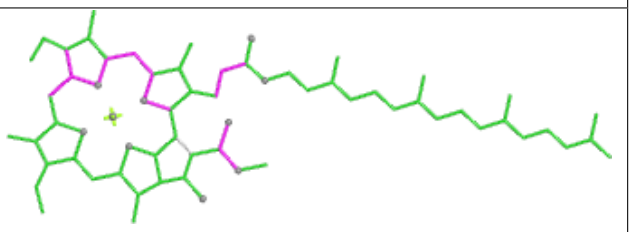
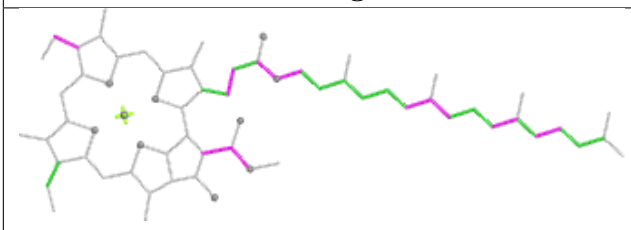


Bond angles



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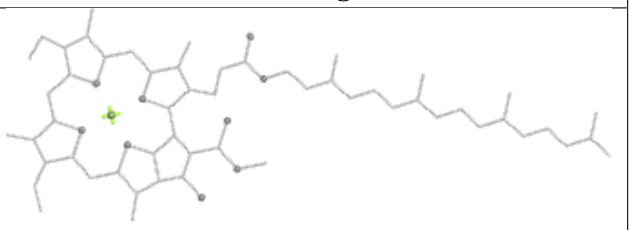
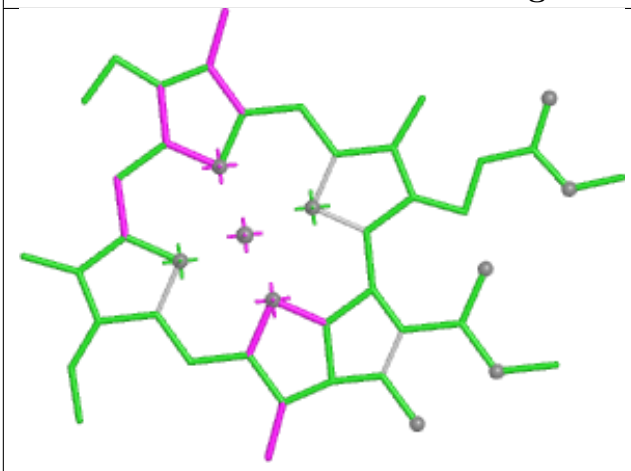


Rings

Ligand CLA 5 319



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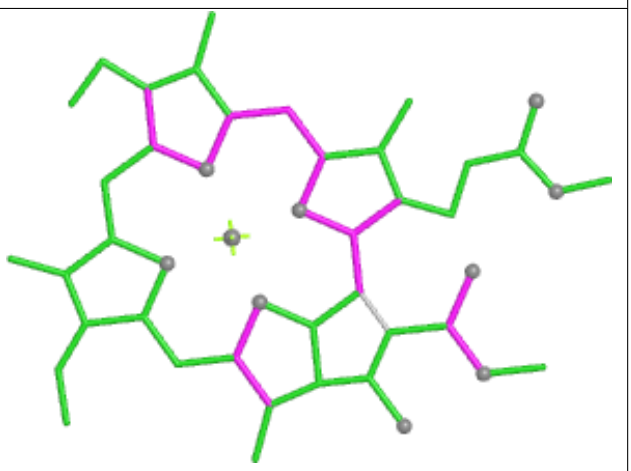
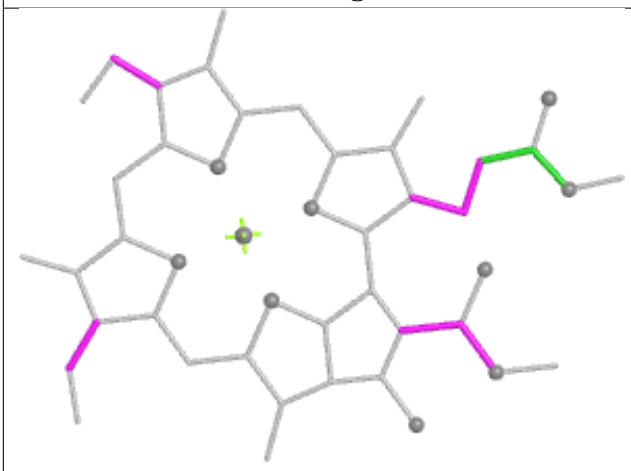


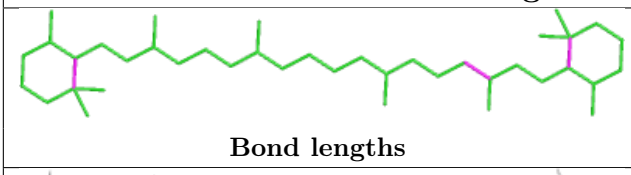
Bond angles



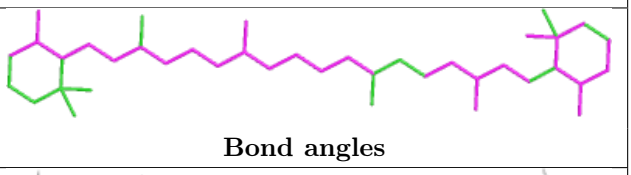
Torsions

Rings

Ligand BCR B 845



Bond lengths



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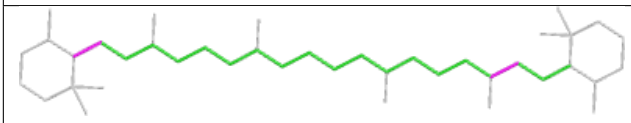

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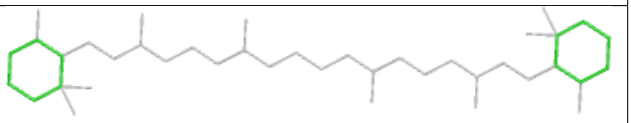
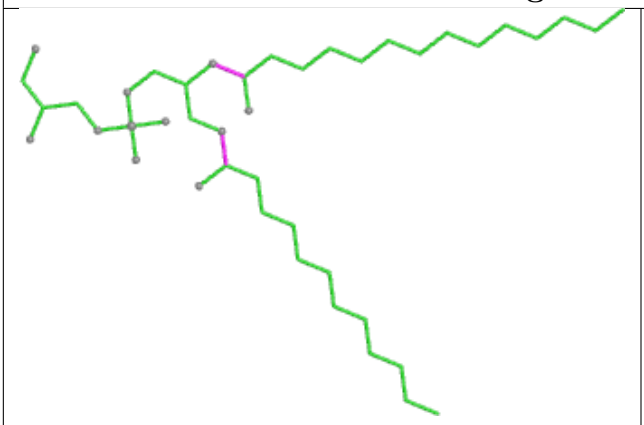


Rings

Ligand LHG 1 618



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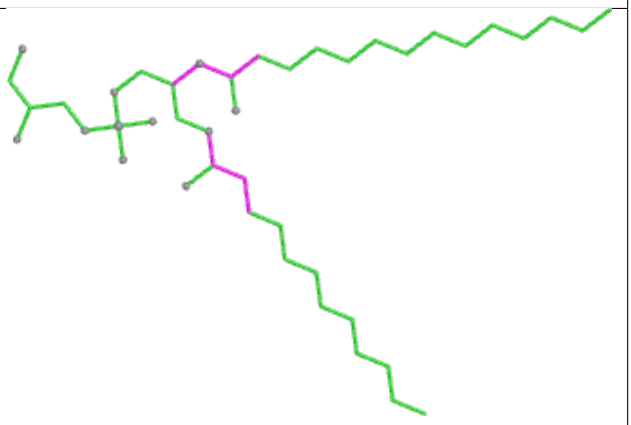
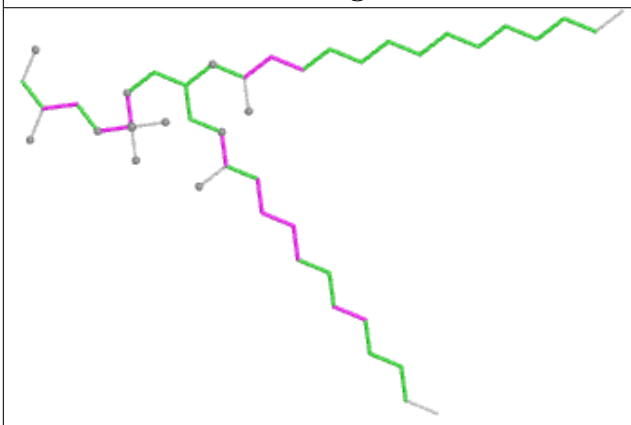


Bond angles



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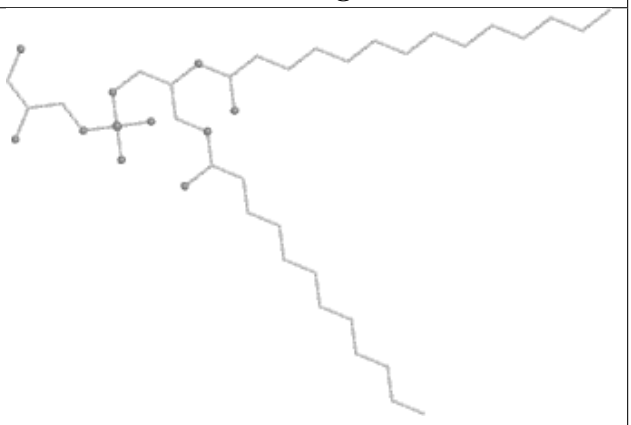
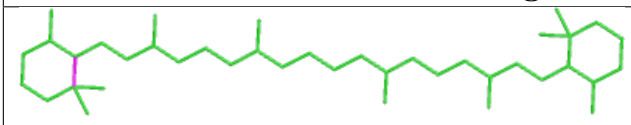
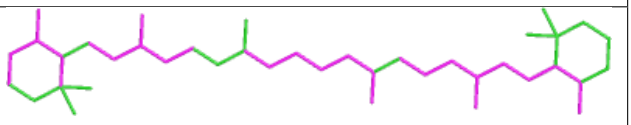


Rings

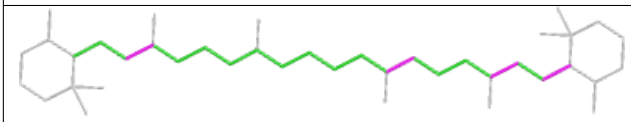
Ligand BCR B 840



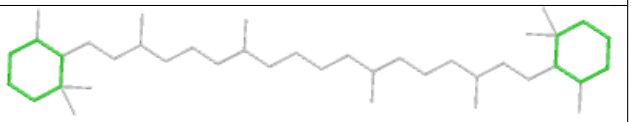
Bond lengths



Bond angles

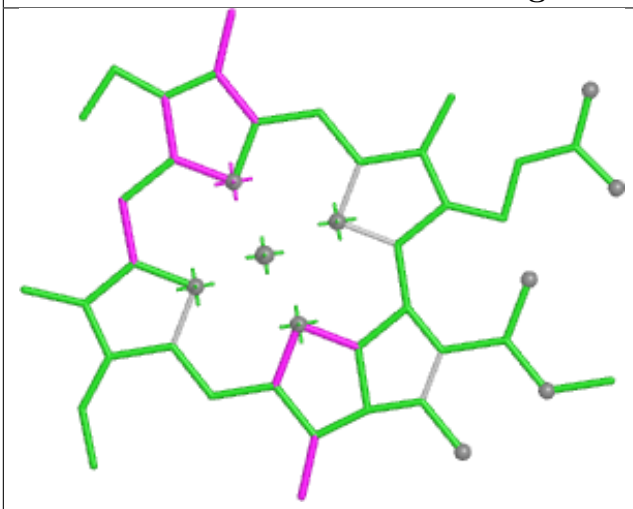


Torsions



Rings

Ligand CLA 4 312



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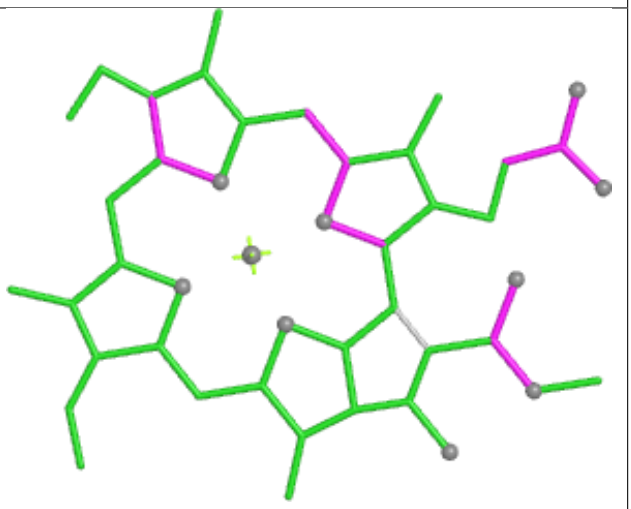
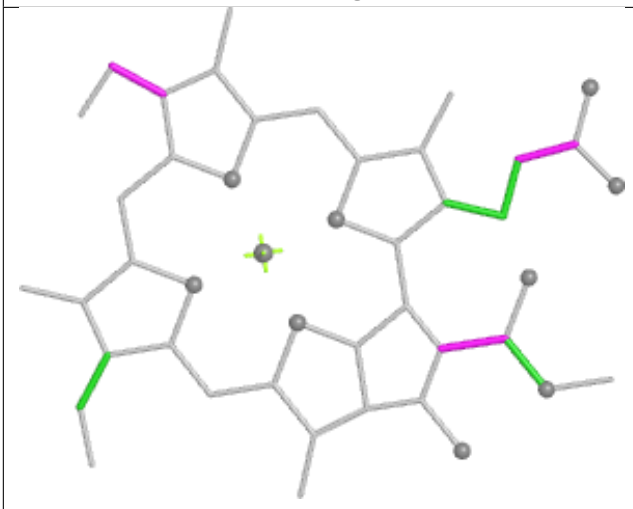


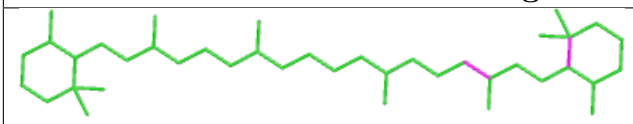
Bond angles



Torsions

Rings

Ligand BCR A 847



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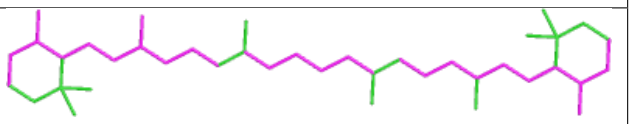
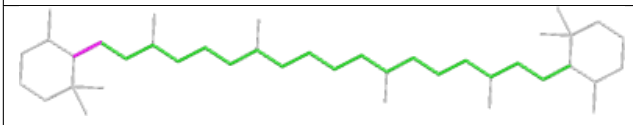
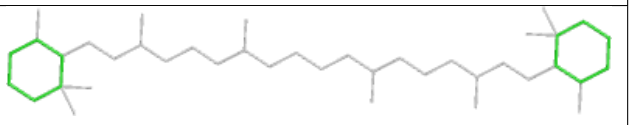


Bond angles

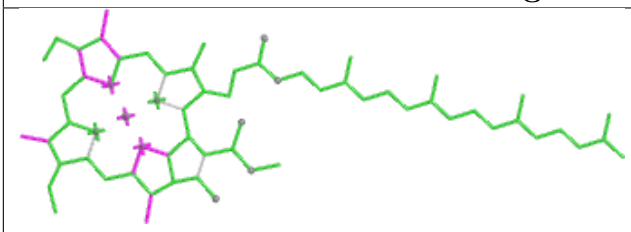


Torsions

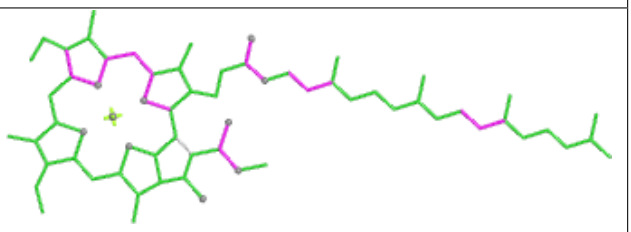


Rings

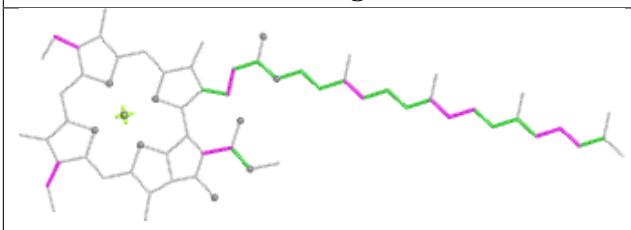
Ligand CLA A 838



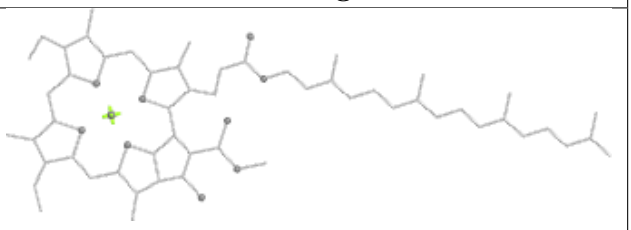
Bond lengths



Bond angles

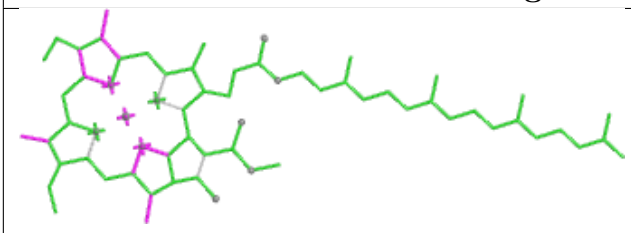


Torsions

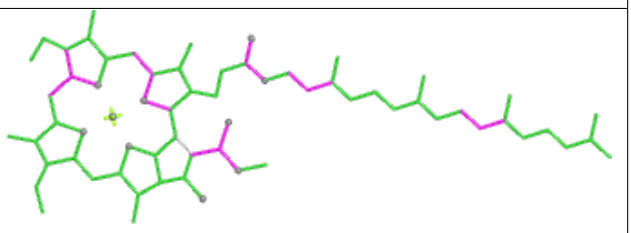


Rings

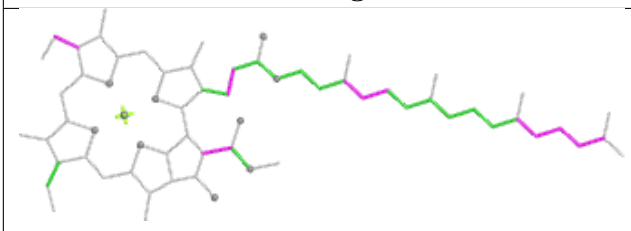
Ligand CLA B 807



Bond lengths



Bond angles



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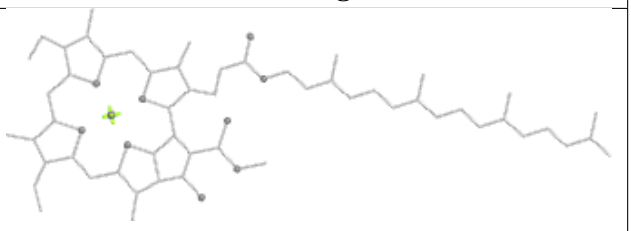
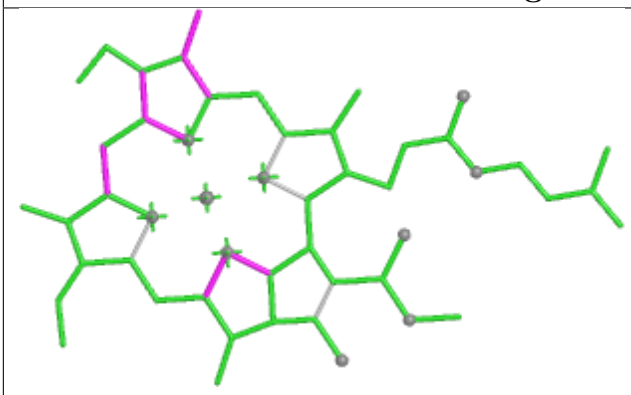


Rings

Ligand CLA T 603



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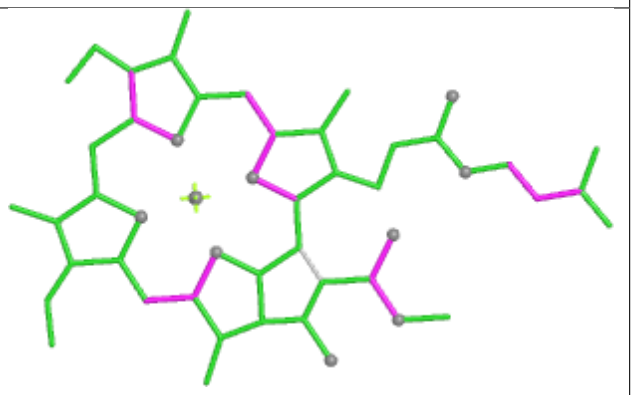

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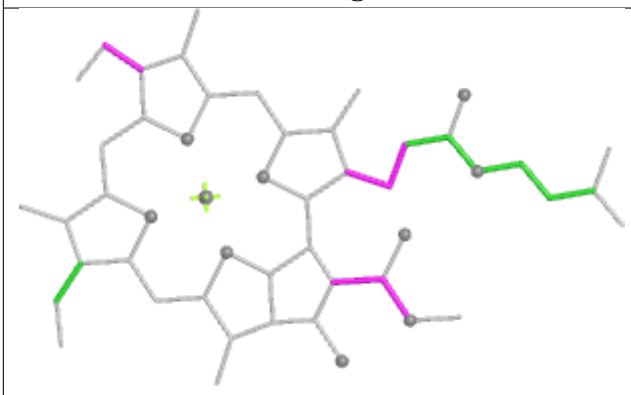

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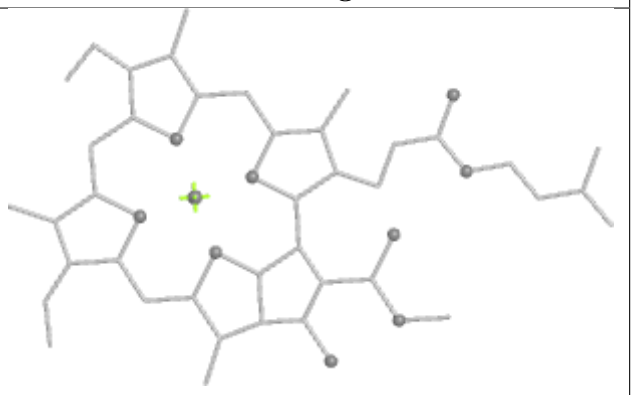
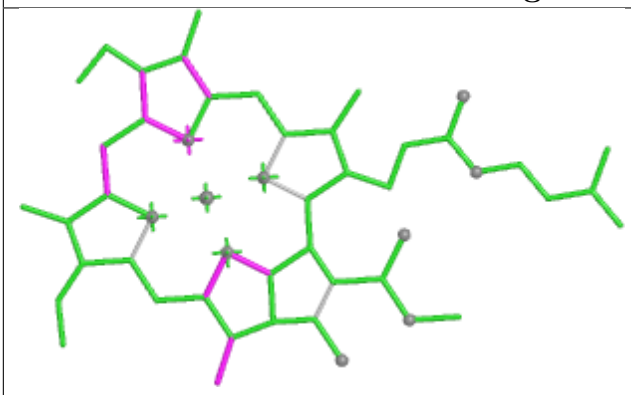


Rings

Ligand CLA Q 604



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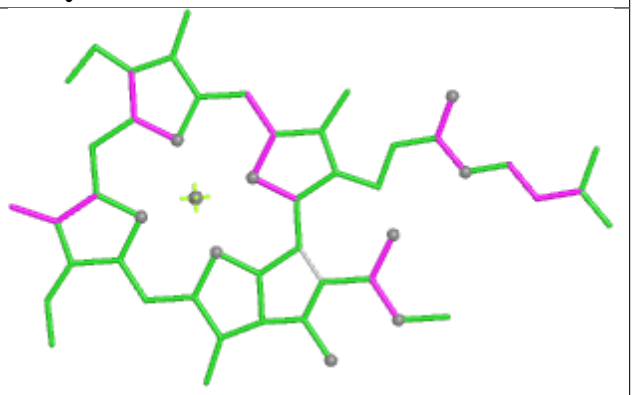

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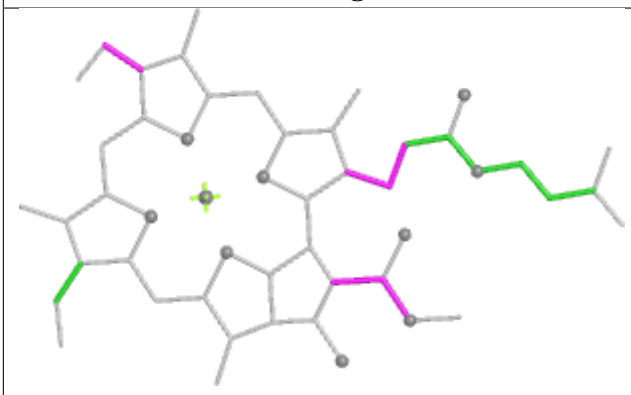

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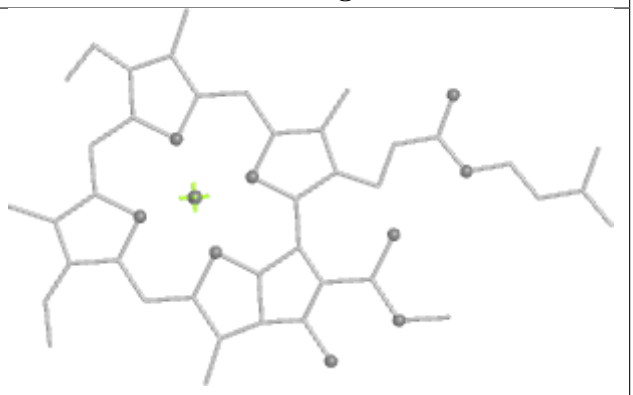
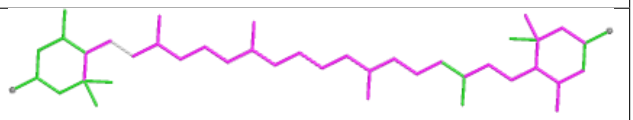


Rings

Ligand LUT 4 315

Bond lengths



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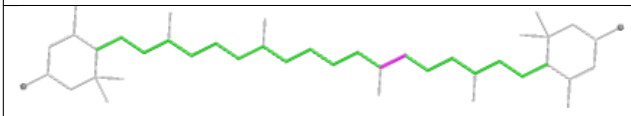

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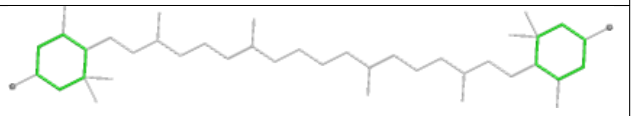
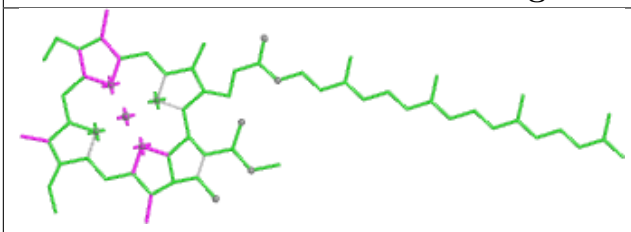


Rings

Ligand CLA 1 603



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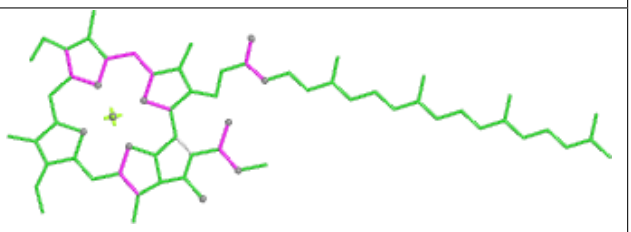

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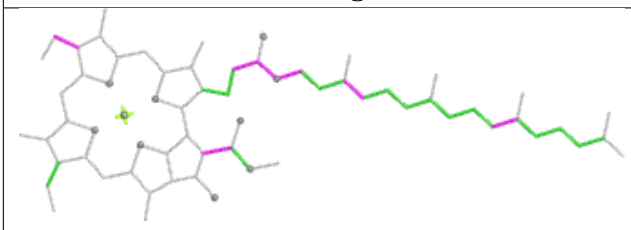

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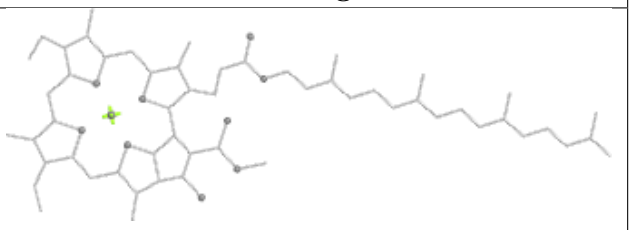
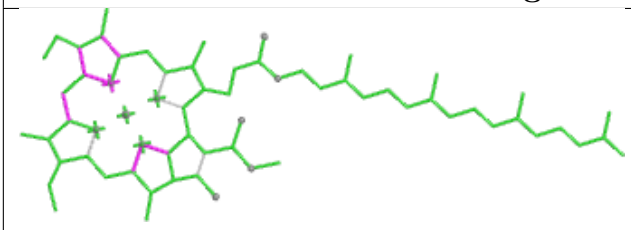


Rings

Ligand CLA R 613



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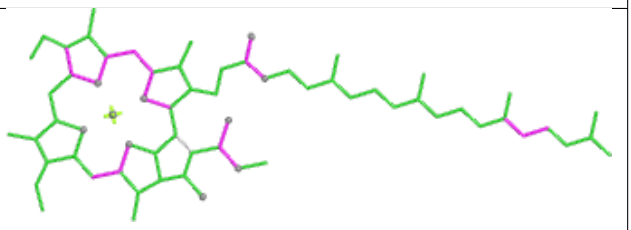

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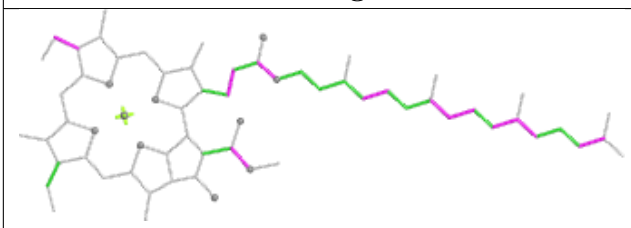

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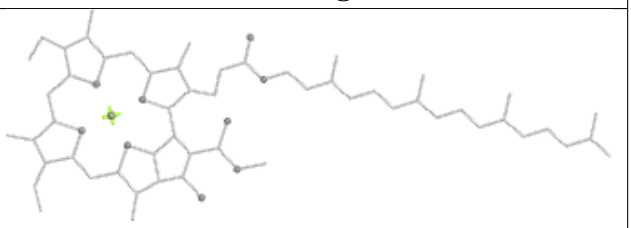
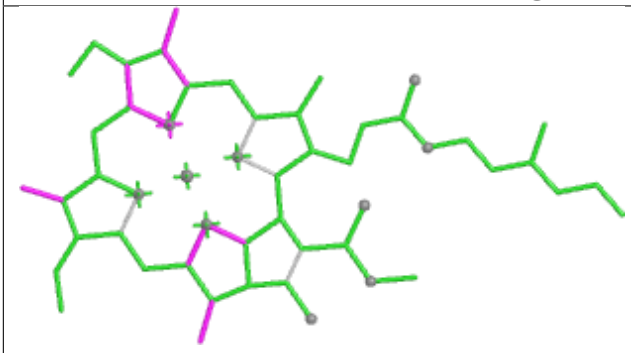


Rings

Ligand CLA 2 305



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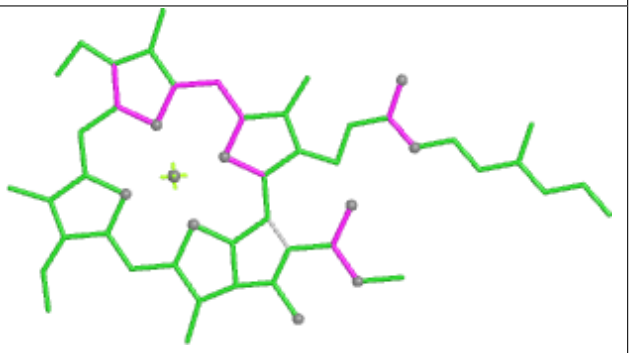

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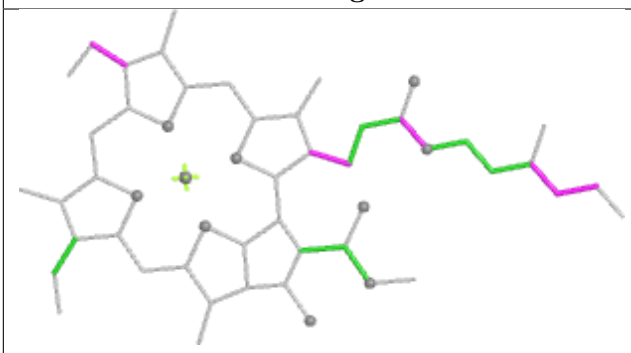

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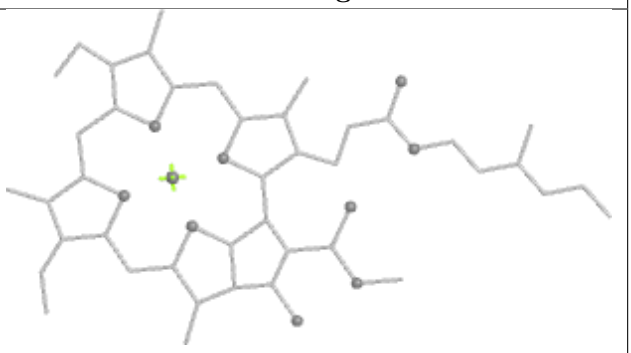
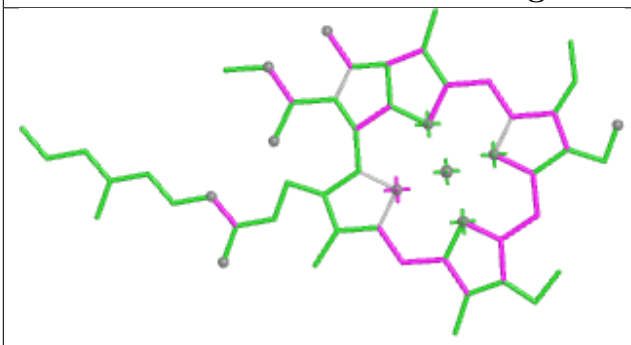


Rings

Ligand CHL 4 322



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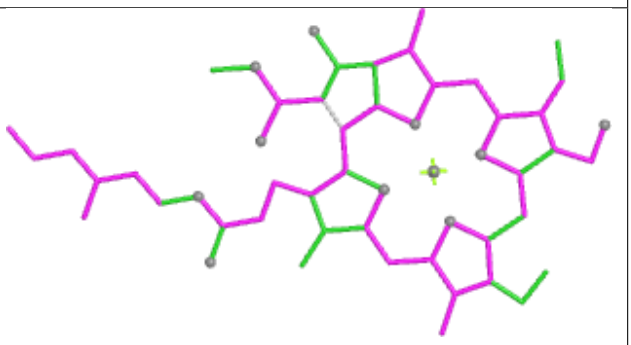
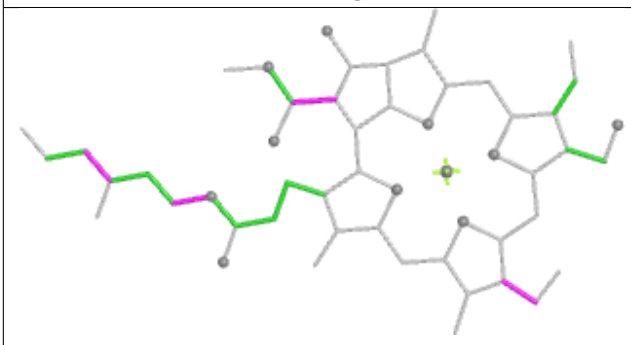


Bond angles



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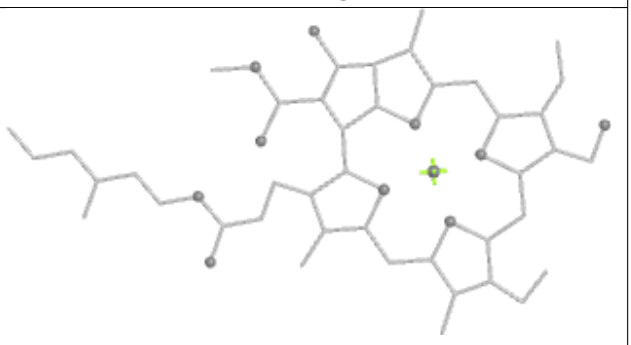
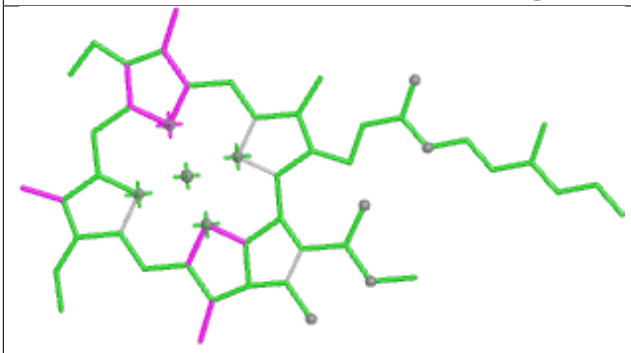
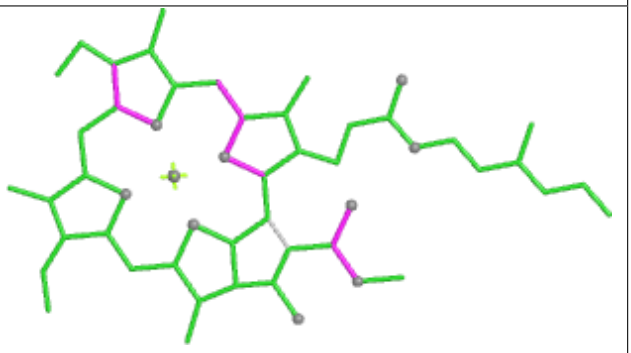
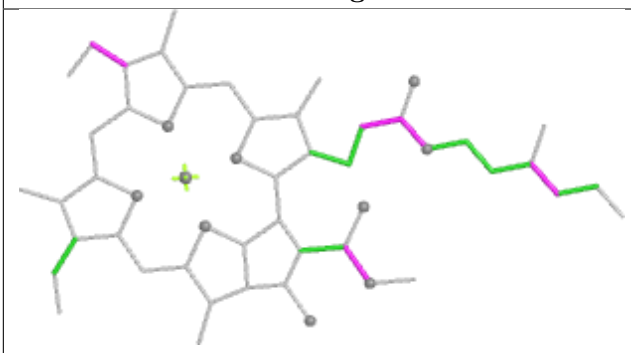
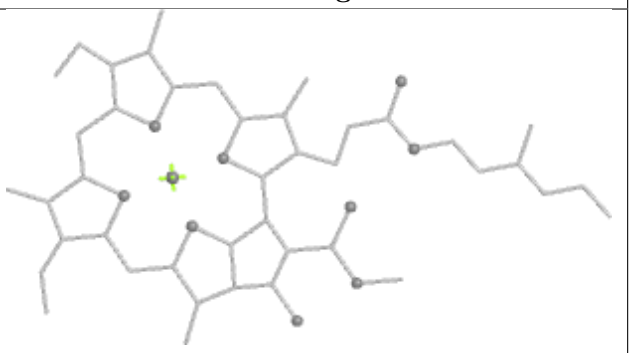
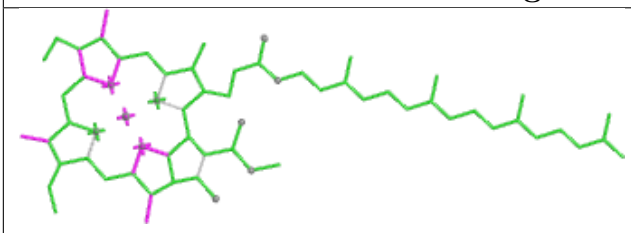
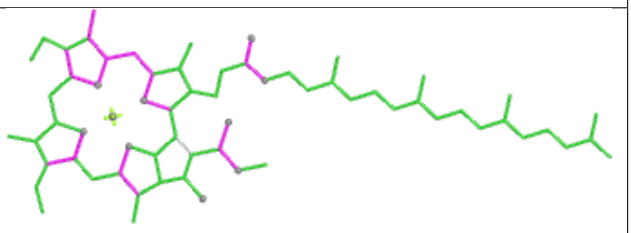
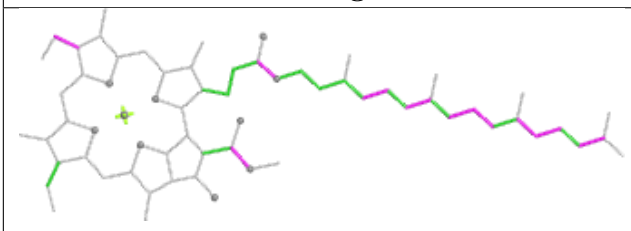
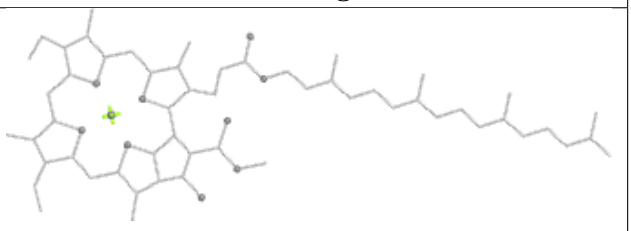
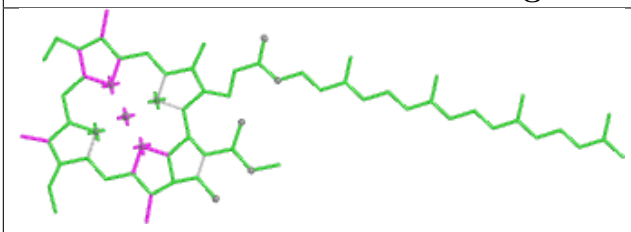


Rings

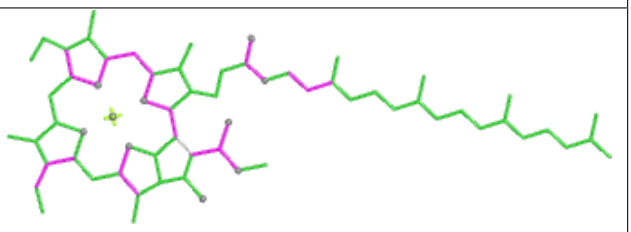
Ligand CLA 8 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

