Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:29 PM UTC

PDB ID	:	9K1E / pdb_00009k1e
EMDB ID	:	EMD-61973
Title	:	Structural insights into photosystem I complex of Bryopsis corticulans
Authors	:	Liu, X.Y.; Wang, W.D.
Deposited on	:	2024-10-16
Resolution	:	2.68 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:

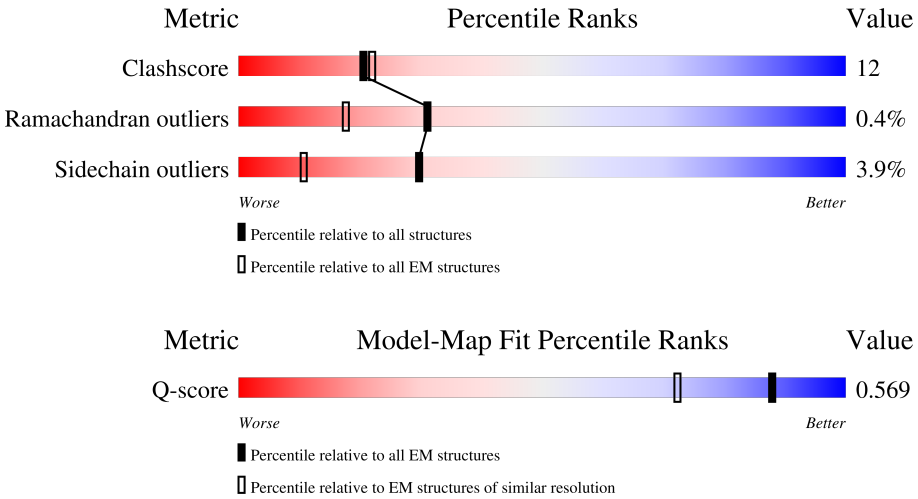
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

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 2.68 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	9255 (2.18 - 3.18)

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	0	245	9% 61% 24% • 13%
2	1	226	• 56% 28% • 14%
2	5	226	6% 62% 22% • 14%
3	2	256	70% 13% • 16%

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Mol	Chain	Length	Quality of chain
4	3	281	62% 18% 19%
5	6	267	69% 16% 14%
6	7	264	66% 19% 14%
7	4	248	48% 29% 6% 17%
7	8	248	59% 21% 17%
8	9	222	60% 18% 6% 15%
9	A	751	72% 26%
10	B	734	76% 23%
11	D	198	55% 17% 28%
12	E	91	62% 8% 30%
13	F	236	58% 11% 30%
14	G	167	36% 16% 44%
15	I	36	6% 67% 28%
16	J	41	63% 34%
17	L	204	9% 64% 15% 21%
18	C	81	77% 22%
19	K	123	55% 9% 35%
20	M	32	84% 12%
21	O	137	6% 57% 9% 33%
22	H	133	13% 59% 11% 29%

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
23	CHL	0	301	X	-	-	-
23	CHL	0	302	X	-	-	-
23	CHL	0	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHL	0	306	X	-	-	-
23	CHL	1	301	X	-	-	-
23	CHL	1	304	X	-	-	-
23	CHL	1	305	X	-	-	-
23	CHL	1	306	X	-	-	-
23	CHL	1	312	X	-	-	-
23	CHL	2	301	X	-	-	-
23	CHL	2	304	X	-	-	-
23	CHL	2	305	X	-	-	-
23	CHL	2	306	X	-	-	-
23	CHL	2	307	X	-	-	-
23	CHL	2	312	X	-	-	-
23	CHL	3	301	X	-	-	-
23	CHL	3	302	X	-	-	-
23	CHL	3	305	X	-	-	-
23	CHL	3	307	X	-	-	-
23	CHL	4	301	X	-	-	-
23	CHL	4	302	X	-	-	-
23	CHL	4	305	X	-	-	-
23	CHL	4	306	X	-	-	-
23	CHL	4	307	X	-	-	-
23	CHL	4	308	X	-	-	-
23	CHL	4	313	X	-	-	-
23	CHL	4	315	X	-	-	-
23	CHL	5	301	X	-	-	-
23	CHL	5	304	X	-	-	-
23	CHL	5	305	X	-	-	-
23	CHL	5	306	X	-	-	-
23	CHL	5	312	X	-	-	-
23	CHL	6	301	X	-	-	-
23	CHL	6	302	X	-	-	-
23	CHL	6	305	X	-	-	-
23	CHL	6	306	X	-	-	-
23	CHL	6	307	X	-	-	-
23	CHL	6	308	X	-	-	-
23	CHL	6	313	X	-	-	-
23	CHL	6	315	X	-	-	-
23	CHL	6	323	X	-	-	-
23	CHL	7	301	X	-	-	-
23	CHL	7	302	X	-	-	-
23	CHL	7	305	X	-	-	-
23	CHL	7	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHL	7	307	X	-	-	-
23	CHL	7	313	X	-	-	-
23	CHL	8	301	X	-	-	-
23	CHL	8	303	X	-	-	-
23	CHL	8	306	X	-	-	-
23	CHL	8	307	X	-	-	-
23	CHL	8	308	X	-	-	-
23	CHL	8	309	X	-	-	-
23	CHL	8	314	X	-	-	-
23	CHL	8	316	X	-	-	-
23	CHL	9	301	X	-	-	-
23	CHL	9	305	X	-	-	-
23	CHL	9	306	X	-	-	-
23	CHL	9	312	X	-	-	-
24	CLA	0	303	X	-	-	-
24	CLA	0	304	X	-	-	-
24	CLA	0	307	X	-	-	-
24	CLA	0	308	X	-	-	-
24	CLA	0	309	X	-	-	-
24	CLA	0	310	X	-	-	-
24	CLA	0	311	X	-	-	-
24	CLA	0	312	X	-	-	-
24	CLA	0	313	X	-	-	-
24	CLA	0	319	X	-	-	-
24	CLA	1	302	X	-	-	-
24	CLA	1	303	X	-	-	-
24	CLA	1	307	X	-	-	-
24	CLA	1	308	X	-	-	-
24	CLA	1	309	X	-	-	-
24	CLA	1	310	X	-	-	-
24	CLA	1	311	X	-	-	-
24	CLA	1	313	X	-	-	-
24	CLA	2	302	X	-	-	-
24	CLA	2	303	X	-	-	-
24	CLA	2	308	X	-	-	-
24	CLA	2	309	X	-	-	-
24	CLA	2	310	X	-	-	-
24	CLA	2	311	X	-	-	-
24	CLA	2	313	X	-	-	-
24	CLA	3	303	X	-	-	-
24	CLA	3	304	X	-	-	-
24	CLA	3	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	3	308	X	-	-	-
24	CLA	3	309	X	-	-	-
24	CLA	3	310	X	-	-	-
24	CLA	3	311	X	-	-	-
24	CLA	3	312	X	-	-	-
24	CLA	3	313	X	-	-	-
24	CLA	3	314	X	-	-	-
24	CLA	3	315	X	-	-	-
24	CLA	4	303	X	-	-	-
24	CLA	4	304	X	-	-	-
24	CLA	4	309	X	-	-	-
24	CLA	4	310	X	-	-	-
24	CLA	4	311	X	-	-	-
24	CLA	4	312	X	-	-	-
24	CLA	4	314	X	-	-	-
24	CLA	5	302	X	-	-	-
24	CLA	5	303	X	-	-	-
24	CLA	5	307	X	-	-	-
24	CLA	5	308	X	-	-	-
24	CLA	5	309	X	-	-	-
24	CLA	5	310	X	-	-	-
24	CLA	5	311	X	-	-	-
24	CLA	5	313	X	-	-	-
24	CLA	6	303	X	-	-	-
24	CLA	6	304	X	-	-	-
24	CLA	6	309	X	-	-	-
24	CLA	6	310	X	-	-	-
24	CLA	6	311	X	-	-	-
24	CLA	6	312	X	-	-	-
24	CLA	6	314	X	-	-	-
24	CLA	6	316	X	-	-	-
24	CLA	6	317	X	-	-	-
24	CLA	6	318	X	-	-	-
24	CLA	7	303	X	-	-	-
24	CLA	7	304	X	-	-	-
24	CLA	7	308	X	-	-	-
24	CLA	7	309	X	-	-	-
24	CLA	7	310	X	-	-	-
24	CLA	7	311	X	-	-	-
24	CLA	7	312	X	-	-	-
24	CLA	7	314	X	-	-	-
24	CLA	7	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	7	316	X	-	-	-
24	CLA	7	317	X	-	-	-
24	CLA	8	304	X	-	-	-
24	CLA	8	305	X	-	-	-
24	CLA	8	310	X	-	-	-
24	CLA	8	311	X	-	-	-
24	CLA	8	312	X	-	-	-
24	CLA	8	313	X	-	-	-
24	CLA	8	315	X	-	-	-
24	CLA	9	302	X	-	-	-
24	CLA	9	303	X	-	-	-
24	CLA	9	304	X	-	-	-
24	CLA	9	307	X	-	-	-
24	CLA	9	308	X	-	-	-
24	CLA	9	309	X	-	-	-
24	CLA	9	310	X	-	-	-
24	CLA	9	311	X	-	-	-
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	803	X	-	-	-
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	806	X	-	-	-
24	CLA	A	807	X	-	-	-
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	814	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	818	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	830	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	832	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	839	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	848	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	B	801	X	-	-	-
24	CLA	B	802	X	-	-	-
24	CLA	B	804	X	-	-	-
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	807	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	817	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	819	X	-	-	-
24	CLA	B	820	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	827	X	-	-	-
24	CLA	B	828	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	839	X	-	-	-
24	CLA	B	840	X	-	-	-
24	CLA	B	841	X	-	-	-
24	CLA	F	302	X	-	-	-
24	CLA	F	303	X	-	-	-
24	CLA	G	101	X	-	-	-
24	CLA	G	102	X	-	-	-
24	CLA	G	103	X	-	-	-
24	CLA	H	201	X	-	-	-
24	CLA	H	202	X	-	-	-
24	CLA	H	203	X	-	-	-
24	CLA	H	204	X	-	-	-
24	CLA	H	205	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	K	101	X	-	-	-
24	CLA	K	102	X	-	-	-
24	CLA	K	103	X	-	-	-
24	CLA	K	104	X	-	-	-
24	CLA	L	201	X	-	-	-
24	CLA	L	202	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	206	X	-	-	-
24	CLA	O	201	X	-	-	-
24	CLA	O	204	X	-	-	-
24	CLA	O	205	X	-	-	-
24	CLA	O	206	X	-	-	-
24	CLA	O	209	X	-	-	-
32	CL0	A	852	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 54077 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	213	Total	C	N	O	S	0	0
			1640	1063	270	296	11		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	195	Total	C	N	O	S	0	0
			1478	950	243	273	12		
2	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	216	Total	C	N	O	S	0	0
			1667	1082	269	304	12		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	228	Total	C	N	O	S	0	0
			1768	1141	288	329	10		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		
7	4	207	Total	C	N	O	S	0	0
			1569	1030	257	273	9		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	189	Total	C	N	O	S	0	0
			1453	932	245	267	9		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	746	Total	C	N	O	S	0	0
			5872	3836	998	1016	22		

- Molecule 10 is a protein called photosystem I.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	733	Total	C	N	O	S	0	0
			5824	3824	979	1002	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	142	Total	C	N	O	S	0	0
			1109	709	193	202	5		

- Molecule 12 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	64	Total	C	N	O	S	0	0
			509	323	90	95	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	165	Total	C	N	O	S	0	0
			1273	810	224	235	4		

- Molecule 14 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	G	93	Total	C	N	O	0	0
			726	471	119	136		

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			262	180	37	43	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	162	Total	C	N	O	S	0	0
			1195	773	192	226	4		

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C	80	Total	C	N	O	S	0	0
			602	370	105	116	11		

- Molecule 19 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	31	Total	C	N	O	0	0
			238	158	37	43		