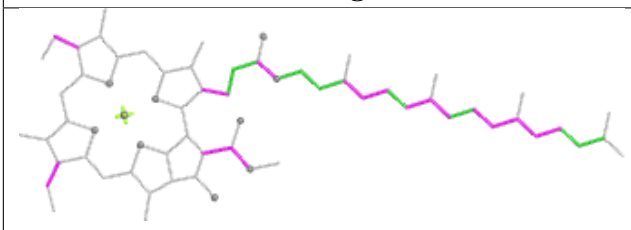
Ligand CLA A 825



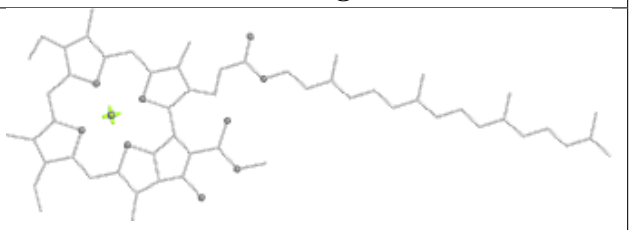
Bond lengths



Bond angles

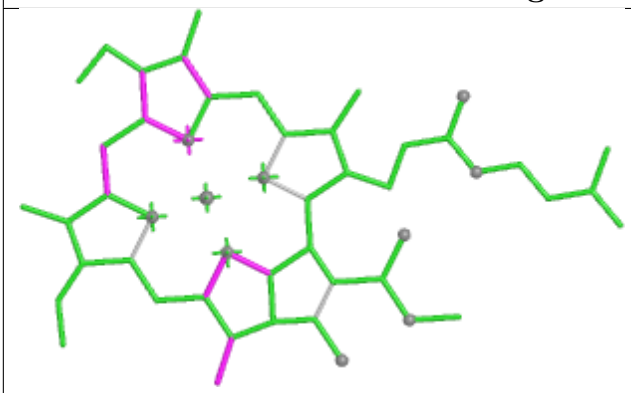


Torsions



Rings

Ligand CLA S 305



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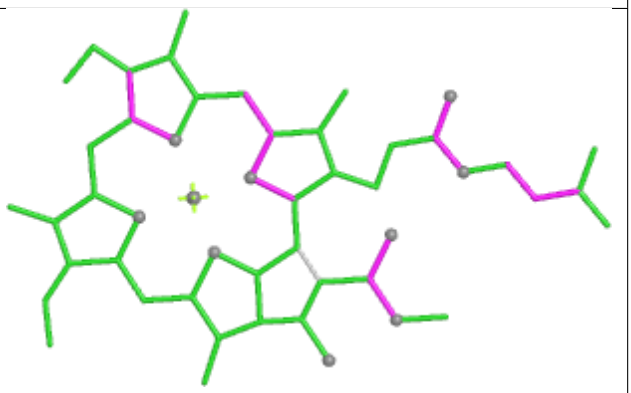
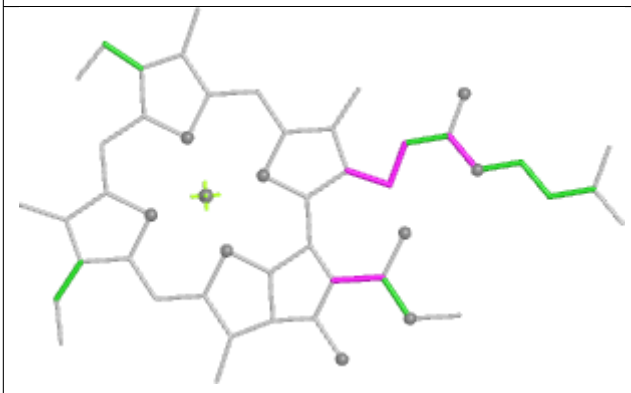
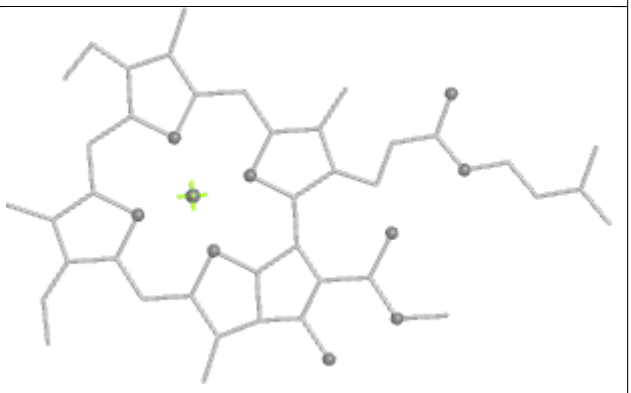


Bond angles

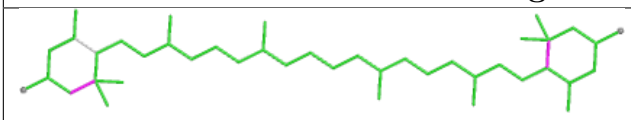


Torsions

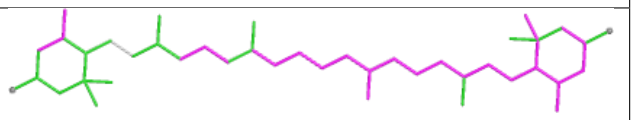


Rings

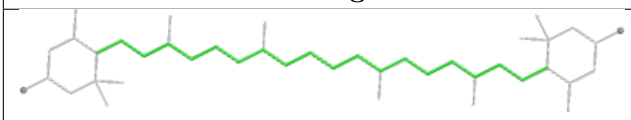
Ligand LUT 3 316



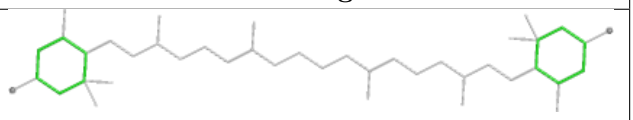
Bond lengths



Bond angles

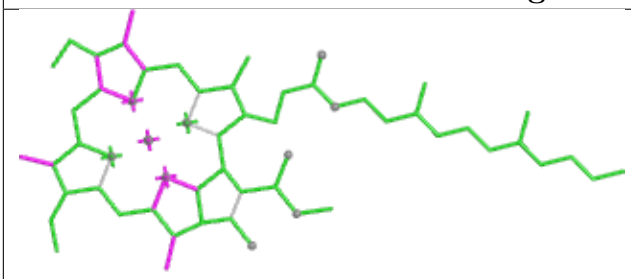


Torsions

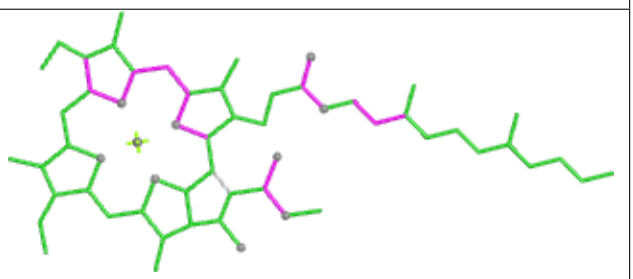


Rings

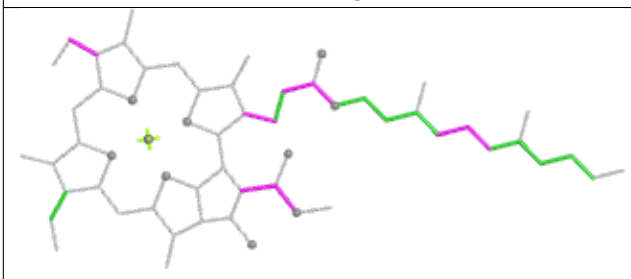
Ligand CLA J 103



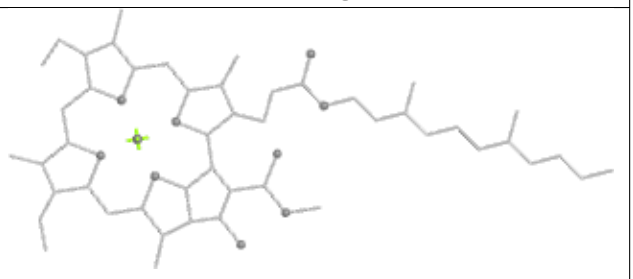
Bond lengths



Bond angles

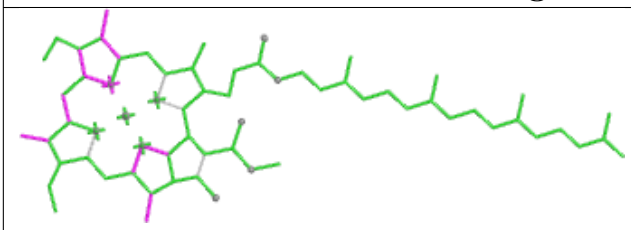


Torsions

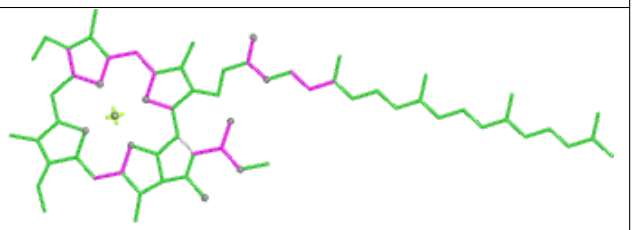


Rings

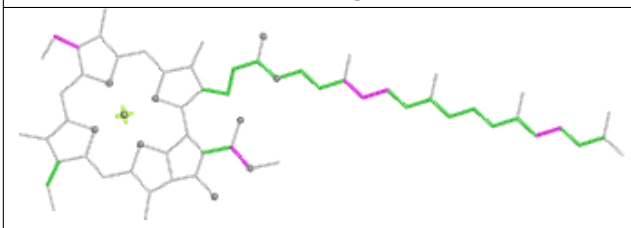
Ligand CLA a 306



Bond lengths



Bond angles



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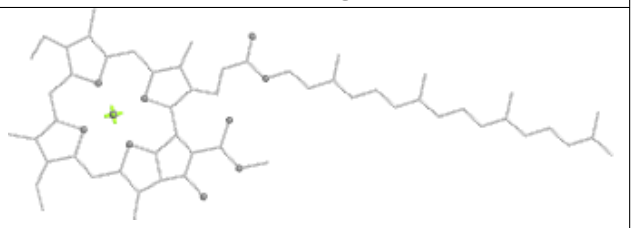
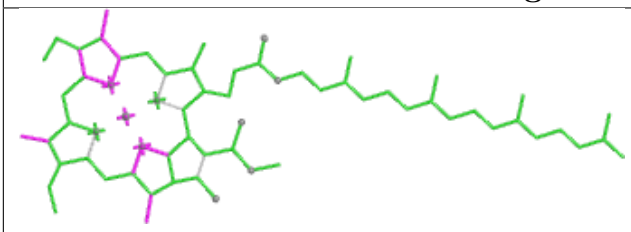


Rings

Ligand CLA B 802



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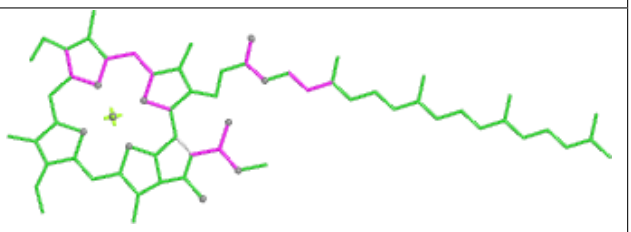
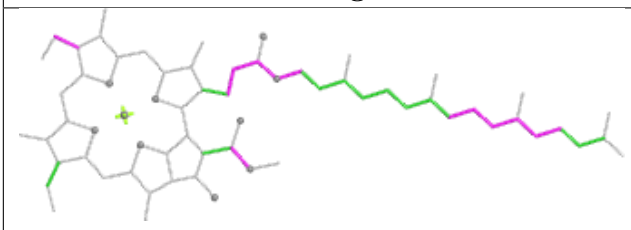


Bond angles



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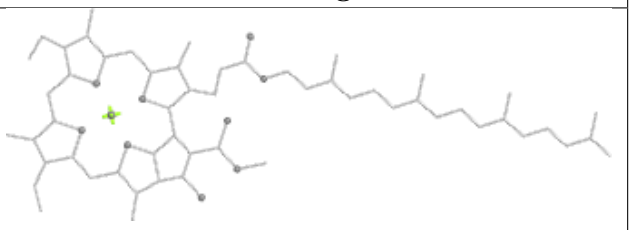
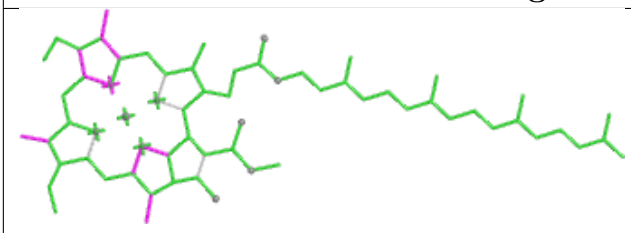


Rings

Ligand CLA a 311



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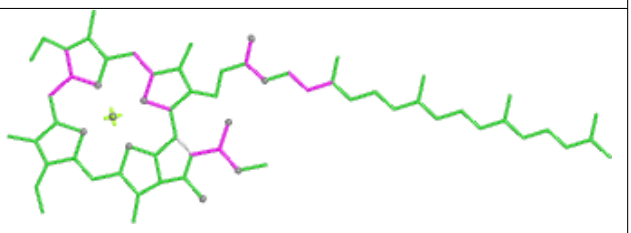
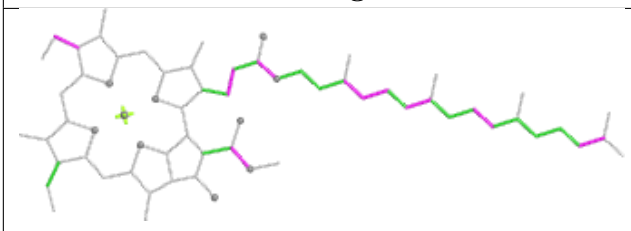


Bond angles



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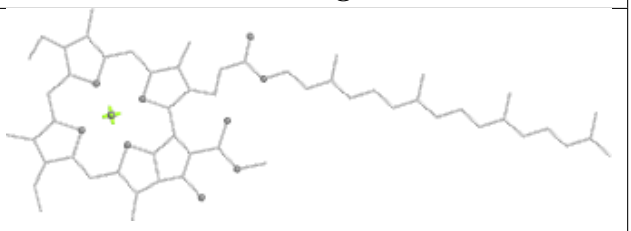
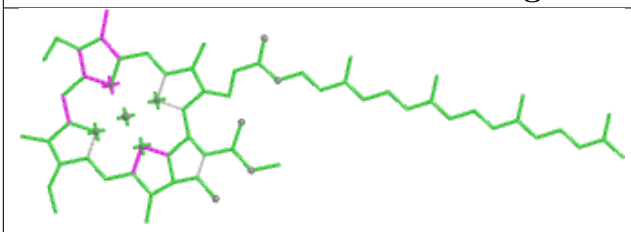


Rings

Ligand CLA Q 609



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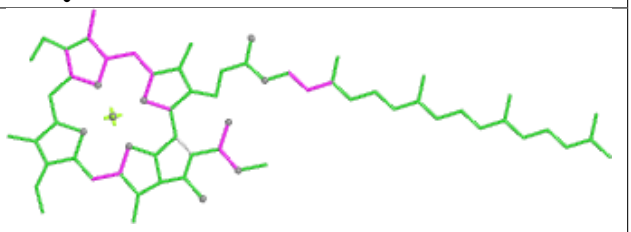
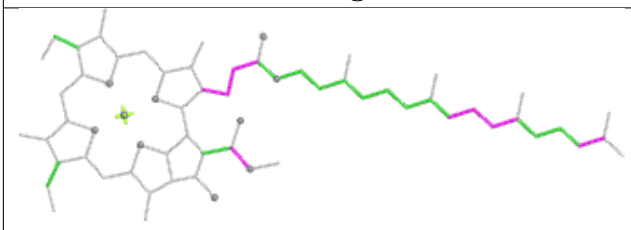


Bond angles



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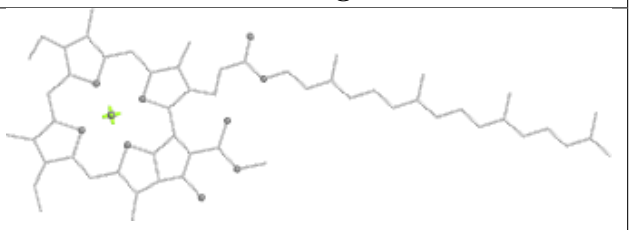
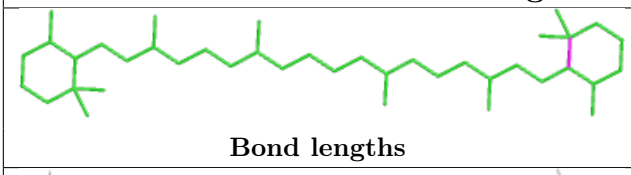


Rings

Ligand BCR 3 318



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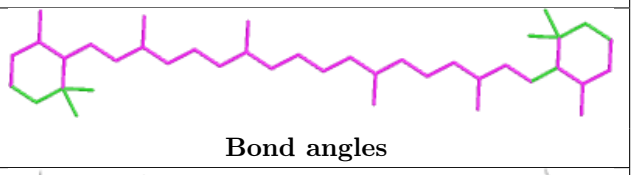
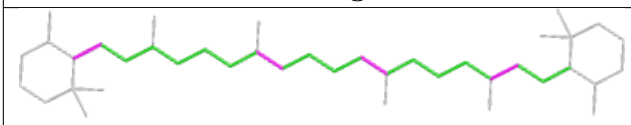


Bond angles



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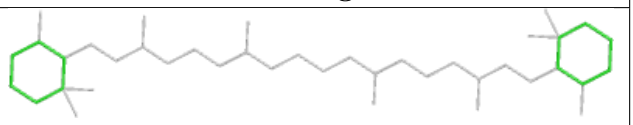
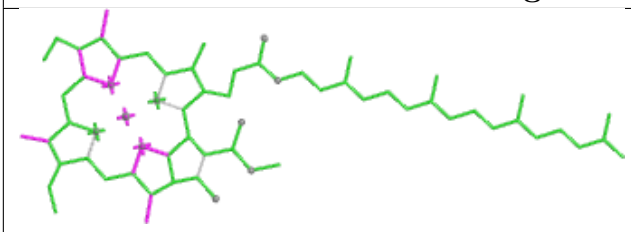


Rings

Ligand CLA A 804



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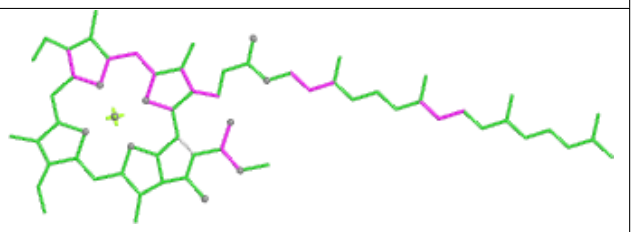
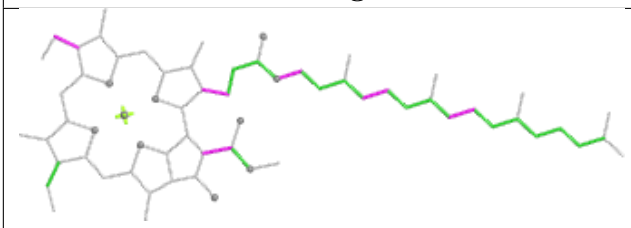


Bond angles



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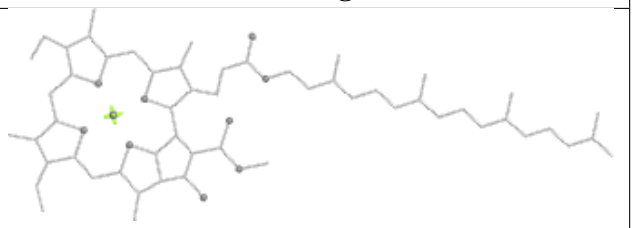
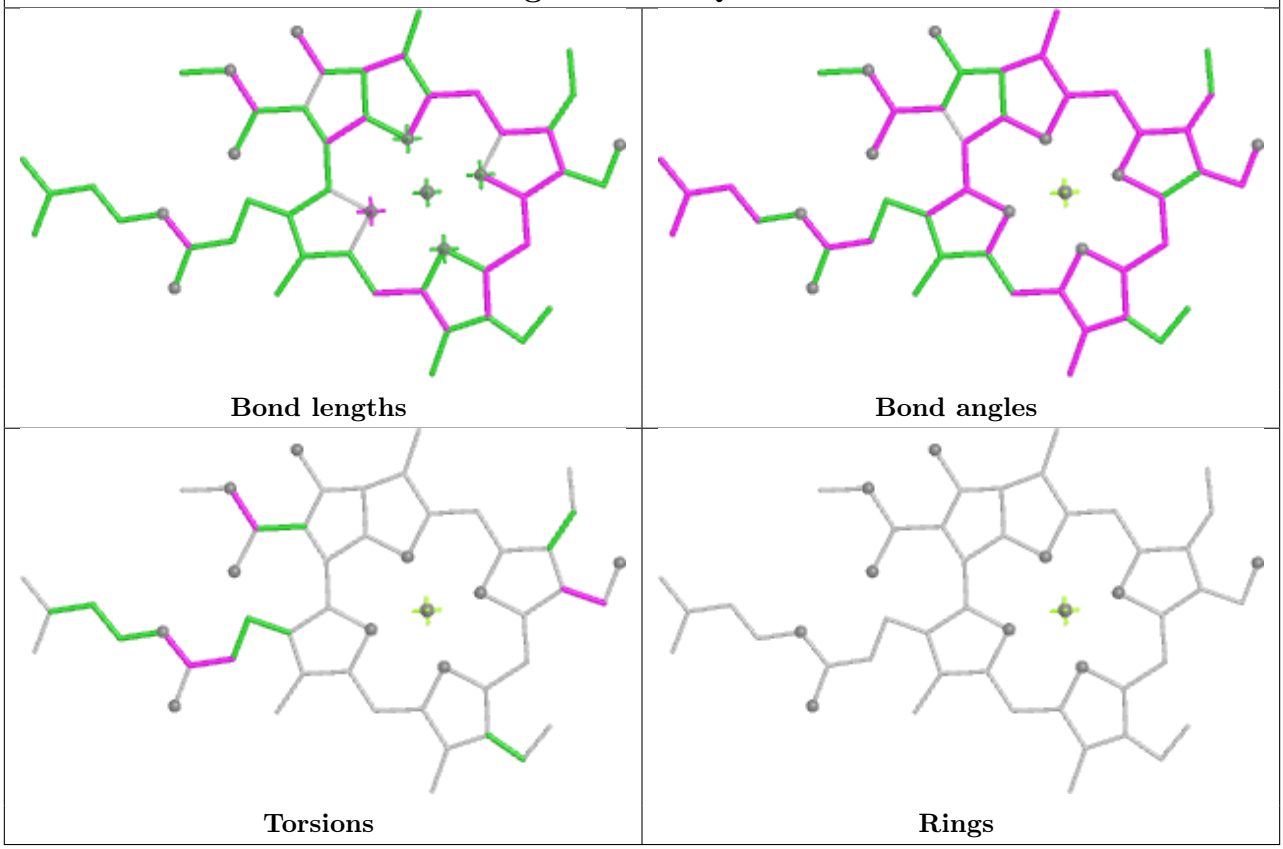
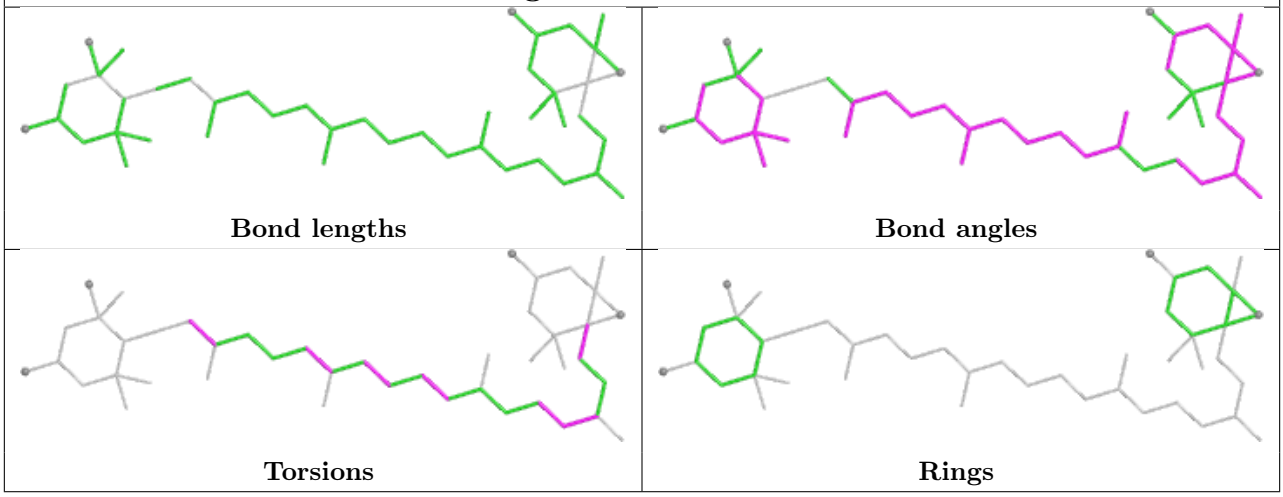


Rings

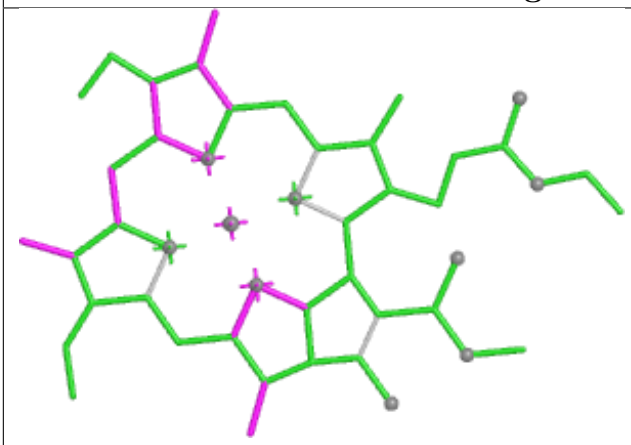
Ligand CHL Q 601



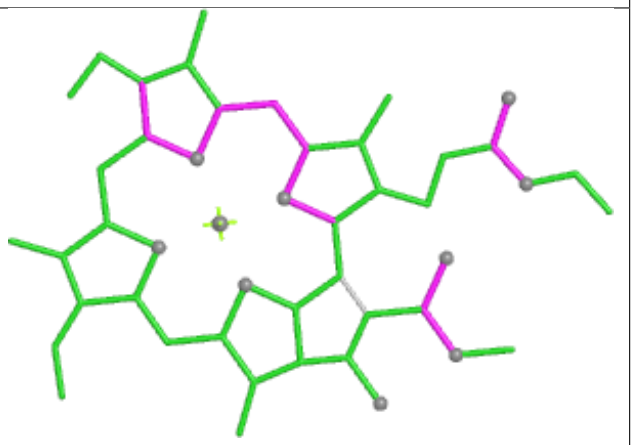
Ligand NEX P 621



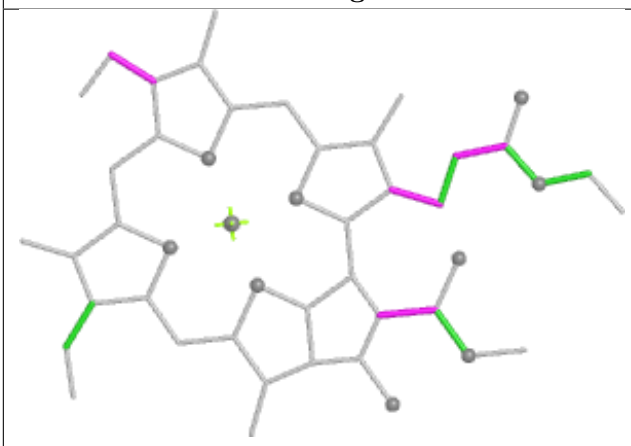
Ligand CLA B 835



Bond lengths



Bond angles



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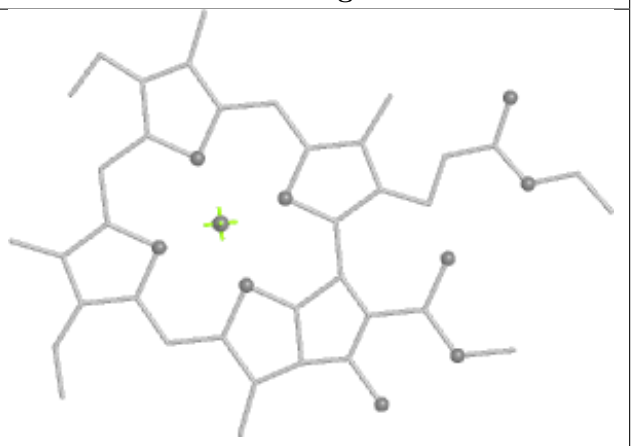
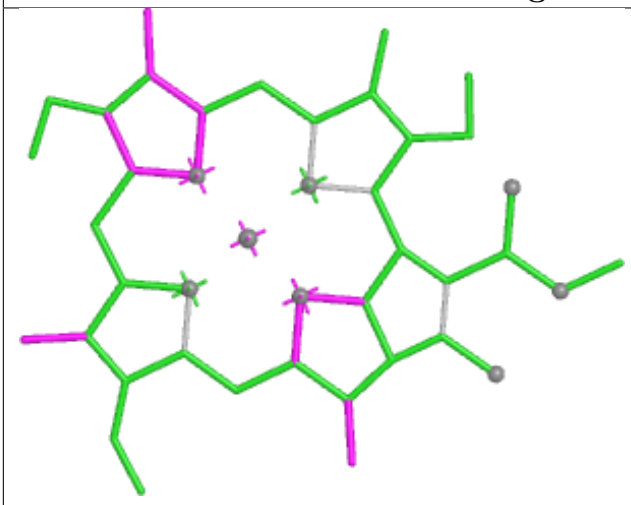


Rings

Ligand CLA 7 304



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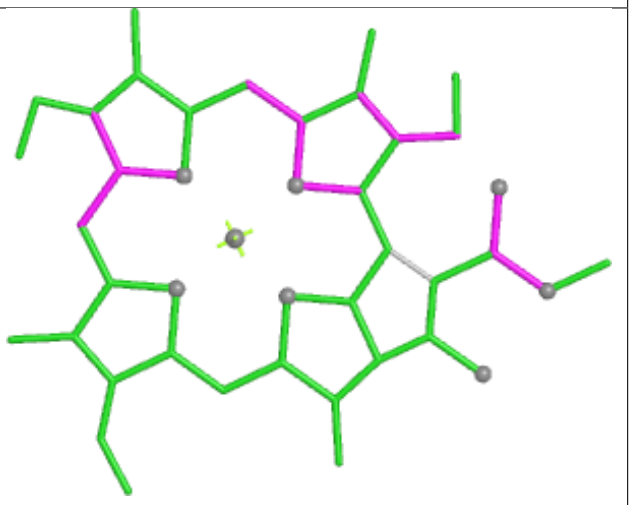

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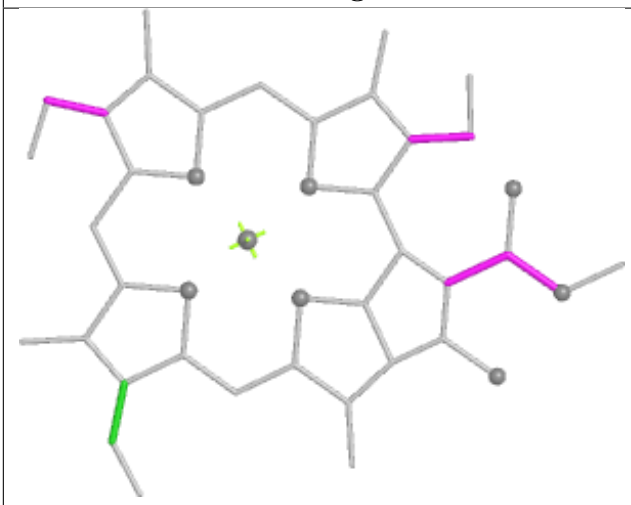
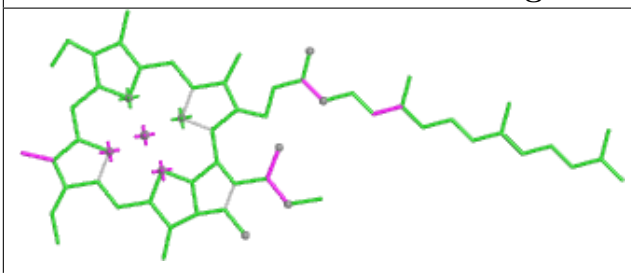


Torsions

Rings

Ligand CLA P 612



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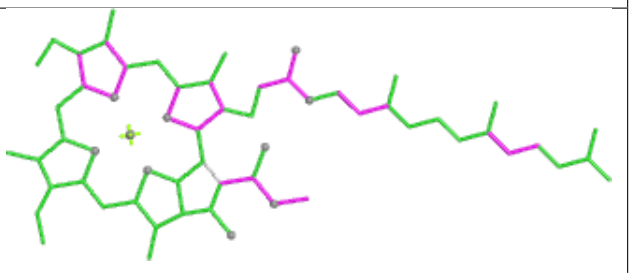

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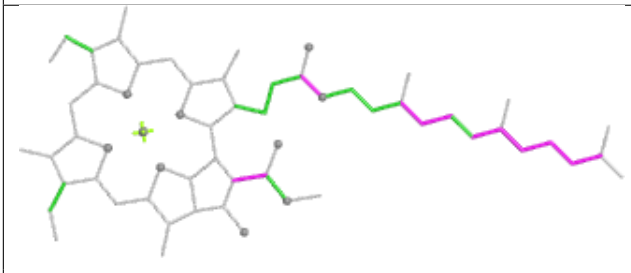

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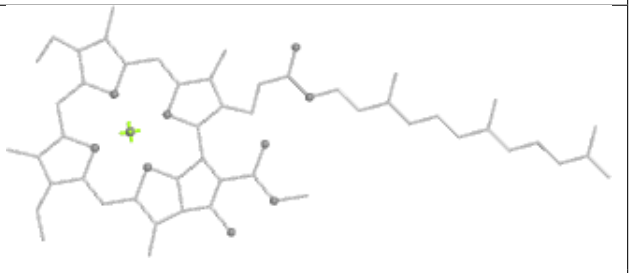
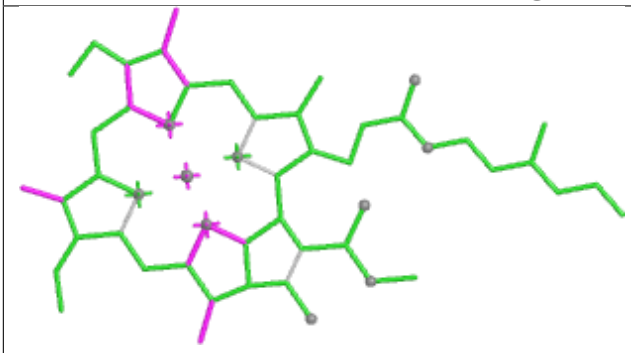


Rings

Ligand CLA 7 310



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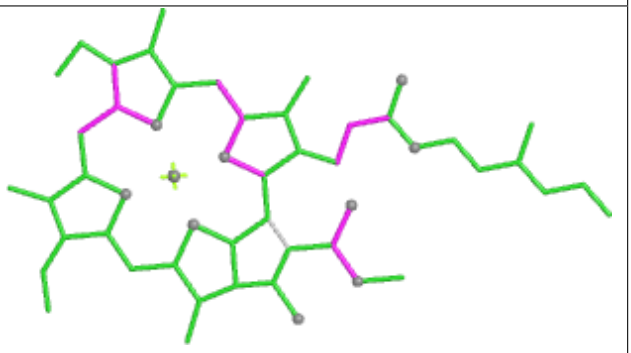
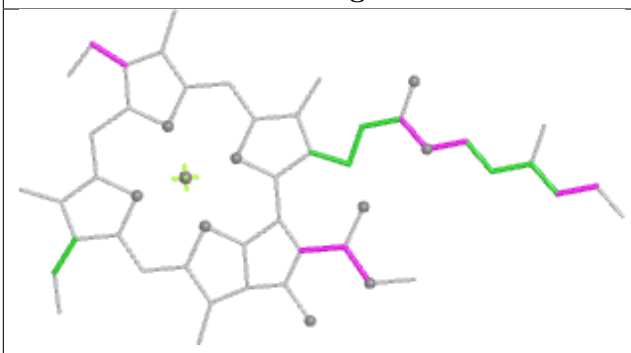


Bond angles



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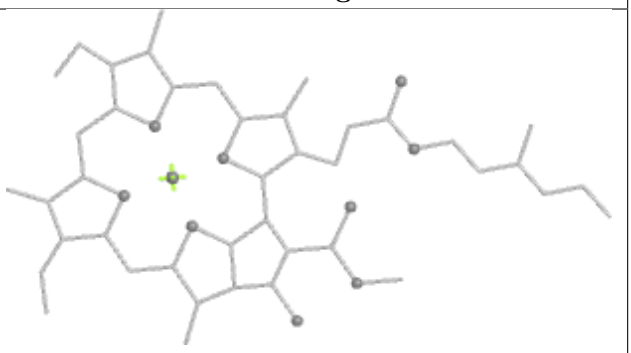
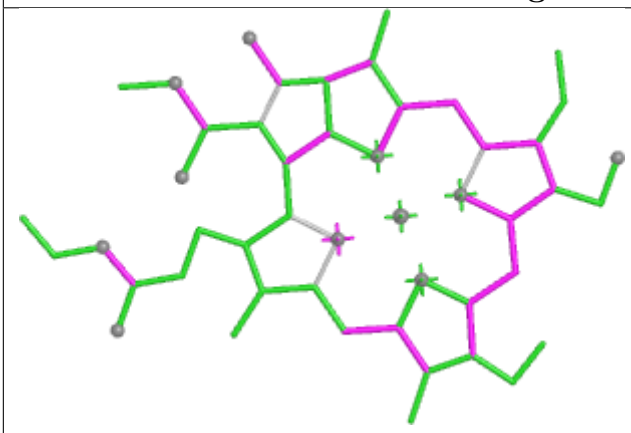
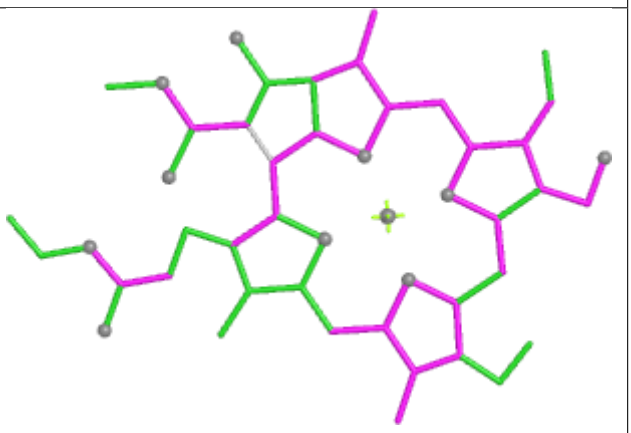


Rings

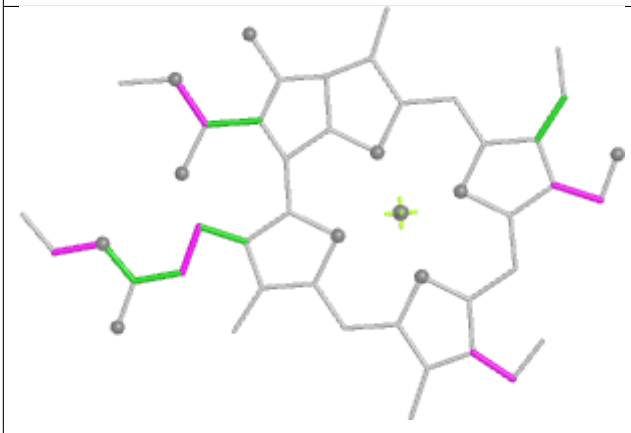
Ligand CHL a 305



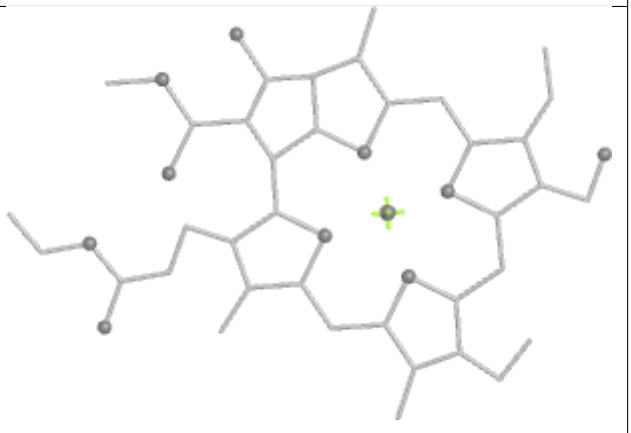
Bond lengths



Bond angles

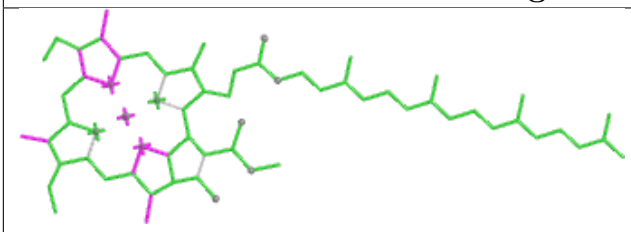


Torsions

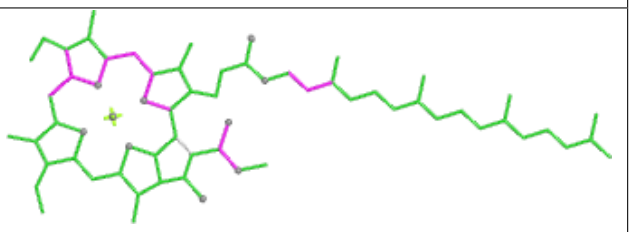


Rings

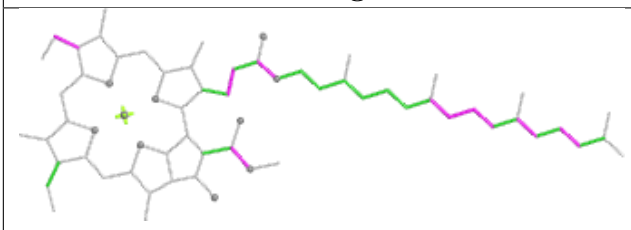
Ligand CLA 6 603



Bond lengths



Bond angles



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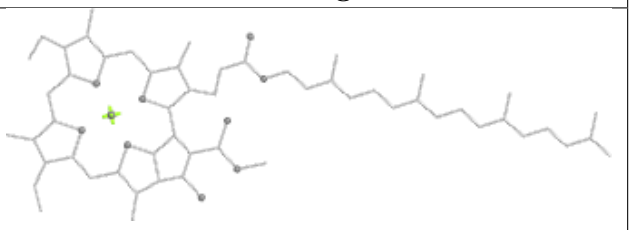
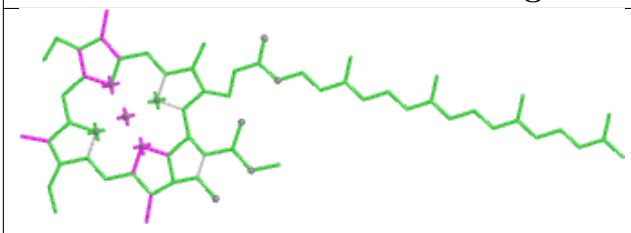
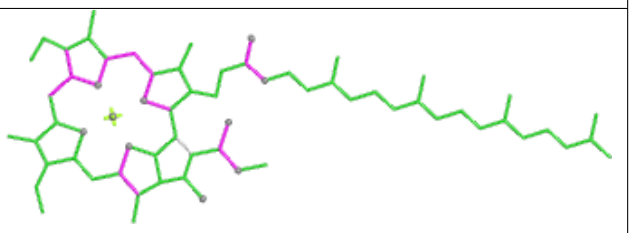


Rings

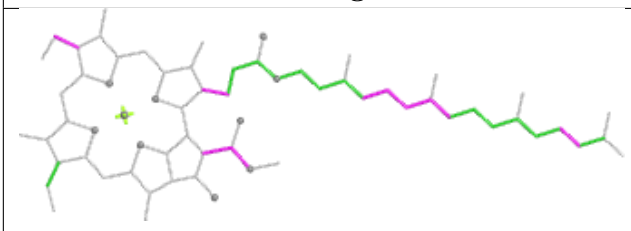
Ligand CLA B 849



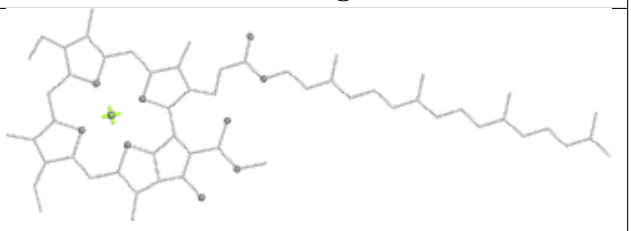
Bond lengths



Bond angles

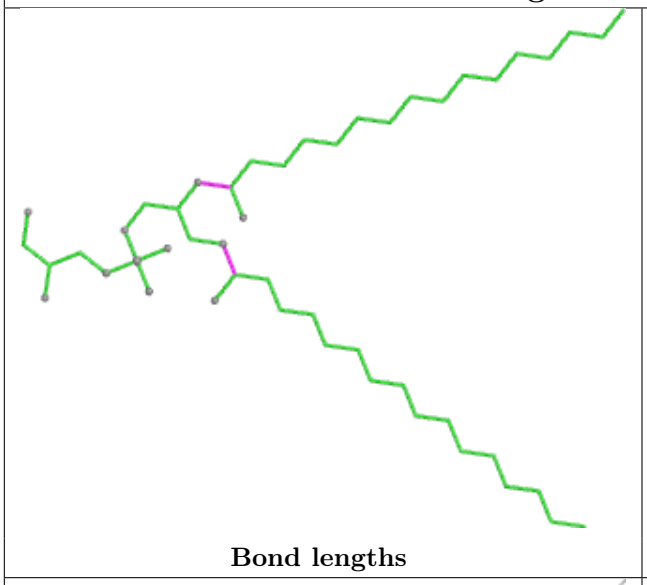


Torsions



Rings

Ligand LHG 6 618



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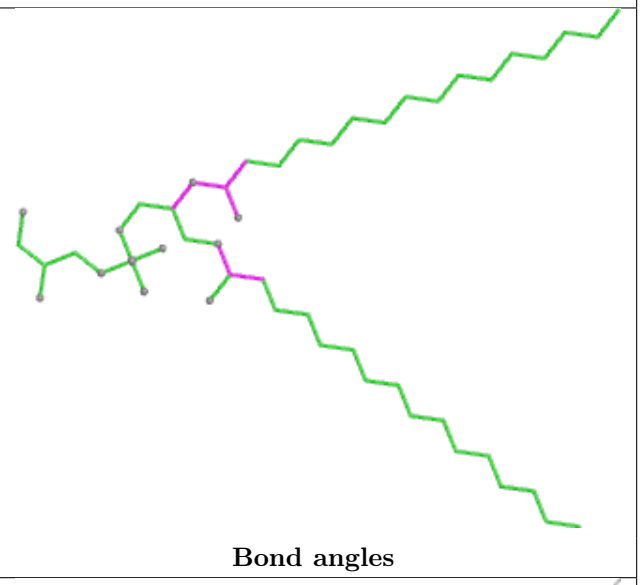

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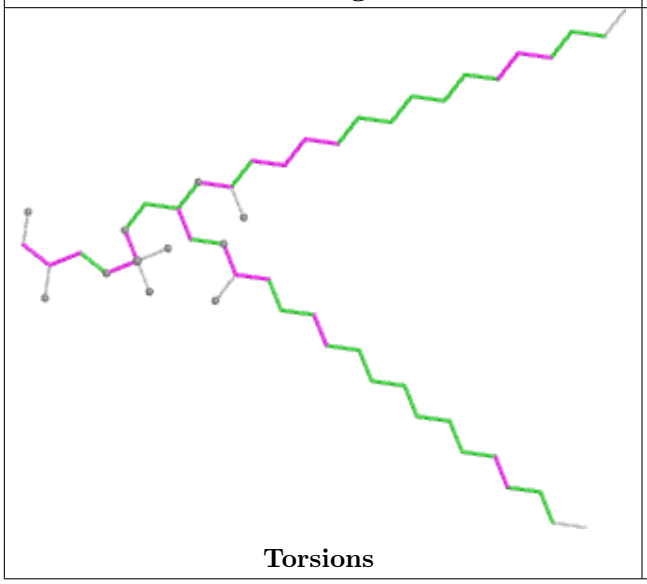

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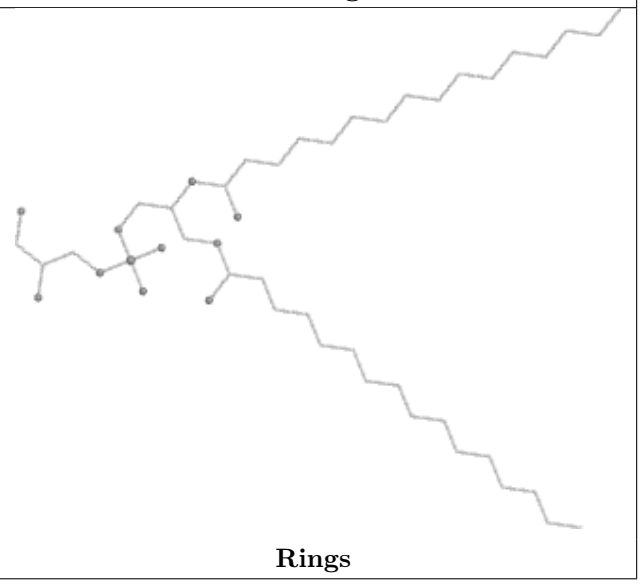
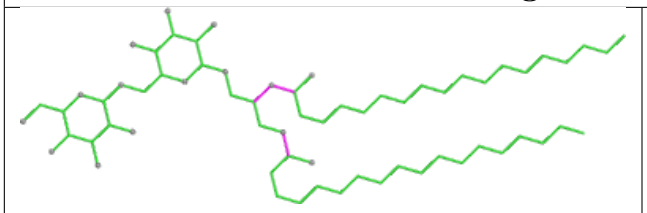


Rings

Ligand DGD B 846



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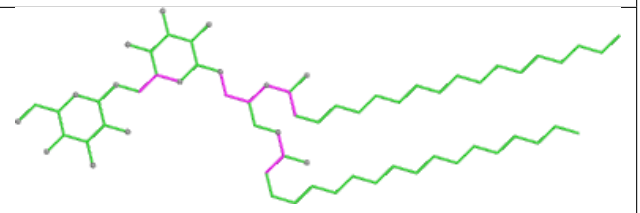
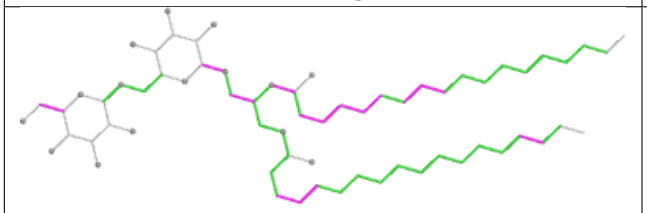


Bond angles



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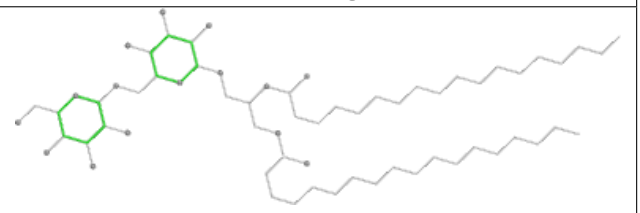
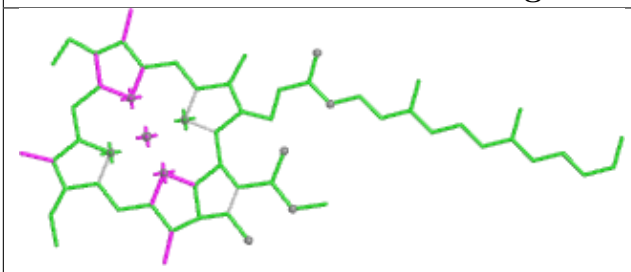


Rings

Ligand CLA B 815



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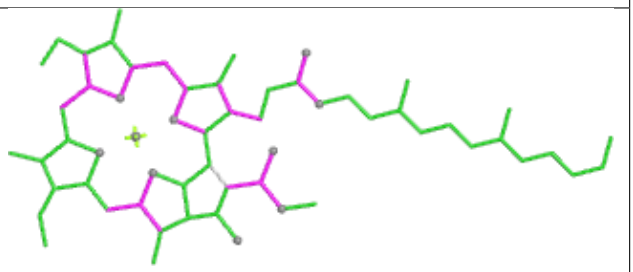
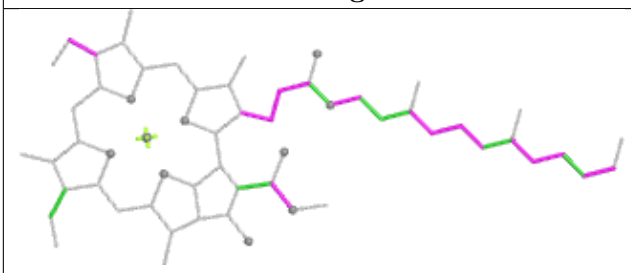


Bond angles



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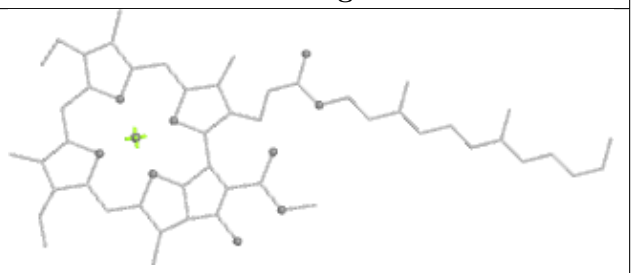
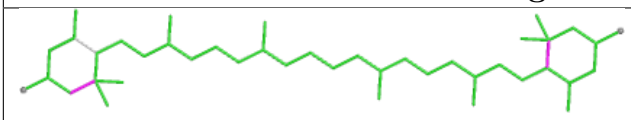


Rings

Ligand LUT 4 316



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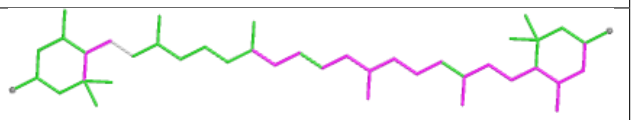
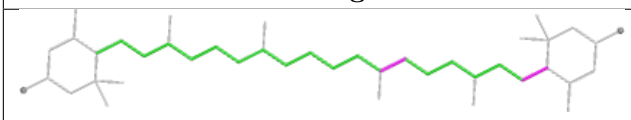


Bond angles



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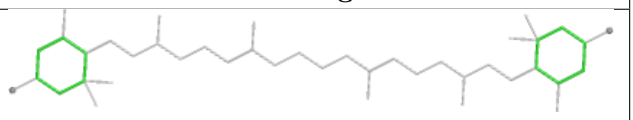
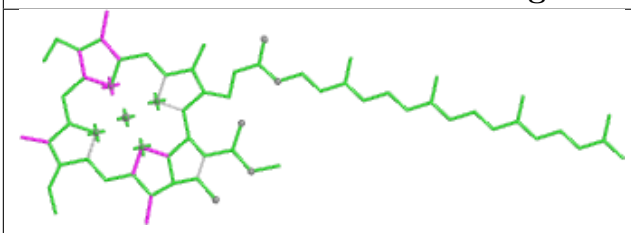


Rings

Ligand CLA 1 607



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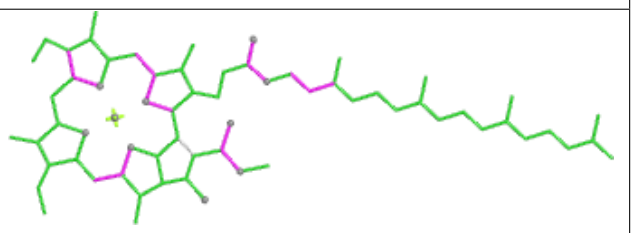
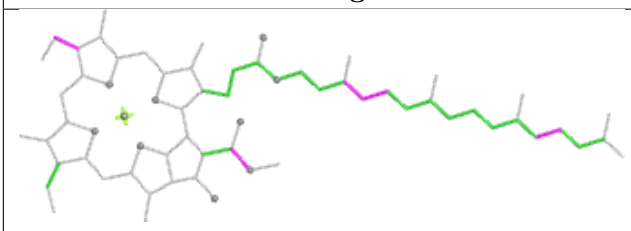


Bond angles



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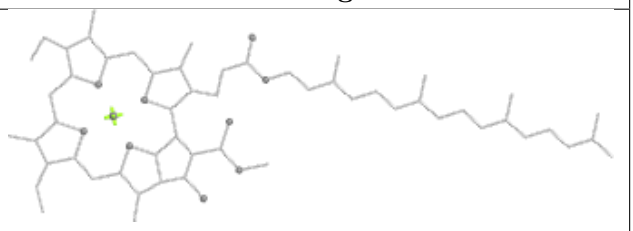
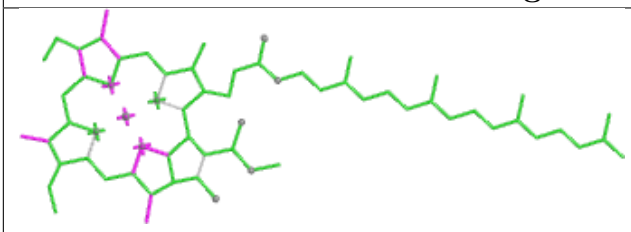
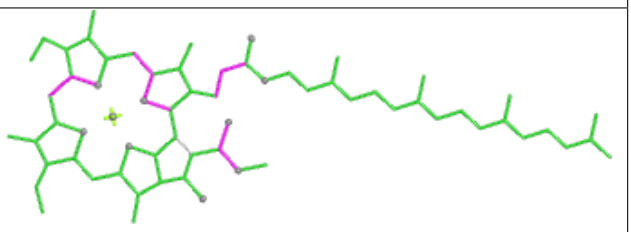


Rings

Ligand CLA A 803



Bond lengths



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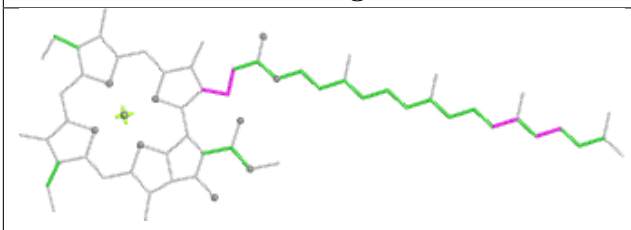

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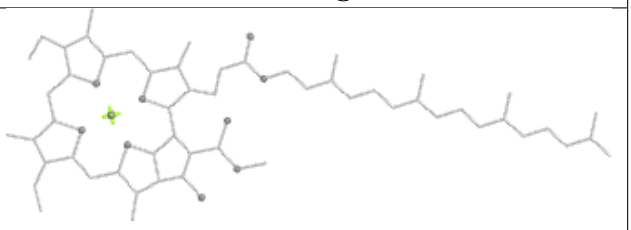
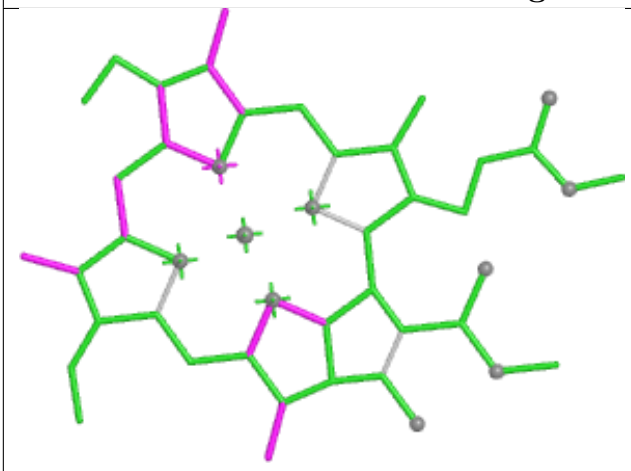


Rings

Ligand CLA 8 309



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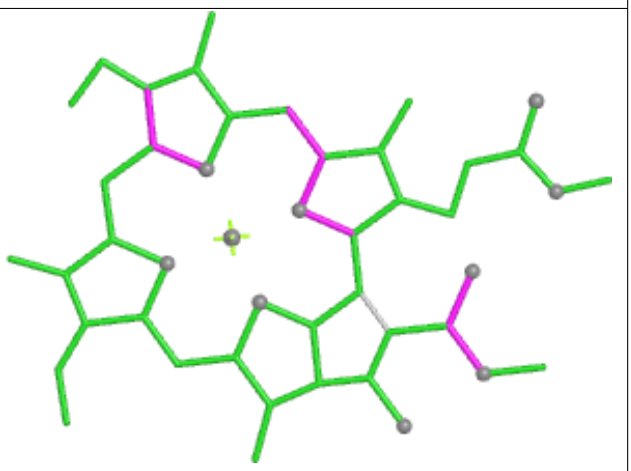
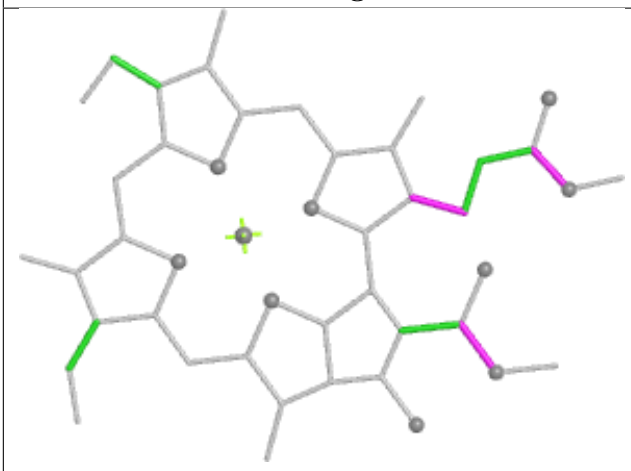


Bond angles



Torsions

Rings

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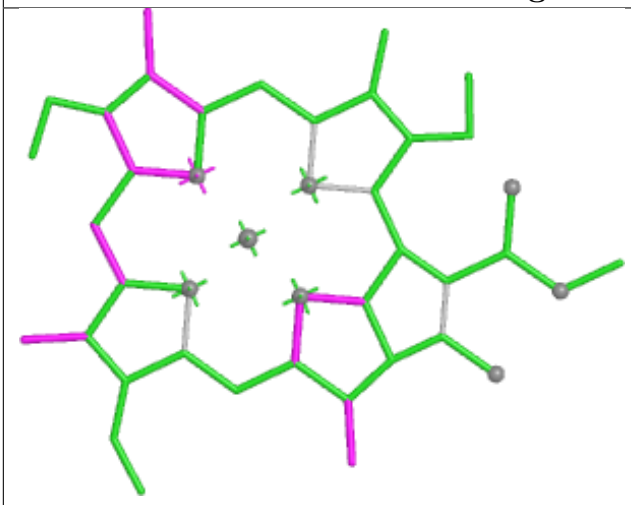

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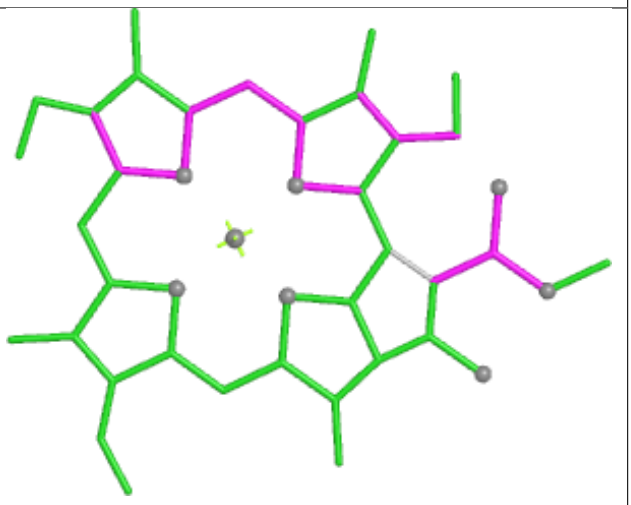
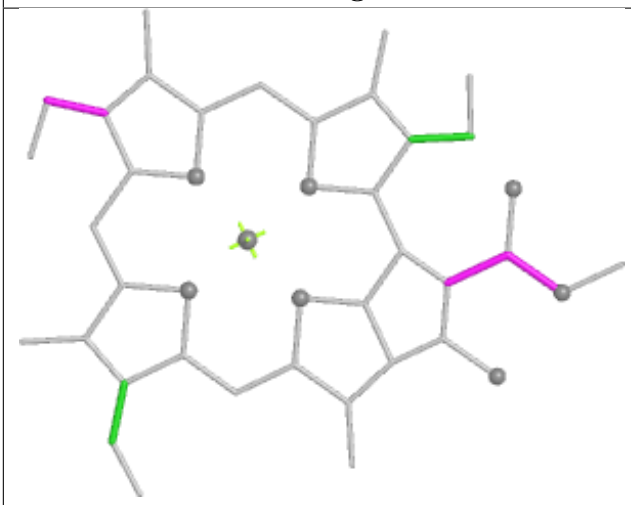


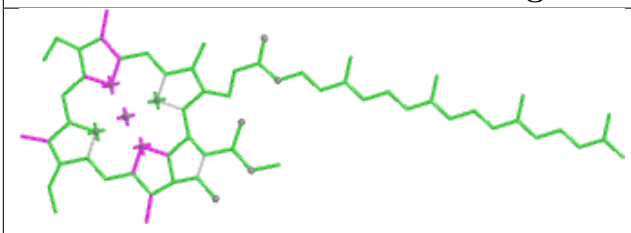
Bond angles



Torsions

Rings

Ligand CLA L 205



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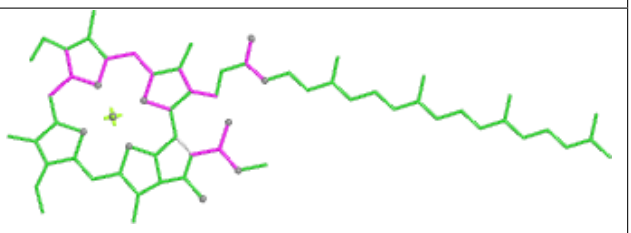
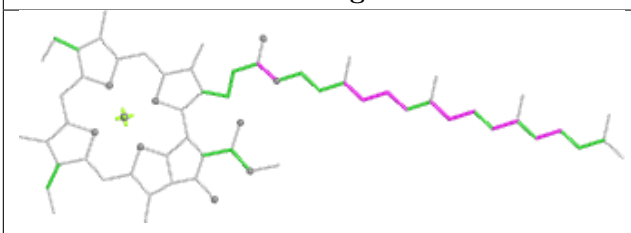


Bond angles



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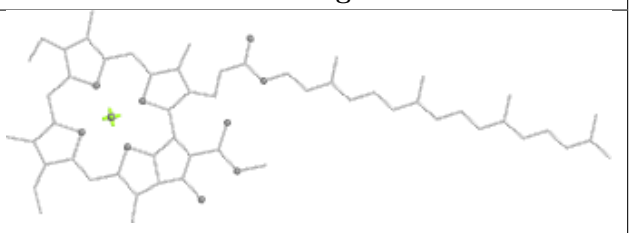
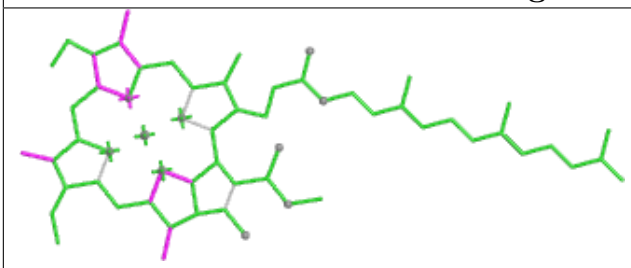


Rings

Ligand CLA 9 309



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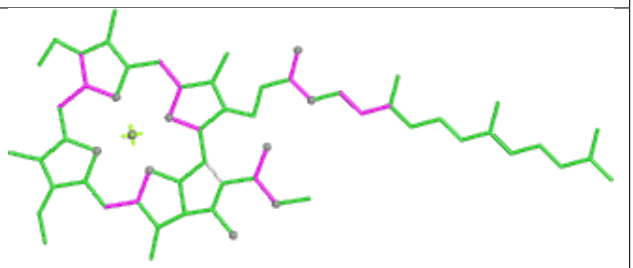
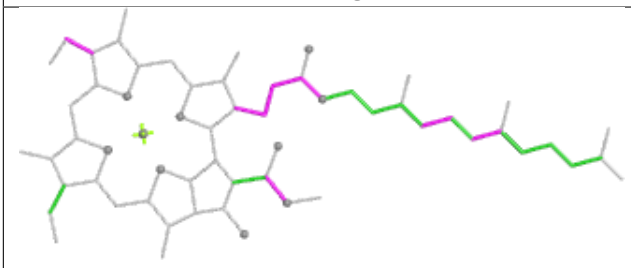


Bond angles



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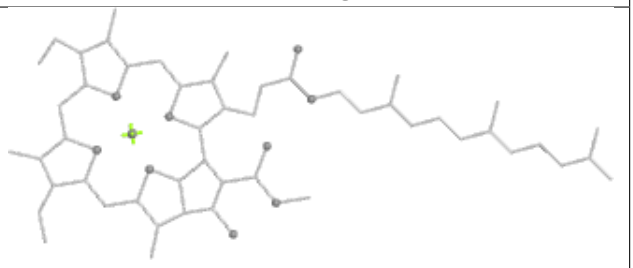
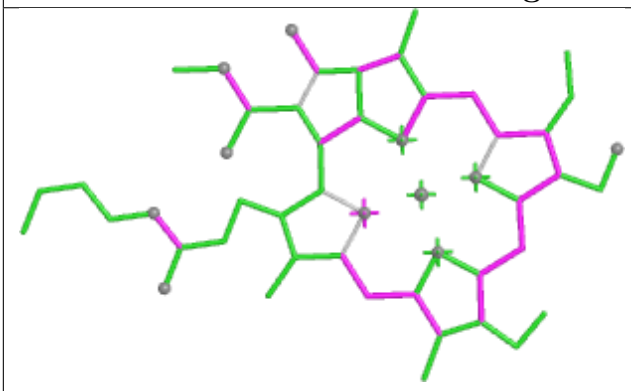


Rings

Ligand CHL U 306



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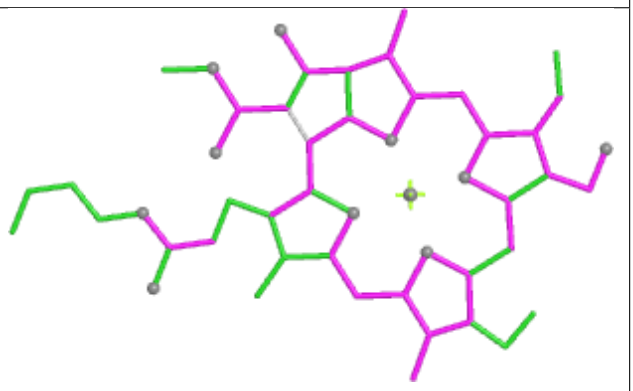
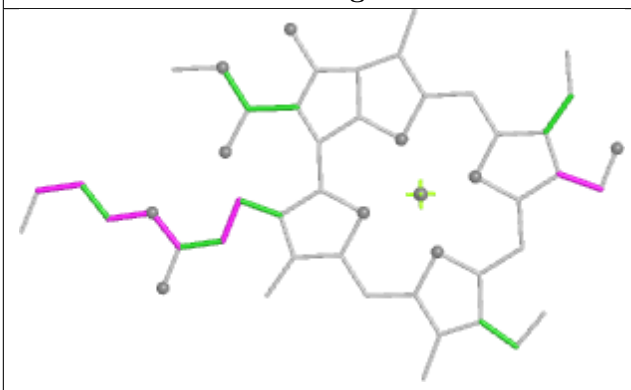


Bond angles



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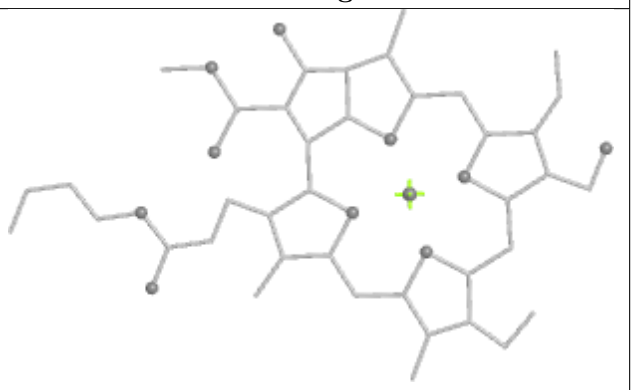
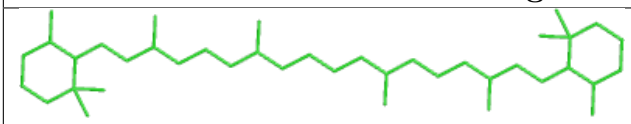


Rings

Ligand BCR 4 317



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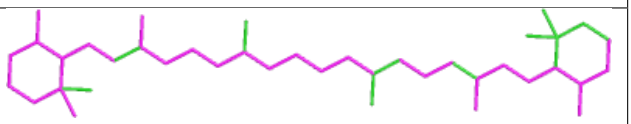
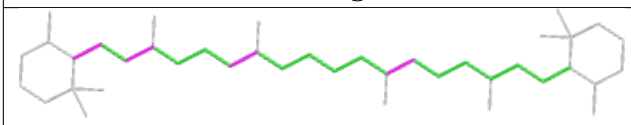


Bond angles



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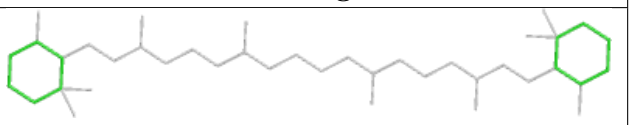
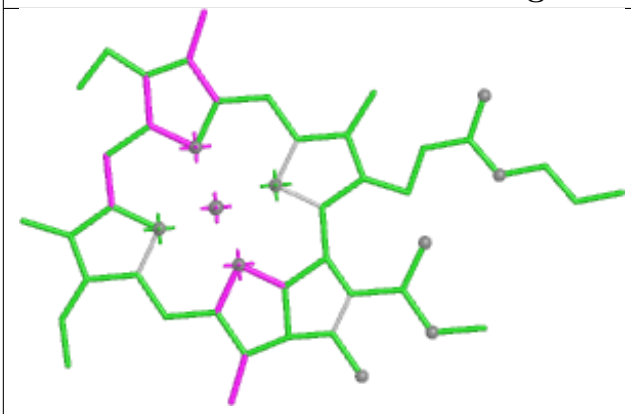


Rings

Ligand CLA S 315



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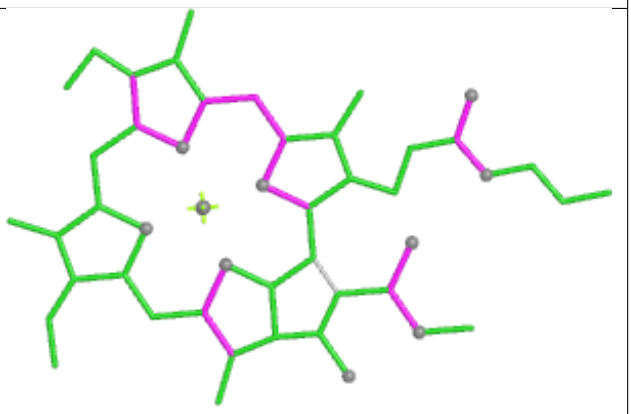
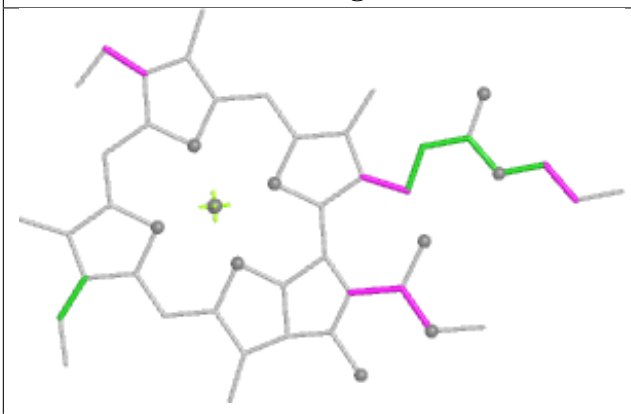


Bond angles



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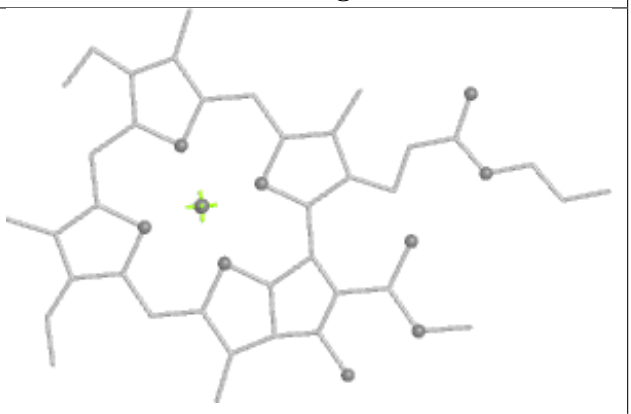
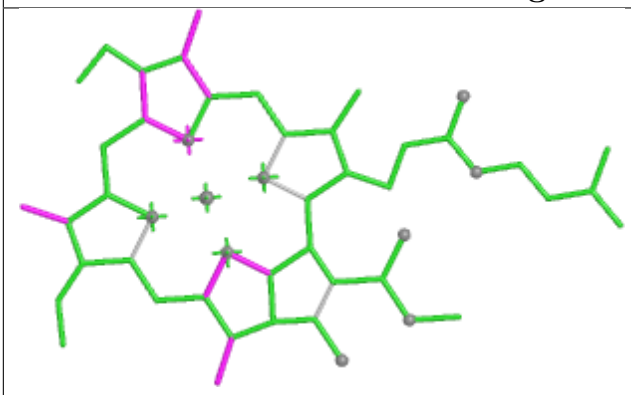


Rings

Ligand CLA 9 305



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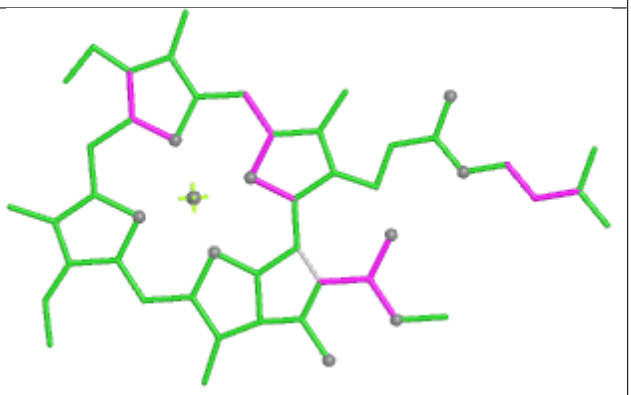
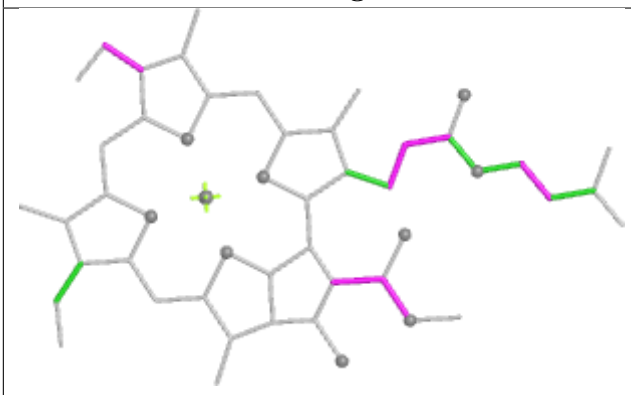
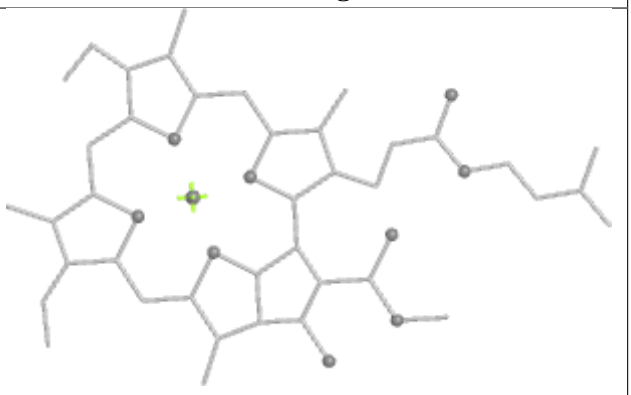


Bond angles



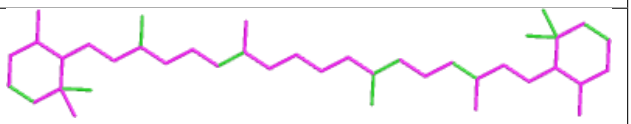
Torsions



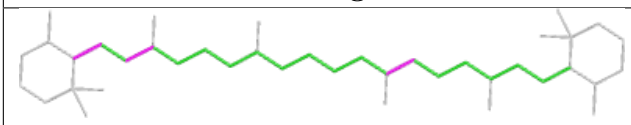
Rings

Ligand BCR 8 318

Bond lengths



Bond angles



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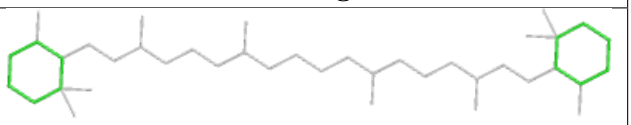
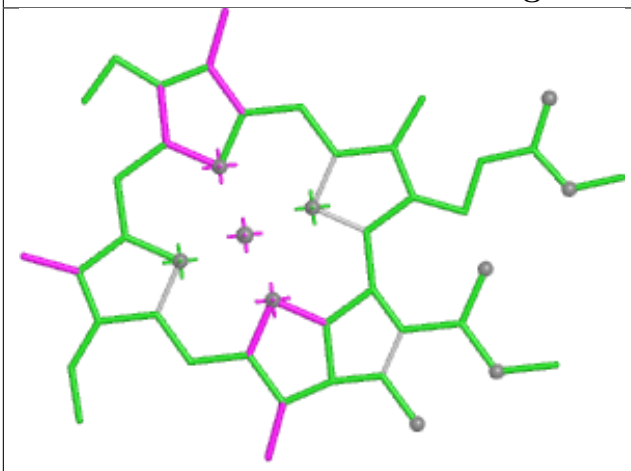


Rings

Ligand CLA H 203



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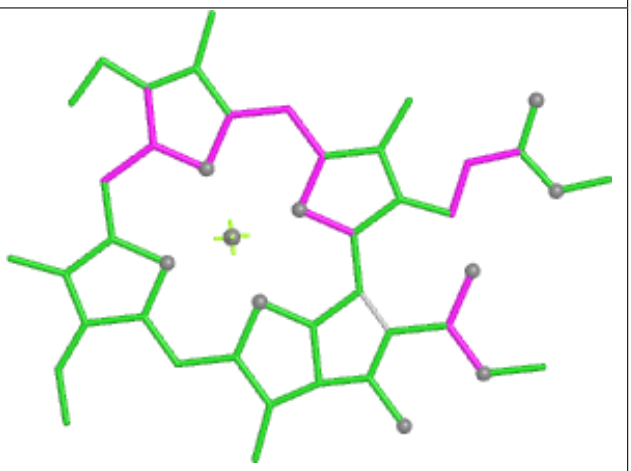
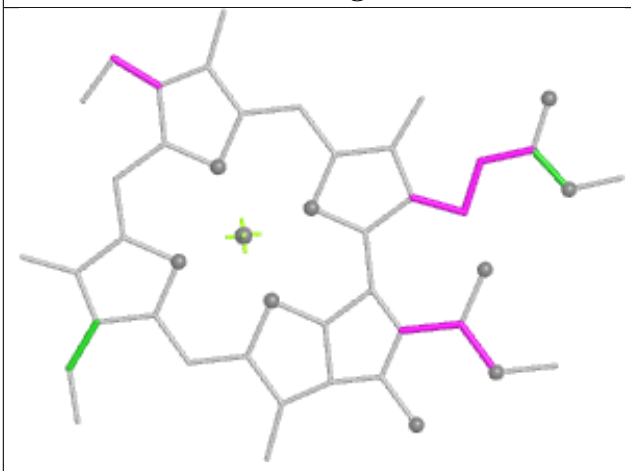


Bond angles



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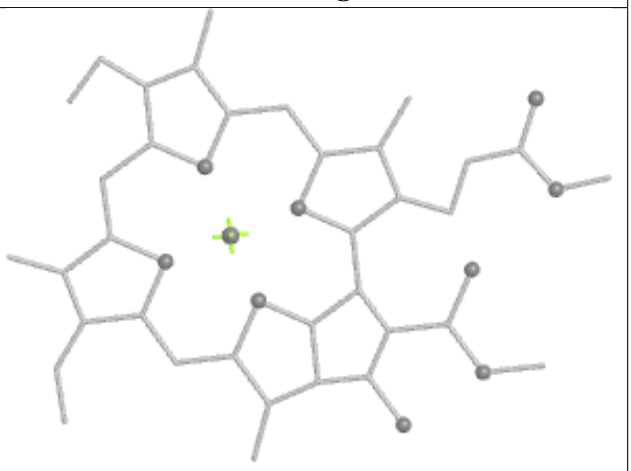
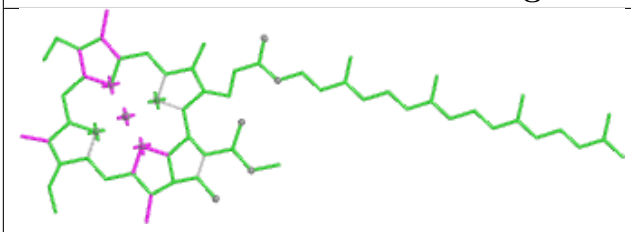


Rings

Ligand CLA A 828



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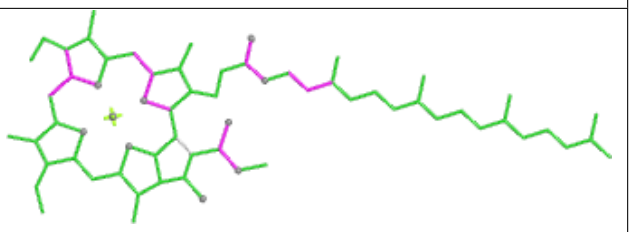
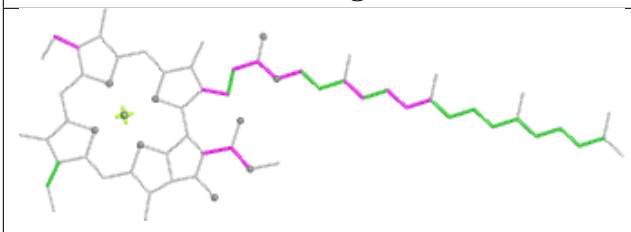
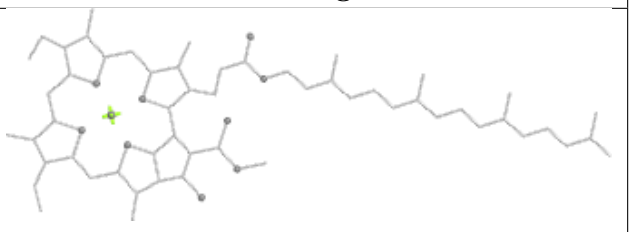


Bond angles

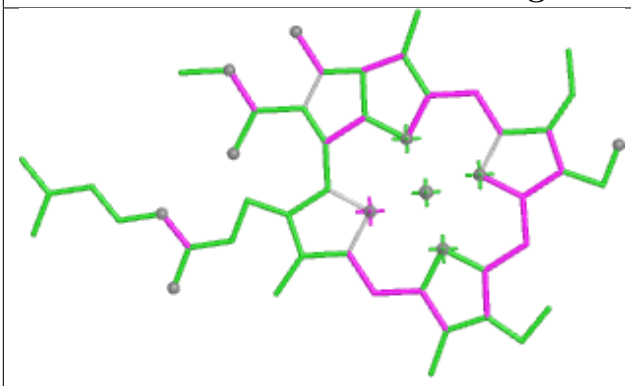


Torsions



Rings

Ligand CHL 6 608



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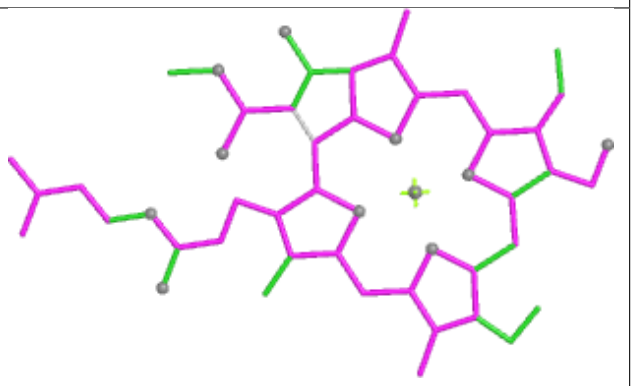
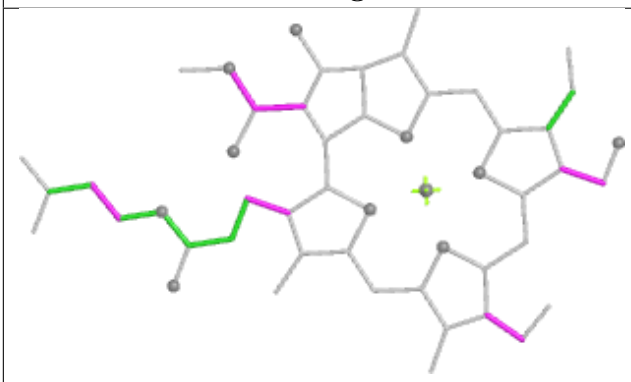


Bond angles



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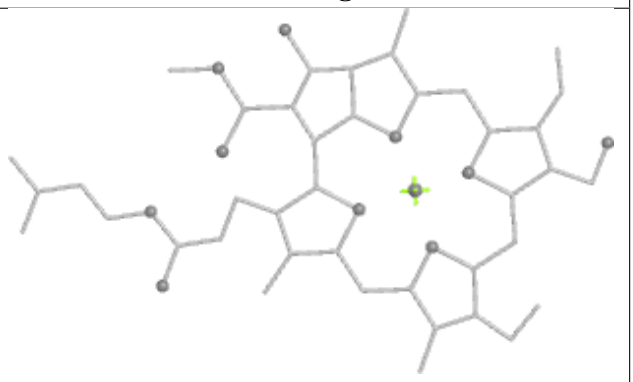
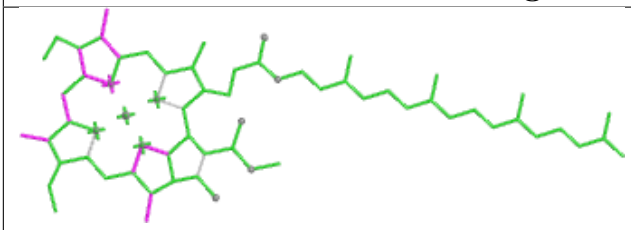