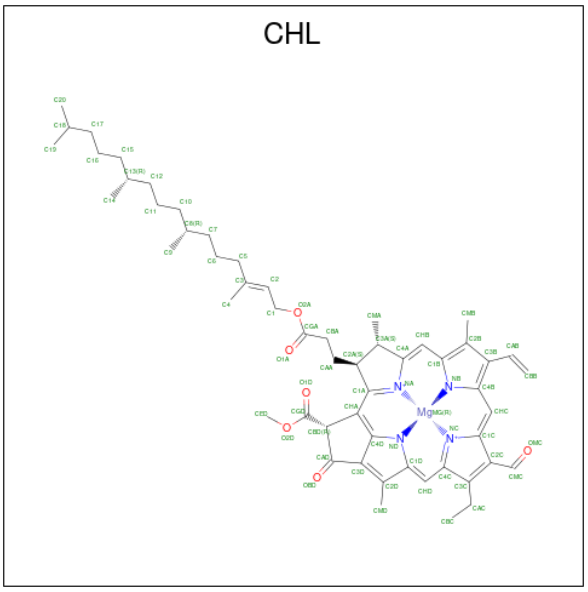
- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			728	488	116	120	4		

- Molecule 22 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	94	Total	C	N	O	S	0	0
			717	451	126	139	1		

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	0	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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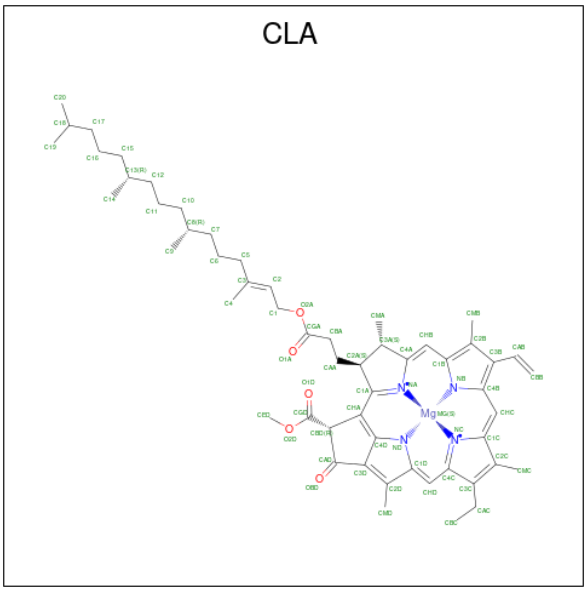
Mol	Chain	Residues	Atoms					AltConf
23	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	0	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
24	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
24	L	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
24	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
24	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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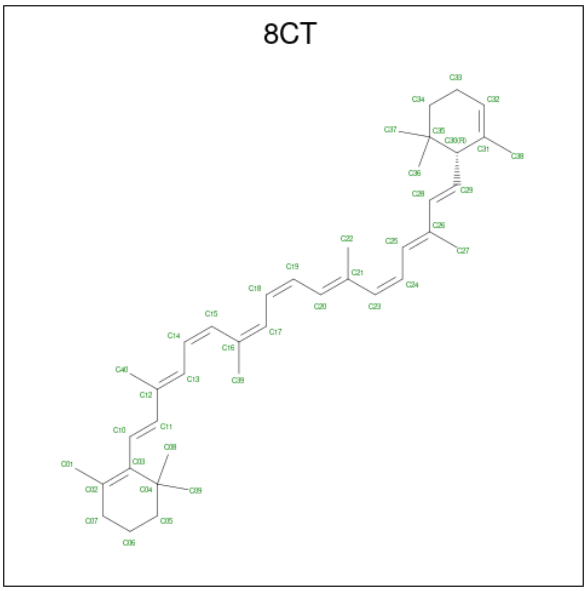
Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
25	0	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	9	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0

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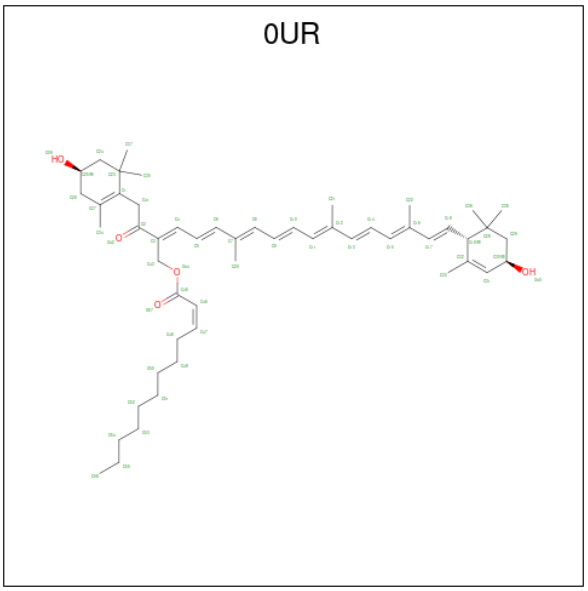
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	4	1	Total C 40 40	0

- Molecule 26 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	0	1	Total C O 52 47 5	0
26	0	1	Total C O 52 47 5	0
26	1	1	Total C O 52 47 5	0
26	1	1	Total C O 52 47 5	0
26	2	1	Total C O 51 46 5	0
26	2	1	Total C O 50 45 5	0
26	3	1	Total C O 51 46 5	0
26	5	1	Total C O 51 46 5	0
26	5	1	Total C O 52 47 5	0
26	6	1	Total C O 51 46 5	0
26	6	1	Total C O 52 47 5	0
26	7	1	Total C O 51 46 5	0
26	8	1	Total C O 51 46 5	0
26	8	1	Total C O 52 47 5	0

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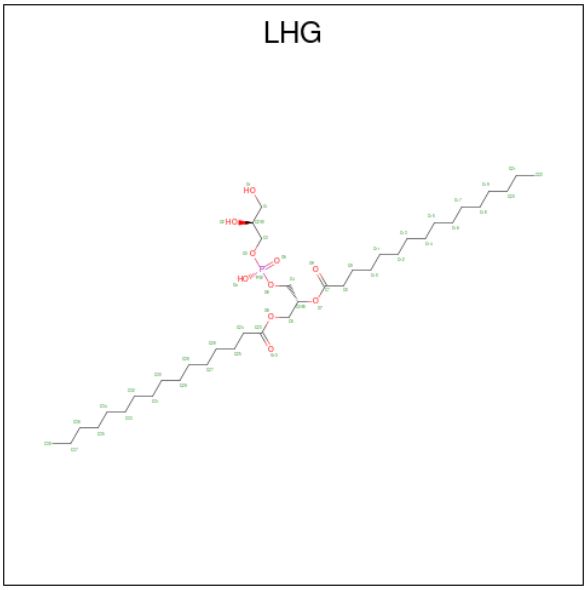
Mol	Chain	Residues	Atoms	AltConf
26	9	1	Total C O 52 47 5	0
26	9	1	Total C O 52 47 5	0
26	O	1	Total C O 52 47 5	0
26	4	1	Total C O 51 46 5	0
26	4	1	Total C O 50 45 5	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
27	0	1	Total C O P 49 38 10 1	0
27	1	1	Total C O P 49 38 10 1	0
27	1	1	Total C O P 43 32 10 1	0
27	2	1	Total C O P 32 21 10 1	0
27	2	1	Total C O P 32 21 10 1	0
27	3	1	Total C O P 36 25 10 1	0

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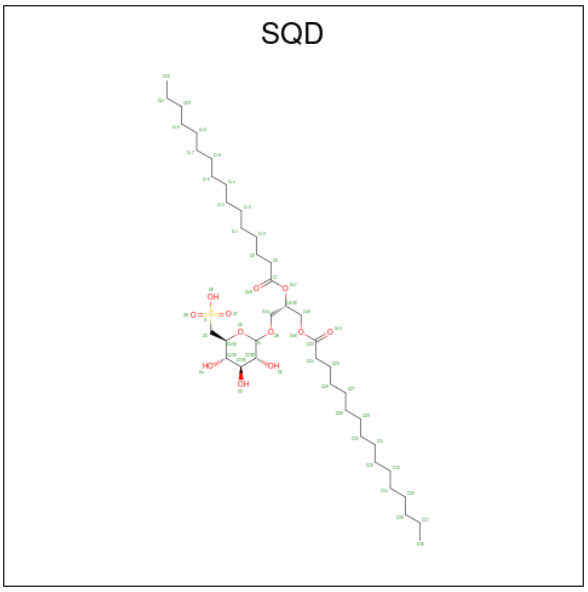
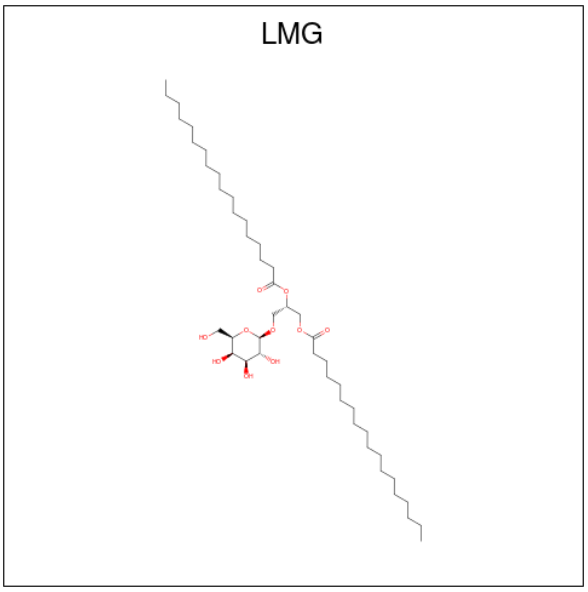
Mol	Chain	Residues	Atoms				AltConf
27	3	1	Total	C	O	P	0
			37	26	10	1	
27	3	1	Total	C	O	P	0
			43	34	8	1	
27	5	1	Total	C	O	P	0
			37	26	10	1	
27	6	1	Total	C	O	P	0
			37	26	10	1	
27	7	1	Total	C	O	P	0
			30	19	10	1	
27	7	1	Total	C	O	P	0
			38	27	10	1	
27	7	1	Total	C	O	P	0
			39	28	10	1	
27	8	1	Total	C	O	P	0
			31	20	10	1	
27	8	1	Total	C	O	P	0
			44	33	10	1	
27	9	1	Total	C	O	P	0
			47	36	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			27	16	10	1	
27	A	1	Total	C	O	P	0
			42	31	10	1	
27	B	1	Total	C	O	P	0
			23	12	10	1	
27	B	1	Total	C	O	P	0
			38	27	10	1	
27	I	1	Total	C	O	P	0
			46	35	10	1	
27	L	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	0	1	Total	C	O	S	0
			36	26	9	1	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			36	26	10	
29	3	1	Total	C	O	0
			36	26	10	

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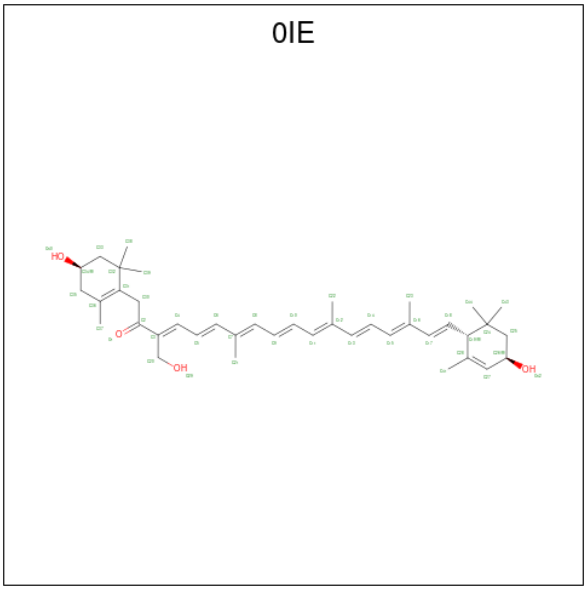
Mol	Chain	Residues	Atoms	AltConf
29	9	1	Total C O 55 45 10	0
29	A	1	Total C O 36 26 10	0
29	A	1	Total C O 37 27 10	0
29	J	1	Total C O 29 19 10	0
29	J	1	Total C O 46 36 10	0
29	M	1	Total C O 42 32 10	0
29	O	1	Total C O 31 21 10	0
29	O	1	Total C O 39 29 10	0