Rings

Ligand CLA A 816



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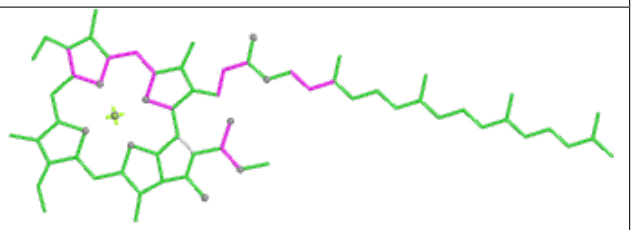
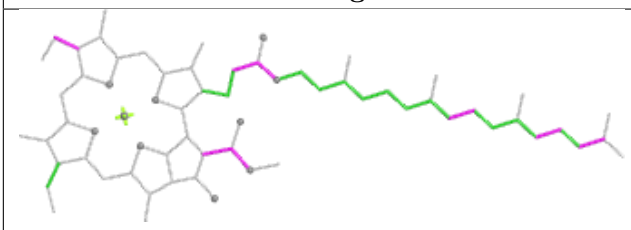


Bond angles



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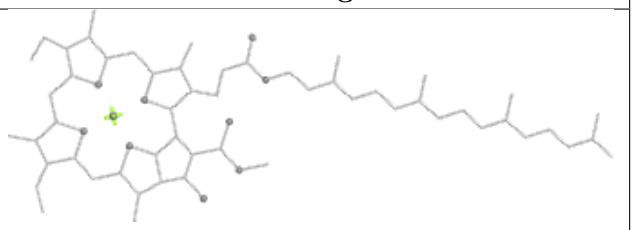
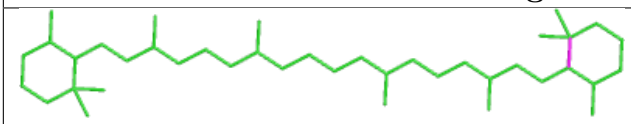


Rings

Ligand BCR 6 621



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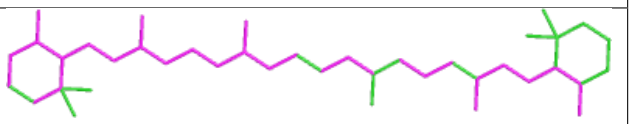
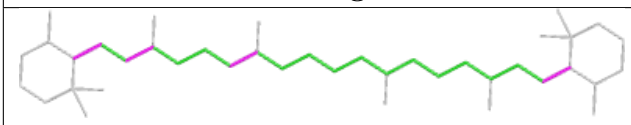


Bond angles



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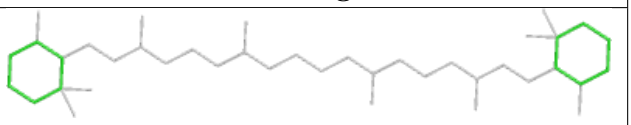
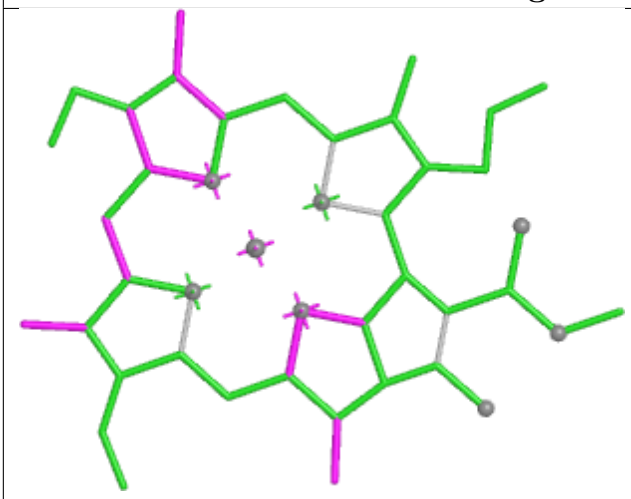


Rings

Ligand CLA 7 312



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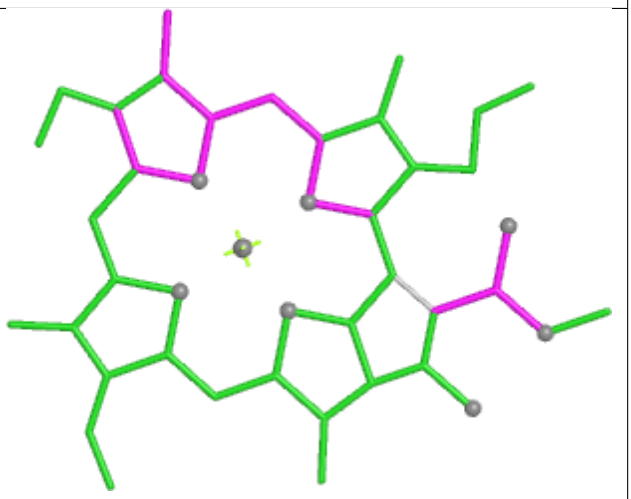

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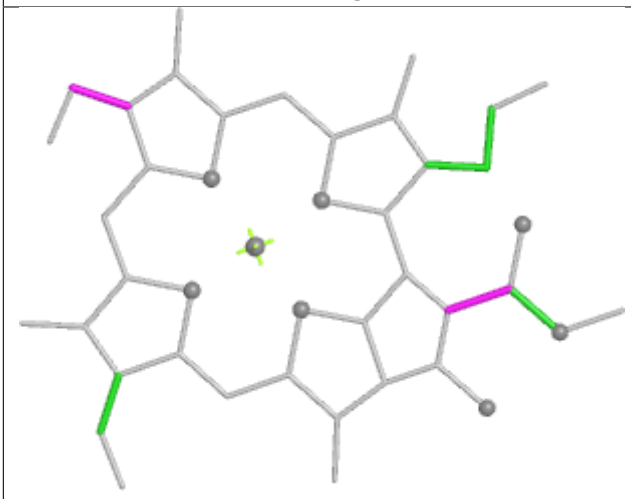

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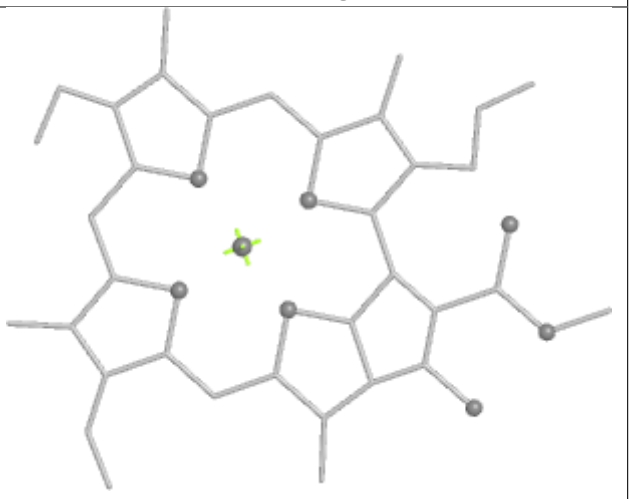
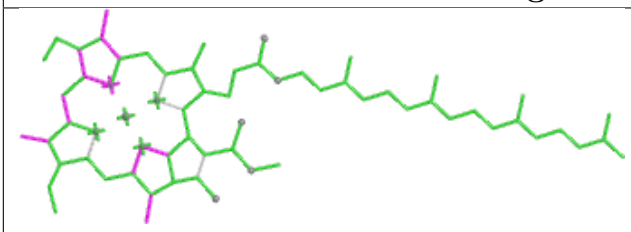


Rings

Ligand CLA S 303



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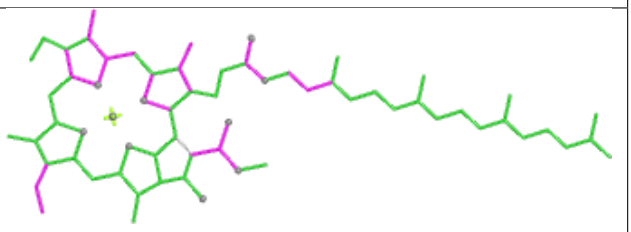
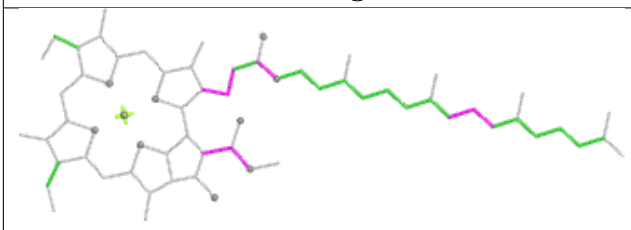


Bond angles



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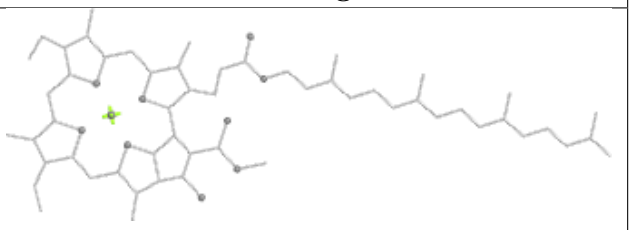
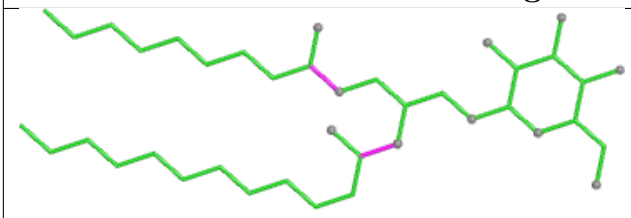


Rings

Ligand LMG 6 602



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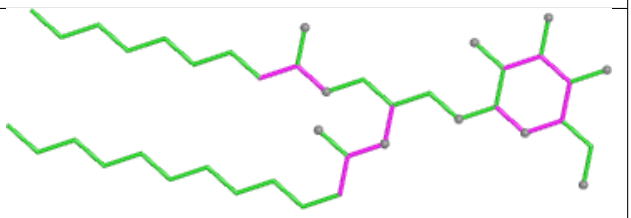
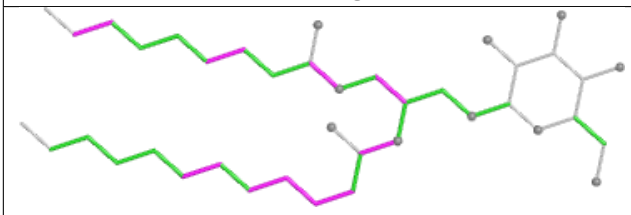


Bond angles



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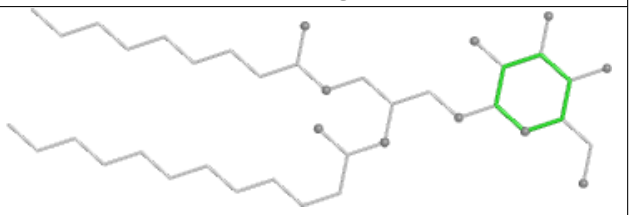
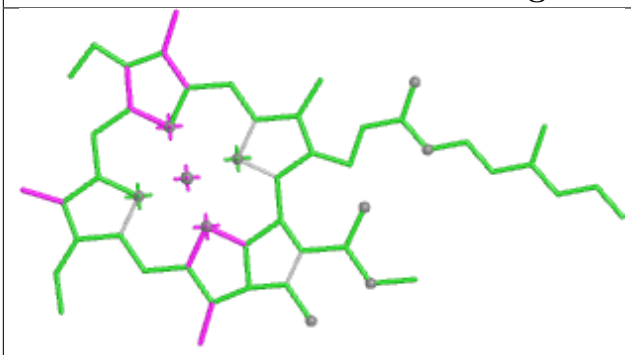


Rings

Ligand CLA 2 311



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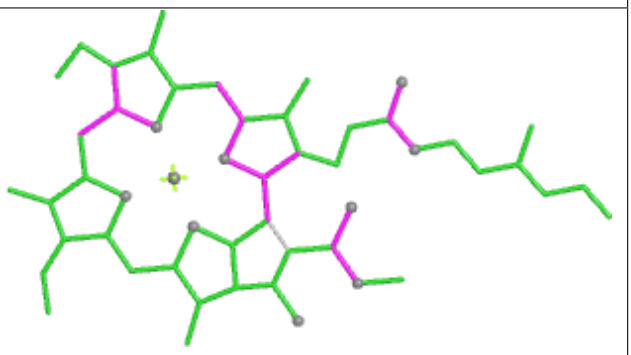
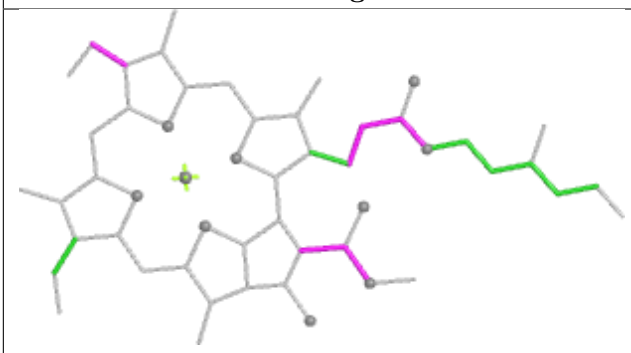


Bond angles



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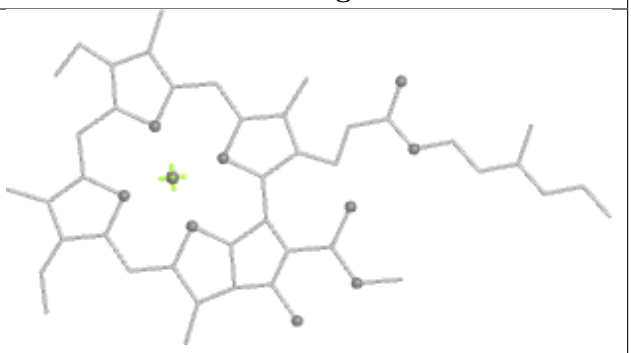
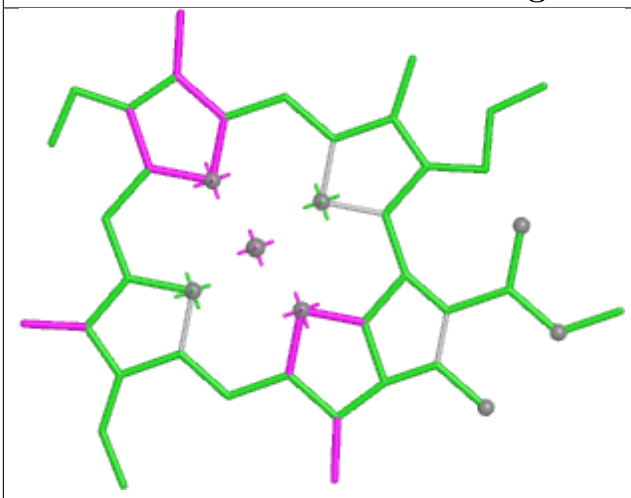


Rings

Ligand CLA 5 316



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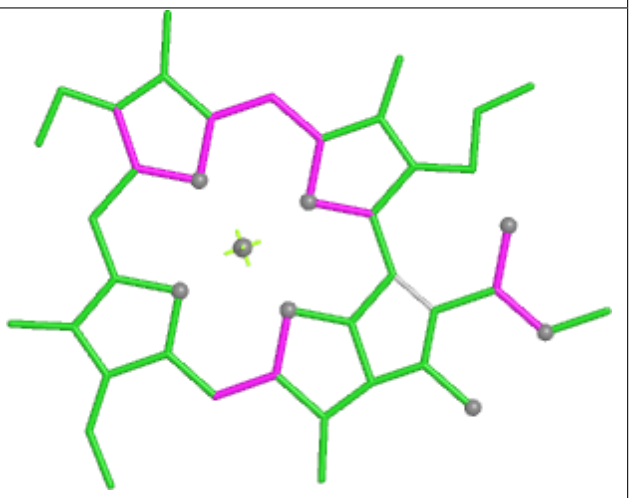
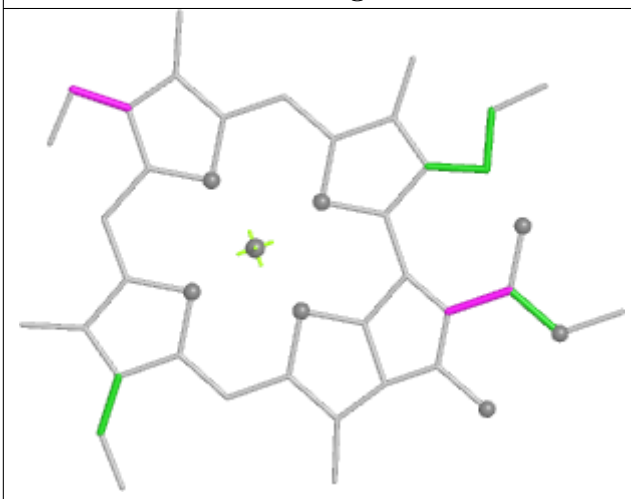


Bond angles



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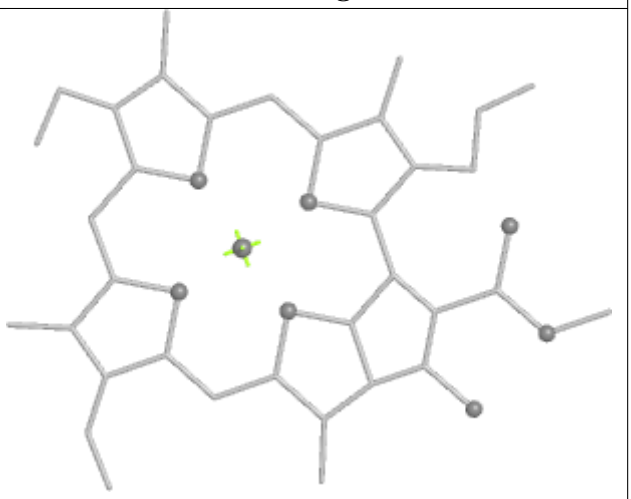
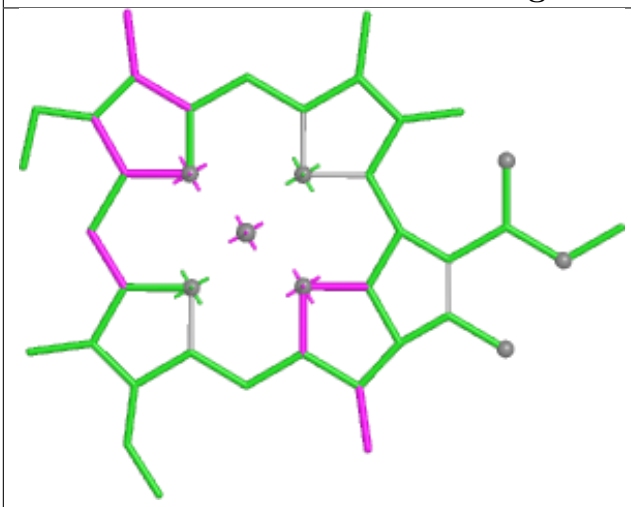


Rings

Ligand CLA 2 310



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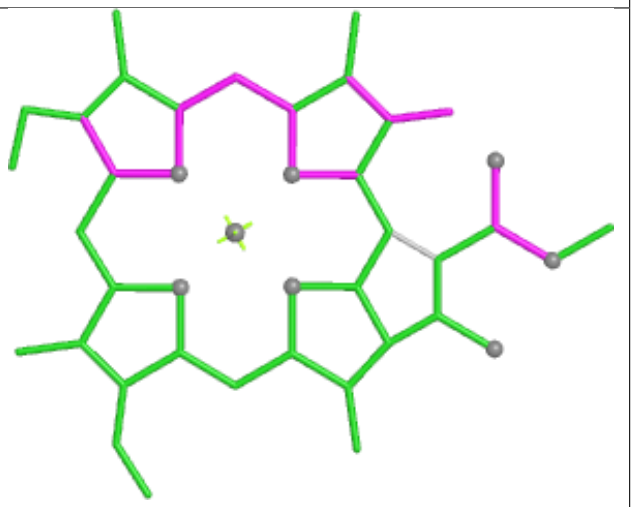
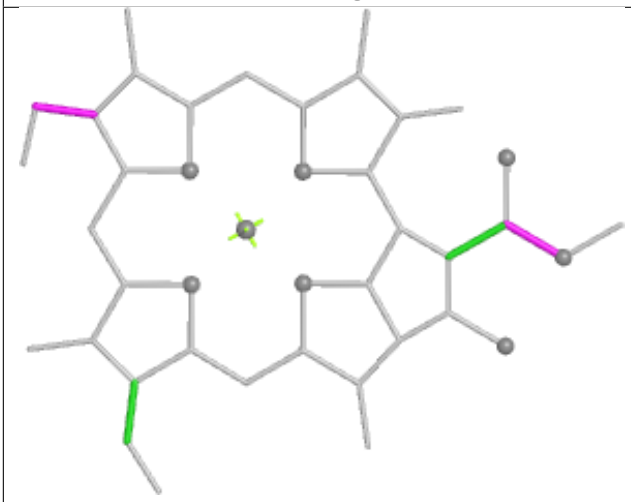
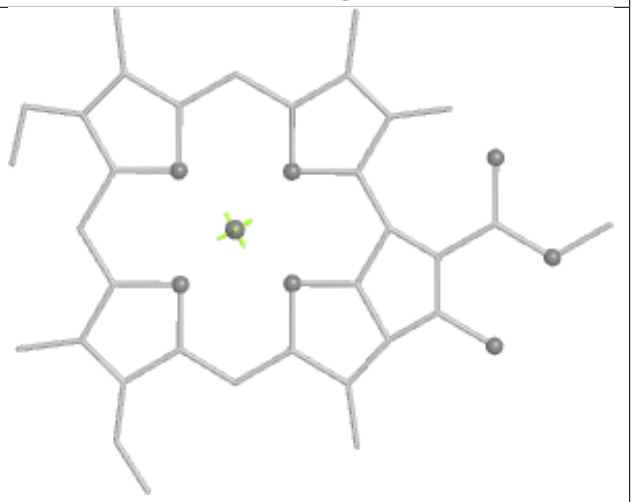


Bond angles

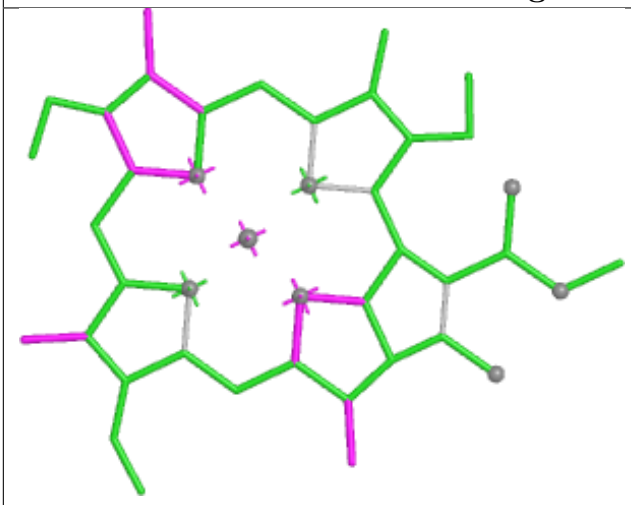


Torsions

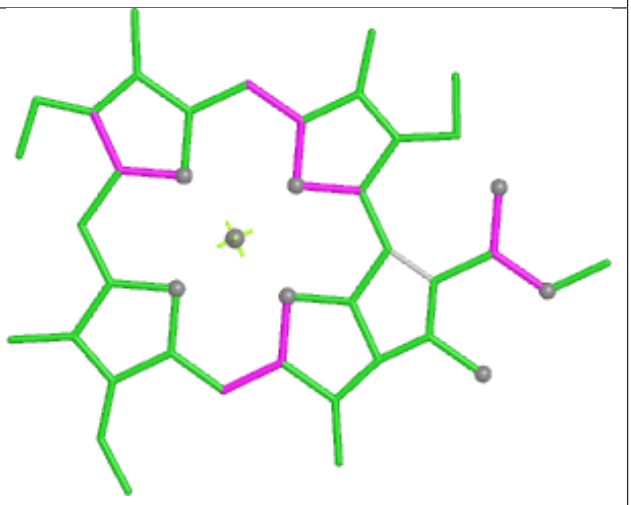


Rings

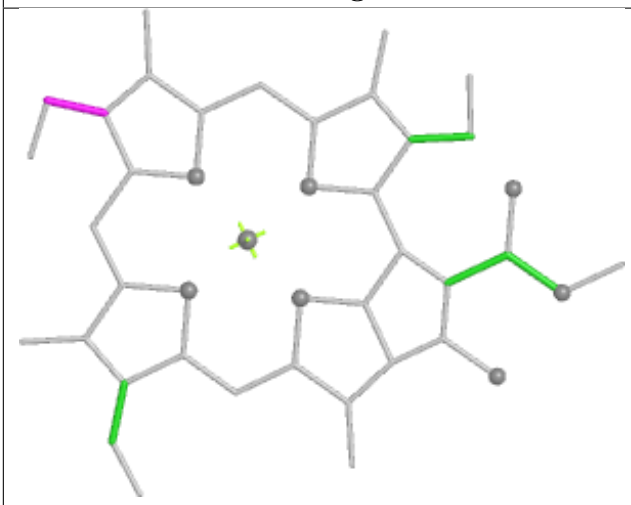
Ligand CLA 3 304



Bond lengths



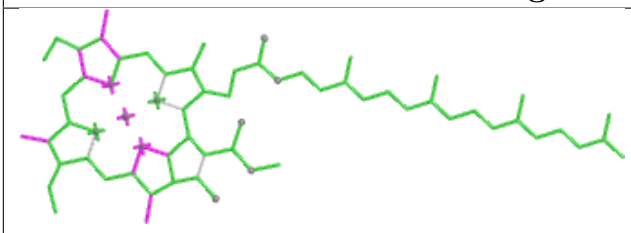
Bond angles



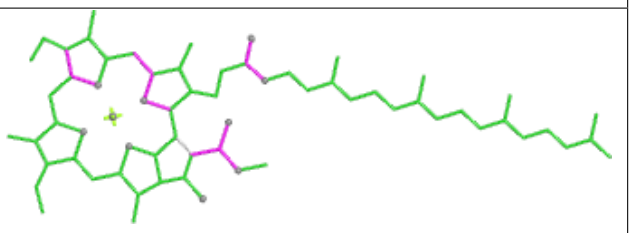
Torsions

Rings

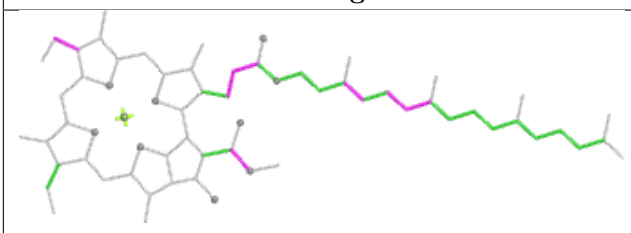
Ligand CLA 1 602



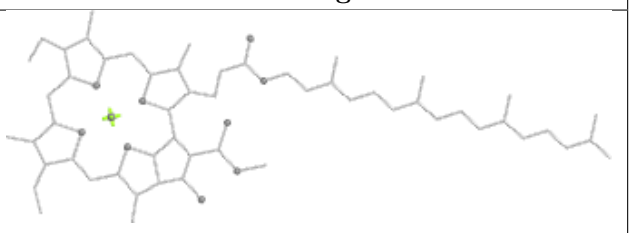
Bond lengths



Bond angles

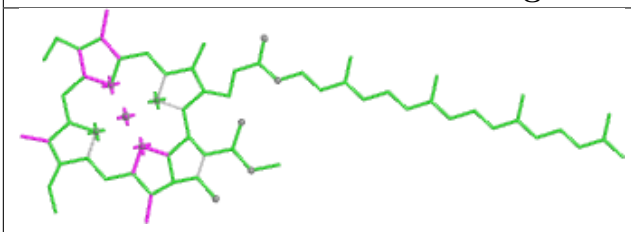


Torsions



Rings

Ligand CLA A 837



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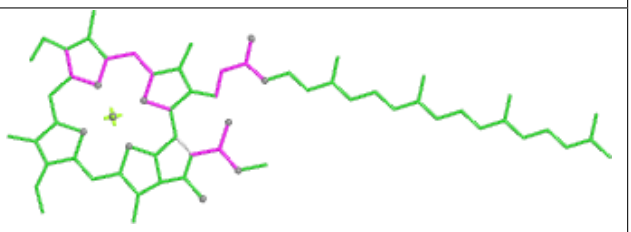

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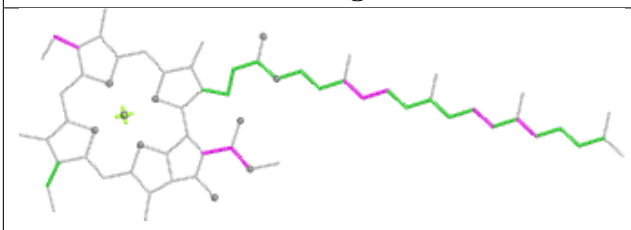
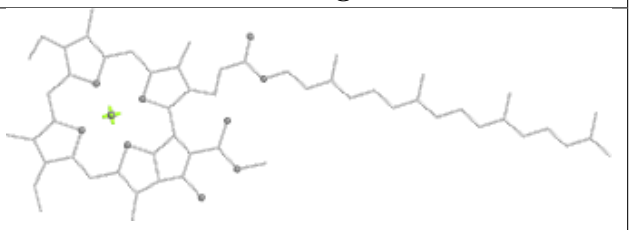
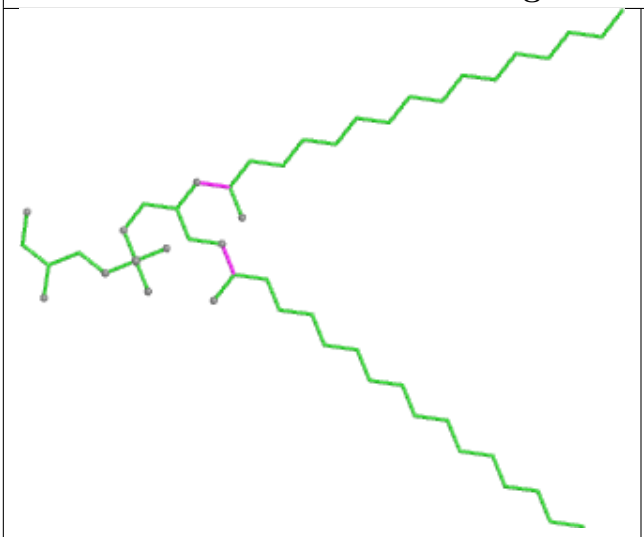


Torsions



Rings

Ligand LHG P 624



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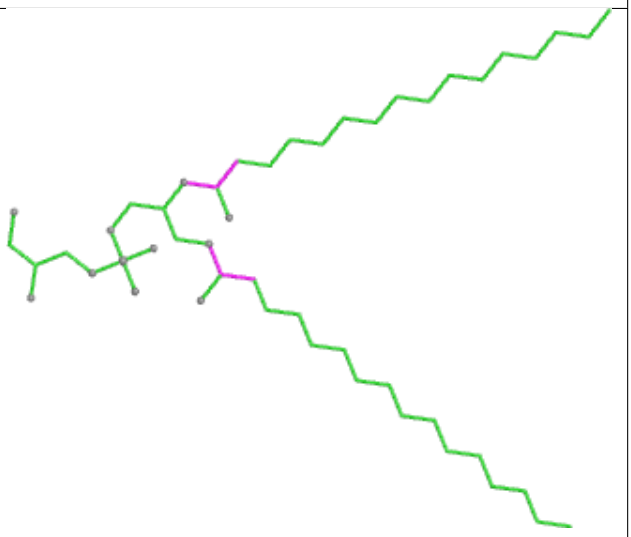
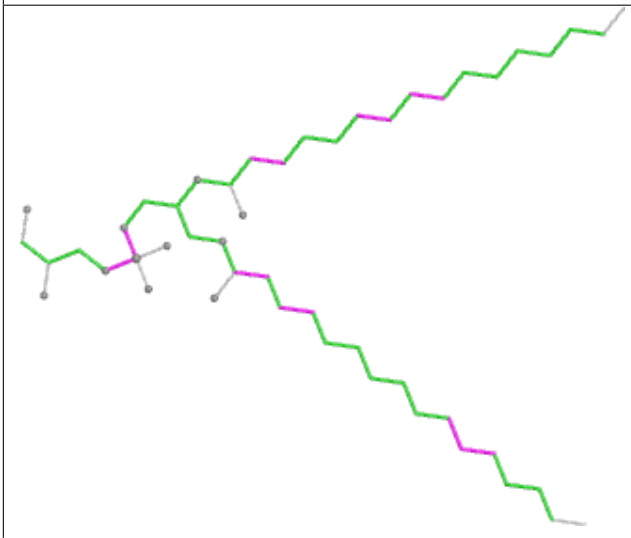
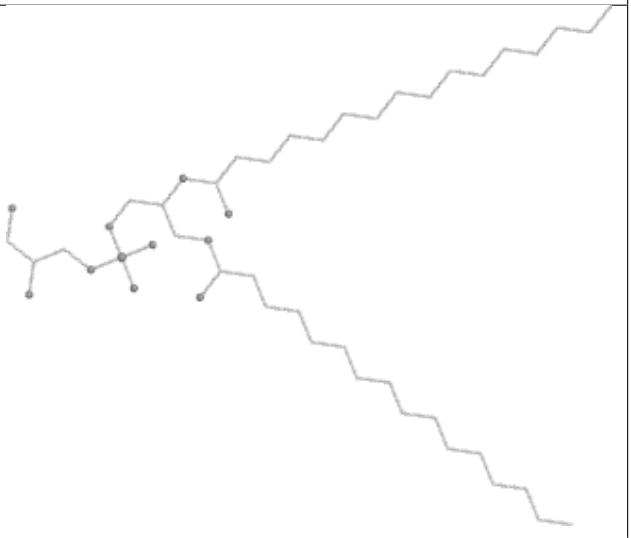


Bond angles

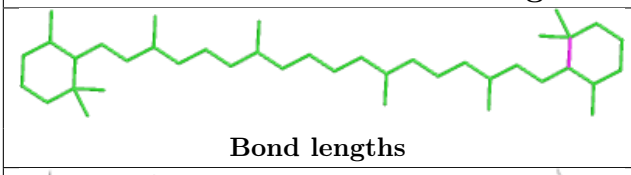


Torsions



Rings

Ligand BCR J 101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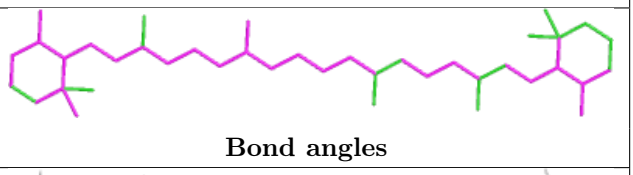
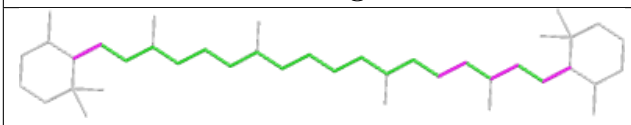
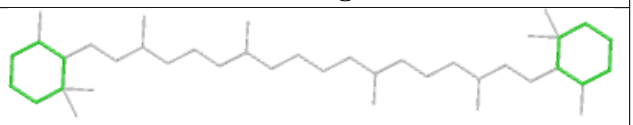
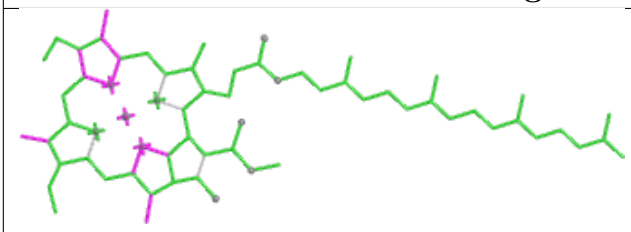

Bond angles


Torsions


Rings

Ligand CLA B 834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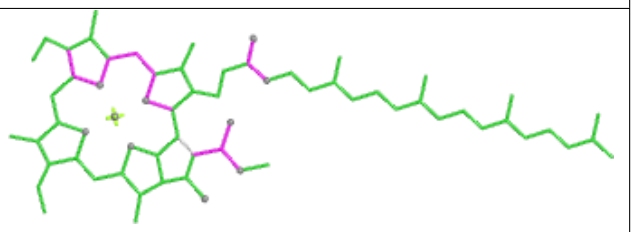
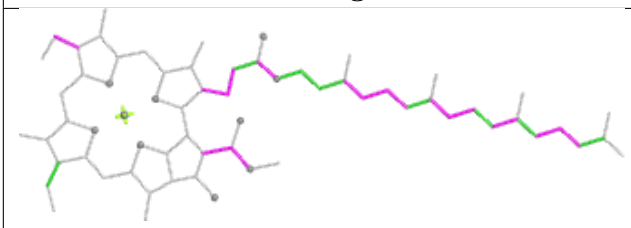

Bond angles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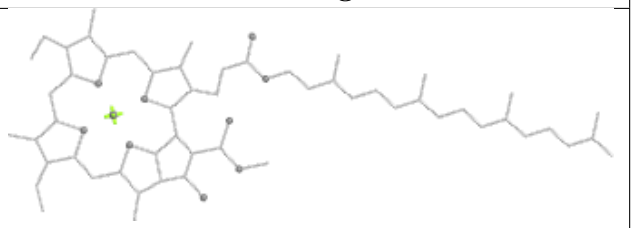
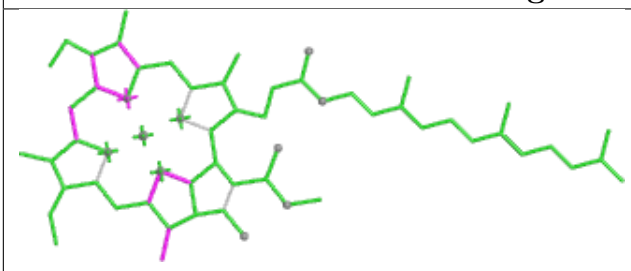

Rings

Ligand CLA S 313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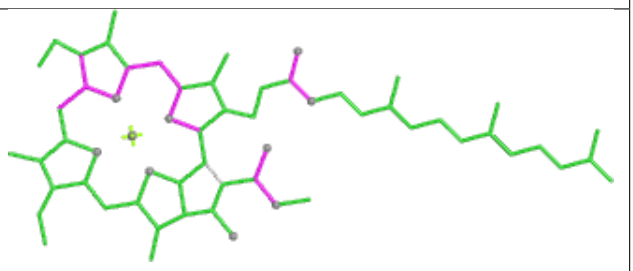
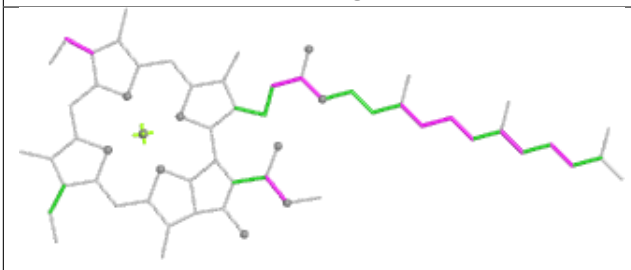

Bond angles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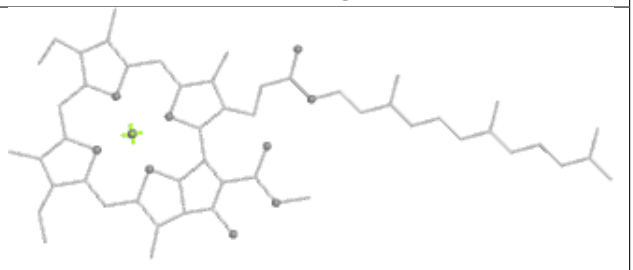
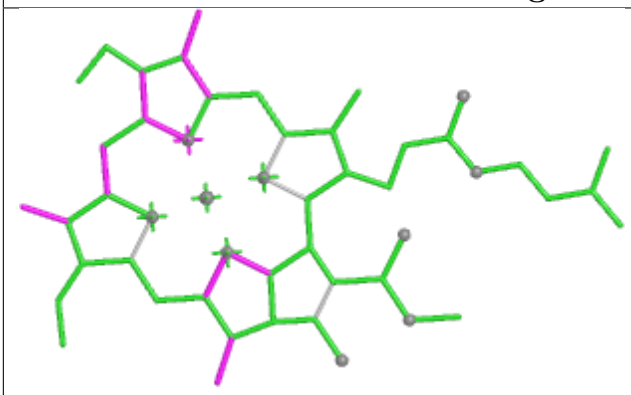

Rings

Ligand CLA 9 310



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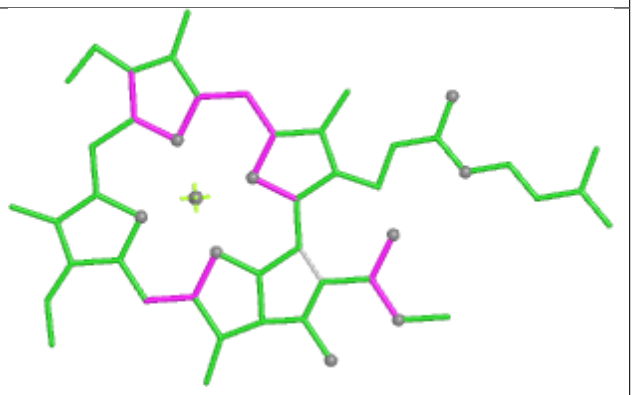

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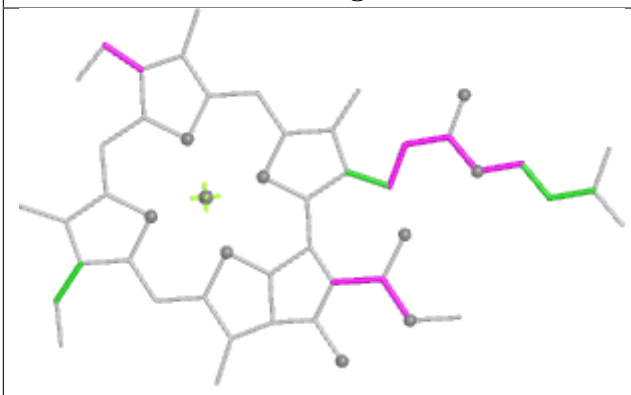

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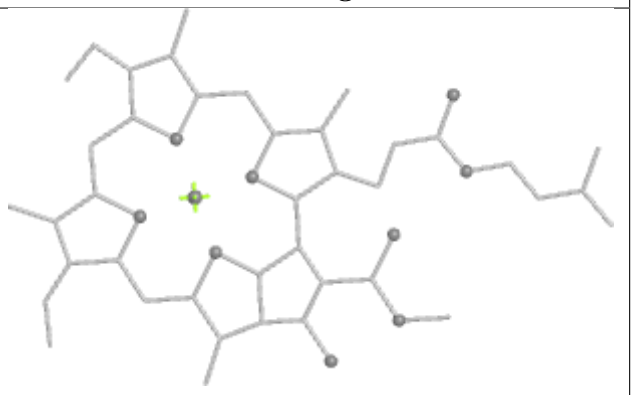
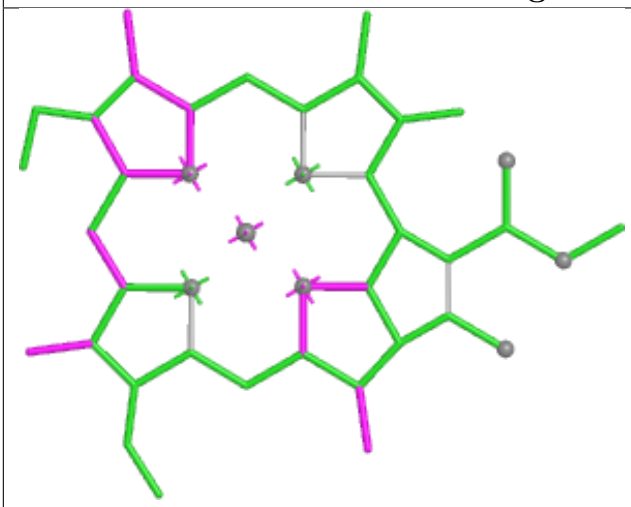