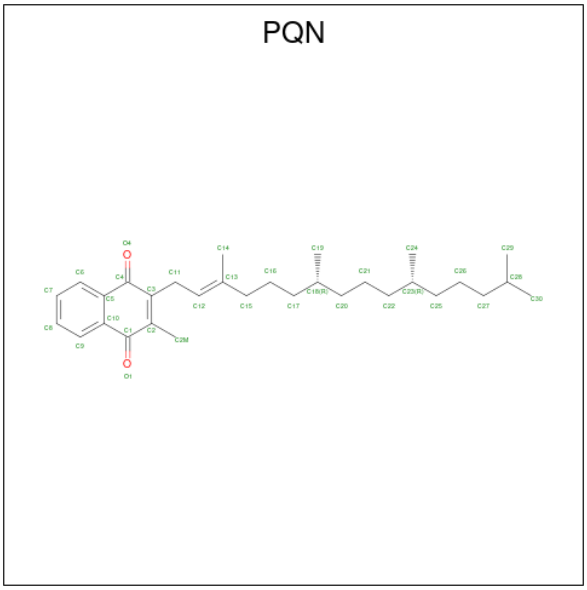
- Molecule 30 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
30	3	1	Total C O 44 40 4	0
30	7	1	Total C O 44 40 4	0

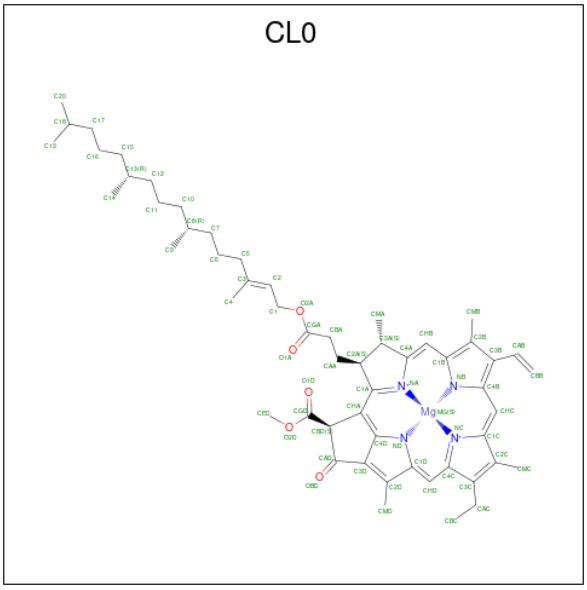
- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Lig-

and of Interest" by depositor).



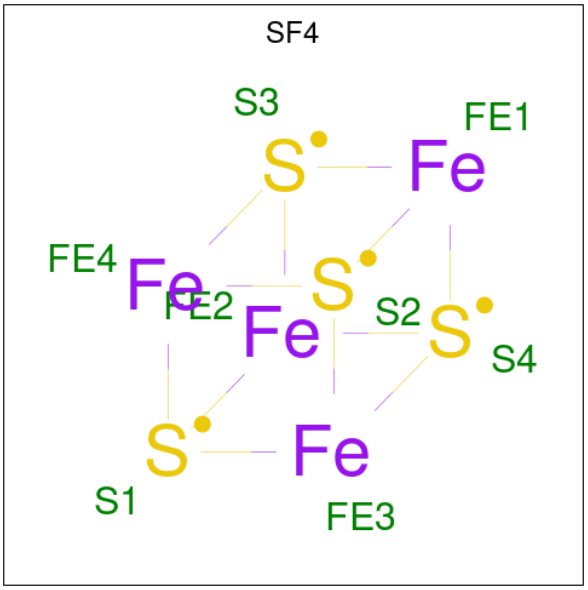
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 33 31 2	0
31	B	1	Total C O 33 31 2	0

- Molecule 32 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



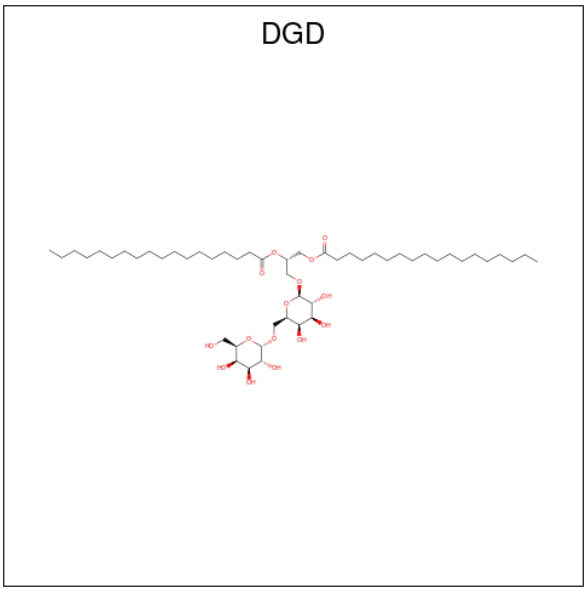
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

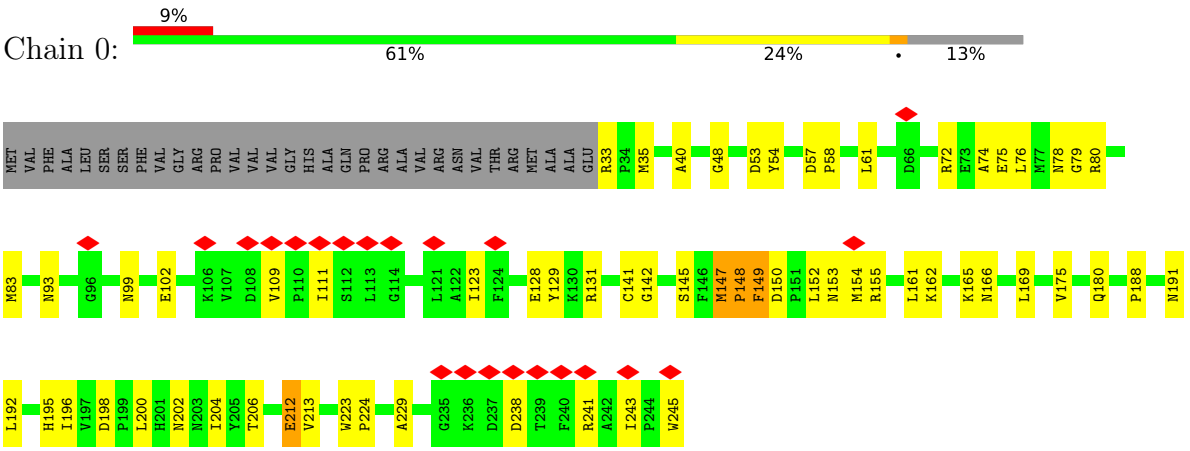


Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			56	41	15	

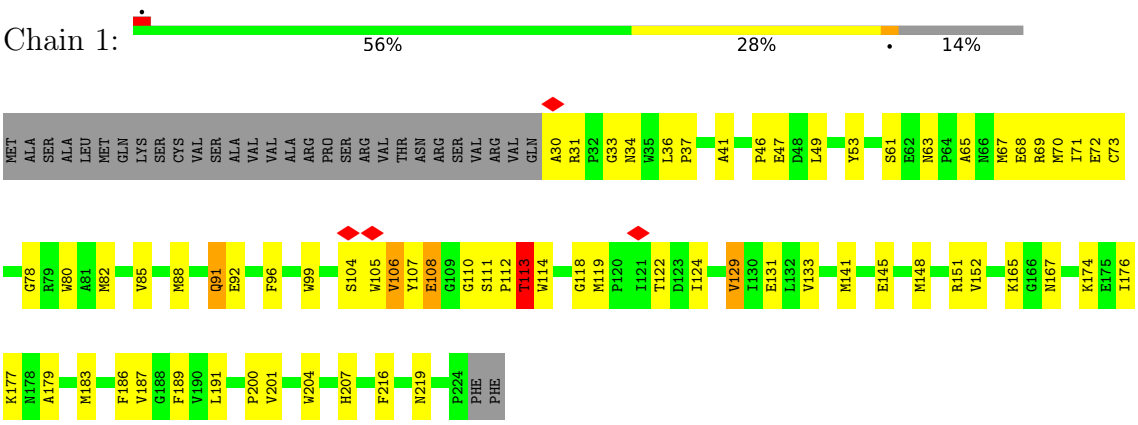
3 Residue-property plots (i)

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.

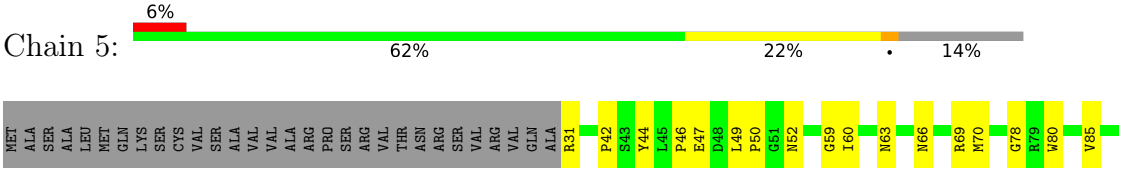
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

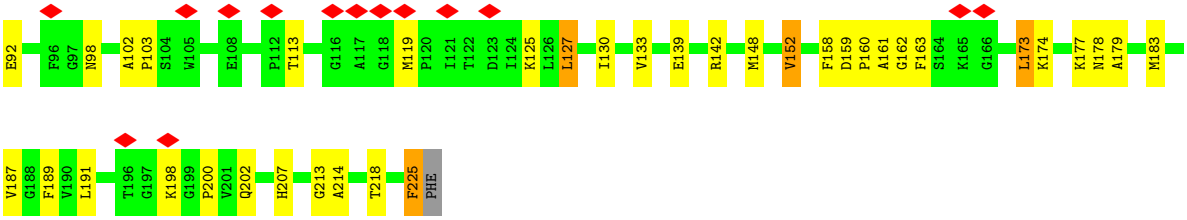


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic



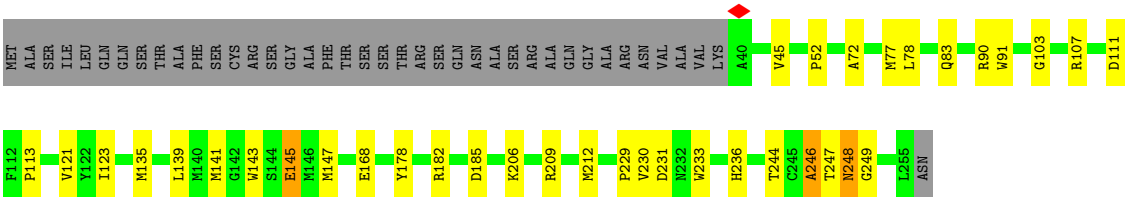
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic





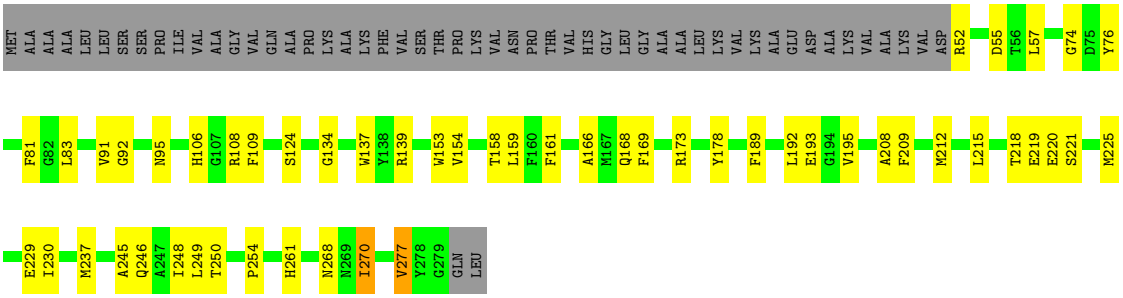
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



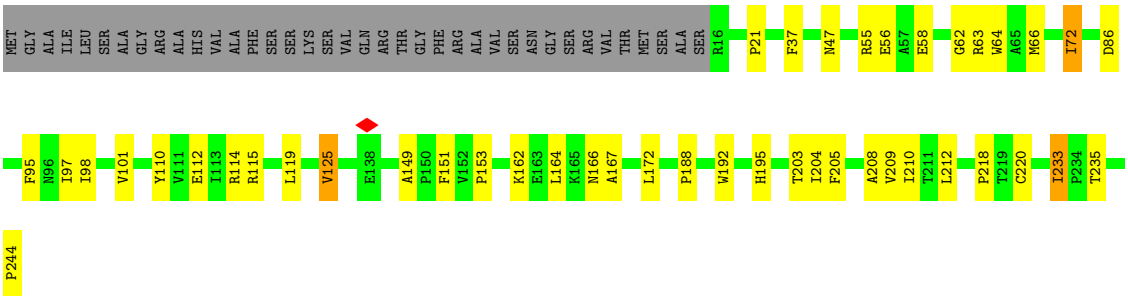
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



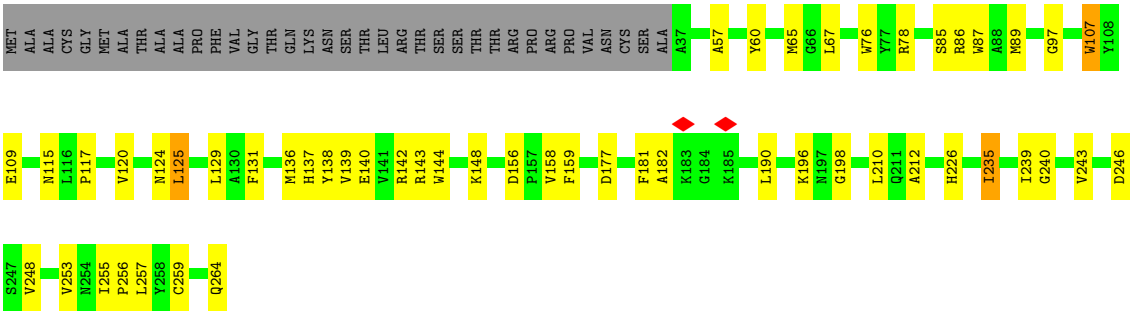
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



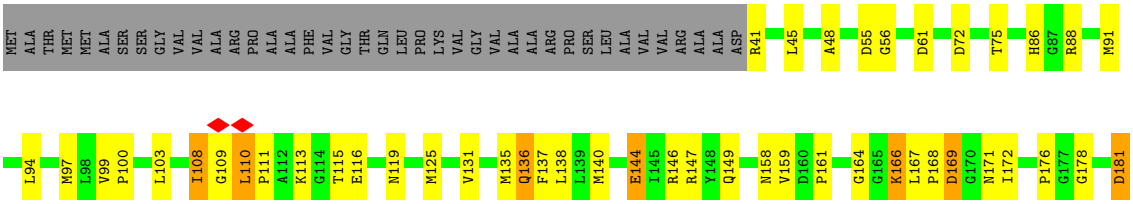
• Molecule 6: Chlorophyll a-b binding protein, chloroplastic

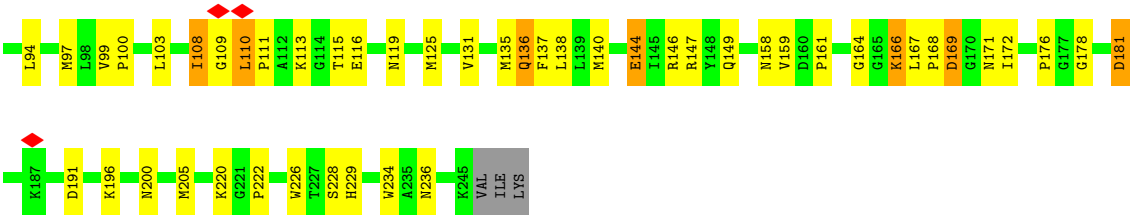
Chain 7:



• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

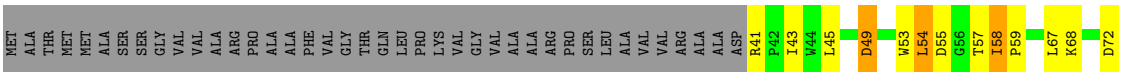
Chain 8:

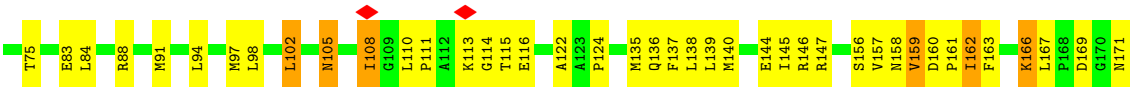




• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

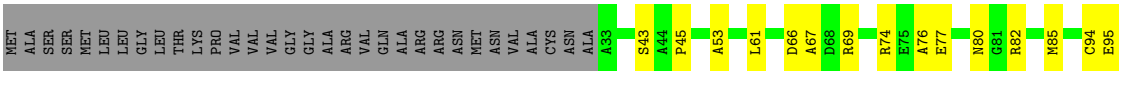
Chain 4:

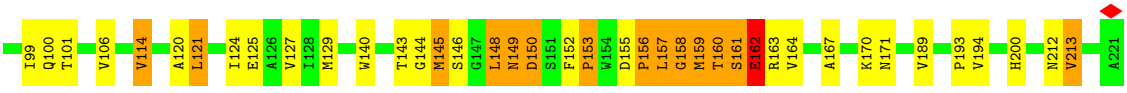




• Molecule 8: Chlorophyll a-b binding protein, chloroplastic

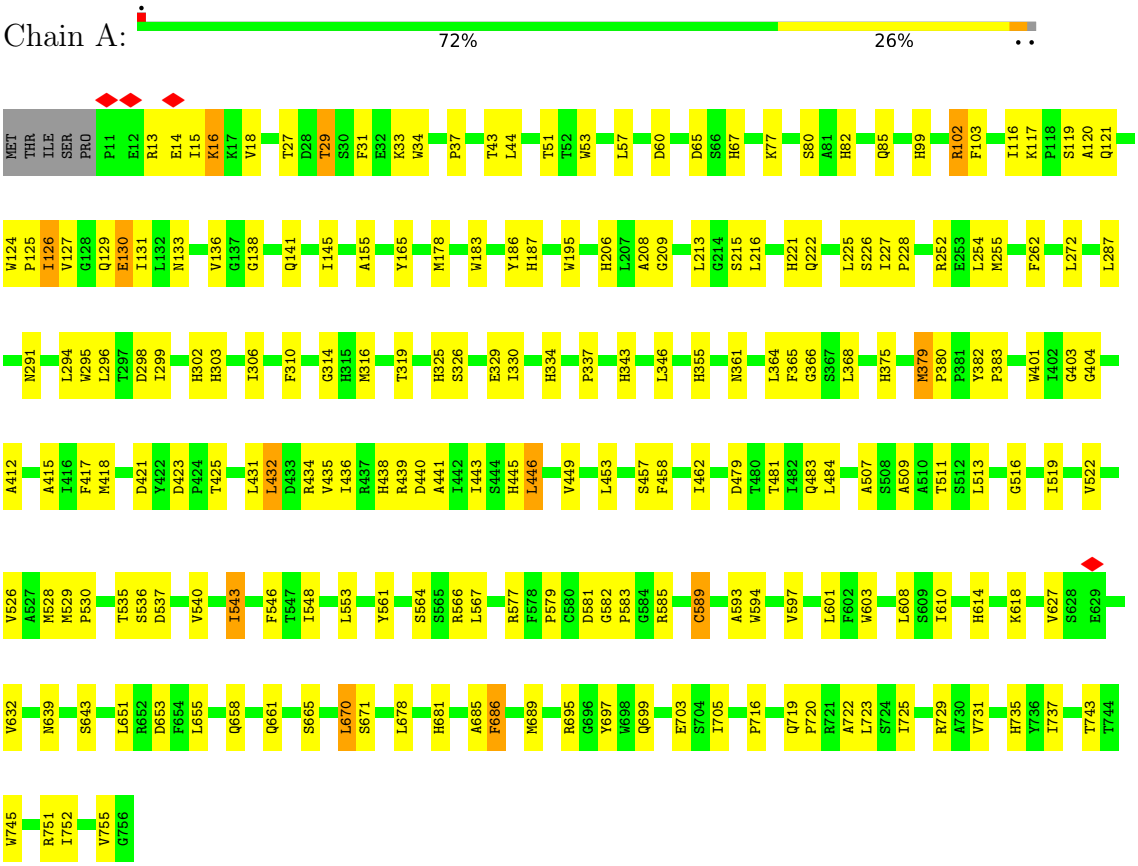
Chain 9:





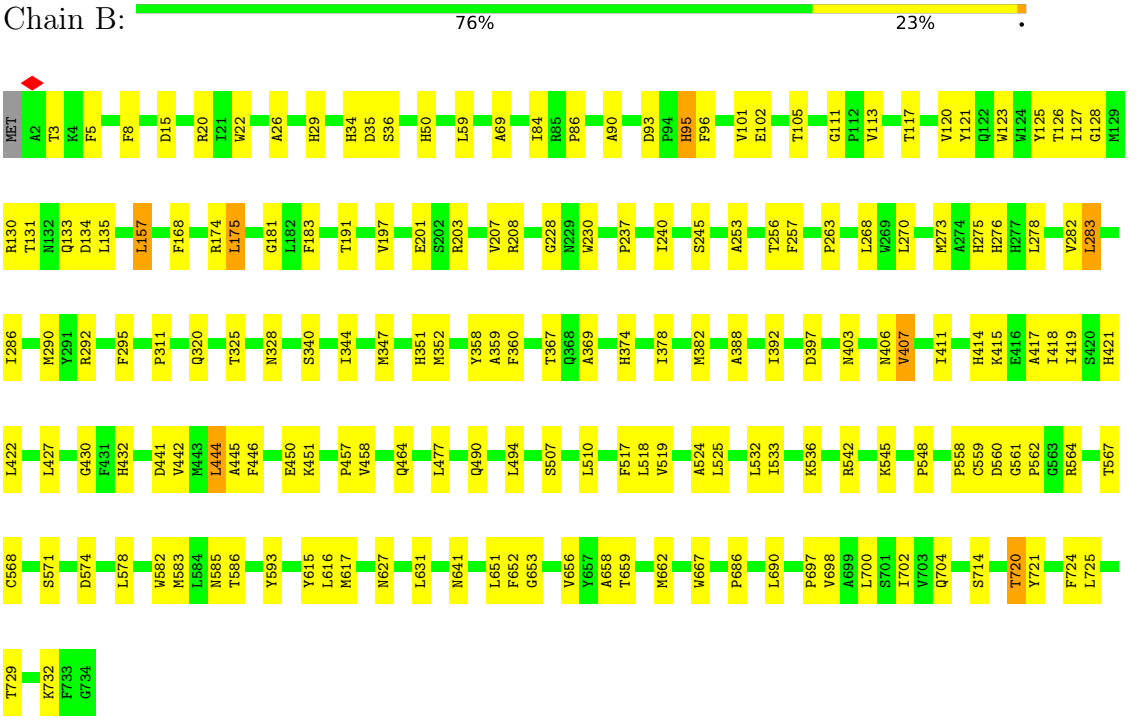
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



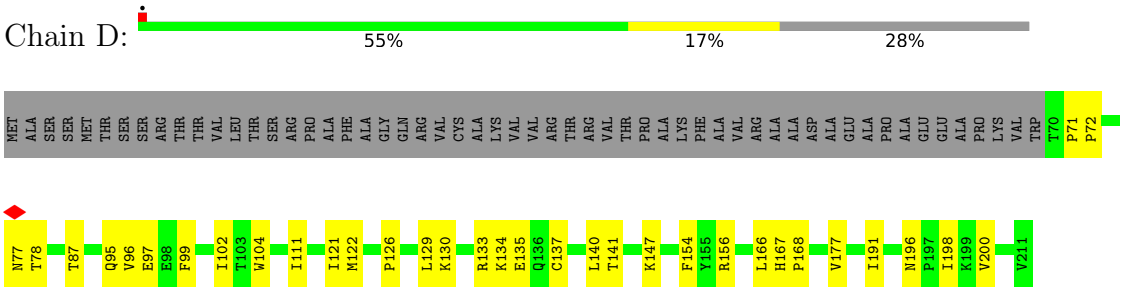
• Molecule 10: photosystem I

Chain B:



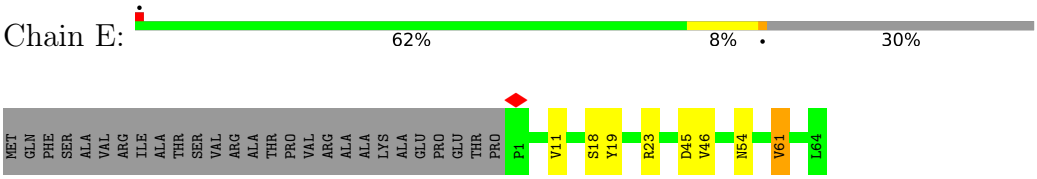
• Molecule 11: Photosystem I reaction center subunit II, chloroplastic