Rings

Ligand CLA 7 309



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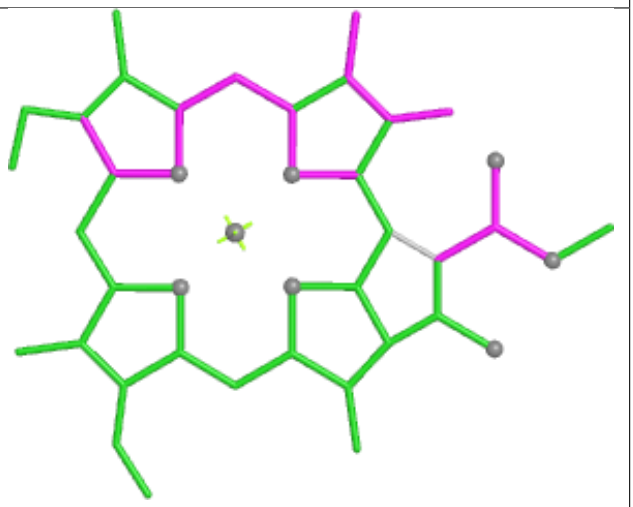

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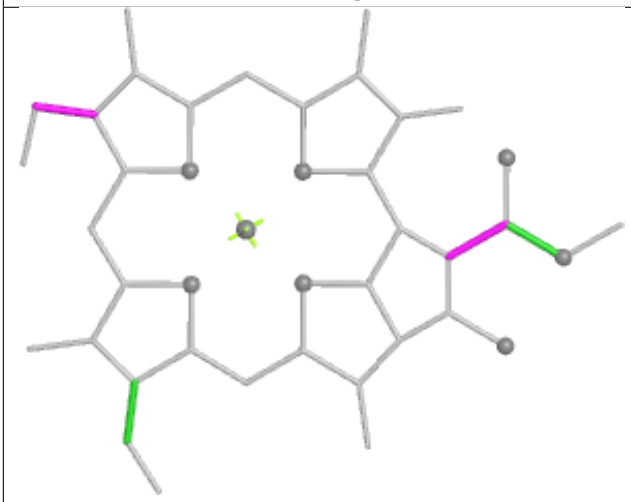

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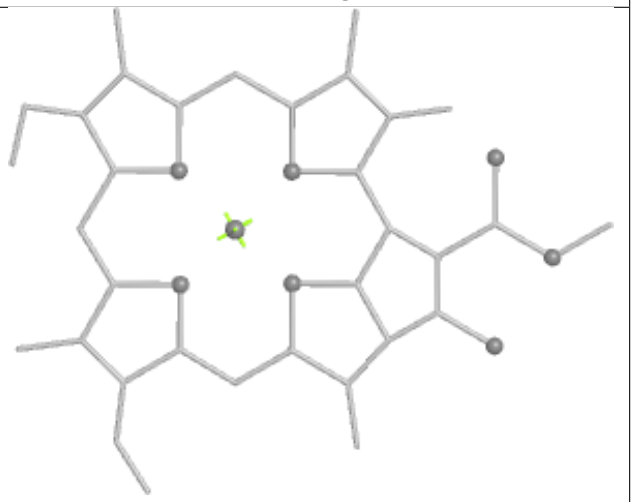
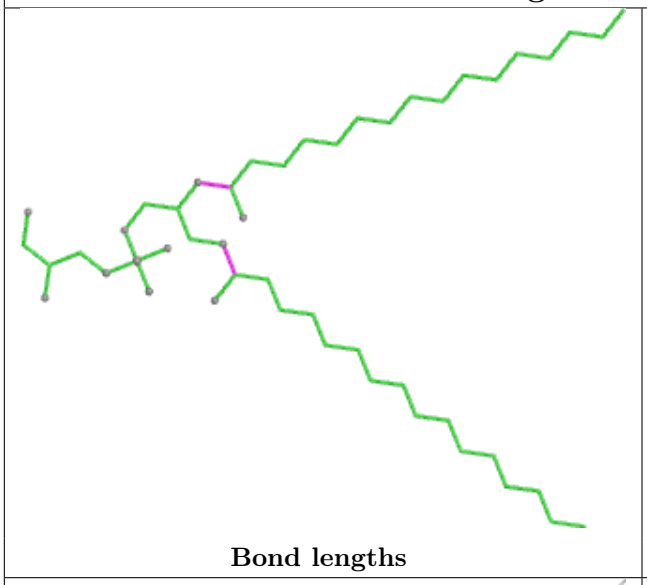


Rings

Ligand LHG 4 318



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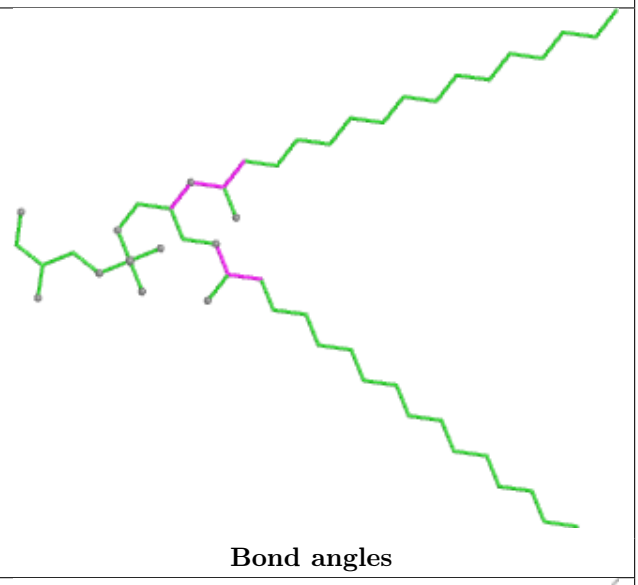
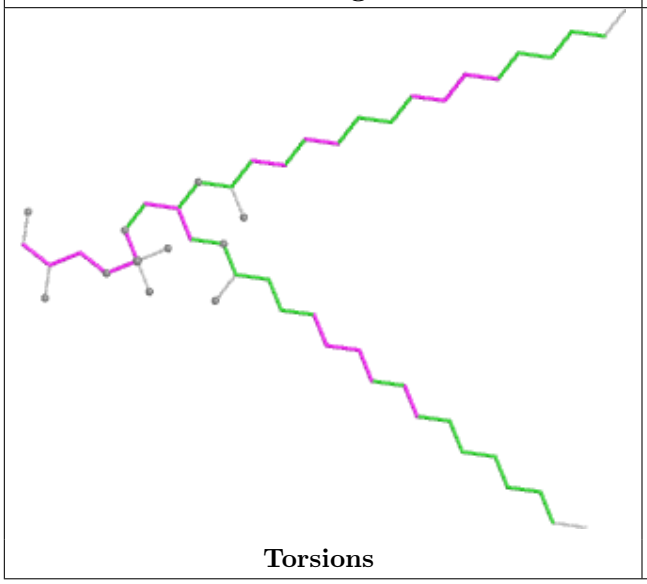


Bond angles



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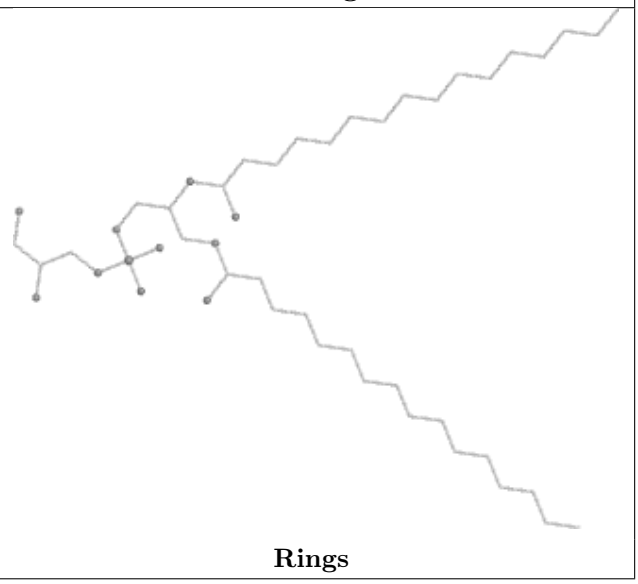
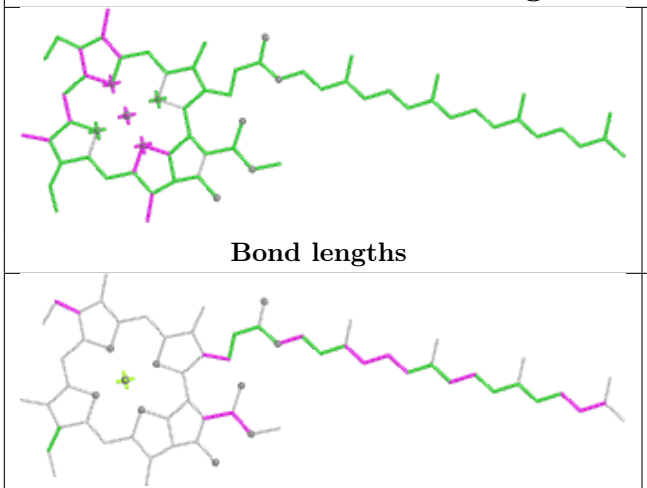


Rings

Ligand CLA A 853



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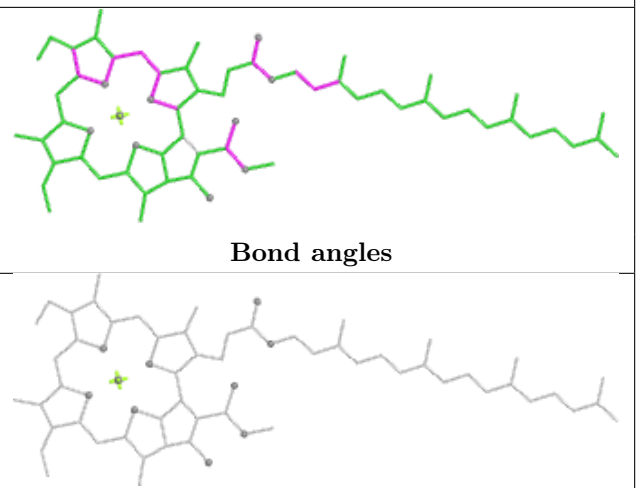
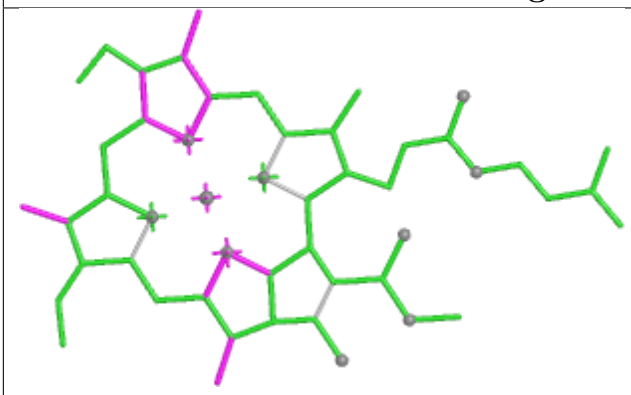


Bond angles

Torsions

Rings

Ligand CLA 3 307



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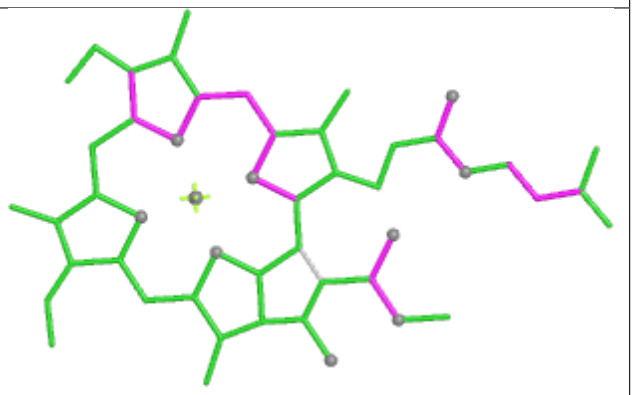
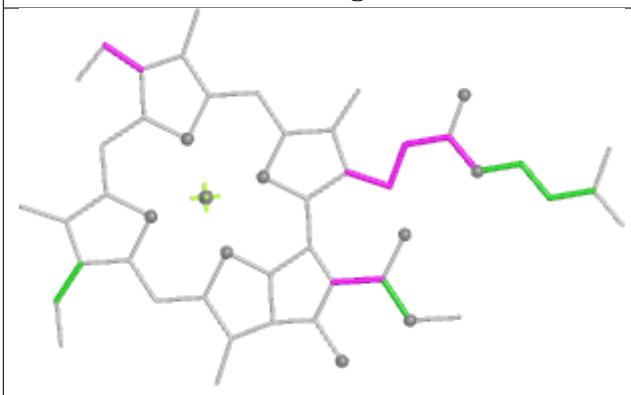


Bond angles



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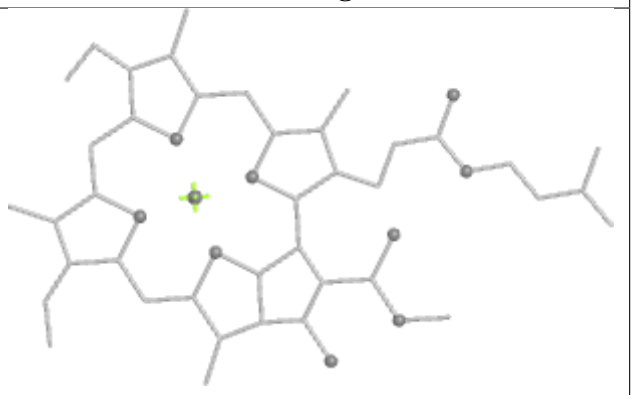
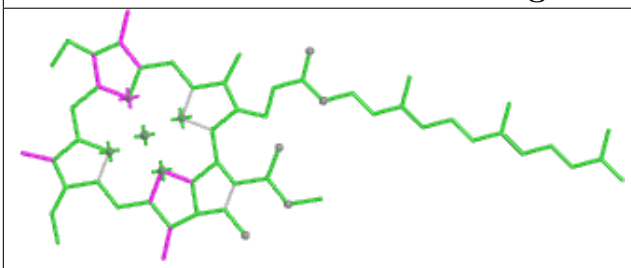


Rings

Ligand CLA 6 623



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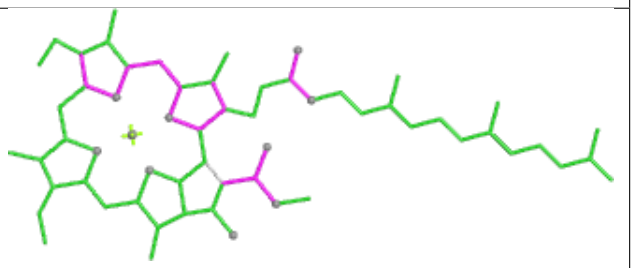
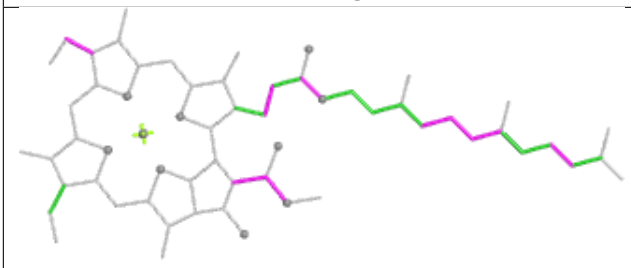


Bond angles



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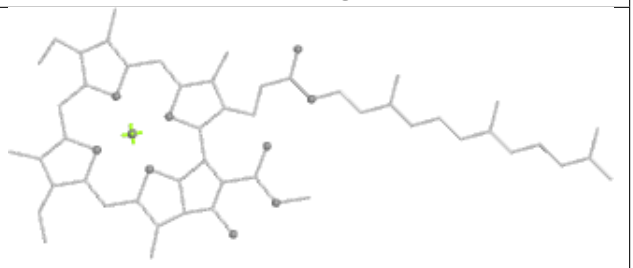
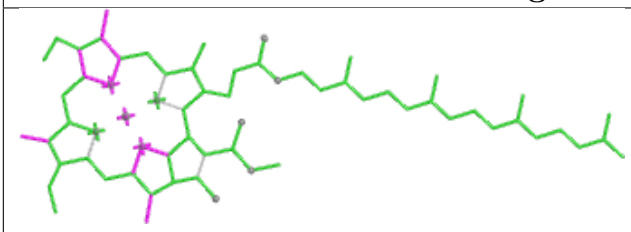
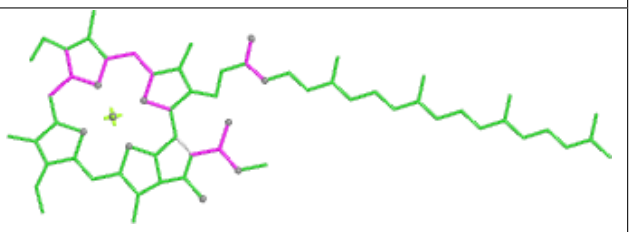
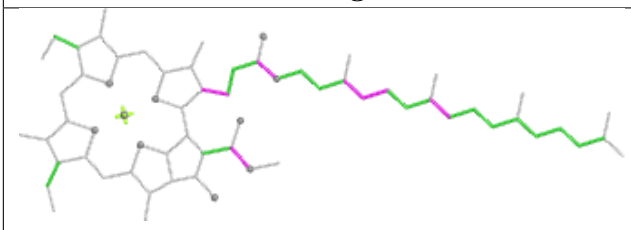
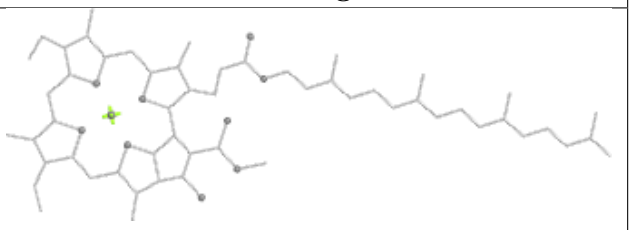
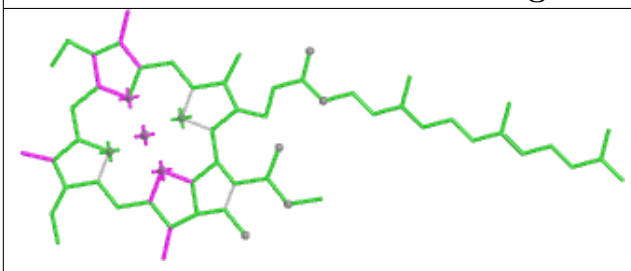
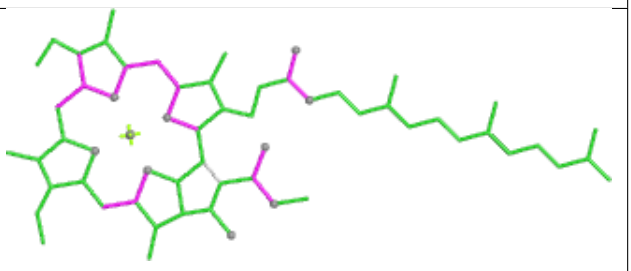
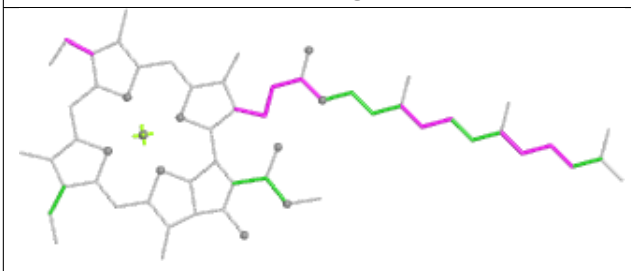
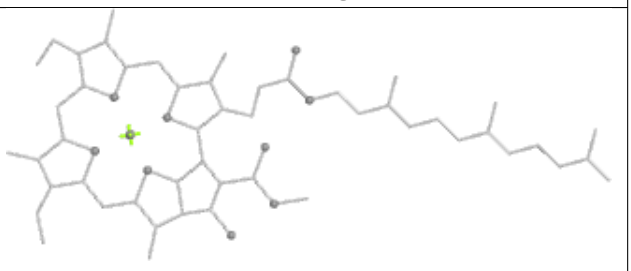
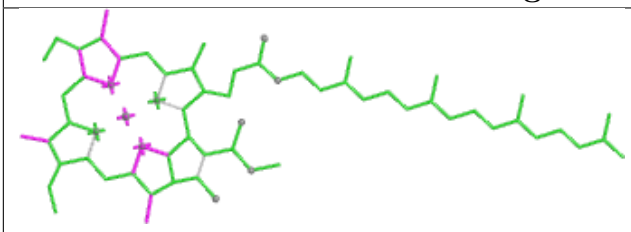


Rings

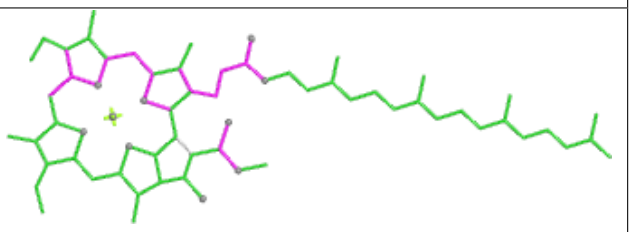
Ligand CLA 3 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

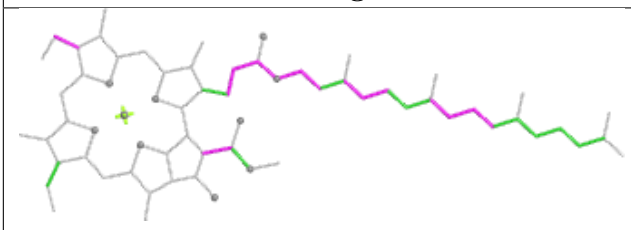
Ligand CLA A 806



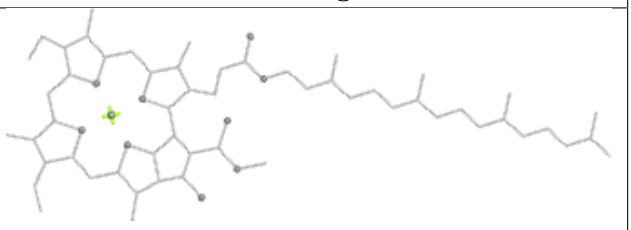
Bond lengths



Bond angles

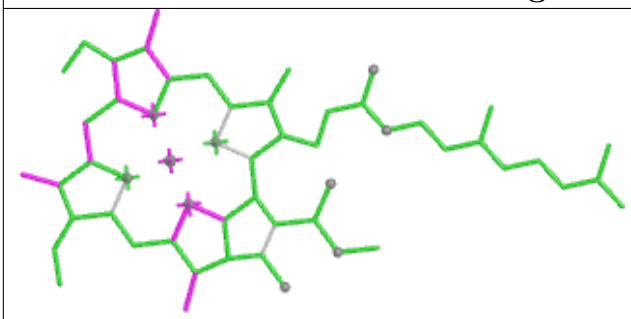


Torsions

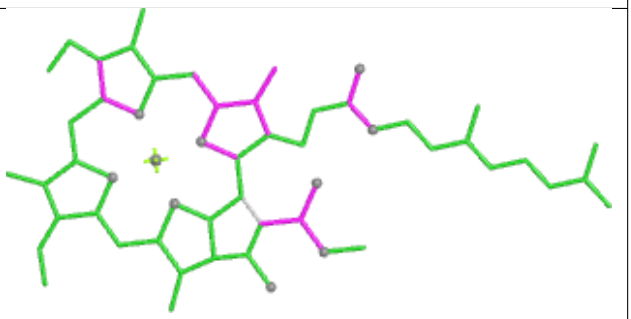


Rings

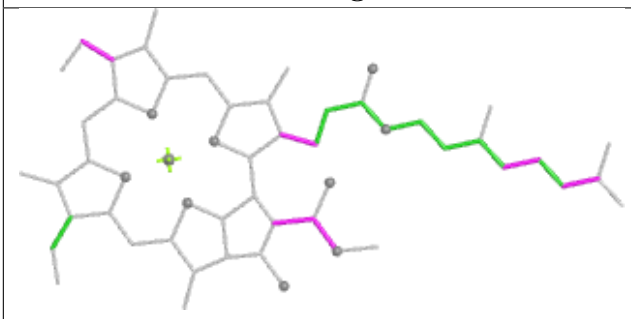
Ligand CLA 8 314



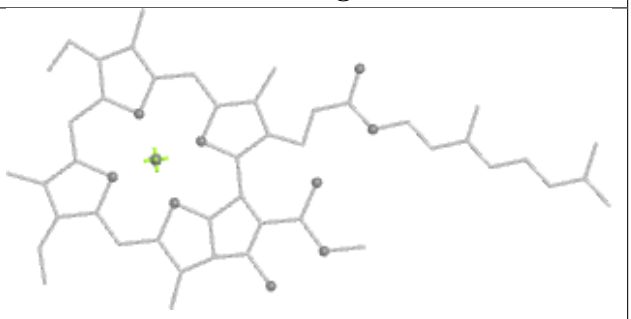
Bond lengths



Bond angles

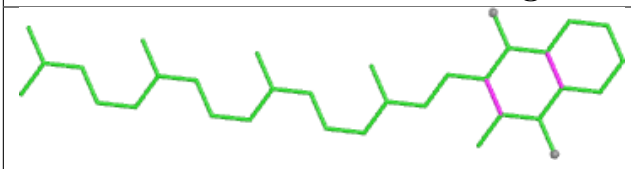


Torsions

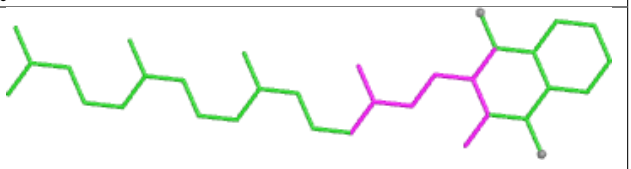


Rings

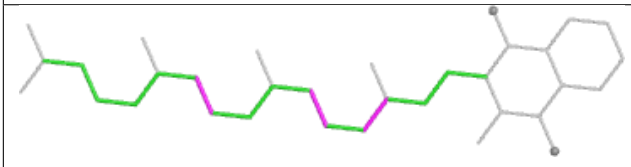
Ligand PQN B 839



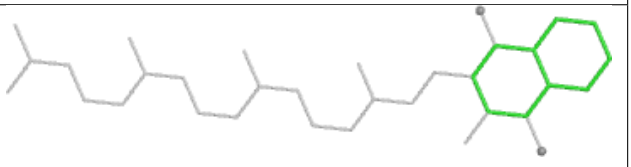
Bond lengths



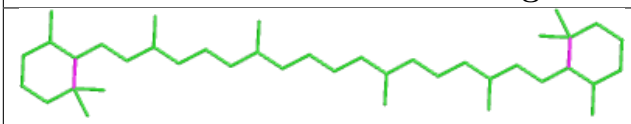
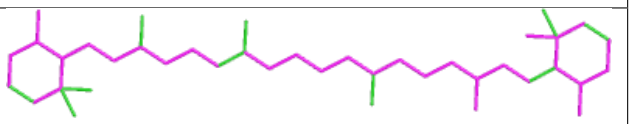
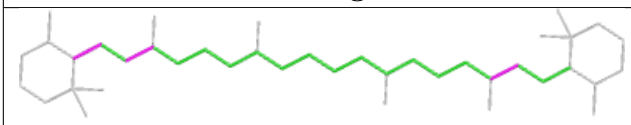
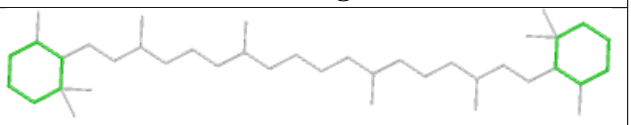
Bond angles

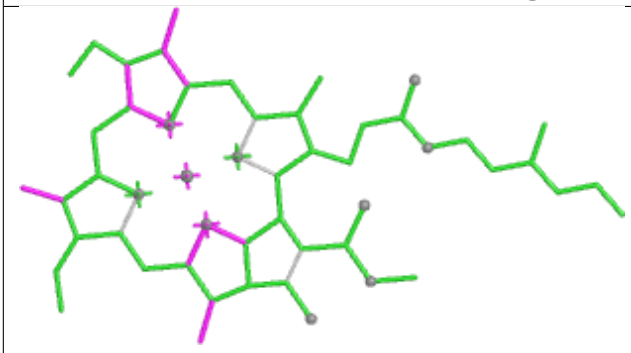
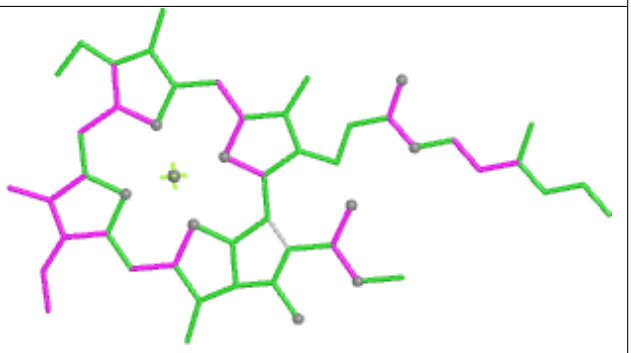
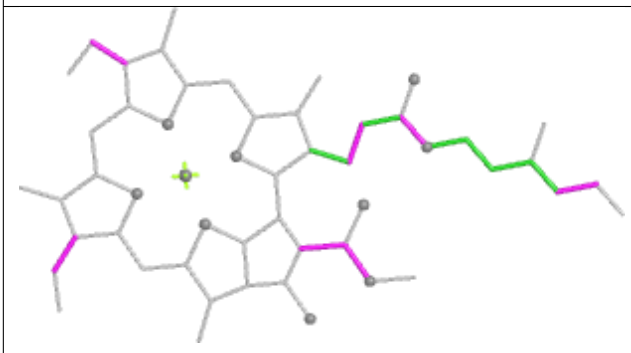
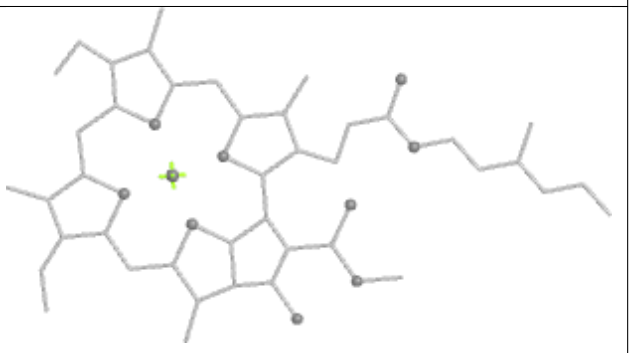


Torsions

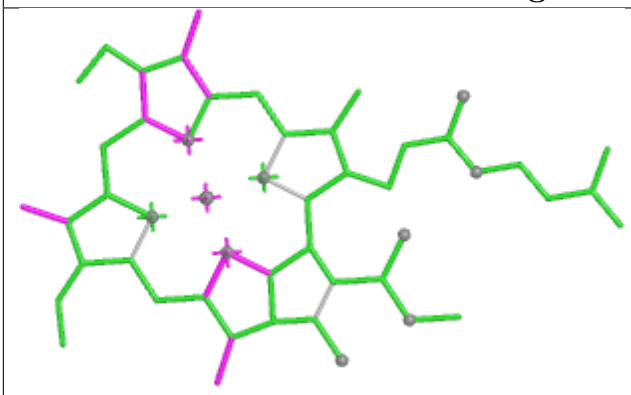


Rings

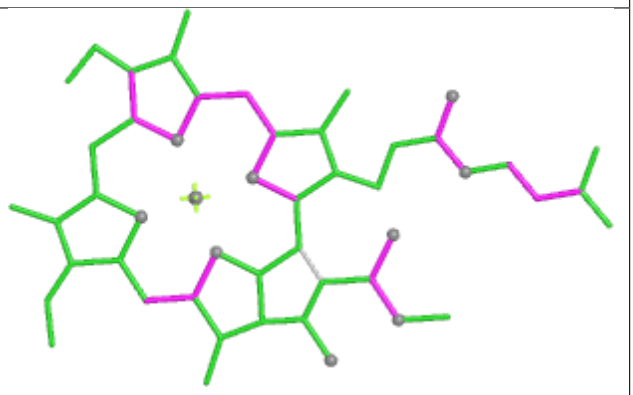
Ligand BCR O 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

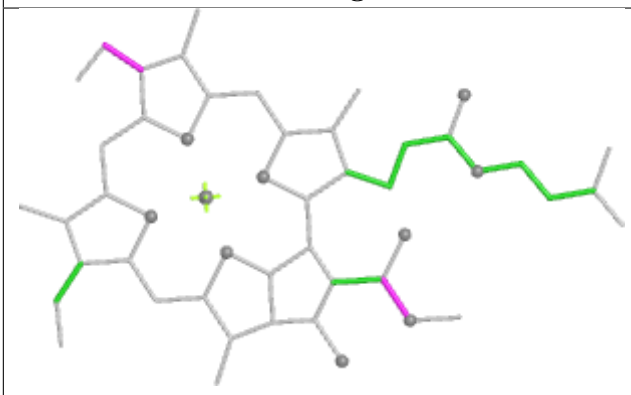
Ligand CLA 7 306



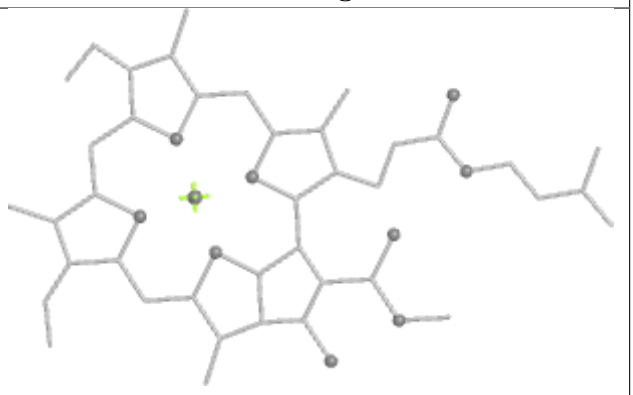
Bond lengths



Bond angles

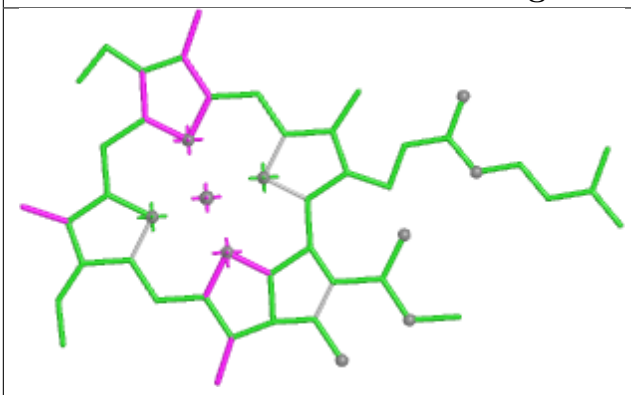


Torsions



Rings

Ligand CLA 5 309



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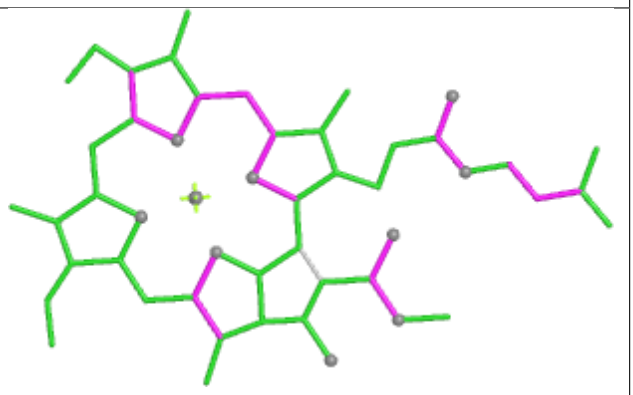
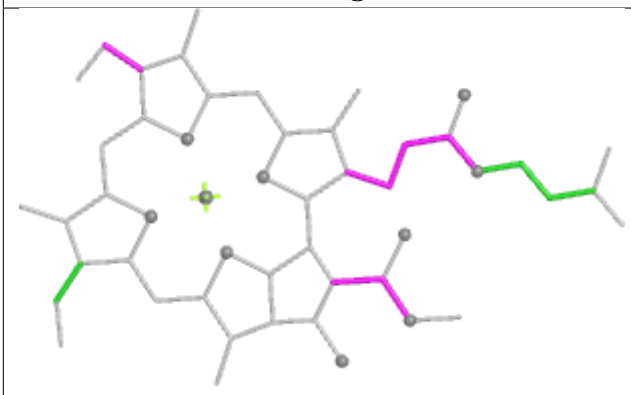


Bond angles



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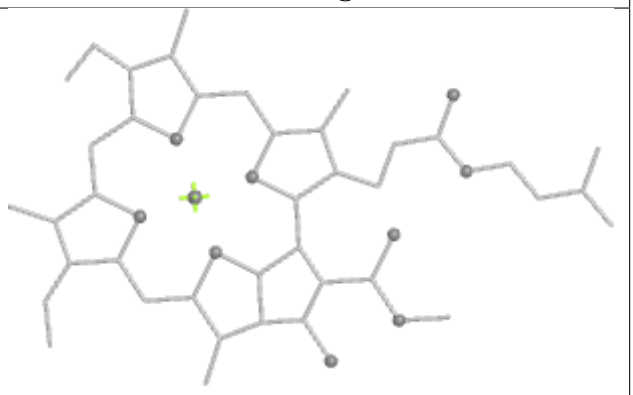
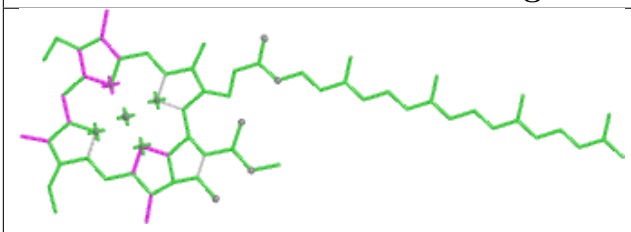


Rings

Ligand CLA A 808



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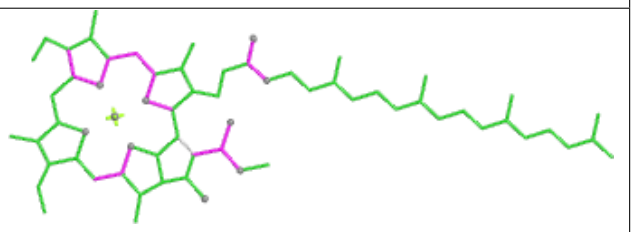
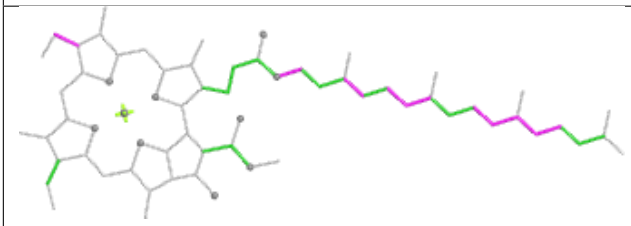


Bond angles



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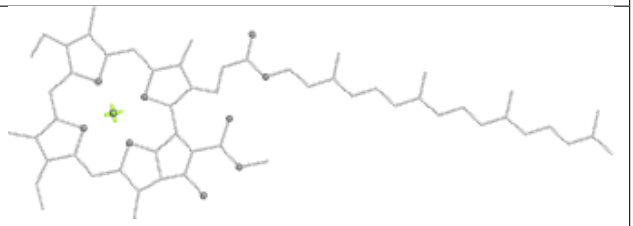
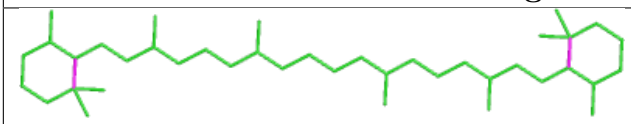


Rings

Ligand BCR L 207



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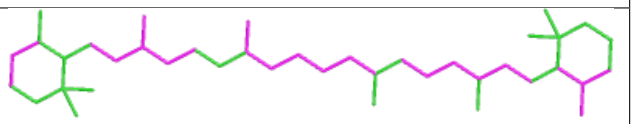
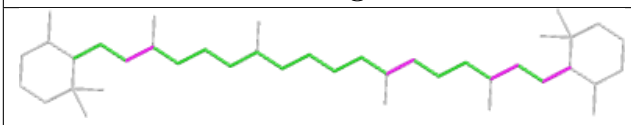


Bond angles



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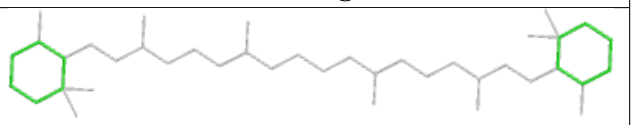
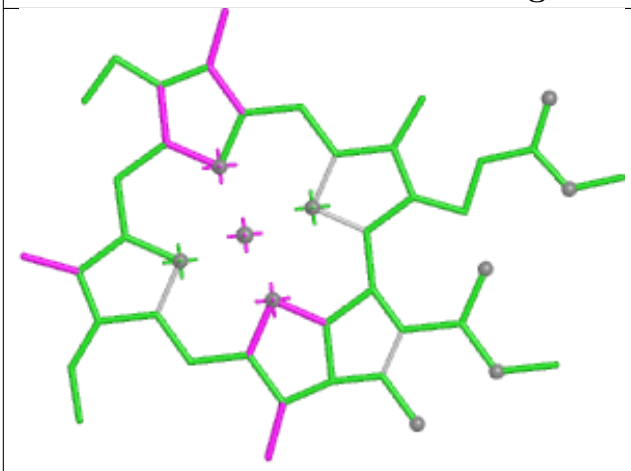


Rings

Ligand CLA 8 315



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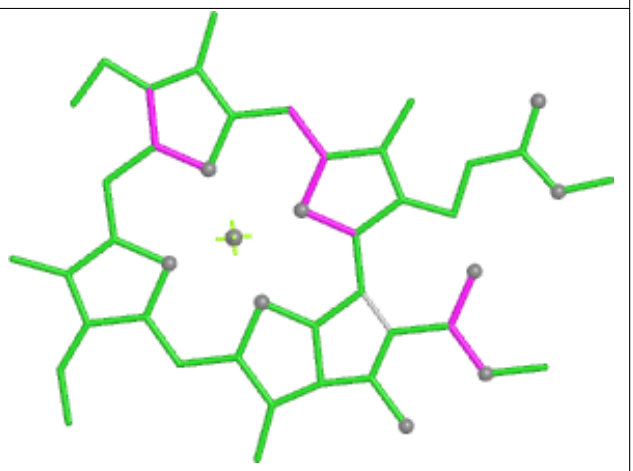
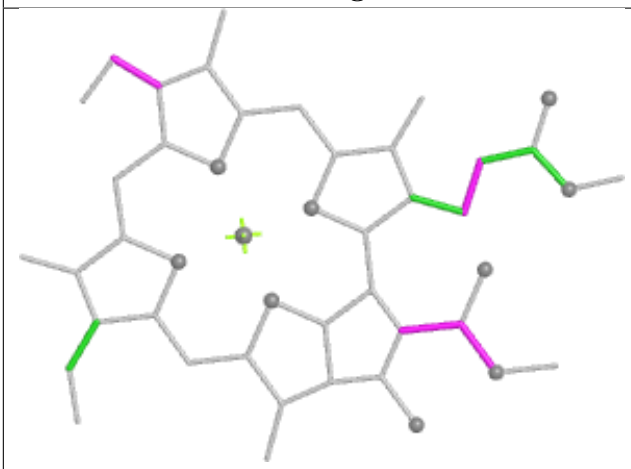


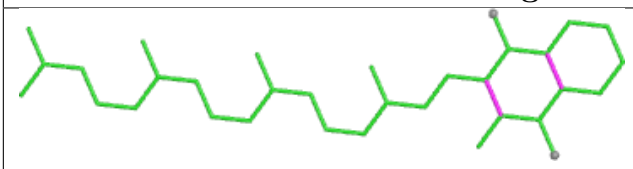
Bond angles



Torsions

Rings

Ligand PQN A 841



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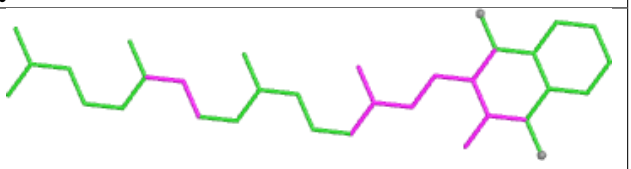
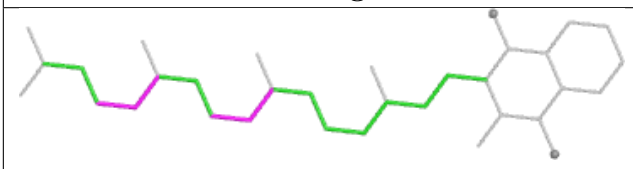
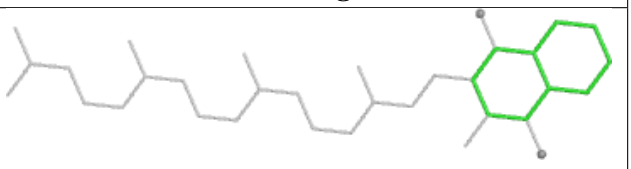


Bond angles

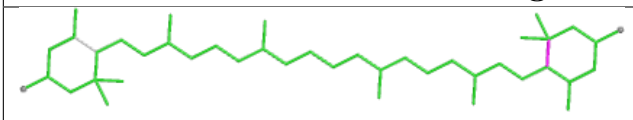


Torsions



Rings

Ligand LUT 8 316



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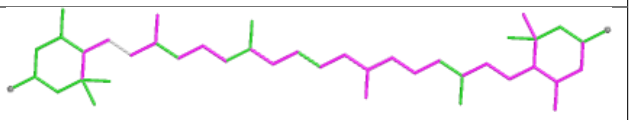
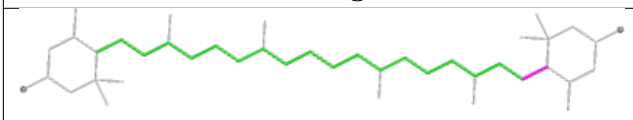
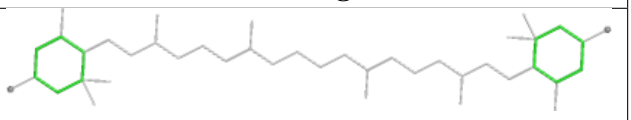


Bond angles

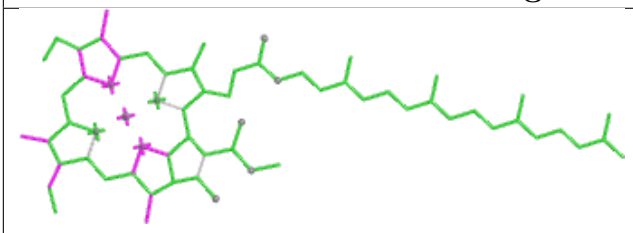


Torsions



Rings

Ligand CLA B 805



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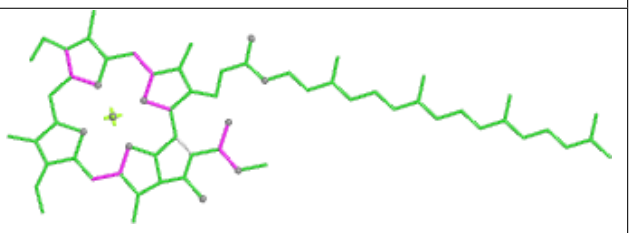
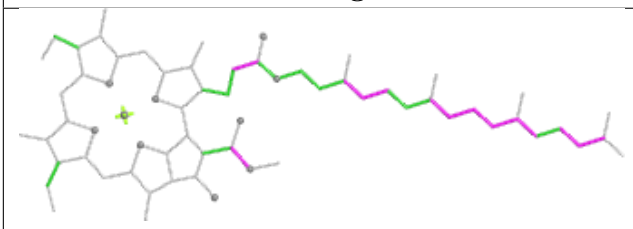
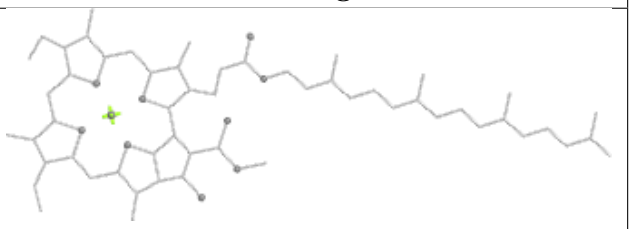


Bond angles

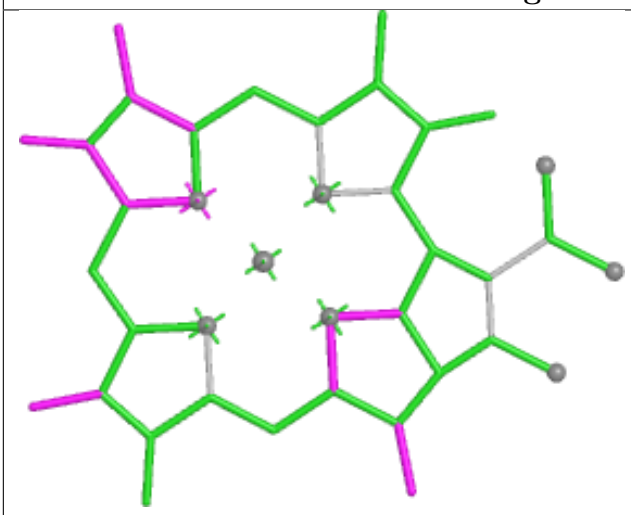


Torsions



Rings

Ligand CLA O 203



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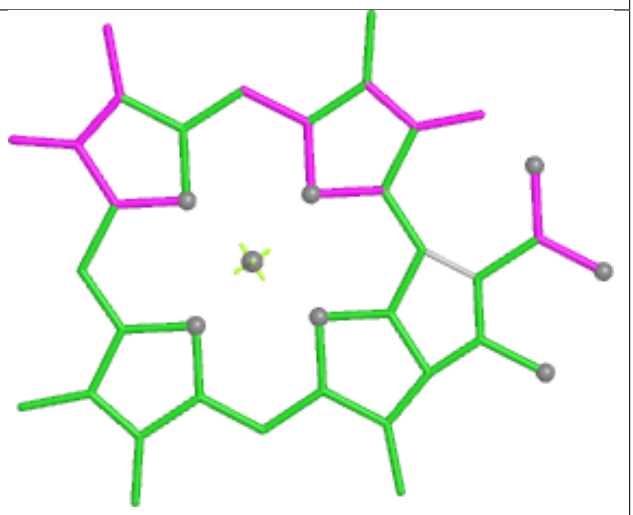
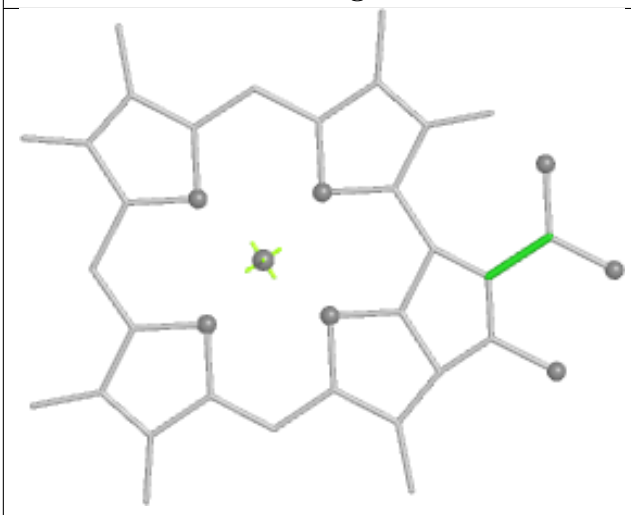
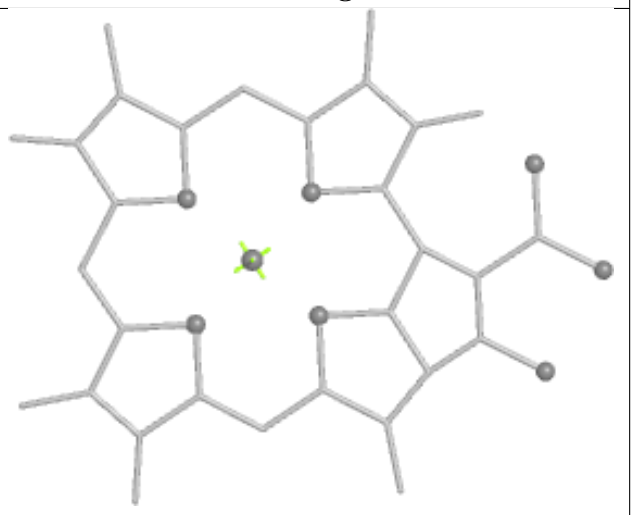


Bond angles

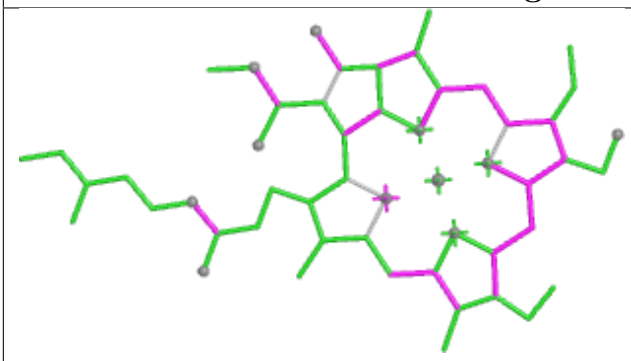


Torsions

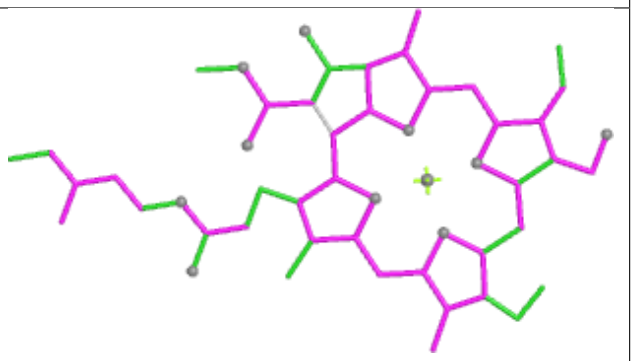


Rings

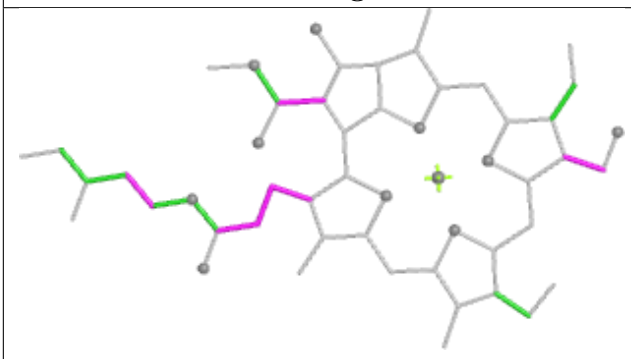
Ligand CHL P 619



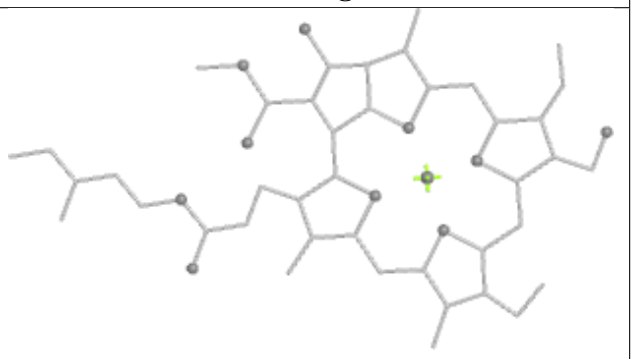
Bond lengths



Bond angles

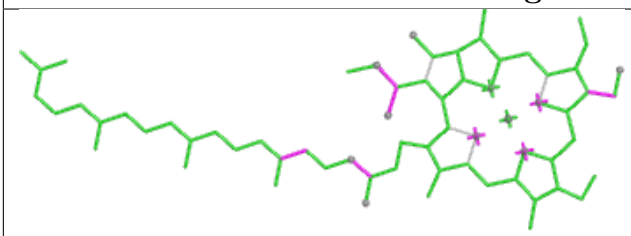


Torsions

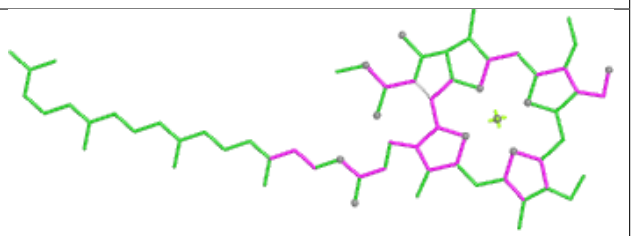


Rings

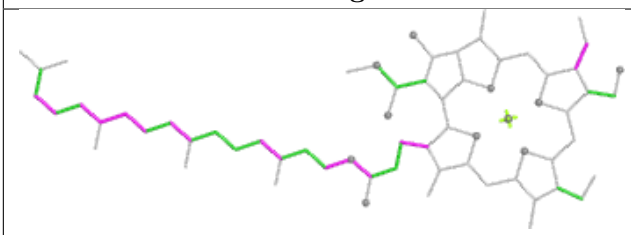
Ligand CHL P 609



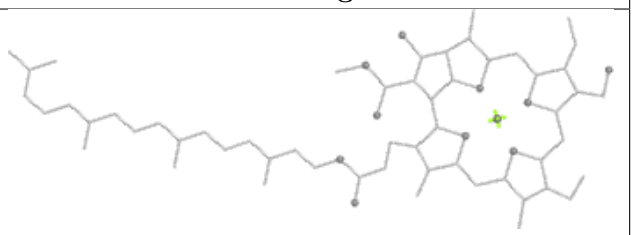
Bond lengths



Bond angles

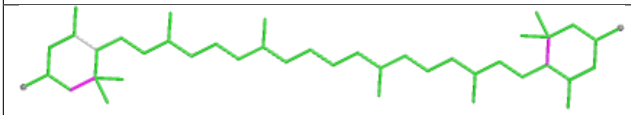


Torsions



Rings

Ligand LUT 3 315



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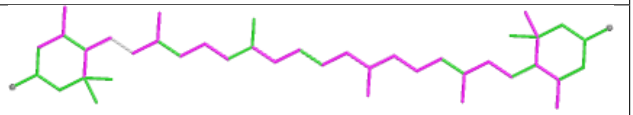
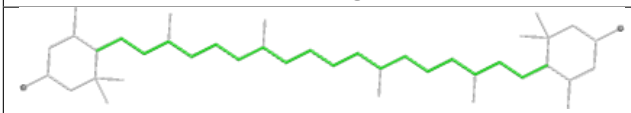


Bond angles



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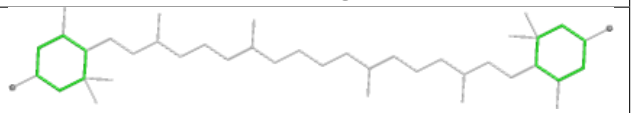
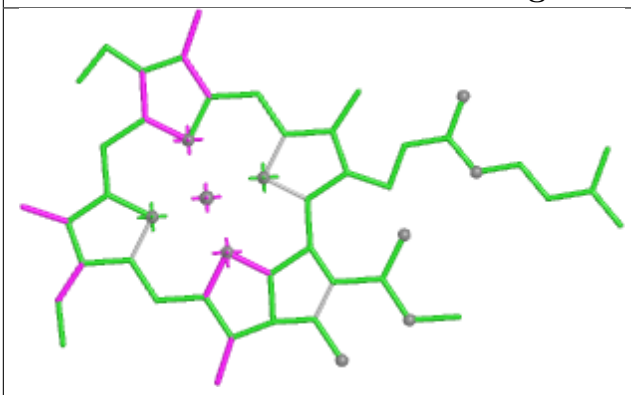


Rings

Ligand CLA 8 308



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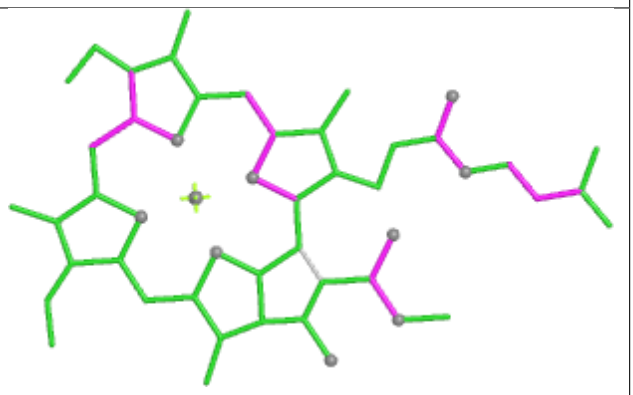
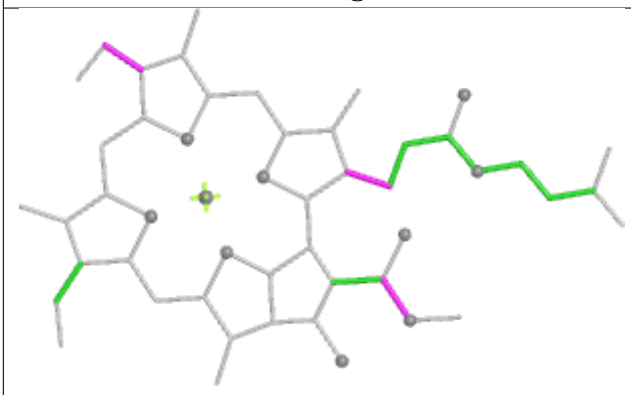


Bond angles



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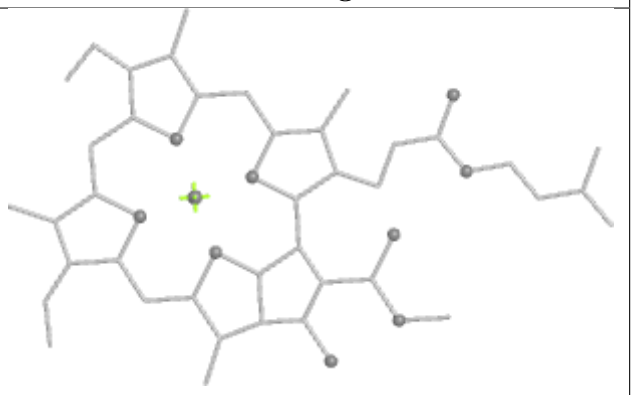
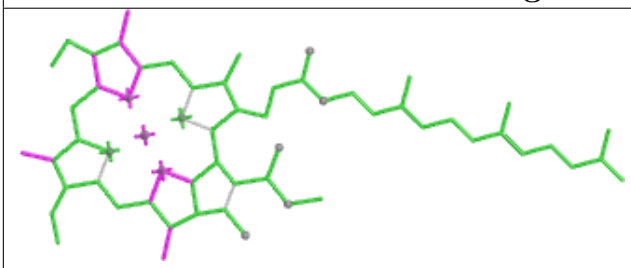
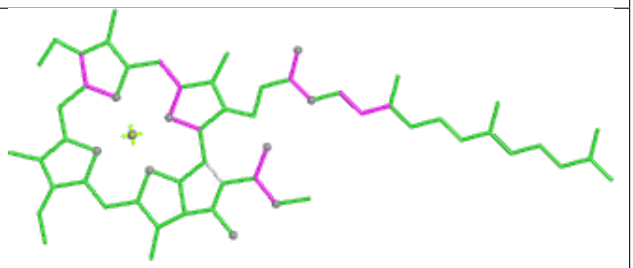


Rings

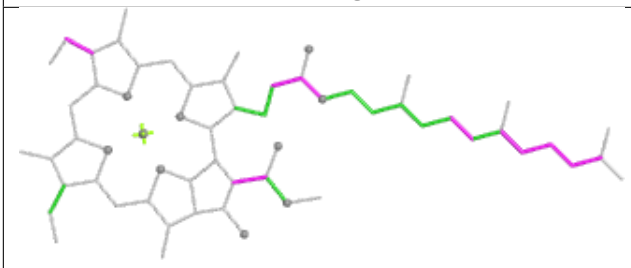
Ligand CLA A 815



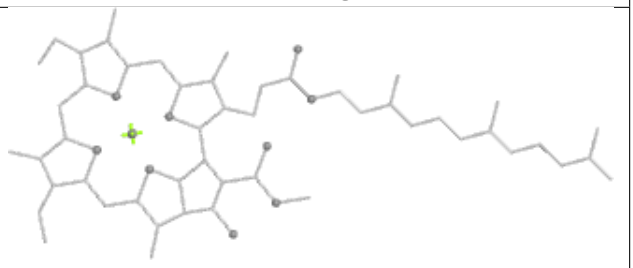
Bond lengths



Bond angles

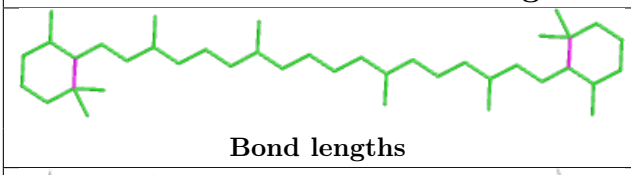


Torsions



Rings

Ligand BCR A 849



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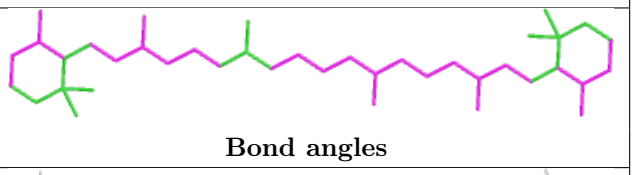
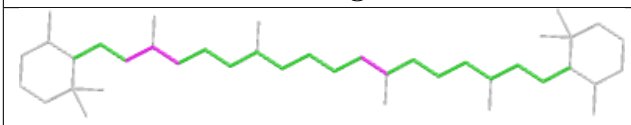


Bond angles



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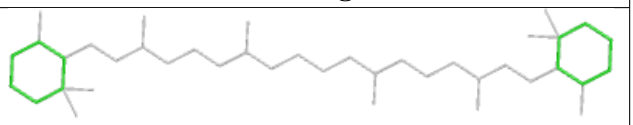
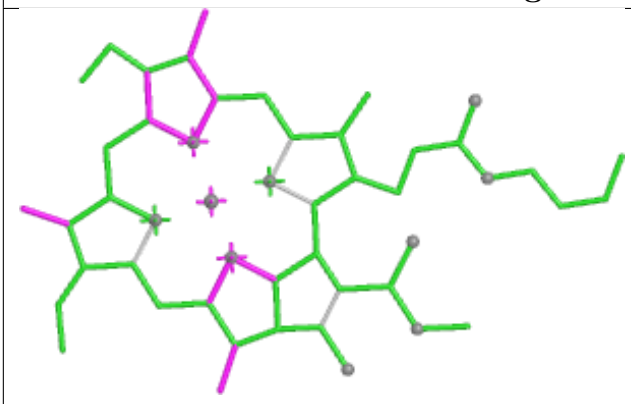


Rings

Ligand CLA B 829



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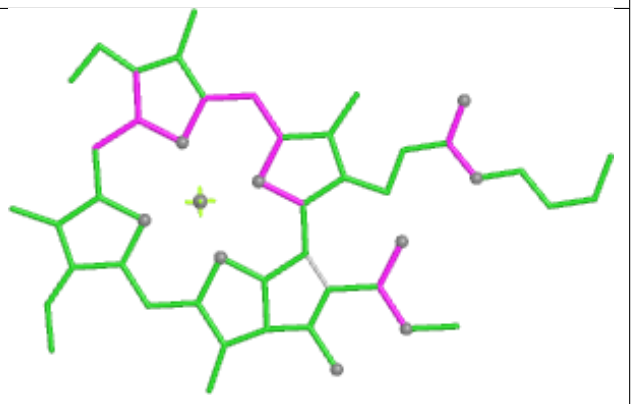
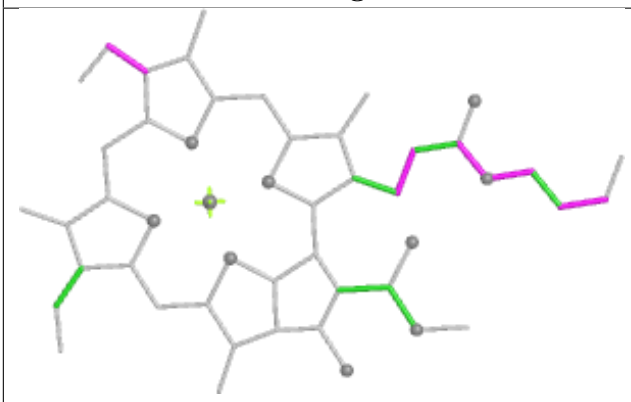
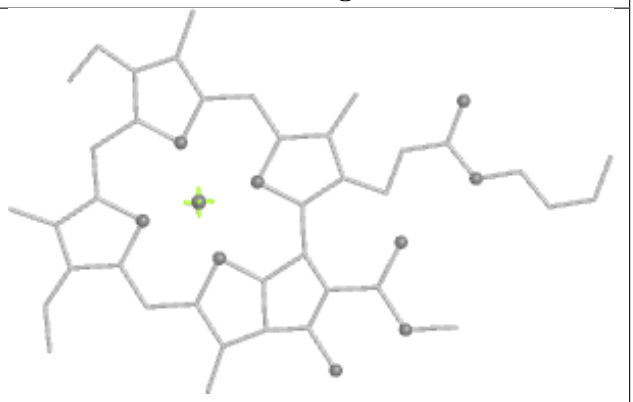


Bond angles

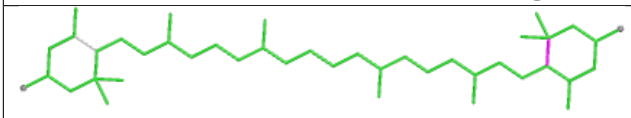


Torsions



Rings

Ligand LUT 9 313



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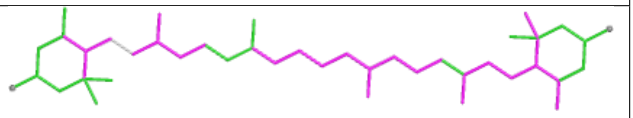
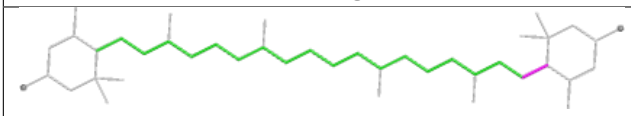


Bond angles



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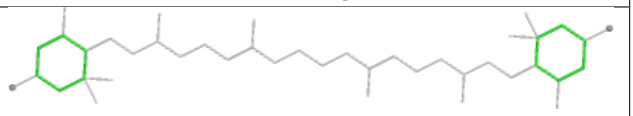
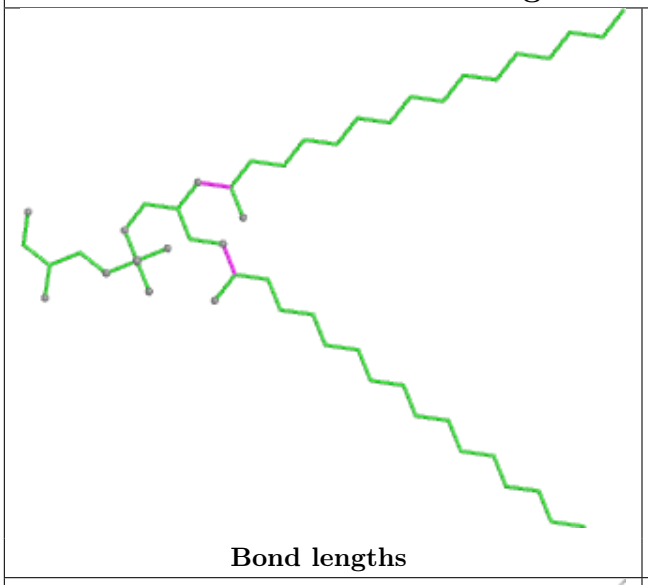


Rings

Ligand LHG R 618



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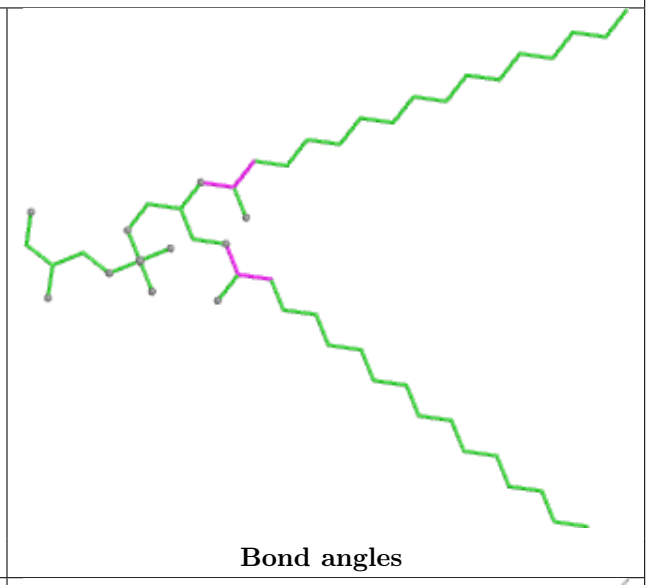
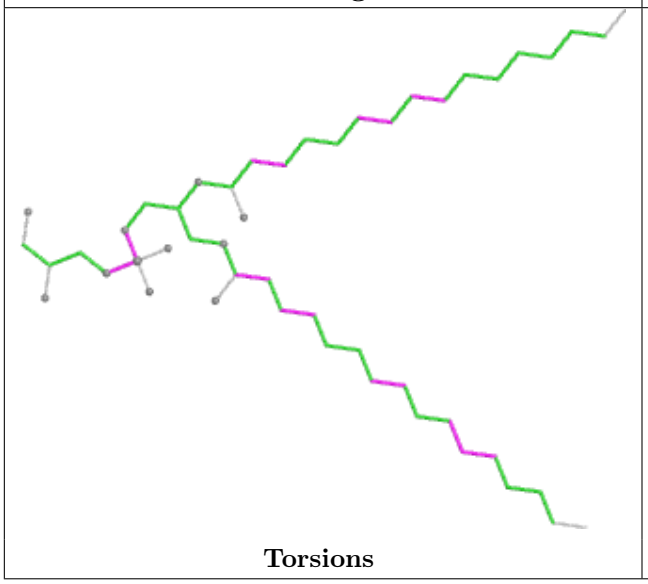
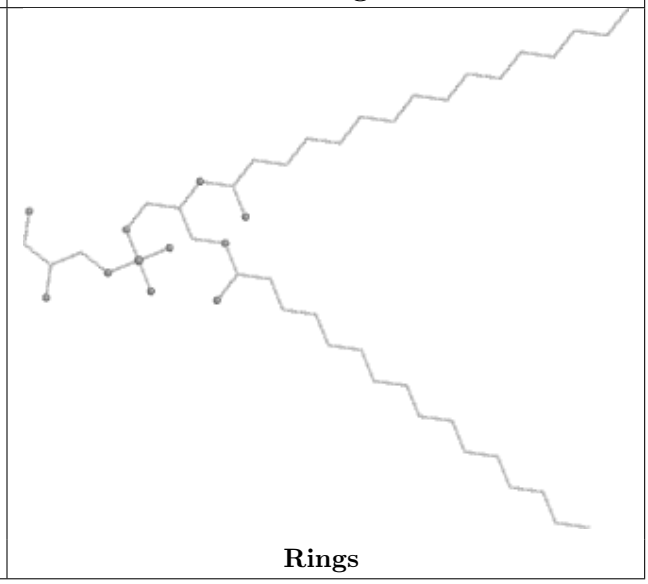


Bond angles

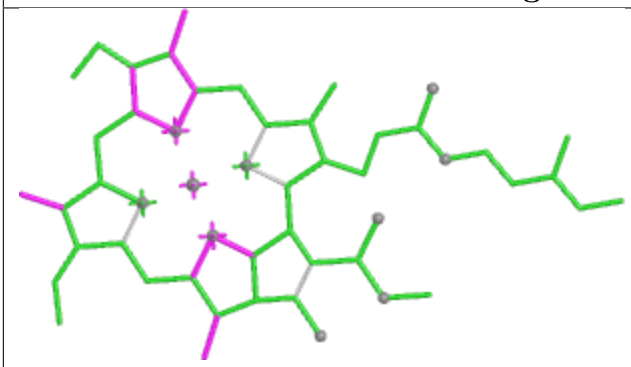


Torsions



Rings

Ligand CLA K 201



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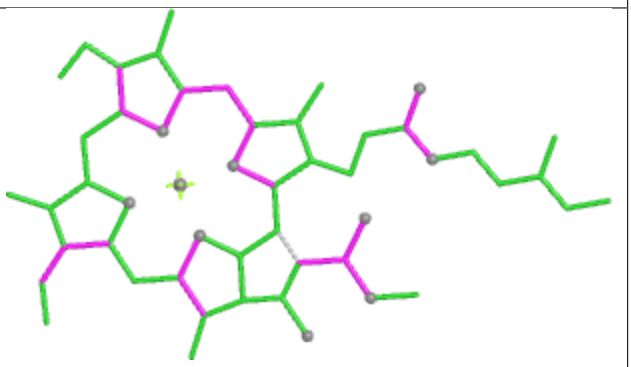
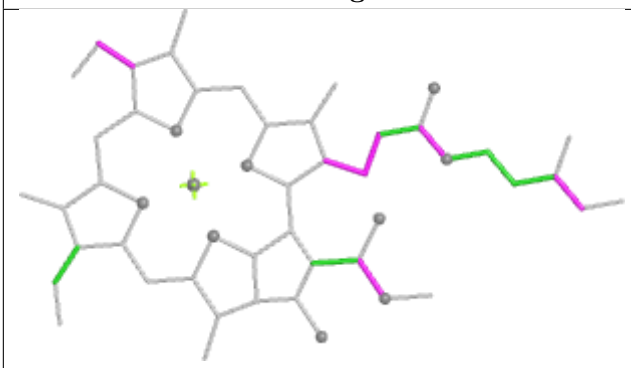


Bond angles



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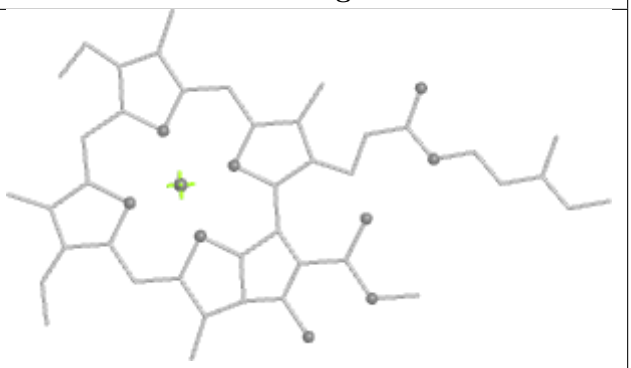
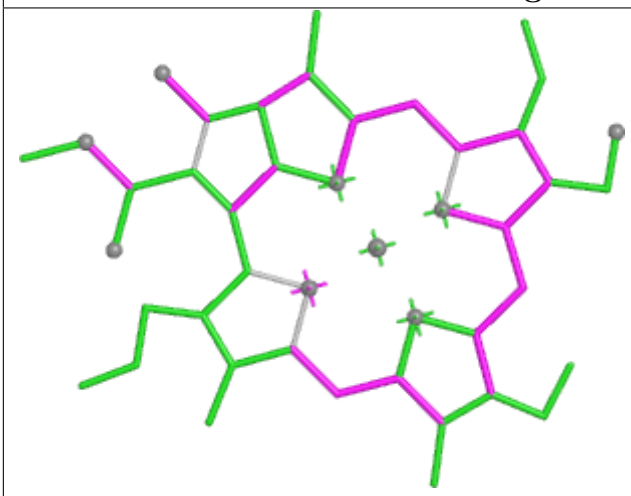


Rings

Ligand CHL P 608



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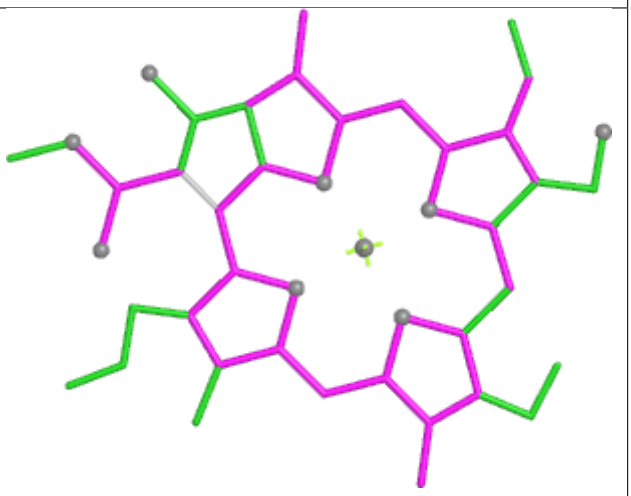
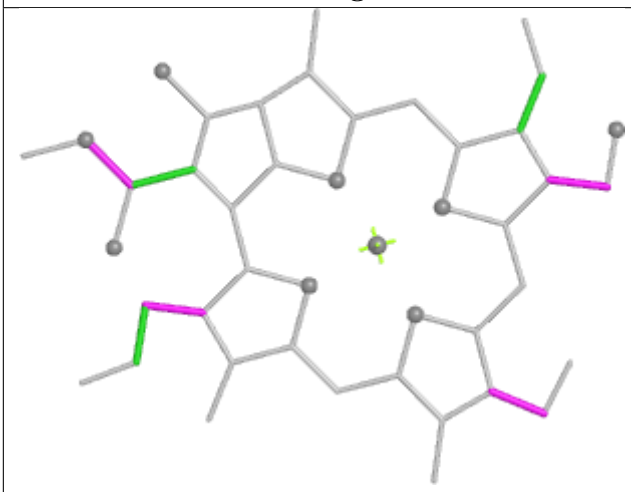
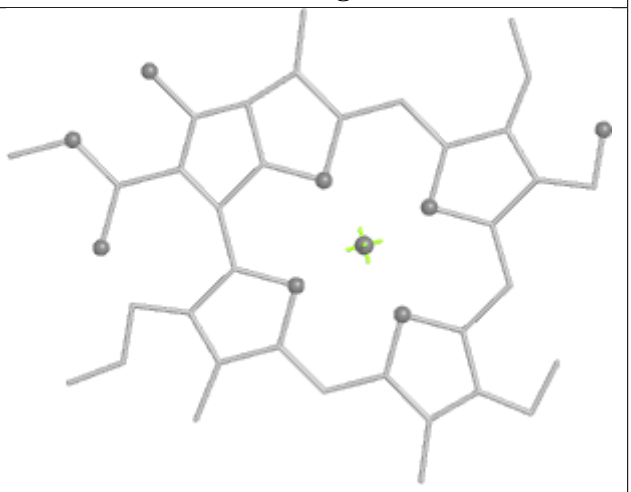


Bond angles

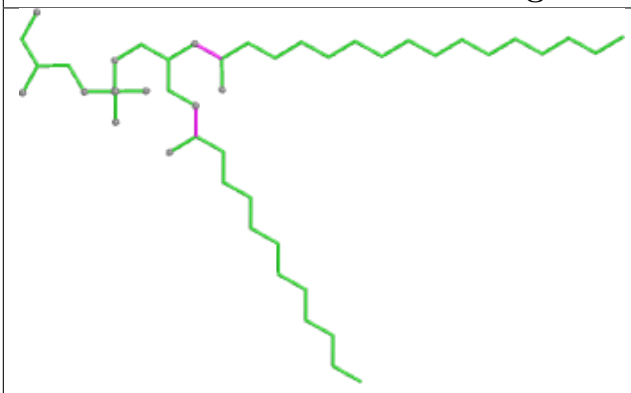


Torsions



Rings

Ligand LHG 5 301



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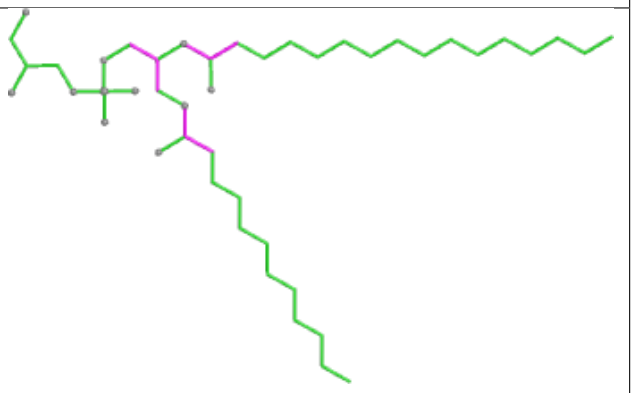
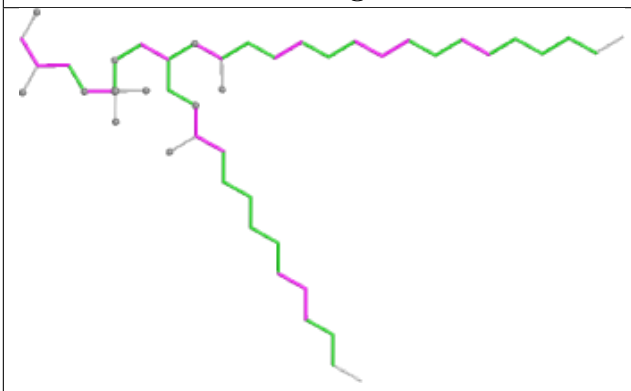


Bond angles



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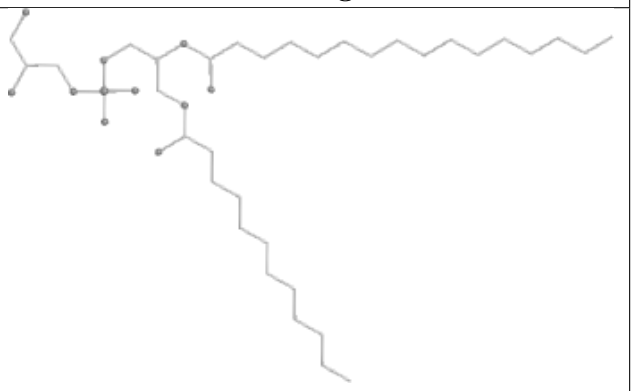
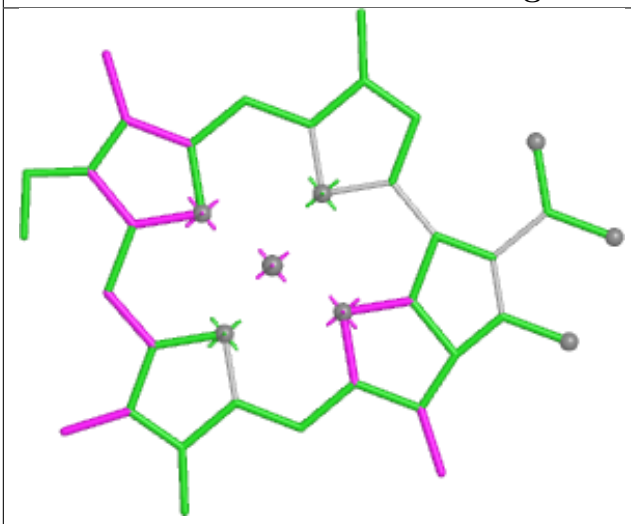
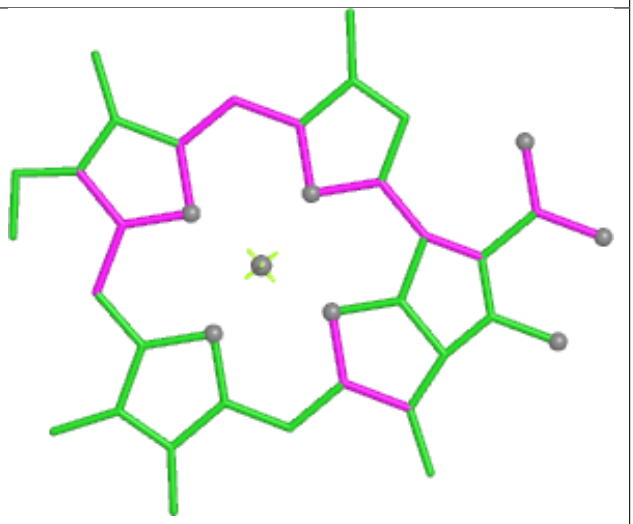