Chain D:



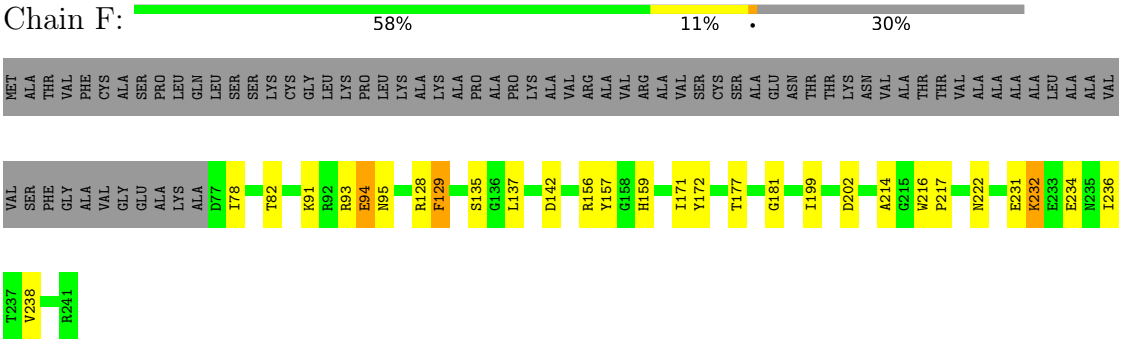
• Molecule 12: PsaE

Chain E:



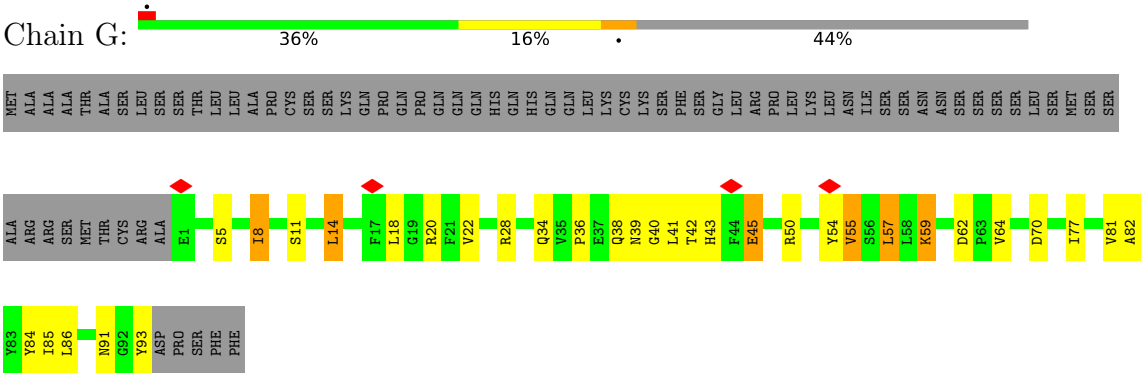
• Molecule 13: Photosystem I reaction center subunit III

Chain F:



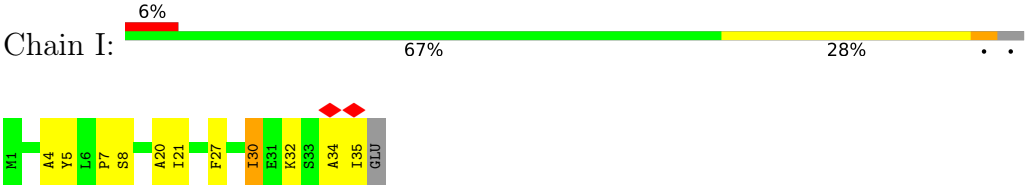
• Molecule 14: PsaG

Chain G:



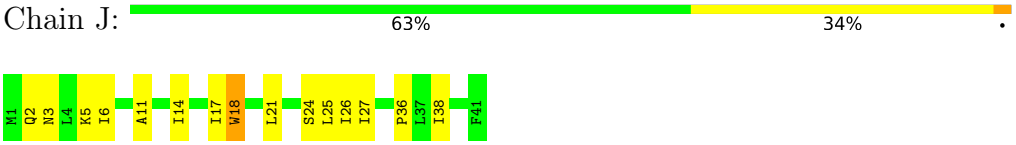
• Molecule 15: Photosystem I reaction center subunit VIII

Chain I:



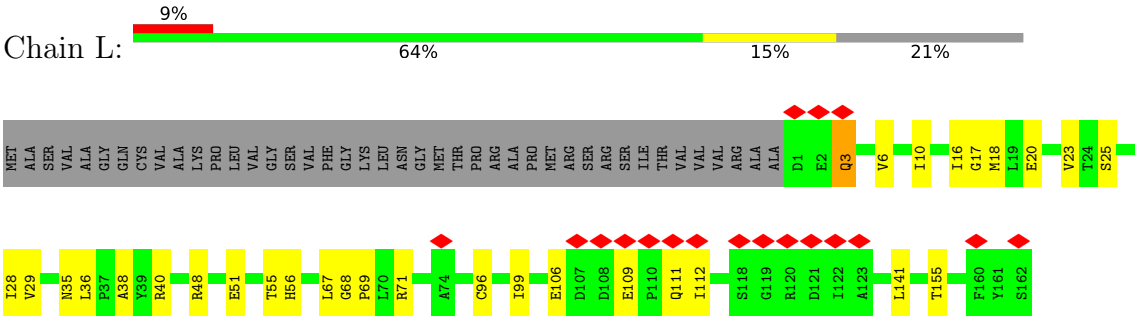
• Molecule 16: Photosystem I reaction center subunit IX

Chain J:



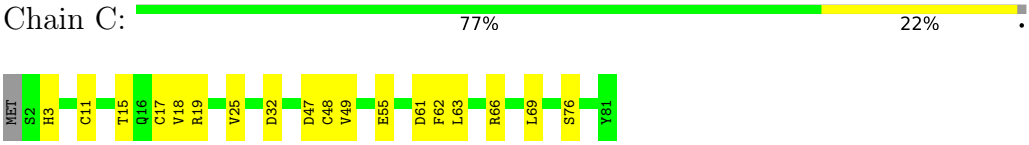
• Molecule 17: PSI subunit V

Chain L:



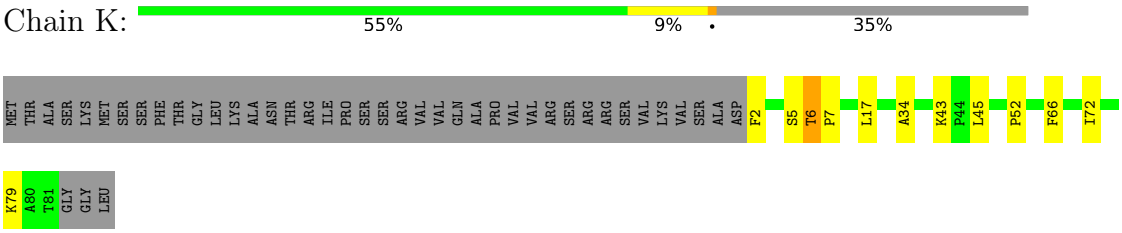
• Molecule 18: Photosystem I iron-sulfur center

Chain C:



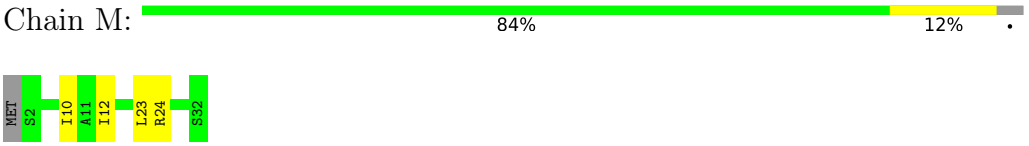
• Molecule 19: PsaK

Chain K:



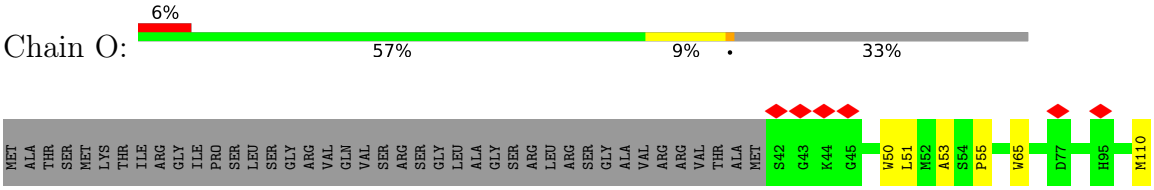
• Molecule 20: Photosystem I reaction center subunit XII

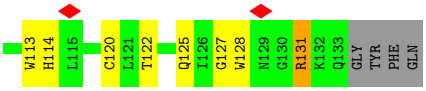
Chain M:



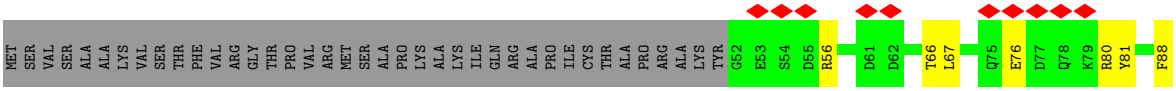
• Molecule 21: PsaO

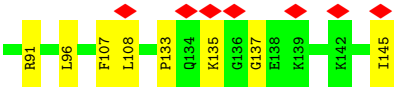
Chain O:





• Molecule 22: PsaH





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.536	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.203	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, SF4, DGD, 0IE, PQN, CHL, 0UR, 8CT, LHG, SQD, LMG, CLA

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	0	0.27	0/1685	0.38	0/2285
2	1	0.41	1/1523 (0.1%)	0.45	1/2073 (0.0%)
2	5	0.21	0/1530	0.41	0/2082
3	2	0.47	2/1727 (0.1%)	0.42	2/2351 (0.1%)
4	3	0.25	0/1818	0.32	0/2466
5	6	0.22	0/1862	0.30	0/2542
6	7	0.22	0/1812	0.31	0/2468
7	4	0.34	0/1619	0.62	1/2206 (0.0%)
7	8	0.20	0/1627	0.41	2/2217 (0.1%)
8	9	0.53	0/1492	0.48	1/2036 (0.0%)
9	A	0.42	1/6069 (0.0%)	0.35	1/8267 (0.0%)
10	B	0.37	0/6034	0.35	0/8239
11	D	0.21	0/1135	0.34	0/1533
12	E	0.20	0/521	0.26	0/706
13	F	0.21	0/1298	0.31	0/1748
14	G	0.25	0/743	0.41	0/1010
15	I	0.60	0/269	0.45	0/367
16	J	0.25	0/346	0.37	0/472
17	L	0.22	0/1224	0.34	0/1673
18	C	0.25	0/612	0.37	0/830
19	K	0.20	0/567	0.27	0/769
20	M	0.66	0/241	0.34	0/325
21	O	0.22	0/760	0.32	0/1042
22	H	0.18	0/729	0.34	0/979
All	All	0.34	4/37243 (0.0%)	0.38	8/50686 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	246	ALA	CA-C	-5.28	1.46	1.52
9	A	689	MET	CA-C	-5.25	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	113	THR	CA-C	-5.14	1.46	1.53
3	2	247	THR	N-CA	-5.12	1.39	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	4	180	PHE	N-CA-C	-13.95	96.82	112.72
8	9	163	ARG	N-CA-C	-8.43	102.05	111.07
7	8	109	GLY	CA-C-N	6.63	129.47	123.10
7	8	109	GLY	C-N-CA	6.63	129.47	123.10
2	1	108	GLU	N-CA-C	-6.22	104.39	112.23
3	2	248	ASN	N-CA-C	-5.76	105.92	113.12
3	2	247	THR	N-CA-C	-5.38	104.50	111.71
9	A	686	PHE	N-CA-C	-5.25	104.98	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1640	0	1609	47	0
2	1	1478	0	1423	55	0
2	5	1484	0	1427	40	0
3	2	1667	0	1562	26	0
4	3	1768	0	1702	45	0
5	6	1797	0	1752	37	0
6	7	1758	0	1701	46	0
7	4	1569	0	1551	67	0
7	8	1574	0	1550	48	0
8	9	1453	0	1404	45	0
9	A	5872	0	5715	162	0
10	B	5824	0	5603	147	0
11	D	1109	0	1124	27	0
12	E	509	0	506	8	0
13	F	1273	0	1290	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	726	0	717	33	0
15	I	262	0	279	10	0
16	J	336	0	355	14	0
17	L	1195	0	1187	25	0
18	C	602	0	591	20	0
19	K	558	0	591	9	0
20	M	238	0	248	4	0
21	O	728	0	699	16	0
22	H	717	0	684	18	0
23	0	215	0	172	14	0
23	1	291	0	262	16	0
23	2	304	0	230	15	0
23	3	240	0	223	10	0
23	4	408	0	308	28	0
23	5	252	0	189	13	0
23	6	486	0	404	28	0
23	7	334	0	280	20	0
23	8	411	0	314	23	0
23	9	193	0	132	5	0
24	0	524	0	459	22	0
24	1	434	0	386	17	0
24	2	389	0	356	8	0
24	3	603	0	554	18	0
24	4	371	0	324	12	0
24	5	409	0	340	13	0
24	6	527	0	456	15	0
24	7	569	0	496	27	0
24	8	364	0	314	10	0
24	9	438	0	403	18	0
24	A	2547	0	2613	127	0
24	B	2368	0	2356	147	0
24	F	92	0	68	4	0
24	G	141	0	105	2	0
24	H	246	0	193	6	0
24	J	42	0	31	2	0
24	K	209	0	176	6	0
24	L	214	0	188	9	0
24	O	220	0	151	10	0
25	0	40	0	0	0	0
25	1	40	0	0	0	0
25	2	40	0	0	0	0
25	3	120	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	4	40	0	0	1	0
25	6	80	0	0	0	0
25	7	80	0	0	0	0
25	8	40	0	0	1	0
25	9	40	0	0	0	0
25	A	200	0	0	1	0
25	B	280	0	0	1	0
25	F	80	0	0	1	0
25	G	40	0	0	0	0
25	I	40	0	0	0	0
25	J	80	0	0	1	0
25	K	40	0	0	0	0
25	L	120	0	0	1	0
25	M	40	0	0	0	0
25	O	80	0	0	0	0
26	0	104	0	0	1	0
26	1	104	0	0	1	0
26	2	101	0	0	3	0
26	3	51	0	0	1	0
26	4	101	0	0	3	0
26	5	103	0	0	4	0
26	6	103	0	0	1	0
26	7	51	0	0	2	0
26	8	103	0	0	2	0
26	9	104	0	0	3	0
26	O	52	0	0	2	0
27	0	49	0	74	2	0
27	1	92	0	133	7	0
27	2	64	0	68	2	0
27	3	116	0	144	7	0
27	5	37	0	44	1	0
27	6	37	0	44	5	0
27	7	107	0	127	5	0
27	8	75	0	90	0	0
27	9	47	0	63	5	0
27	A	118	0	152	11	0
27	B	61	0	62	2	0
27	I	46	0	65	4	0
27	L	31	0	32	0	0
28	0	36	0	41	2	0
29	2	36	0	42	0	0
29	3	36	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	9	55	0	86	4	0
29	A	73	0	86	7	0
29	J	75	0	93	3	0
29	M	42	0	54	1	0
29	O	70	0	80	1	0
30	3	44	0	0	0	0
30	7	44	0	0	0	0
31	A	33	0	46	4	0
31	B	33	0	46	1	0
32	A	65	0	72	8	0
33	B	8	0	0	1	0
33	C	16	0	0	0	0
34	B	56	0	70	3	0
All	All	54077	0	49609	1253	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 12.