Rings

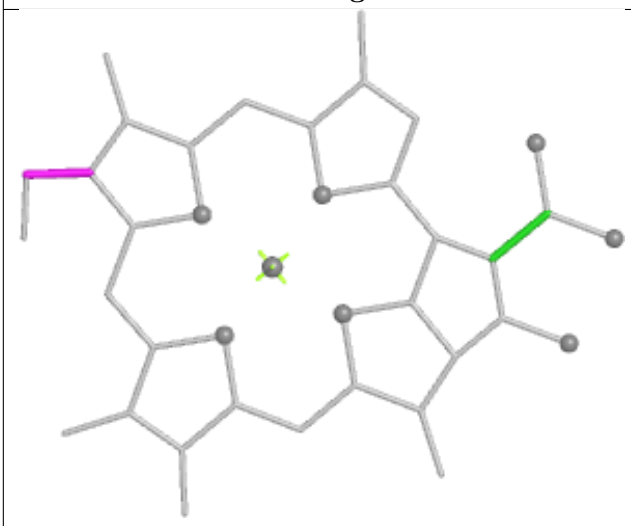
Ligand CLA O 202



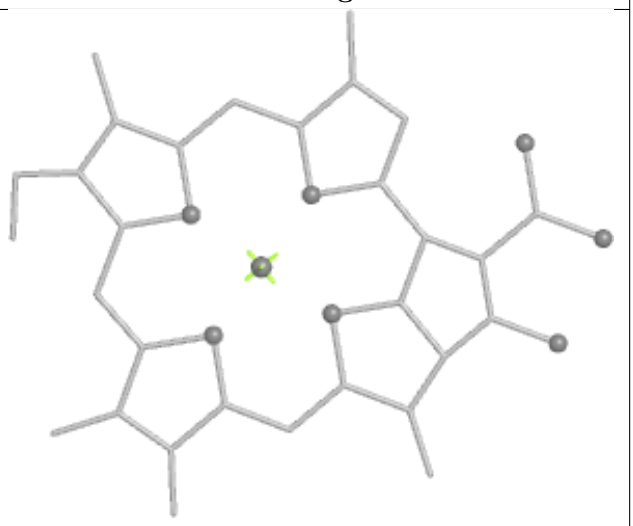
Bond lengths



Bond angles

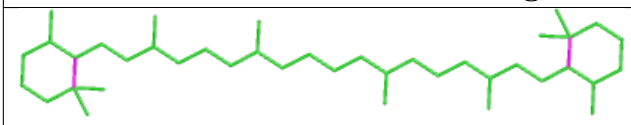


Torsions

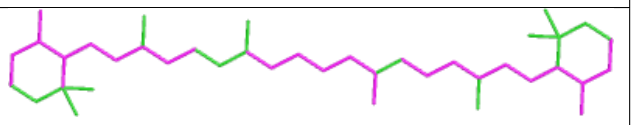


Rings

Ligand BCR B 851

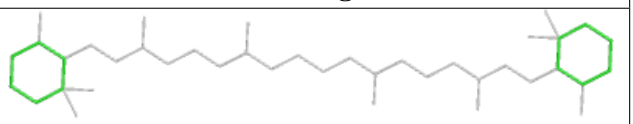


Bond lengths



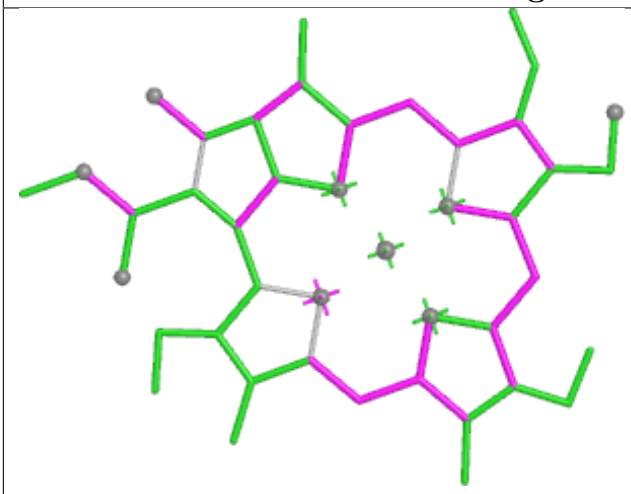
Bond angles

Torsions

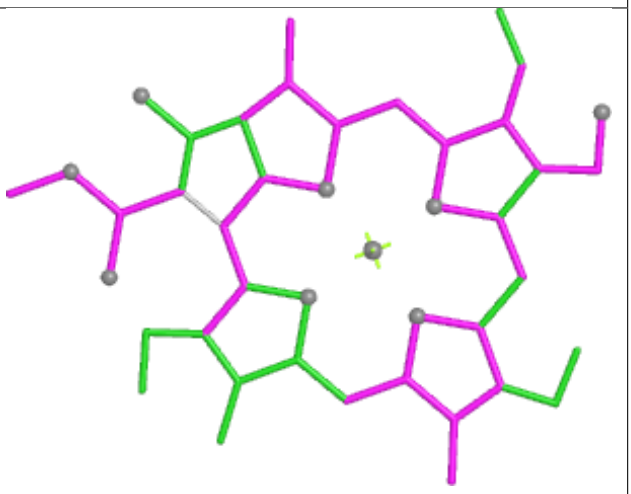


Rings

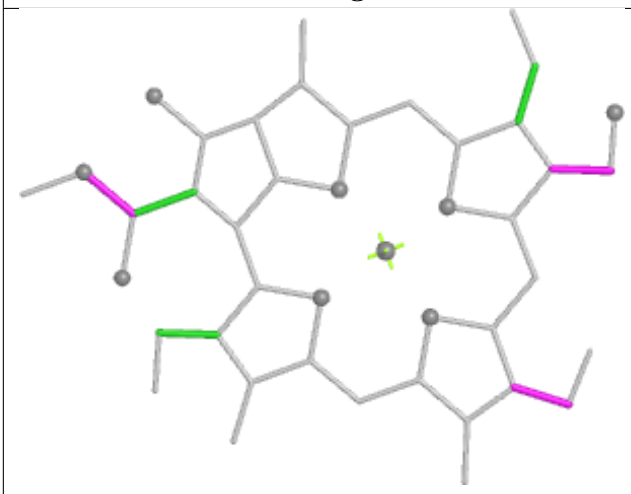
Ligand CHL 4 314



Bond lengths



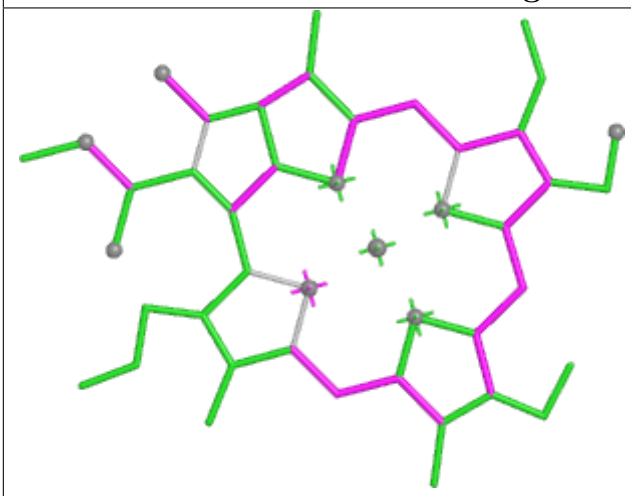
Bond angles



Torsions

Rings

Ligand CHL U 308



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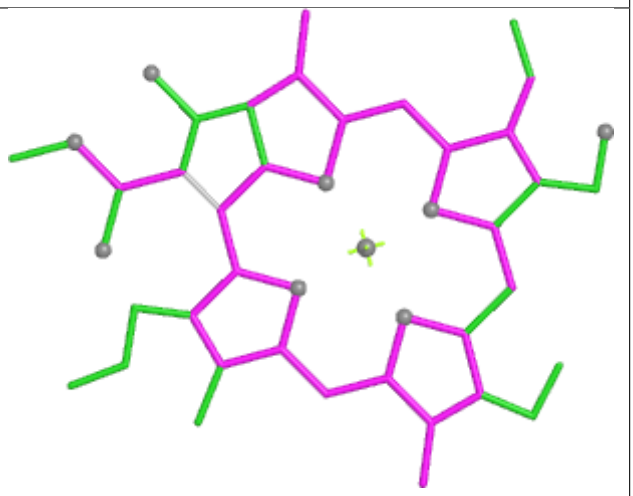

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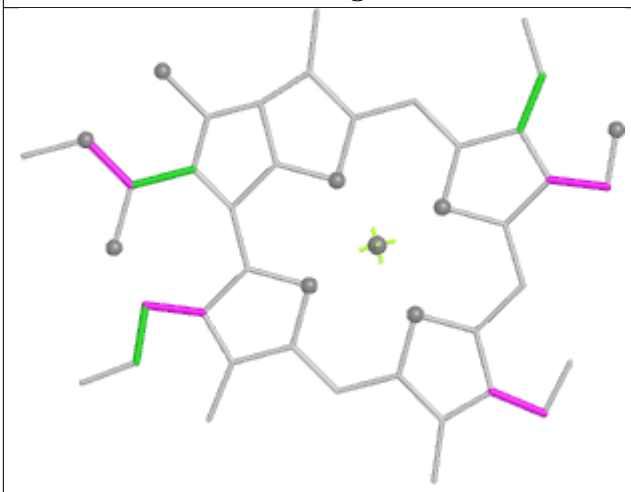
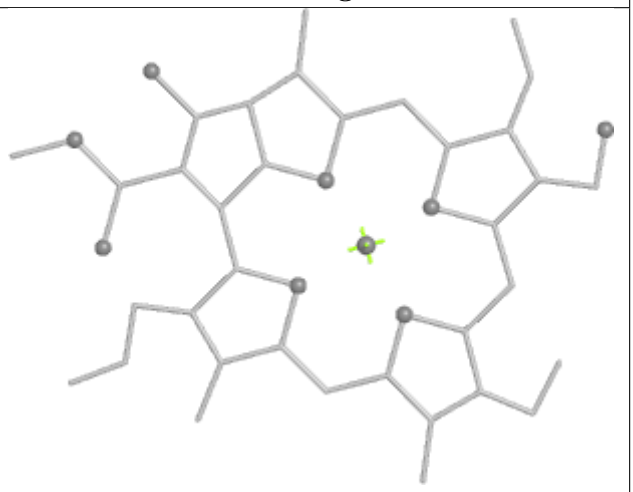
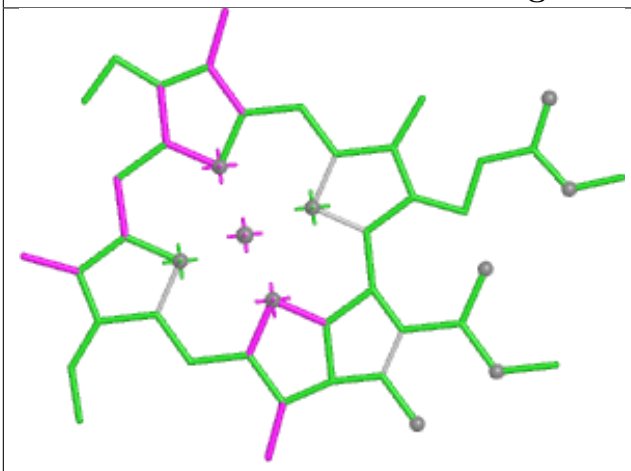


Torsions



Rings

Ligand CLA 2 302



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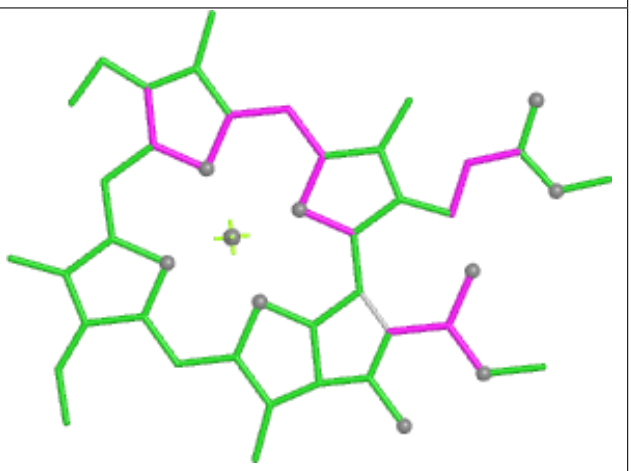

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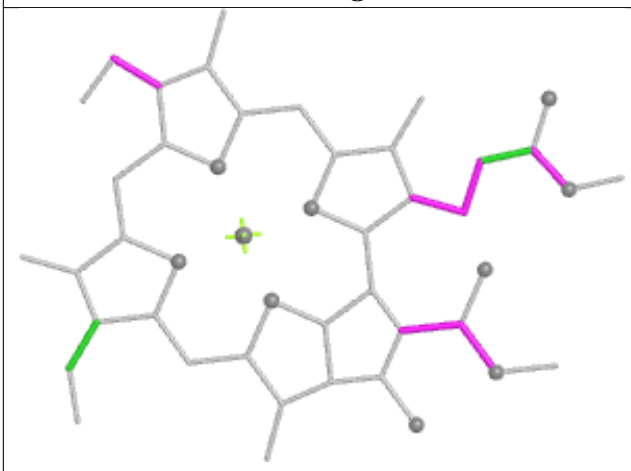

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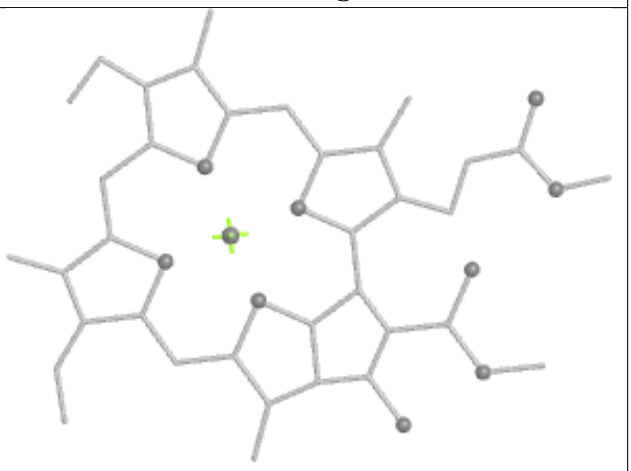
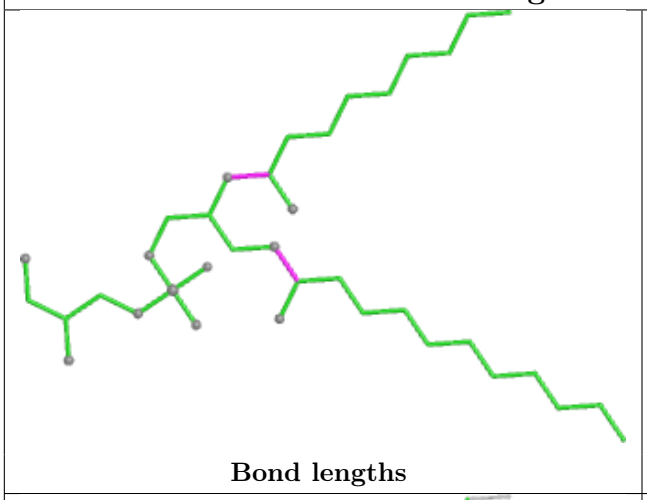


Rings

Ligand LHG 7 317



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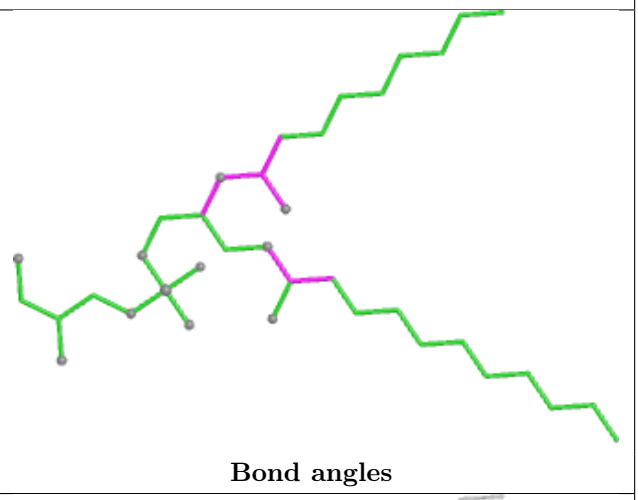

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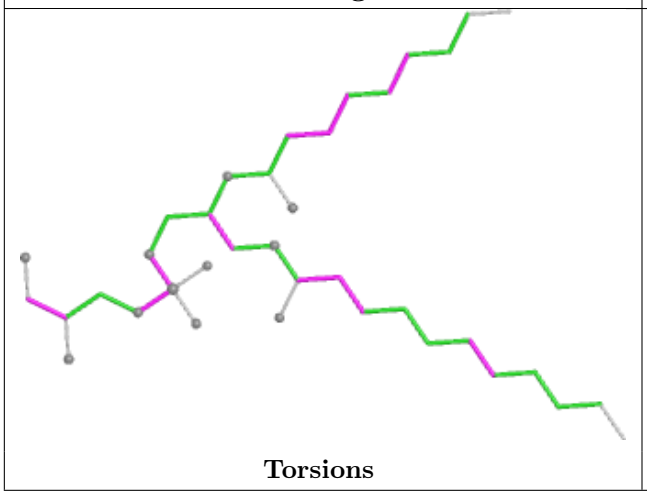

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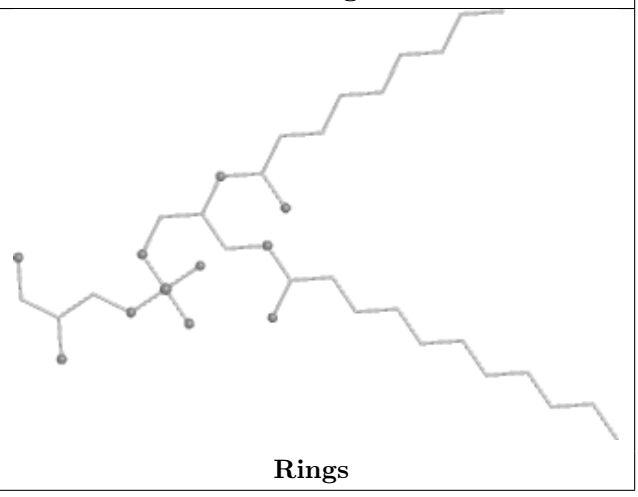
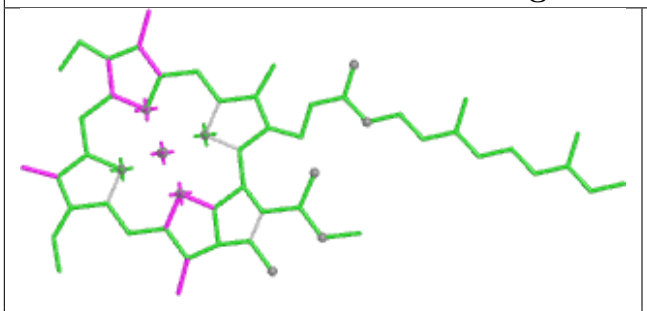


Rings

Ligand CLA 3 314



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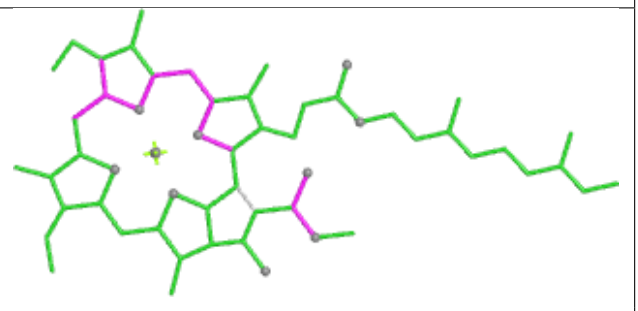
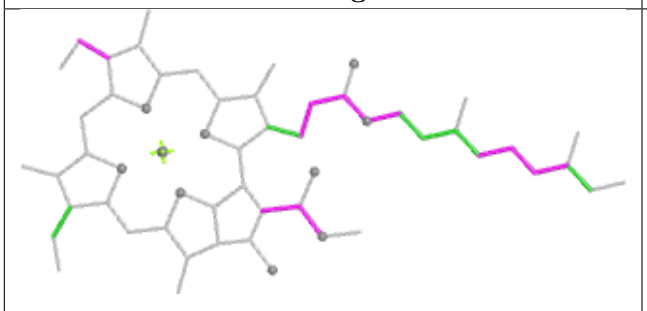


Bond angles



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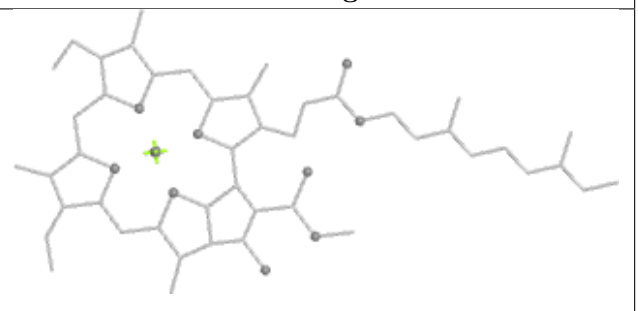
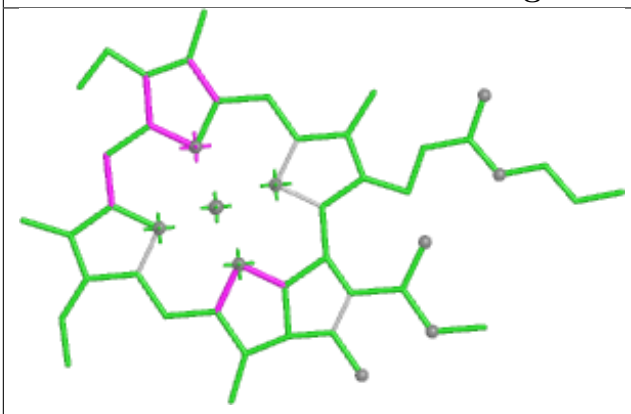


Rings

Ligand CLA R 614



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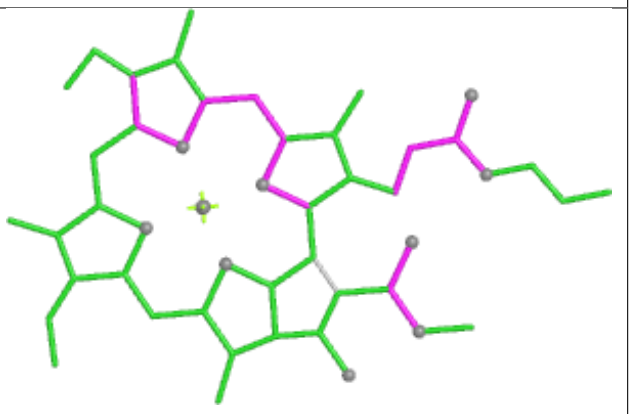
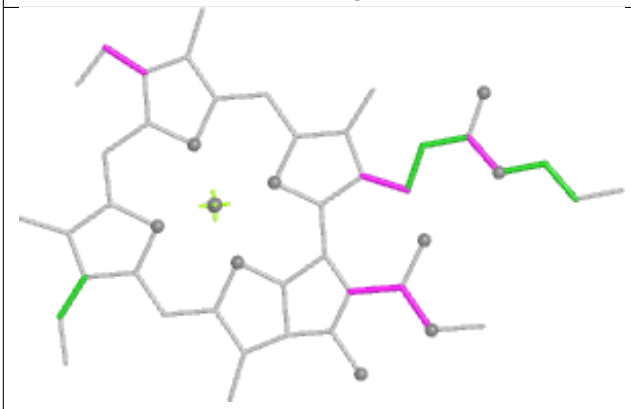


Bond angles



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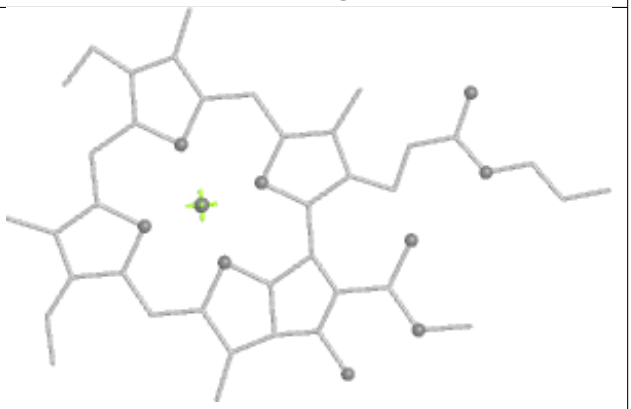
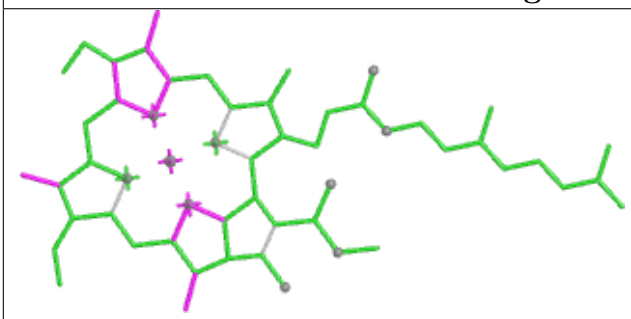


Rings

Ligand CLA A 824



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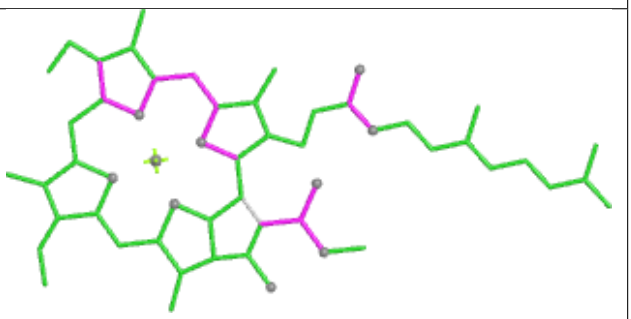

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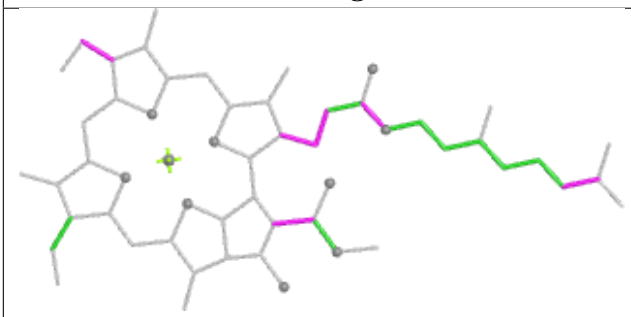

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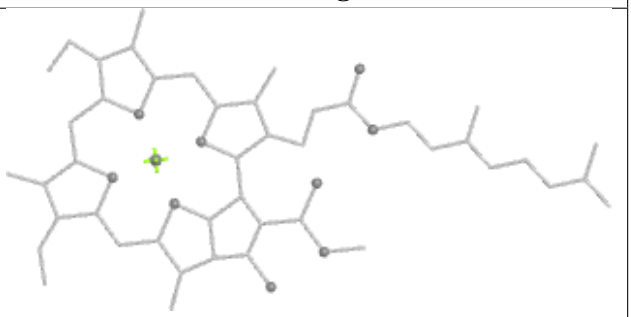
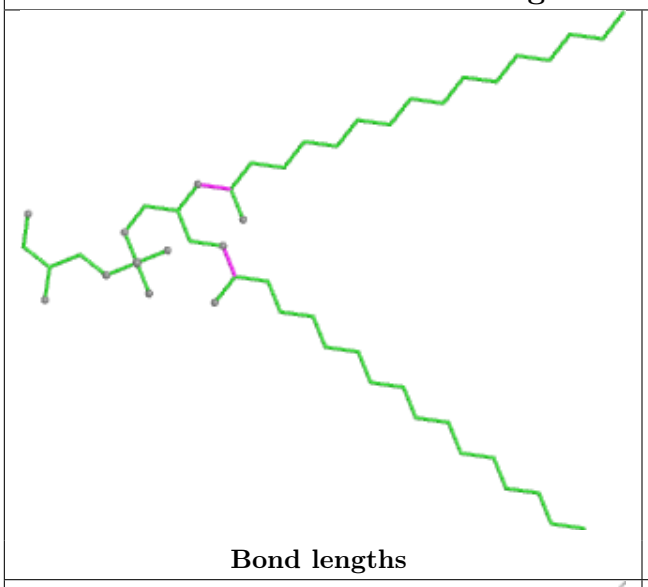


Rings

Ligand LHG 2 317



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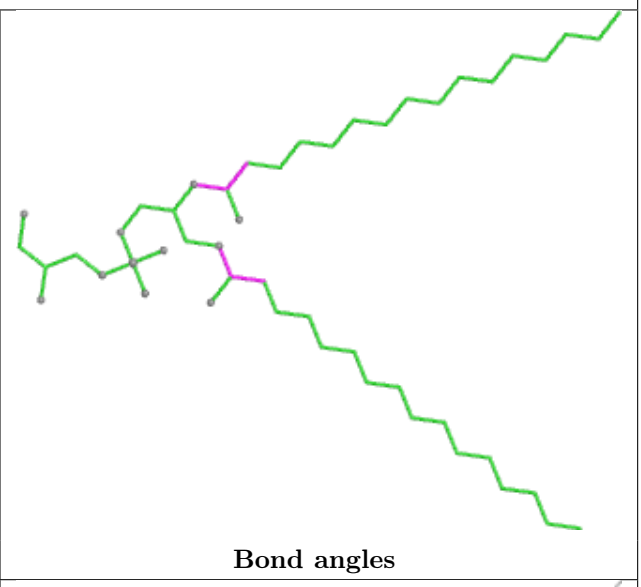

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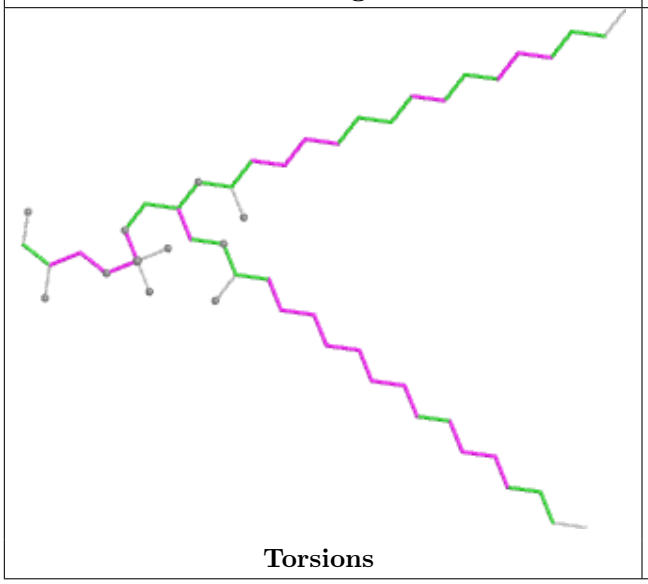

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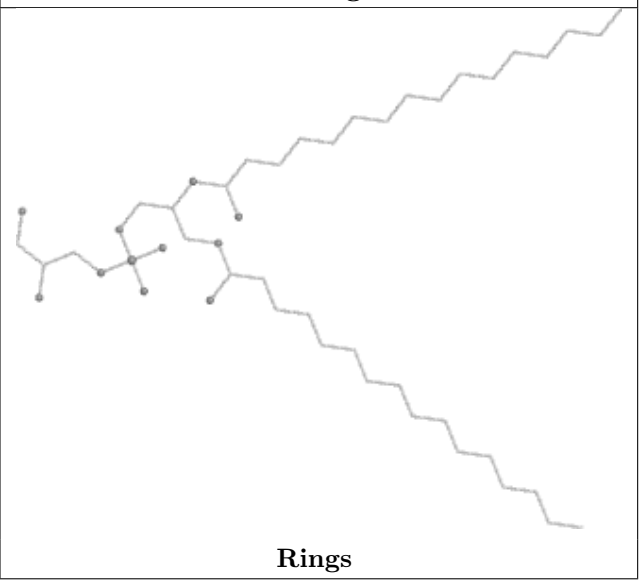
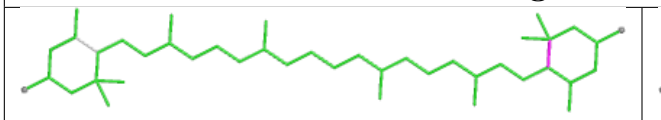


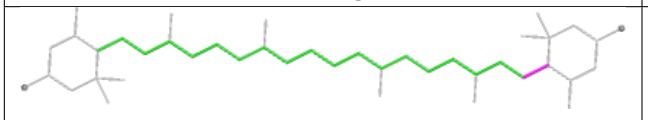
Rings

Ligand LUT 6 619



Bond lengths

Bond angles



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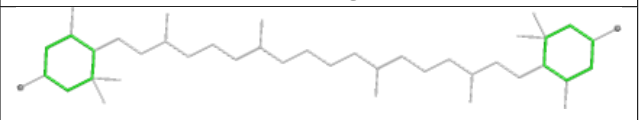
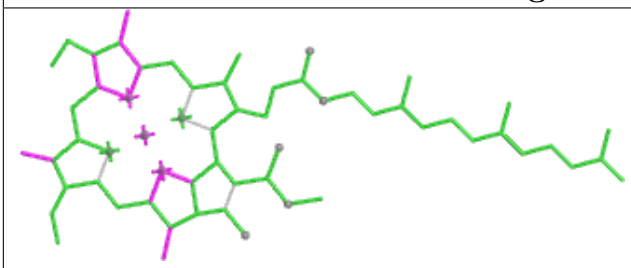


Rings

Ligand CLA 9 303



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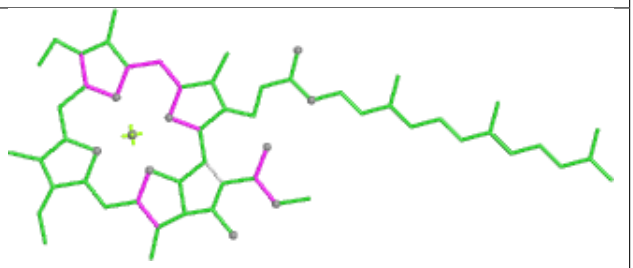
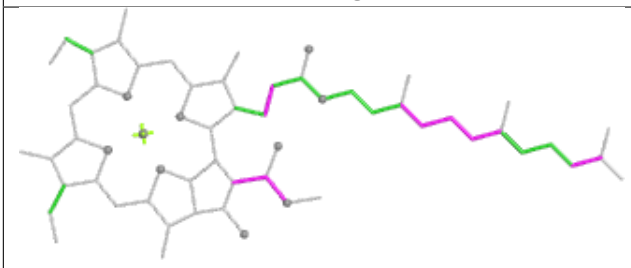


Bond angles



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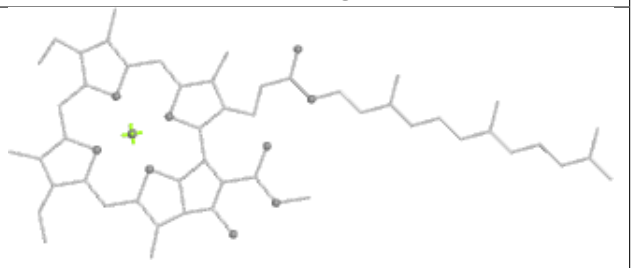
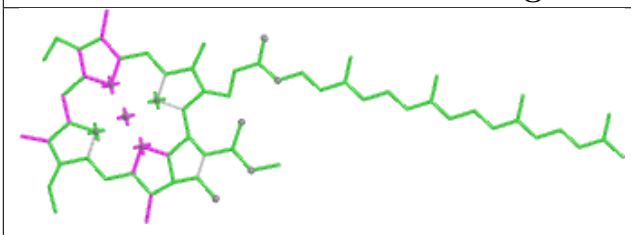


Rings

Ligand CLA B 838



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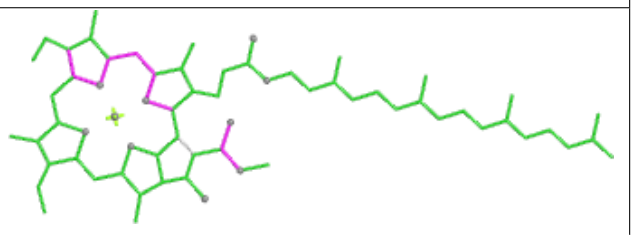
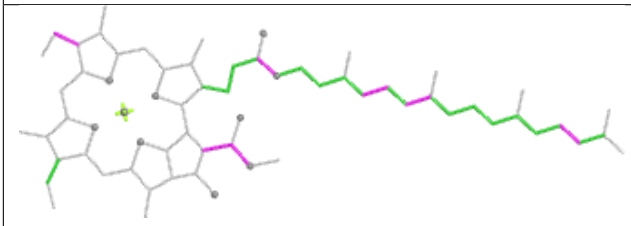
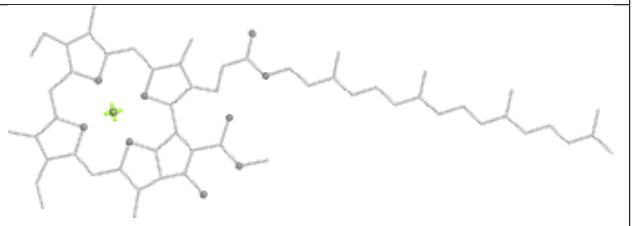


Bond angles

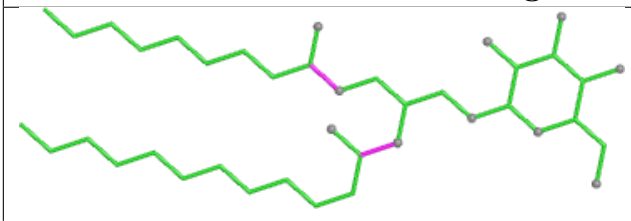


Torsions



Rings

Ligand LMG J 102



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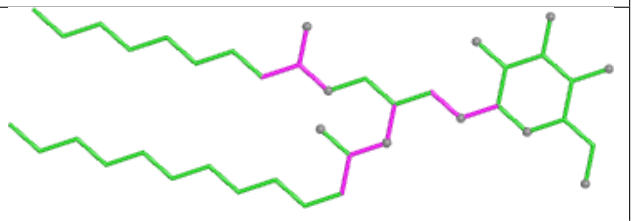
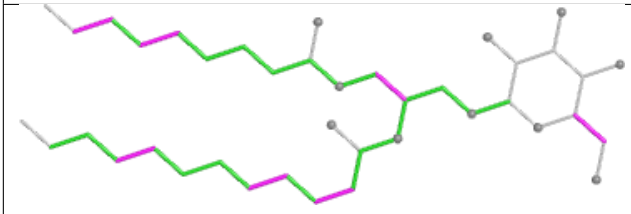


Bond angles



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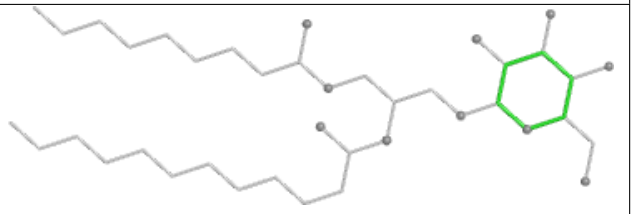
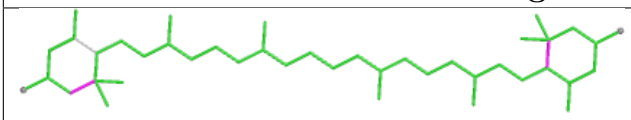


Rings

Ligand LUT 7 314



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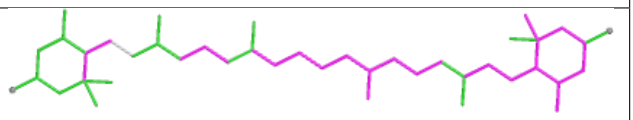
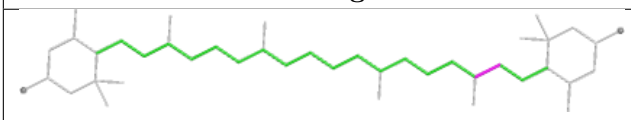


Bond angles



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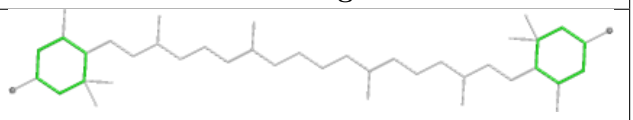
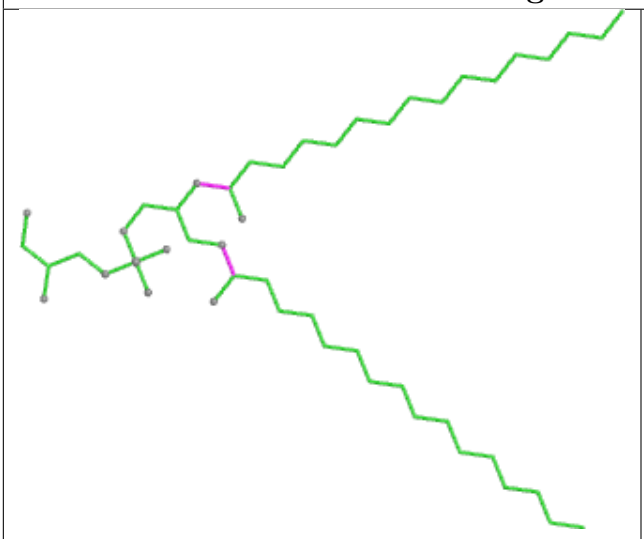


Rings

Ligand LHG 8 319



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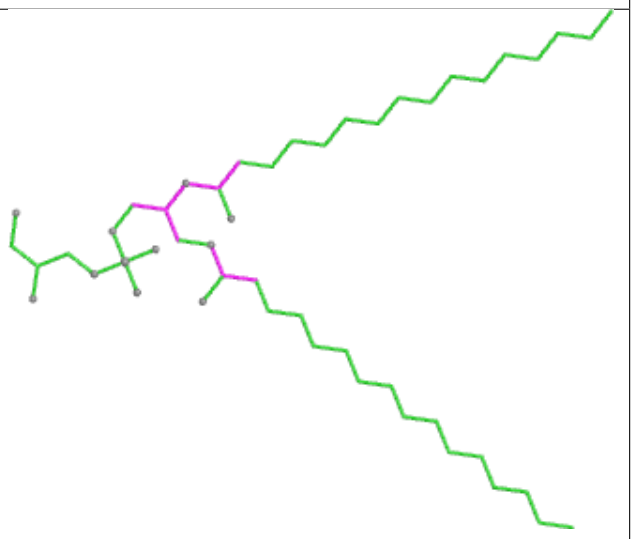
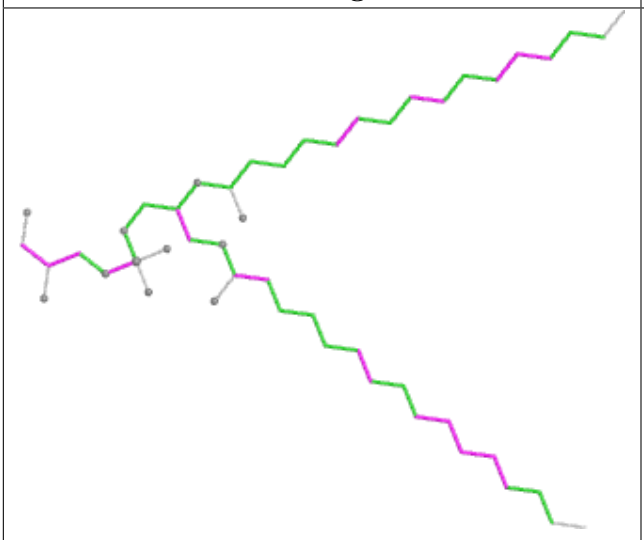
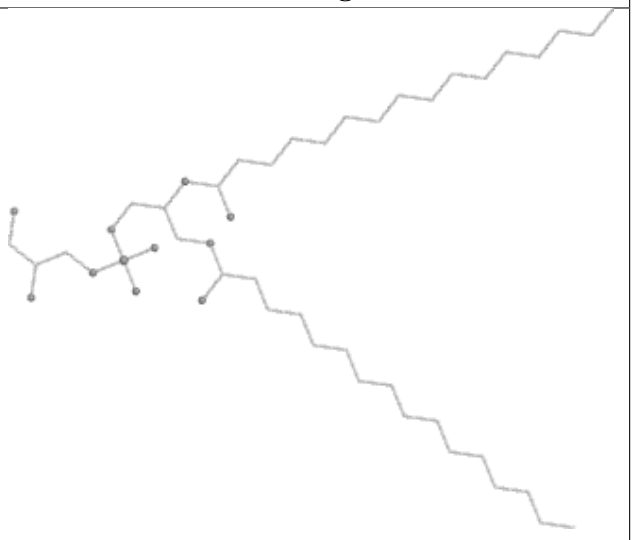