All (1253) 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)
2:5:160:PRO:HD2	26:5:314:0UR:C30	1.90	1.01
1:0:147:MET:HB3	1:0:148:PRO:HD2	1.42	1.01
24:A:804:CLA:H11	24:A:805:CLA:HBB1	1.51	0.91
32:A:852:CL0:H15	24:B:804:CLA:HED1	1.52	0.89
9:A:29:THR:HG21	9:A:183:TRP:HE1	1.39	0.88
8:9:145:MET:HB3	8:9:153:PRO:HD3	1.58	0.84
2:1:174:LYS:HD3	24:1:310:CLA:HBA1	1.64	0.80
2:1:78:GLY:HA3	2:1:179:ALA:HB1	1.61	0.80
10:B:415:LYS:HZ3	13:F:238:VAL:HG21	1.49	0.77
24:B:804:CLA:HHB	24:B:805:CLA:H202	1.66	0.76
7:8:146:ARG:O	7:8:158:ASN:ND2	2.20	0.74
9:A:65:ASP:OD2	9:A:355:HIS:NE2	2.20	0.74
24:B:824:CLA:H52	24:B:825:CLA:H142	1.67	0.74
23:9:306:CHL:HHC	23:9:306:CHL:HBB1	1.68	0.74
24:A:831:CLA:HBB2	17:L:67:LEU:HD13	1.69	0.74
17:L:35:ASN:HB3	24:H:201:CLA:HAC1	1.68	0.73
8:9:152:PHE:O	8:9:153:PRO:C	2.29	0.73
24:A:808:CLA:HAB	24:B:833:CLA:HMD2	1.69	0.73
5:6:114:ARG:NH1	23:6:323:CHL:OBD	2.22	0.73
2:5:78:GLY:HA3	2:5:179:ALA:HB1	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:115:ARG:NH2	23:6:308:CHL:O1D	2.21	0.73
6:7:85:SER:HB2	6:7:198:GLY:HA3	1.70	0.72
2:1:204:TRP:HE1	23:1:312:CHL:HMC	1.55	0.72
7:4:146:ARG:NH1	23:4:315:CHL:OBD	2.20	0.72
23:4:315:CHL:HHC	23:4:315:CHL:HBB1	1.70	0.72
1:0:147:MET:O	1:0:148:PRO:C	2.31	0.72
23:7:306:CHL:HHC	23:7:306:CHL:HBB1	1.72	0.72
23:4:301:CHL:HHC	23:4:301:CHL:HBB1	1.70	0.72
7:8:88:ARG:NH1	23:8:308:CHL:OBD	2.20	0.72
23:8:306:CHL:HBB1	23:8:306:CHL:HHC	1.72	0.71
9:A:206:HIS:HB3	24:A:824:CLA:HED2	1.71	0.71
9:A:601:LEU:HD21	24:A:829:CLA:HBC1	1.71	0.71
8:9:152:PHE:CB	8:9:153:PRO:HD2	2.21	0.71
9:A:252:ARG:NH1	9:A:262:PHE:O	2.22	0.71
9:A:577:ARG:NH1	27:A:842:LHG:O10	2.23	0.71
24:A:803:CLA:H61	24:A:808:CLA:H202	1.71	0.71
27:1:317:LHG:H122	23:4:315:CHL:H2	1.73	0.70
23:0:301:CHL:HBB2	23:0:302:CHL:HHD	1.71	0.70
24:A:824:CLA:HBA1	24:A:828:CLA:H203	1.73	0.70
7:8:149:GLN:HB2	7:8:158:ASN:HD21	1.56	0.70
9:A:511:THR:HG21	24:A:826:CLA:HAB	1.74	0.70
2:1:113:THR:HG21	23:1:304:CHL:HMD3	1.71	0.70
5:6:203:THR:HG22	5:6:205:PHE:H	1.56	0.70
13:F:202:ASP:HA	29:J:102:LMG:HC61	1.73	0.70
27:I:102:LHG:H111	17:L:99:ILE:HD11	1.74	0.69
23:6:301:CHL:O1A	6:7:137:HIS:ND1	2.25	0.69
23:4:306:CHL:HHC	23:4:306:CHL:HBB1	1.74	0.69
7:4:43:ILE:HG22	7:4:45:LEU:H	1.57	0.69
14:G:11:SER:HB3	14:G:81:VAL:HG13	1.74	0.69
8:9:170:LYS:NZ	27:9:316:LHG:O4	2.21	0.69
23:6:323:CHL:HHC	23:6:323:CHL:HBB1	1.74	0.69
10:B:290:MET:HB2	24:B:822:CLA:HBC3	1.75	0.69
18:C:15:THR:OG1	18:C:19:ARG:NH1	2.24	0.69
7:4:49:ASP:N	7:4:49:ASP:OD1	2.26	0.69
27:0:317:LHG:HC91	27:0:317:LHG:H281	1.74	0.69
5:6:101:VAL:HG22	23:6:306:CHL:HBC1	1.73	0.69
6:7:86:ARG:NH1	23:7:307:CHL:OBD	2.24	0.69
1:0:147:MET:HB3	1:0:148:PRO:CD	2.22	0.68
11:D:167:HIS:HB3	11:D:168:PRO:HD3	1.75	0.68
24:5:302:CLA:HBC1	24:5:307:CLA:HAC1	1.76	0.68
10:B:120:VAL:HG21	24:B:811:CLA:HED1	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:8:305:CLA:H192	23:8:308:CHL:HAA2	1.75	0.68
7:4:226:TRP:CZ3	23:4:313:CHL:HMC	2.29	0.68
9:A:13:ARG:HE	19:K:43:LYS:HE3	1.58	0.68
7:4:226:TRP:HZ3	23:4:313:CHL:HMC	1.58	0.68
9:A:543:ILE:HD13	32:A:852:CL0:H59	1.75	0.68
7:8:161:PRO:HG2	7:8:166:LYS:HG3	1.76	0.67
2:1:30:ALA:N	2:1:47:GLU:O	2.27	0.67
23:8:301:CHL:HHC	23:8:301:CHL:HBB1	1.77	0.67
14:G:55:VAL:O	14:G:59:LYS:NZ	2.27	0.67
9:A:77:LYS:NZ	24:A:810:CLA:OBD	2.28	0.66
9:A:209:GLY:O	9:A:213:LEU:HB2	1.95	0.66
7:4:239:TRP:H	7:4:243:LEU:HD11	1.61	0.66
13:F:137:LEU:HD21	16:J:38:ILE:HG21	1.77	0.66
7:4:84:LEU:HD12	7:4:176:PRO:HG2	1.77	0.66
1:0:147:MET:CB	1:0:148:PRO:HD2	2.23	0.66
8:9:160:THR:HA	24:9:308:CLA:HAA2	1.78	0.66
7:4:182:PRO:HD2	26:4:317:0UR:C30	2.25	0.66
10:B:230:TRP:O	24:B:817:CLA:H3A	1.95	0.66
2:1:88:MET:HB3	2:1:99:TRP:HB3	1.77	0.65
24:A:818:CLA:HAB	24:A:818:CLA:H8	1.76	0.65
24:A:821:CLA:HAA2	19:K:34:ALA:HB3	1.78	0.65
1:0:33:ARG:NH2	1:0:53:ASP:O	2.30	0.65
2:5:113:THR:OG1	2:5:119:MET:SD	2.53	0.65
2:5:92:GLU:HB2	2:5:98:ASN:HA	1.77	0.65
23:0:305:CHL:HHC	23:0:305:CHL:HBB1	1.77	0.65
24:8:305:CLA:H2A	24:8:305:CLA:HED2	1.78	0.65
5:6:208:ALA:HB2	5:6:218:PRO:HD3	1.77	0.65
2:1:216:PHE:HB3	24:1:311:CLA:H12	1.79	0.65
13:F:231:GLU:HG3	13:F:232:LYS:H	1.62	0.65
6:7:97:GLY:HA3	24:7:304:CLA:HBC3	1.78	0.65
9:A:379:MET:HE3	24:A:817:CLA:HBD	1.79	0.65
23:2:305:CHL:HBB1	23:2:305:CHL:HHC	1.78	0.64
5:6:55:ARG:NH1	5:6:58:GLU:OE1	2.29	0.64
2:5:174:LYS:O	2:5:178:ASN:ND2	2.28	0.64
9:A:441:ALA:O	9:A:445:HIS:ND1	2.26	0.64
1:0:54:TYR:OH	1:0:165:LYS:NZ	2.31	0.64
4:3:124:SER:HB2	4:3:134:GLY:HA3	1.79	0.64
9:A:272:LEU:HD11	19:K:72:ILE:HG23	1.80	0.64
23:8:308:CHL:HHC	23:8:308:CHL:HBB1	1.80	0.64
9:A:375:HIS:ND1	24:A:817:CLA:OBD	2.27	0.64
10:B:130:ARG:NH2	10:B:245:SER:OG	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:63:ARG:NH1	23:6:307:CHL:OBD	2.27	0.63
2:1:129:VAL:HG13	14:G:14:LEU:HD22	1.80	0.63
5:6:62:GLY:HA3	5:6:167:ALA:HB1	1.79	0.63
6:7:148:LYS:NZ	24:7:316:CLA:O1D	2.31	0.63
7:4:198:VAL:O	7:4:202:ARG:HG2	1.98	0.63
2:1:70:MET:HA	2:1:73:CYS:SG	2.38	0.63
9:A:671:SER:HB2	10:B:445:ALA:HB1	1.81	0.63
2:1:177:LYS:NZ	27:1:317:LHG:O4	2.31	0.63
24:5:308:CLA:HAB	26:5:314:0UR:C13	2.28	0.63
3:2:168:GLU:OE2	3:2:182:ARG:NH2	2.28	0.63
24:6:311:CLA:HHC	24:6:311:CLA:HBB1	1.81	0.63
3:2:139:LEU:HB3	23:4:301:CHL:H43	1.82	0.62
5:6:192:TRP:HE1	23:6:313:CHL:HMC	1.63	0.62
7:8:171:ASN:ND2	7:8:176:PRO:O	2.30	0.62
9:A:31:PHE:O	16:J:3:ASN:HB3	1.99	0.62
10:B:125:TYR:O	10:B:130:ARG:NH1	2.32	0.62
16:J:14:ILE:HD12	16:J:17:ILE:HD11	1.81	0.62
23:7:307:CHL:HBB1	23:7:307:CHL:HHC	1.81	0.62
5:6:56:GLU:HG2	5:6:119:LEU:HD22	1.81	0.62
1:0:93:ASN:ND2	1:0:99:ASN:OD1	2.32	0.62
28:0:318:SQD:H45	20:M:24:ARG:HD2	1.79	0.62
2:1:124:ILE:HG21	14:G:91:ASN:HA	1.80	0.62
5:6:244:PRO:HB3	24:6:316:CLA:HAB	1.82	0.62
6:7:57:ALA:O	6:7:78:ARG:NH2	2.33	0.62
24:A:838:CLA:HAB	24:A:838:CLA:H122	1.81	0.62
14:G:11:SER:HA	14:G:14:LEU:HD23	1.82	0.62
2:1:165:LYS:HG3	2:1:167:ASN:H	1.66	0.61
7:8:220:LYS:NZ	7:8:228:SER:OG	2.32	0.61
27:9:316:LHG:H311	27:9:316:LHG:H122	1.82	0.61
9:A:457:SER:HB2	9:A:543:ILE:HG13	1.81	0.61
10:B:627:ASN:OD1	10:B:732:LYS:NZ	2.32	0.61
9:A:82:HIS:ND1	24:A:812:CLA:OBD	2.31	0.61
6:7:140:GLU:OE1	6:7:143:ARG:NH2	2.28	0.61
7:8:147:ARG:NH2	23:8:309:CHL:O1D	2.32	0.61
10:B:690:LEU:HD11	17:L:38:ALA:HB1	1.82	0.61
17:L:55:THR:HG21	24:L:202:CLA:HED2	1.82	0.61
7:4:53:TRP:HZ2	7:4:68:LYS:HG3	1.66	0.61
4:3:52:ARG:NH1	4:3:55:ASP:OD2	2.33	0.61
9:A:479:ASP:O	9:A:483:GLN:NE2	2.33	0.61
9:A:661:GLN:OE1	9:A:751:ARG:NH1	2.34	0.61
11:D:134:LYS:NZ	18:C:47:ASP:OD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:3:THR:HB	15:I:34:ALA:HA	1.82	0.61
10:B:105:THR:HG21	22:H:133:PRO:HB3	1.83	0.61
7:4:83:GLU:OE2	7:4:202:ARG:NE	2.34	0.61
9:A:368:LEU:HD11	24:A:818:CLA:H72	1.83	0.61
10:B:50:HIS:HE1	24:B:808:CLA:H171	1.66	0.61
24:B:809:CLA:H2	24:B:809:CLA:HED3	1.83	0.60
11:D:87:THR:HA	17:L:17:GLY:O	2.00	0.60
8:9:200:HIS:CG	24:9:311:CLA:HAA2	2.36	0.60
2:1:207:HIS:CG	24:1:311:CLA:HAA2	2.36	0.60
1:0:35:MET:HB3	1:0:40:ALA:HB3	1.84	0.60
2:1:37:PRO:HB3	7:4:162:ILE:HG13	1.82	0.60
7:8:138:LEU:HD12	23:8:301:CHL:H42	1.84	0.60
24:0:312:CLA:HBB2	8:9:120:ALA:HB1	1.81	0.60
9:A:287:LEU:HD21	9:A:380:PRO:HD2	1.84	0.60
4:3:83:LEU:HD12	23:3:302:CHL:H11	1.83	0.60
7:4:156:SER:HB3	7:4:158:ASN:H	1.67	0.60
7:8:226:TRP:HE1	23:8:314:CHL:HMC	1.67	0.60
24:9:307:CLA:H43	29:9:317:LMG:H381	1.84	0.60
2:5:46:PRO:HG2	2:5:49:LEU:HB2	1.84	0.59
24:A:836:CLA:H141	24:L:202:CLA:H141	1.85	0.59
24:B:817:CLA:HBD	24:B:817:CLA:HBA1	1.83	0.59
12:E:18:SER:OG	18:C:61:ASP:OD2	2.21	0.59
9:A:446:LEU:HD13	9:A:553:LEU:HA	1.83	0.59
14:G:36:PRO:HB2	14:G:43:HIS:CD2	2.36	0.59
1:0:129:TYR:OH	22:H:91:ARG:NH2	2.36	0.59
6:7:156:ASP:OD1	6:7:159:PHE:N	2.30	0.59
7:4:157:VAL:HG21	23:4:307:CHL:HMC	1.85	0.59
4:3:108:ARG:NH1	23:3:307:CHL:OBD	2.31	0.59
11:D:111:ILE:HG12	11:D:121:ILE:HG12	1.85	0.59
29:A:854:LMG:H131	24:L:203:CLA:HBA2	1.84	0.59
2:5:66:ASN:O	2:5:70:MET:HG2	2.03	0.58
9:A:404:GLY:HA3	9:A:608:LEU:HD11	1.84	0.58
24:A:827:CLA:H162	24:A:827:CLA:H101	1.84	0.58
11:D:130:LYS:NZ	22:H:66:THR:O	2.33	0.58
24:4:309:CLA:HAB	26:4:317:0UR:C13	2.32	0.58
9:A:566:ARG:NH2	11:D:87:THR:O	2.37	0.58
7:8:229:HIS:CG	24:8:313:CLA:HAA2	2.39	0.58
7:8:168:PRO:HB3	7:8:178:GLY:HA3	1.86	0.58
17:L:109:GLU:OE2	17:L:111:GLN:NE2	2.36	0.58
2:5:139:GLU:OE1	2:5:142:ARG:NH2	2.32	0.58
6:7:196:LYS:NZ	27:7:322:LHG:O5	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:20:ARG:HD3	24:G:103:CLA:HBB1	1.84	0.58
21:O:127:GLY:O	24:O:206:CLA:HMA1	2.04	0.58
2:5:148:MET:O	2:5:152:VAL:HG12	2.04	0.58
4:3:52:ARG:HB3	4:3:57:LEU:HD21	1.85	0.57
7:8:125:MET:HE2	23:8:306:CHL:HHD	1.85	0.57
3:2:45:VAL:HG11	3:2:52:PRO:HG3	1.85	0.57
6:7:226:HIS:CG	24:7:312:CLA:HAA2	2.39	0.57
9:A:745:TRP:NE1	24:A:827:CLA:O1A	2.38	0.57
9:A:627:VAL:HG22	9:A:632:VAL:HG22	1.85	0.57
23:2:312:CHL:HED3	4:3:158:THR:HG23	1.85	0.57