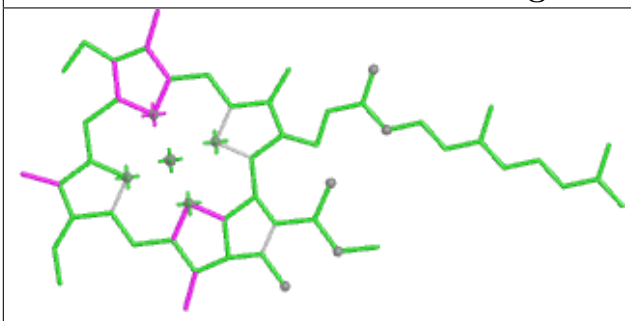
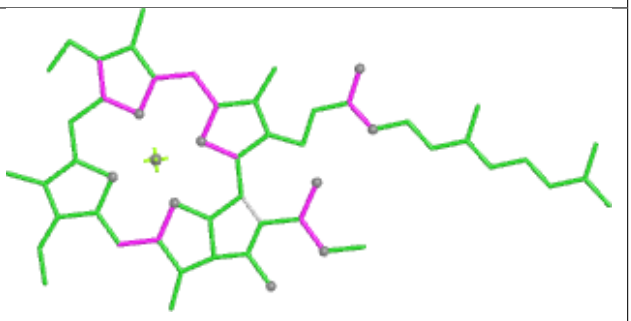
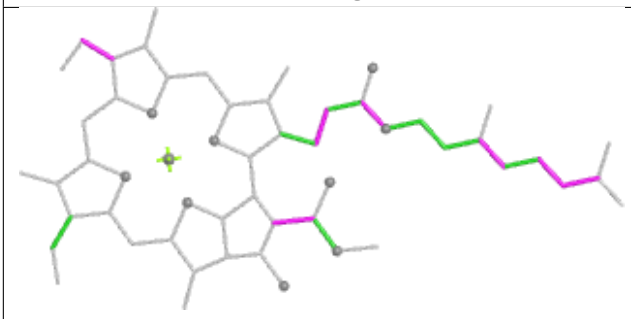
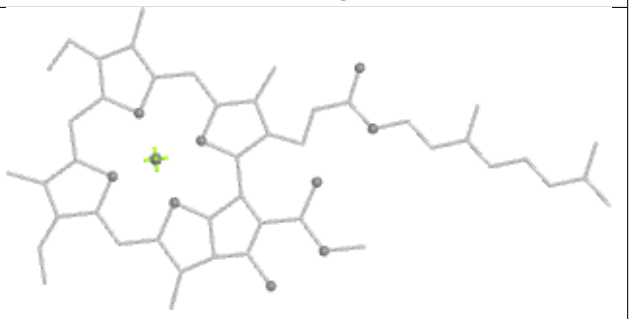
Bond angles

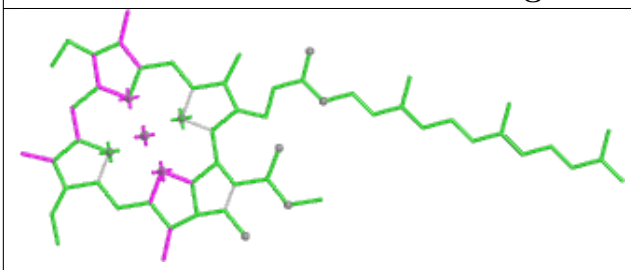
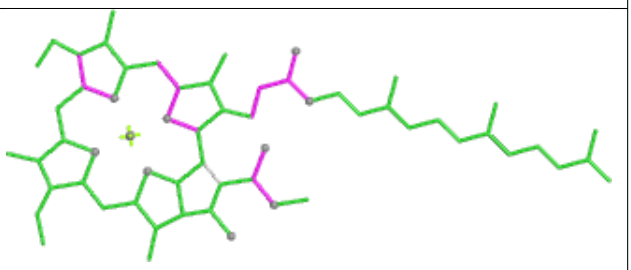
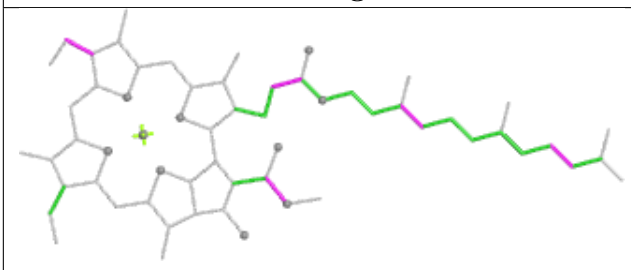
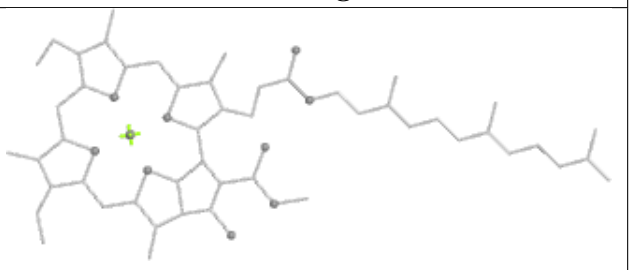


Torsions

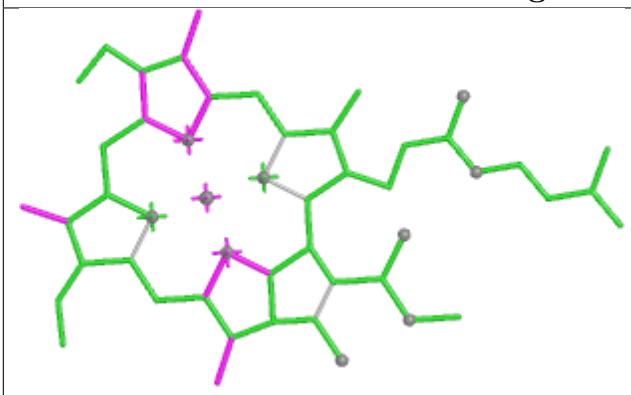


Rings

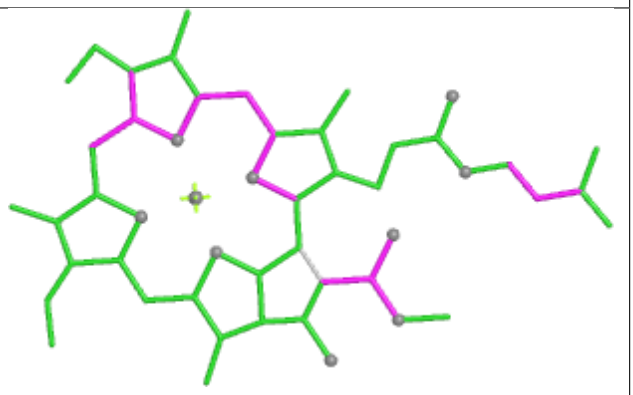
Ligand CLA 3 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

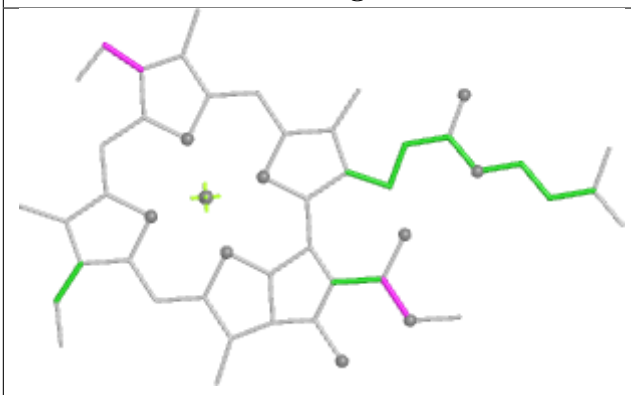
Ligand CLA 5 305



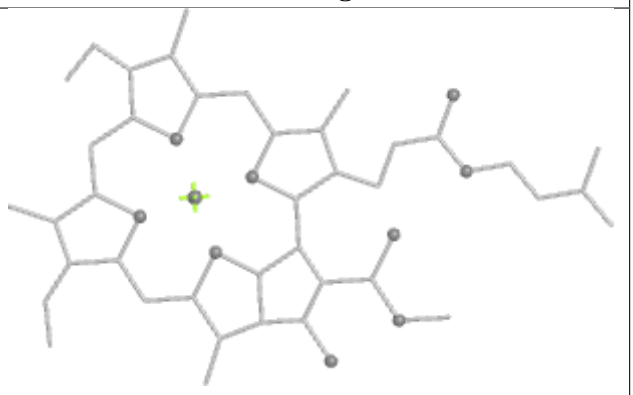
Bond lengths



Bond angles

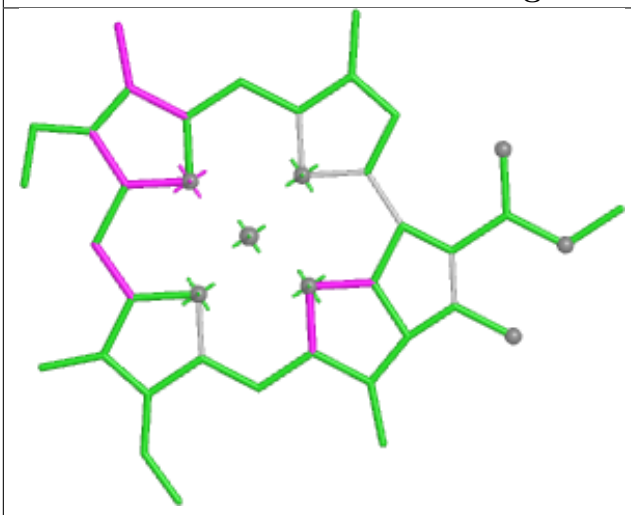


Torsions

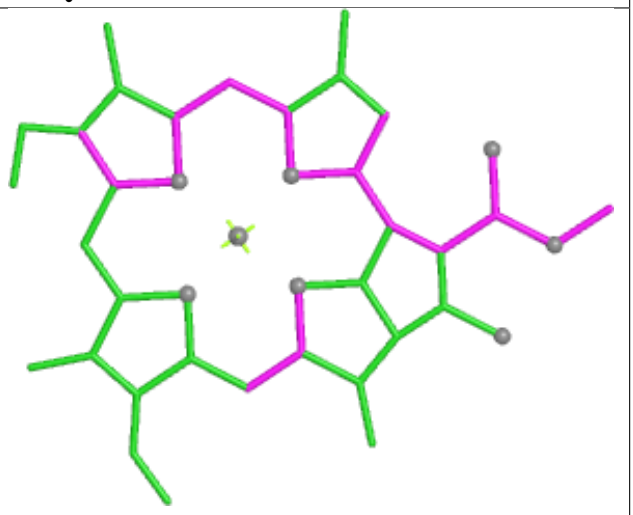


Rings

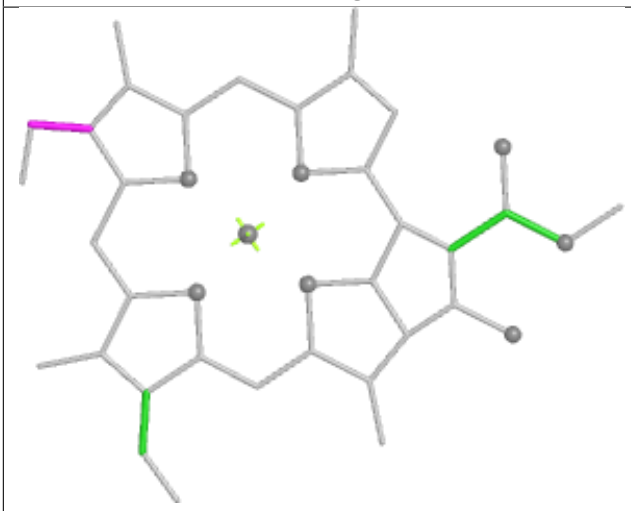
Ligand CLA Q 610



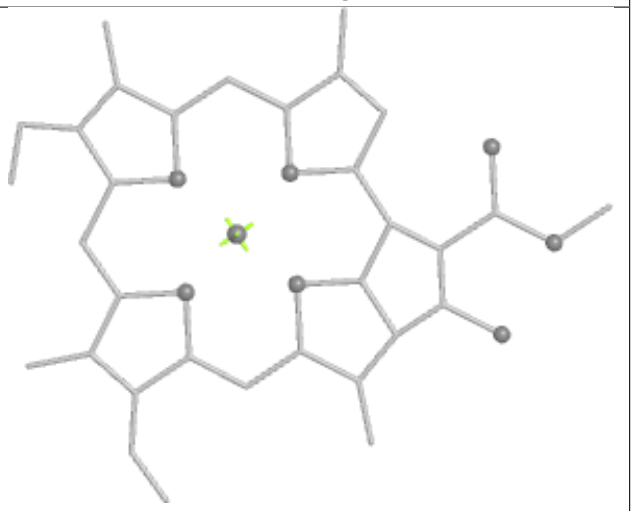
Bond lengths



Bond angles

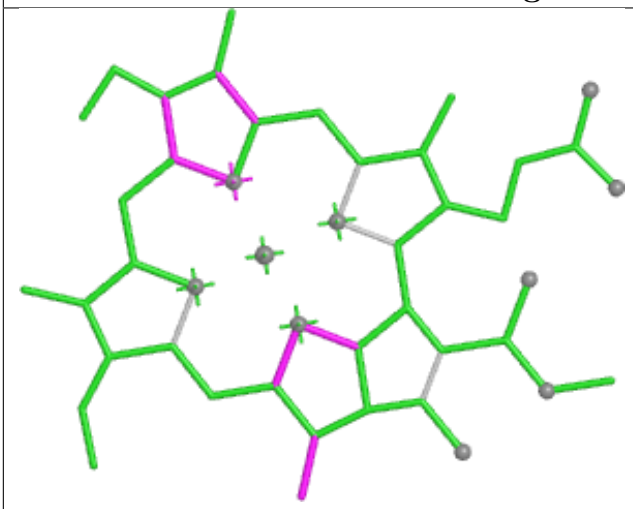


Torsions

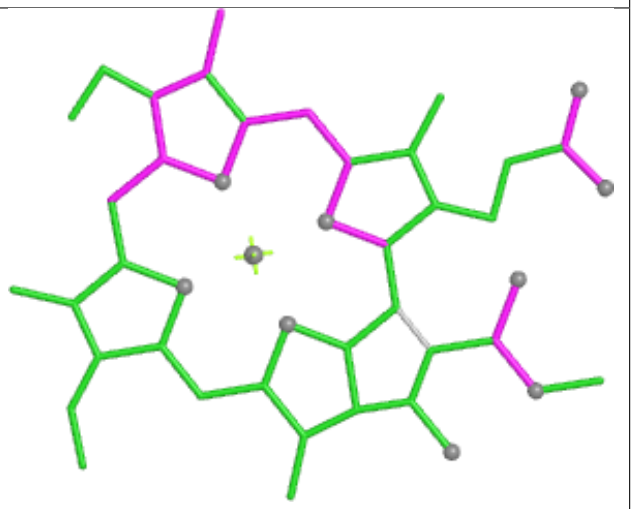


Rings

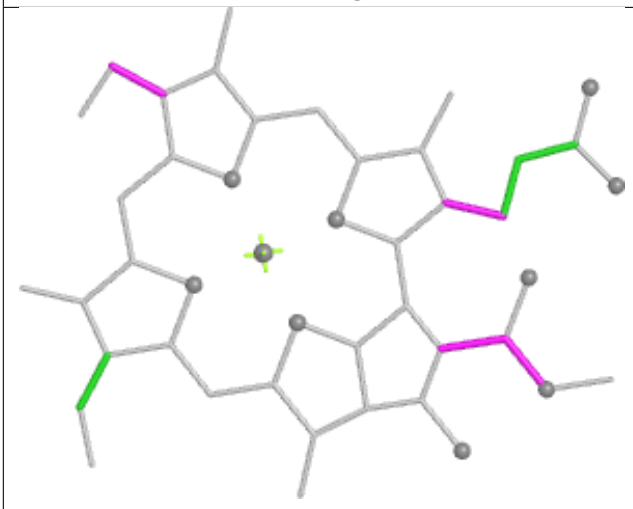
Ligand CLA U 313



Bond lengths



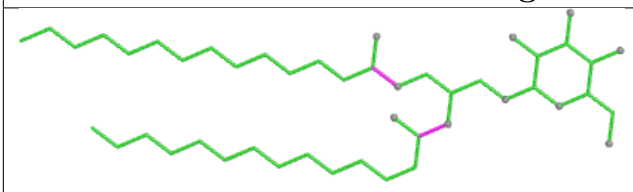
Bond angles



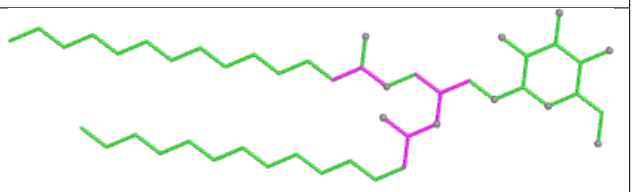
Torsions

Rings

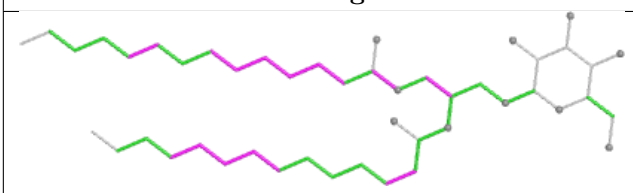
Ligand LMG H 204



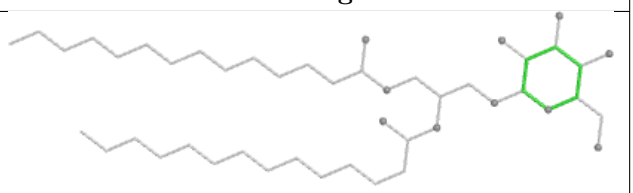
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

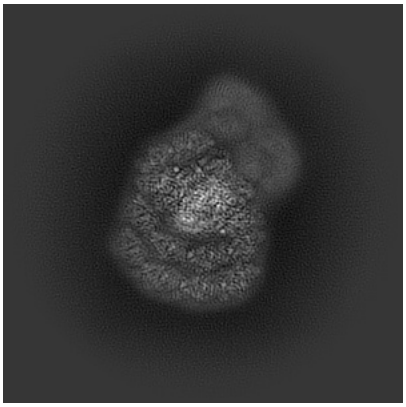
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30536. These allow visual inspection of the internal detail of the map and identification of artifacts.

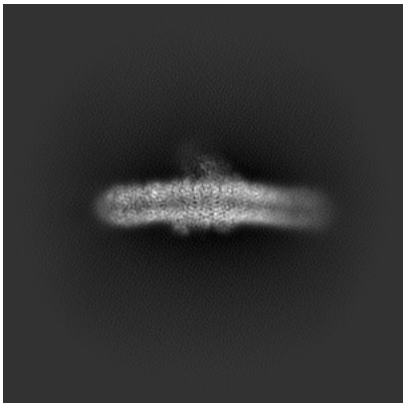
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

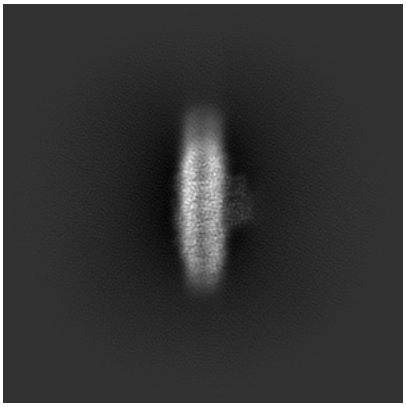
6.1.1 Primary map



X



Y

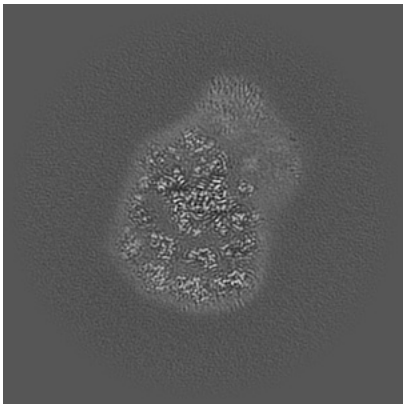


Z

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

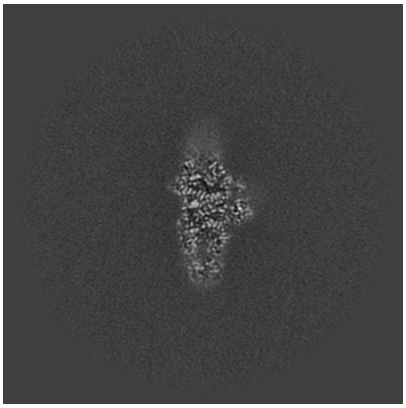
6.2 Central slices

6.2.1 Primary map



X Index: 180

Y Index: 180

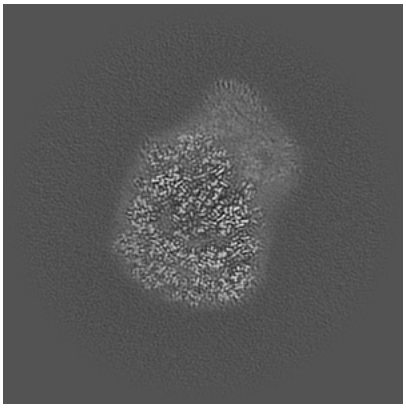


Z Index: 180

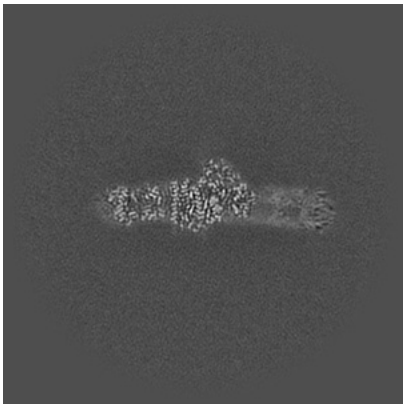
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

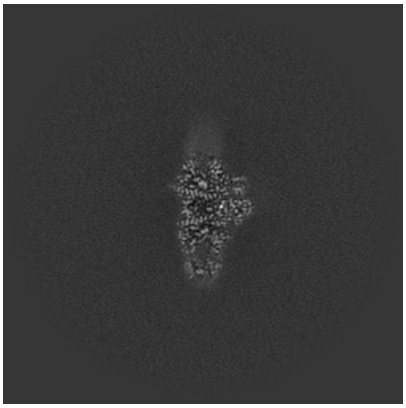
6.3.1 Primary map



X Index: 187



Y Index: 198

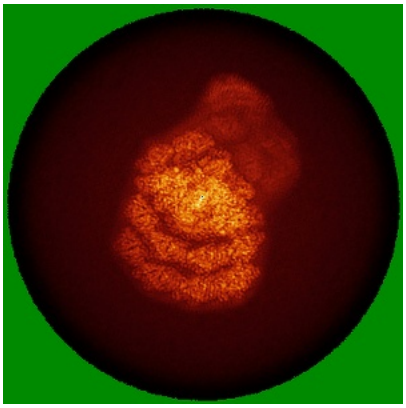


Z Index: 182

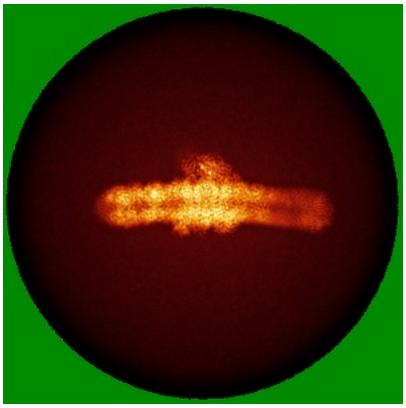
The images above show the largest variance slices of the map in three orthogonal directions.

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

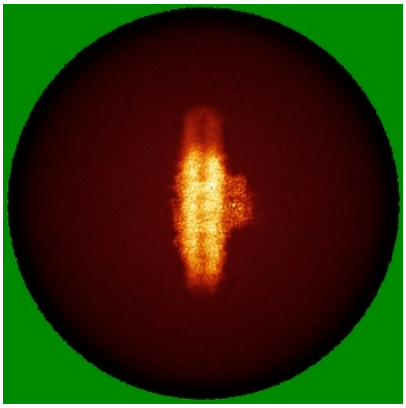
6.4.1 Primary map



X



Y

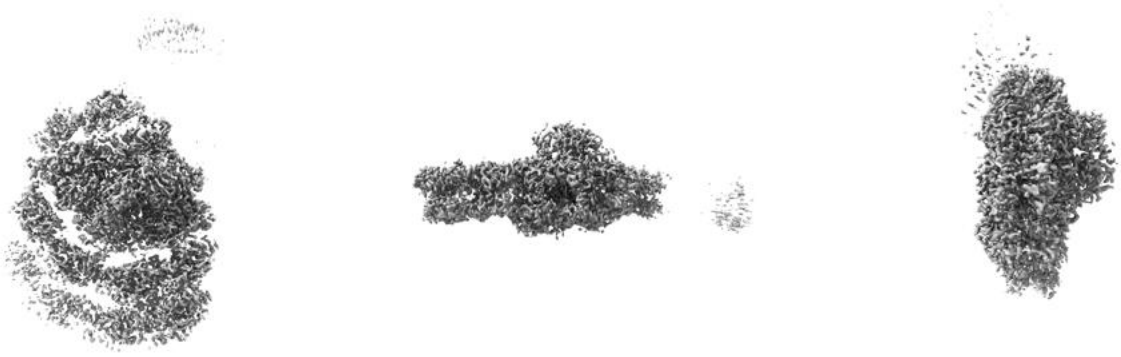


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

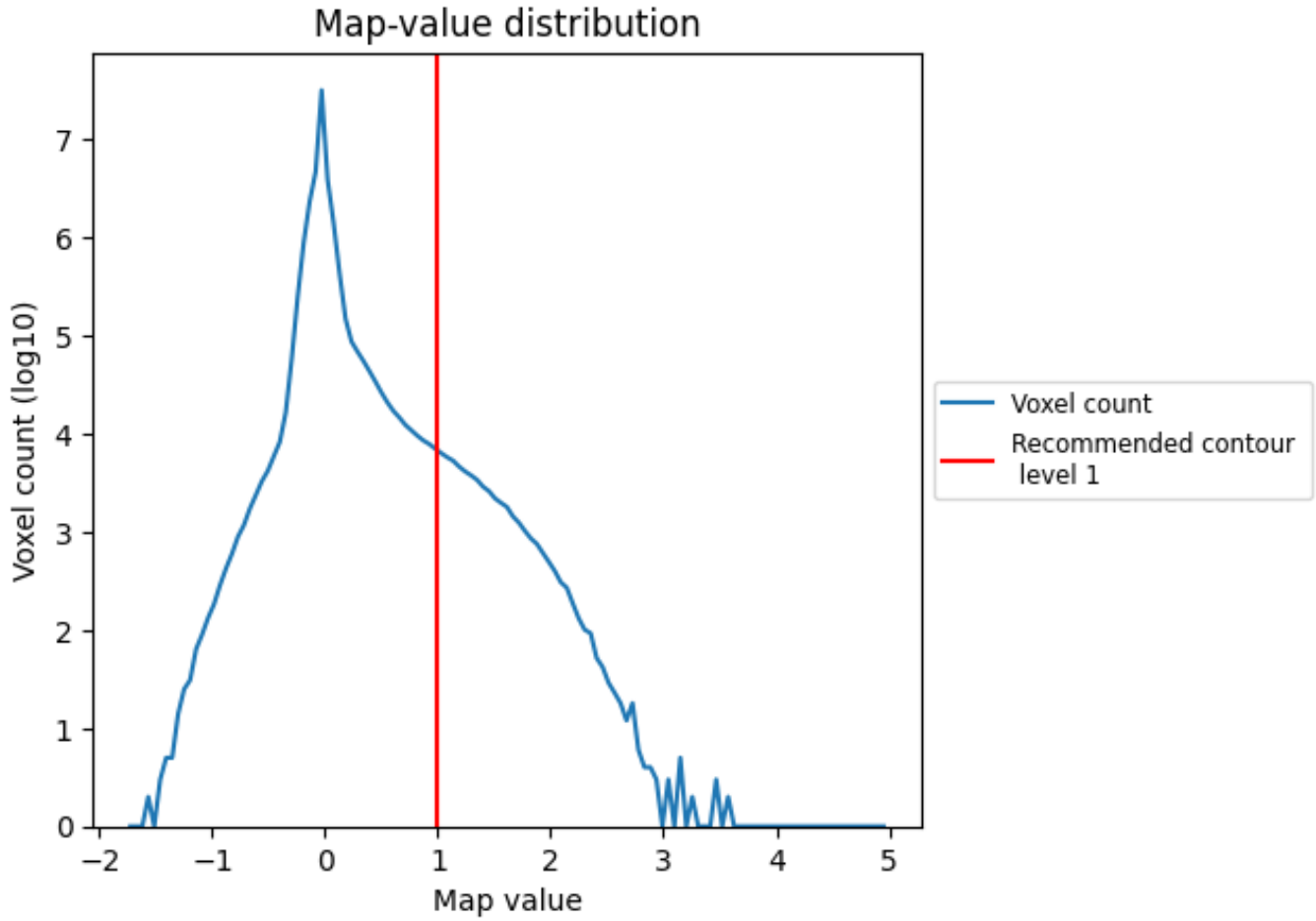
6.6 Mask visualisation (i)

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

7 Map analysis

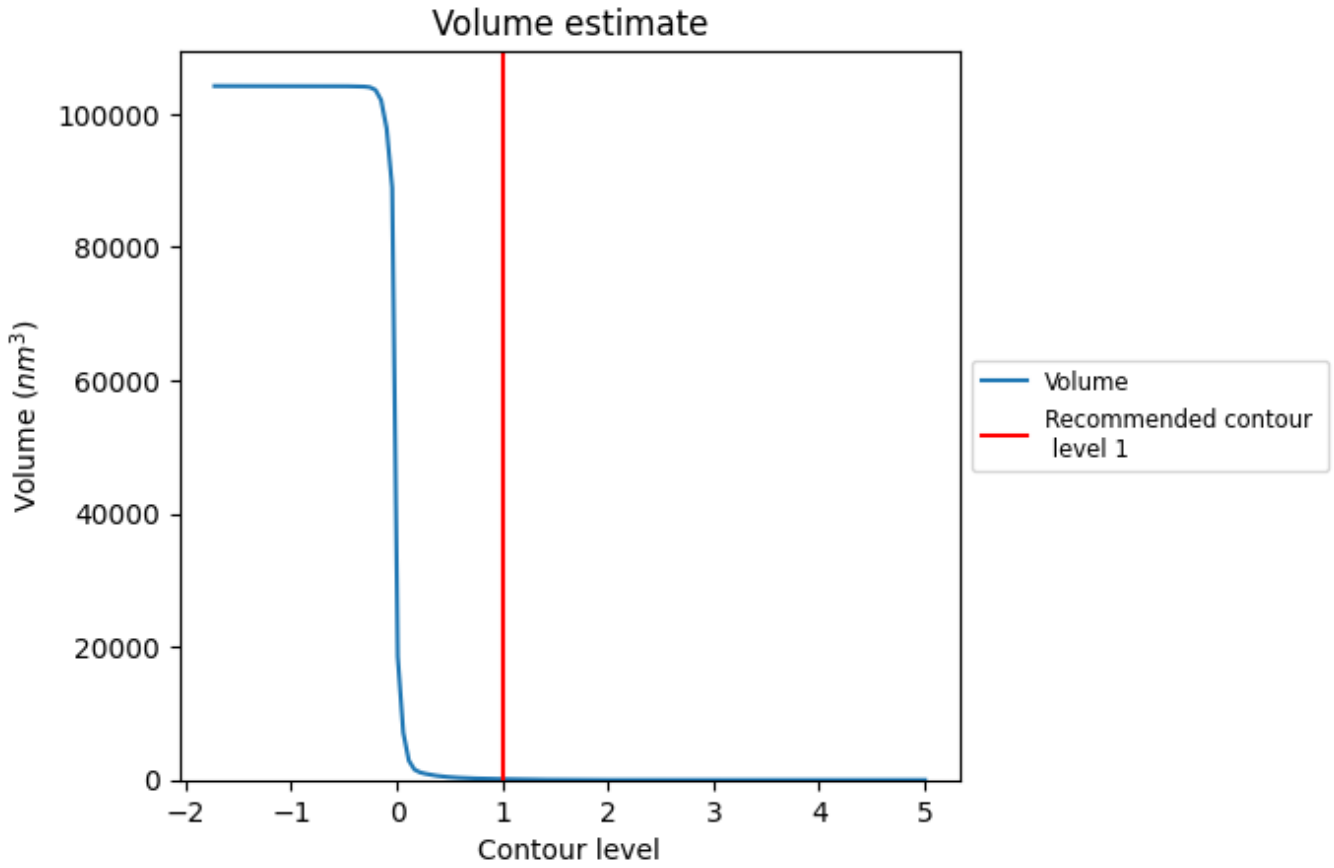
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

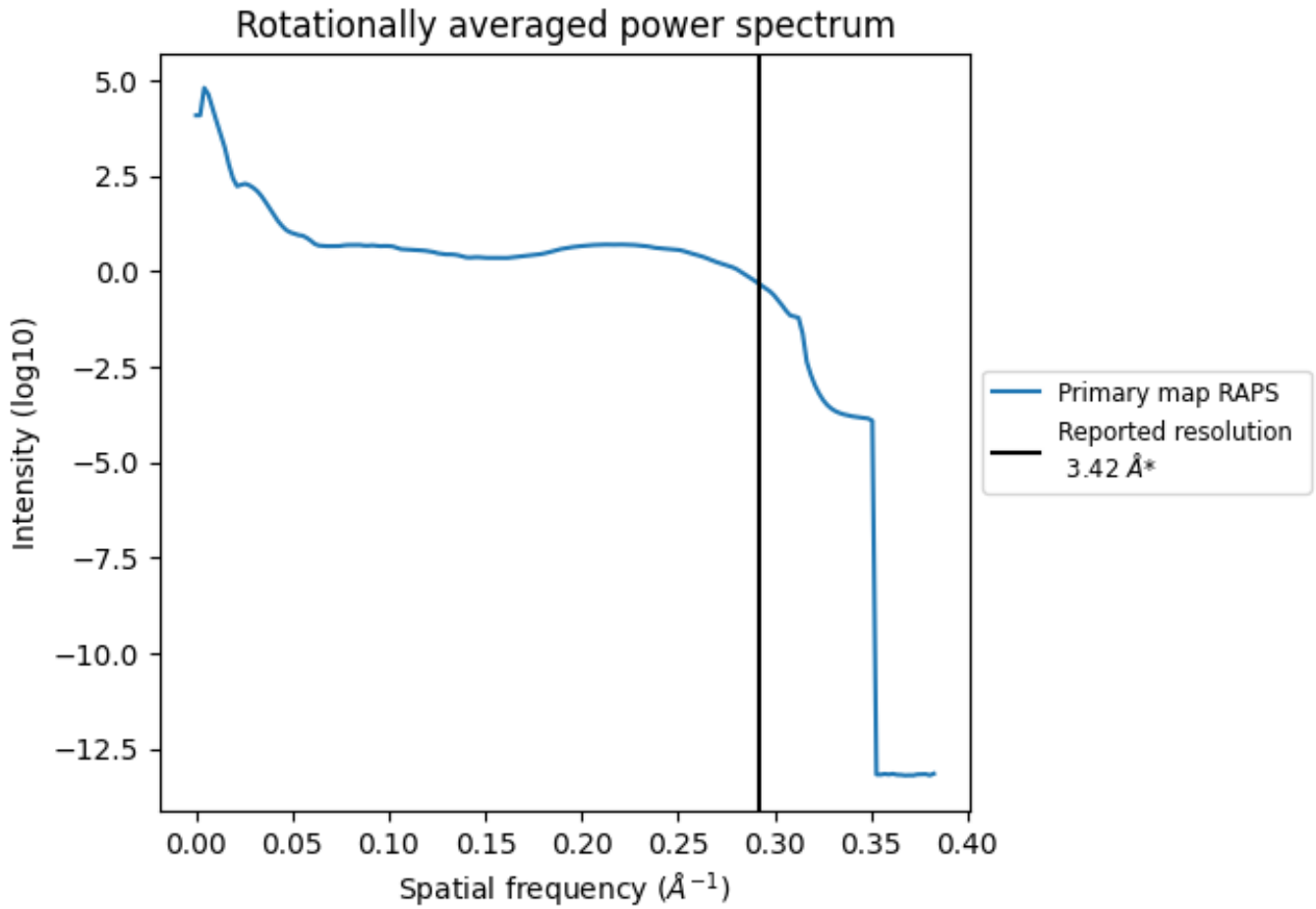
7.2 Volume estimate



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 115 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 0.292 $Å^{-1}$

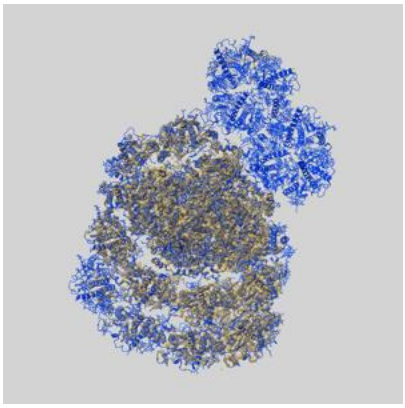
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

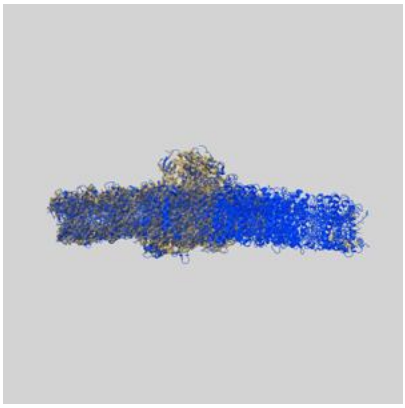
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30536 and PDB model 7D0J. Per-residue inclusion information can be found in section 3 on page 37.

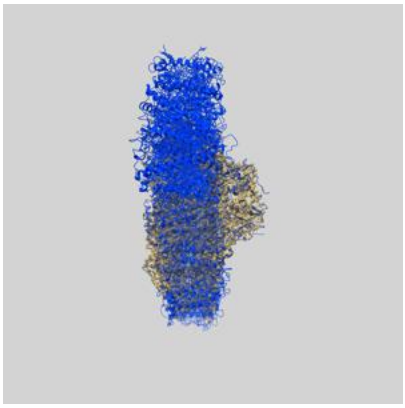
9.1 Map-model overlay



X



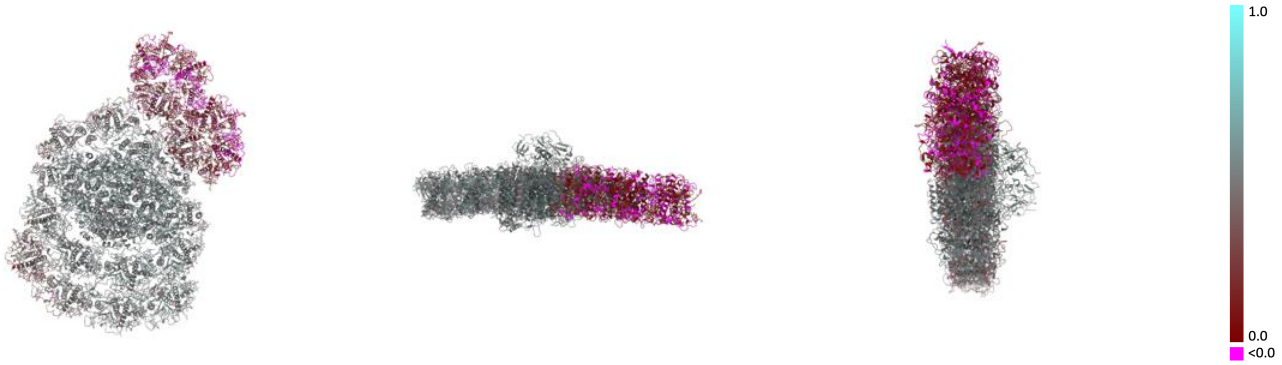
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

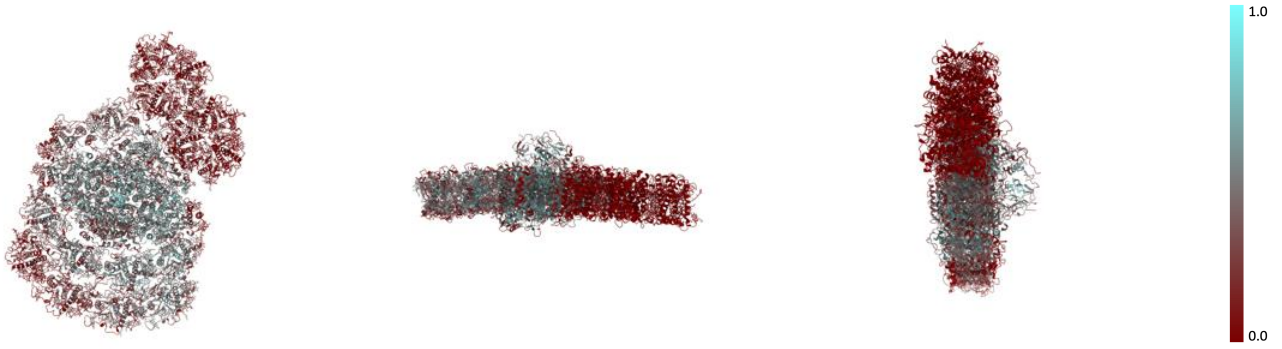
9.2 Q-score mapped to coordinate model



X Y Z

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

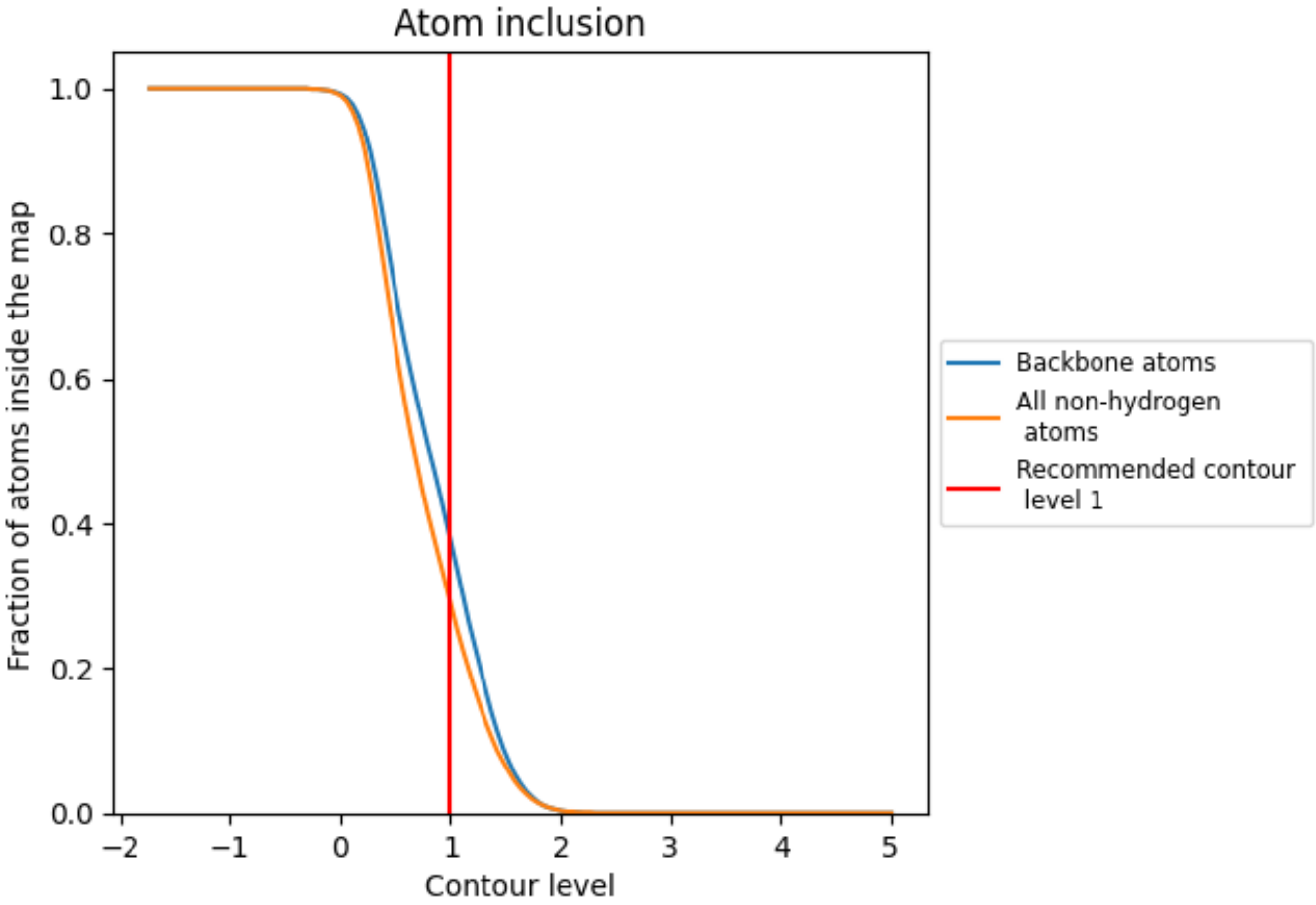
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2900	0.4070
1	0.3150	0.4760
2	0.2700	0.4450
3	0.4270	0.5110
4	0.1240	0.4380
5	0.3910	0.4980
6	0.2670	0.4690
7	0.4370	0.5110
8	0.3670	0.4930
9	0.2290	0.4440
A	0.5310	0.5300
B	0.5200	0.5290
C	0.5710	0.5210
D	0.3740	0.5140
E	0.3710	0.5020
F	0.2700	0.4750
G	0.1380	0.4410
H	0.3030	0.4750
I	0.4730	0.5110
J	0.2900	0.5190
K	0.1580	0.4560
L	0.4360	0.5030
O	0.3060	0.4670
P	0.0000	0.1620
Q	0.0020	0.0510
R	0.0050	0.0630
S	0.0030	0.2360
T	0.0000	0.1130
U	0.0000	0.1020
a	0.0570	0.3750