6:7:182:ALA:HB2	24:7:309:CLA:HAA2	1.86	0.57
9:A:665:SER:HB2	9:A:670:LEU:HB2	1.86	0.57
12:E:54:ASN:CG	18:C:61:ASP:HB2	2.29	0.57
24:A:831:CLA:H143	31:B:842:PQN:H191	1.87	0.57
10:B:311:PRO:HG2	27:B:851:LHG:HC31	1.87	0.57
4:3:178:TYR:HE2	27:3:322:LHG:HC41	1.70	0.57
2:5:103:PRO:HG3	23:5:304:CHL:HMC	1.87	0.57
10:B:457:PRO:HG3	10:B:517:PHE:HB2	1.86	0.57
18:C:3:HIS:CE1	18:C:76:SER:HB2	2.40	0.57
14:G:36:PRO:HB2	14:G:43:HIS:HD2	1.69	0.57
24:A:820:CLA:HMB2	24:A:824:CLA:HMA3	1.86	0.56
10:B:406:ASN:OD1	10:B:407:VAL:N	2.36	0.56
11:D:95:GLN:HA	22:H:67:LEU:HD13	1.87	0.56
23:2:312:CHL:HBB2	5:6:212:LEU:HD13	1.87	0.56
23:2:312:CHL:HHB	27:7:323:LHG:H101	1.85	0.56
1:0:195:HIS:CG	24:0:311:CLA:HAA2	2.40	0.56
23:0:305:CHL:HBC2	23:0:306:CHL:HHD	1.87	0.56
3:2:90:ARG:NH1	23:2:306:CHL:OBD	2.29	0.56
29:9:317:LMG:H332	29:9:317:LMG:H162	1.88	0.56
9:A:685:ALA:HB3	24:A:853:CLA:HBB2	1.87	0.56
1:0:153:ASN:O	1:0:155:ARG:NH1	2.38	0.56
24:0:303:CLA:H42	22:H:108:LEU:HD21	1.86	0.56
5:6:162:LYS:O	5:6:166:ASN:ND2	2.25	0.56
17:L:51:GLU:OE1	22:H:81:TYR:OH	2.24	0.56
1:0:229:ALA:HB2	29:9:317:LMG:H292	1.87	0.56
5:6:110:TYR:CZ	5:6:114:ARG:HD2	2.40	0.56
24:4:309:CLA:H102	24:4:311:CLA:HMB1	1.88	0.56
8:9:66:ASP:OD1	8:9:67:ALA:N	2.38	0.56
21:O:65:TRP:CD1	21:O:120:CYS:HG	2.23	0.56
24:1:302:CLA:H42	24:B:823:CLA:HMB2	1.88	0.56
3:2:233:TRP:HE1	23:2:312:CHL:HMC	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:304:CLA:HMB2	23:7:305:CHL:HBB1	1.88	0.56
9:A:120:ALA:H	9:A:145:ILE:HG12	1.70	0.56
27:I:102:LHG:O9	27:I:102:LHG:O1	2.23	0.56
27:1:317:LHG:H282	27:1:317:LHG:HC82	1.87	0.56
27:1:318:LHG:H242	24:B:823:CLA:H11	1.88	0.56
2:5:183:MET:HB2	23:5:301:CHL:HMC	1.87	0.56
9:A:418:MET:HE1	9:A:432:LEU:HD21	1.88	0.56
23:2:306:CHL:HHC	23:2:306:CHL:HBB1	1.87	0.56
24:A:839:CLA:C4D	24:A:839:CLA:H11	2.36	0.56
10:B:560:ASP:OD2	10:B:564:ARG:NH2	2.33	0.56
11:D:133:ARG:NH2	11:D:135:GLU:OE1	2.38	0.56
16:J:24:SER:HB2	24:J:103:CLA:HAB	1.88	0.56
1:0:188:PRO:O	26:0:315:0UR:O39	2.24	0.55
9:A:651:LEU:HD22	10:B:651:LEU:HD21	1.87	0.55
24:B:810:CLA:HBC1	20:M:12:ILE:HA	1.88	0.55
11:D:96:VAL:HG23	11:D:97:GLU:HG3	1.87	0.55
24:4:309:CLA:H102	24:4:311:CLA:CMB	2.36	0.55
24:A:838:CLA:HAA2	24:B:802:CLA:HMB1	1.87	0.55
7:4:243:LEU:HD23	24:4:314:CLA:C1D	2.36	0.55
4:3:248:ILE:HD12	24:A:814:CLA:H62	1.87	0.55
27:6:322:LHG:H292	27:6:322:LHG:H112	1.89	0.55
2:1:61:SER:OG	2:1:67:MET:SD	2.53	0.55
6:7:87:TRP:CE2	23:7:307:CHL:HED2	2.42	0.55
9:A:516:GLY:HA2	9:A:530:PRO:HB3	1.88	0.55
17:L:20:GLU:OE1	17:L:25:SER:OG	2.20	0.55
9:A:655:LEU:HD11	32:A:852:CL0:H43	1.88	0.55
10:B:369:ALA:HB1	10:B:725:LEU:HD11	1.89	0.55
1:0:61:LEU:HD11	24:0:303:CLA:H72	1.87	0.55
2:5:50:PRO:HA	2:5:173:LEU:HD22	1.88	0.55
10:B:207:VAL:O	10:B:208:ARG:NH1	2.34	0.55
8:9:66:ASP:HB3	8:9:69:ARG:HB2	1.88	0.55
7:4:179:ILE:C	7:4:181:ASP:H	2.15	0.55
8:9:43:SER:OG	14:G:59:LYS:NZ	2.32	0.55
10:B:328:ASN:ND2	14:G:39:ASN:OD1	2.35	0.55
27:3:322:LHG:HC32	27:3:322:LHG:HC62	1.89	0.54
23:7:301:CHL:HMA3	27:7:322:LHG:H112	1.87	0.54
24:B:839:CLA:H201	15:I:20:ALA:HB2	1.90	0.54
1:0:141:CYS:SG	1:0:142:GLY:N	2.80	0.54
3:2:147:MET:HA	23:4:301:CHL:HED3	1.88	0.54
6:7:235:ILE:HD12	24:7:312:CLA:H42	1.89	0.54
7:4:88:ARG:NH1	23:4:307:CHL:OBD	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:91:VAL:HA	27:3:322:LHG:HC31	1.89	0.54
8:9:161:SER:HB3	8:9:164:VAL:HG22	1.89	0.54
24:A:840:CLA:H71	24:B:839:CLA:H43	1.90	0.54
10:B:542:ARG:NH2	11:D:196:ASN:OD1	2.39	0.54
21:O:51:LEU:O	21:O:53:ALA:N	2.41	0.54
2:5:31:ARG:NH2	2:5:47:GLU:OE1	2.40	0.54
2:5:46:PRO:O	2:5:52:ASN:ND2	2.41	0.54
9:A:294:LEU:HB2	9:A:299:ILE:HD11	1.90	0.54
9:A:415:ALA:HB1	9:A:593:ALA:HB1	1.90	0.54
24:B:824:CLA:HBB1	24:B:831:CLA:HBC2	1.88	0.54
5:6:210:ILE:HD12	24:6:316:CLA:HMC2	1.90	0.54
9:A:302:HIS:HB2	24:A:817:CLA:C1B	2.38	0.54
10:B:168:PHE:O	10:B:174:ARG:NH2	2.39	0.54
1:0:154:MET:HE3	24:0:308:CLA:HED1	1.90	0.54
8:9:148:LEU:O	8:9:149:ASN:C	2.48	0.54
9:A:453:LEU:HB3	9:A:546:PHE:HB2	1.90	0.54
18:C:3:HIS:CD2	18:C:69:LEU:HA	2.43	0.54
2:1:92:GLU:OE1	2:1:201:VAL:N	2.35	0.54
9:A:155:ALA:HB2	9:A:383:PRO:HD2	1.90	0.54
10:B:117:THR:HA	10:B:367:THR:HG22	1.90	0.54
2:1:148:MET:SD	2:1:148:MET:N	2.78	0.54
6:7:117:PRO:HG2	6:7:120:VAL:HG22	1.89	0.54
21:O:128:TRP:HA	24:O:206:CLA:CMA	2.38	0.54
2:1:104:SER:HG	2:1:105:TRP:CD1	2.26	0.53
23:1:306:CHL:HBA1	23:1:306:CHL:H13	1.90	0.53
9:A:228:PRO:HG3	9:A:255:MET:HE1	1.88	0.53
24:A:831:CLA:H41	24:A:840:CLA:HBC2	1.90	0.53
10:B:347:MET:HG3	10:B:351:HIS:CE1	2.43	0.53
13:F:172:TYR:OH	13:F:214:ALA:O	2.25	0.53
7:4:94:LEU:HD11	7:4:207:ALA:HB3	1.90	0.53
7:4:108:ILE:HD13	7:4:108:ILE:H	1.74	0.53
1:0:123:ILE:HD13	23:0:305:CHL:H11	1.90	0.53
2:5:80:TRP:CE2	23:5:306:CHL:HED2	2.43	0.53
7:8:115:THR:OG1	7:8:116:GLU:N	2.39	0.53
8:9:53:ALA:O	8:9:74:ARG:NH2	2.29	0.53
10:B:50:HIS:ND1	24:B:814:CLA:OBD	2.32	0.53
10:B:191:THR:HG21	10:B:278:LEU:HB2	1.90	0.53
10:B:320:GLN:O	10:B:406:ASN:ND2	2.41	0.53
29:3:321:LMG:O3	29:A:851:LMG:O2	2.21	0.53
24:5:303:CLA:HBA1	23:5:304:CHL:C1D	2.38	0.53
5:6:37:PHE:HB2	23:6:302:CHL:HMD1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:41:ARG:NH1	7:8:61:ASP:O	2.41	0.53
7:8:196:LYS:O	7:8:200:ASN:ND2	2.26	0.53
10:B:237:PRO:HB3	10:B:256:THR:HG21	1.90	0.53
21:O:110:MET:HG2	21:O:114:HIS:CE1	2.43	0.53
7:4:53:TRP:CZ2	7:4:68:LYS:HG3	2.43	0.53
4:3:83:LEU:HB2	23:3:302:CHL:O1A	2.09	0.53
6:7:177:ASP:OD1	26:7:320:0UR:O40	2.25	0.53
24:B:818:CLA:H41	24:B:834:CLA:HAA2	1.90	0.53
7:4:110:LEU:HD12	7:4:111:PRO:HD2	1.91	0.53
7:4:144:GLU:OE2	7:4:147:ARG:NH2	2.40	0.53
23:4:305:CHL:HHC	23:4:305:CHL:HBB1	1.90	0.53
9:A:567:LEU:O	11:D:133:ARG:NH1	2.36	0.53
6:7:109:GLU:HG2	23:7:306:CHL:HED2	1.90	0.53
9:A:102:ARG:HD3	9:A:103:PHE:CZ	2.43	0.53
9:A:639:ASN:O	9:A:643:SER:HB3	2.09	0.53
10:B:105:THR:HG22	10:B:111:GLY:C	2.34	0.53
10:B:295:PHE:HA	14:G:57:LEU:HD22	1.91	0.53
24:9:302:CLA:H2A	24:9:302:CLA:HED2	1.90	0.53
10:B:276:HIS:HB2	24:B:818:CLA:C1B	2.38	0.53
24:9:302:CLA:HAB	26:9:315:0UR:C6	2.38	0.53
24:A:801:CLA:H151	24:H:202:CLA:HBC3	1.90	0.53
10:B:450:GLU:OE2	13:F:128:ARG:NH1	2.41	0.53
2:1:34:ASN:HB3	7:4:162:ILE:HD11	1.91	0.53
24:9:302:CLA:HBC1	27:9:316:LHG:H271	1.91	0.53
9:A:102:ARG:HG3	9:A:165:TYR:OH	2.09	0.53
10:B:464:GLN:NE2	24:B:836:CLA:OBD	2.35	0.53
2:5:173:LEU:HD12	2:5:177:LYS:HE3	1.90	0.52
9:A:543:ILE:CD1	32:A:852:CL0:H59	2.39	0.52
10:B:131:THR:HG22	10:B:133:GLN:H	1.73	0.52
11:D:102:ILE:HD13	11:D:140:LEU:HD23	1.91	0.52
21:O:65:TRP:HH2	21:O:113:TRP:HA	1.74	0.52
2:1:80:TRP:CE2	23:1:306:CHL:HED2	2.44	0.52
9:A:519:ILE:HG12	9:A:529:MET:HG3	1.91	0.52
9:A:678:LEU:HD11	10:B:617:MET:HB2	1.90	0.52
9:A:697:TYR:OH	24:A:853:CLA:OBD	2.21	0.52
10:B:268:LEU:HD22	24:B:818:CLA:HBA1	1.92	0.52
24:B:829:CLA:HHC	24:B:829:CLA:HBB1	1.92	0.52
12:E:23:ARG:NH2	12:E:45:ASP:OD2	2.42	0.52
7:4:158:ASN:O	7:4:158:ASN:ND2	2.43	0.52
10:B:417:ALA:O	10:B:421:HIS:ND1	2.36	0.52
3:2:141:MET:HE2	23:2:307:CHL:C2C	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:248:VAL:HG12	6:7:255:ILE:HB	1.92	0.52
22:H:88:PHE:HB2	24:H:204:CLA:HBC3	1.90	0.52
7:8:161:PRO:HG3	23:8:316:CHL:C4C	2.40	0.52
9:A:80:SER:OG	9:A:186:TYR:HB2	2.09	0.52
4:3:261:HIS:CG	24:3:312:CLA:HAA2	2.45	0.52
8:9:100:GLN:HG2	8:9:106:VAL:HB	1.91	0.52
8:9:167:ALA:O	8:9:171:ASN:ND2	2.29	0.52
2:1:69:ARG:HH21	27:1:318:LHG:HC5	1.74	0.52
9:A:537:ASP:OD1	9:A:618:LYS:NZ	2.39	0.52
1:0:198:ASP:OD1	1:0:202:ASN:ND2	2.39	0.52
6:7:109:GLU:O	6:7:115:ASN:ND2	2.35	0.52
24:9:307:CLA:H43	29:9:317:LMG:H402	1.92	0.52
10:B:26:ALA:HA	24:B:830:CLA:H43	1.92	0.52
7:4:196:LYS:HD3	24:4:311:CLA:HAA2	1.91	0.52
1:0:128:GLU:OE1	1:0:131:ARG:NH2	2.39	0.51
23:0:305:CHL:NC	23:0:306:CHL:HBC3	2.25	0.51
13:F:91:LYS:HE3	13:F:95:ASN:HD21	1.75	0.51
7:4:245:LYS:O	7:4:247:ILE:N	2.38	0.51
10:B:270:LEU:HD23	10:B:273:MET:HE3	1.92	0.51
24:B:809:CLA:H151	24:B:829:CLA:HBB2	1.93	0.51
2:1:106:VAL:HG23	2:1:107:TYR:CG	2.45	0.51
5:6:151:PHE:CE2	5:6:153:PRO:HG3	2.45	0.51
9:A:126:ILE:HG22	9:A:129:GLN:OE1	2.10	0.51
10:B:411:ILE:HA	10:B:414:HIS:CE1	2.45	0.51
10:B:616:LEU:HD12	24:B:804:CLA:H11	1.91	0.51
20:M:10:ILE:HG21	29:M:101:LMG:H121	1.92	0.51
24:7:309:CLA:HAB	26:7:320:0UR:C13	2.41	0.51
9:A:343:HIS:CE1	27:A:843:LHG:HC12	2.45	0.51
10:B:174:ARG:HB2	24:B:814:CLA:HBC2	1.92	0.51
17:L:10:ILE:HG21	17:L:16:ILE:HB	1.91	0.51
7:4:202:ARG:HD2	23:4:302:CHL:C4C	2.41	0.51
10:B:29:HIS:ND1	24:B:809:CLA:O1A	2.31	0.51
10:B:477:LEU:HD13	24:B:834:CLA:HMD1	1.93	0.51
2:5:125:LYS:H	2:5:125:LYS:HD2	1.75	0.51
6:7:235:ILE:HG13	24:7:312:CLA:H11	1.92	0.51
24:A:853:CLA:CGA	24:A:853:CLA:H3A	2.39	0.51
11:D:191:ILE:HG21	18:C:62:PHE:HD2	1.75	0.51
24:5:308:CLA:H121	24:5:310:CLA:HBC1	1.91	0.51
23:6:301:CHL:H2	6:7:138:TYR:HB2	1.92	0.51
9:A:382:TYR:OH	24:A:828:CLA:OBD	2.25	0.51
32:A:852:CL0:H14	24:B:805:CLA:NA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:560:ASP:OD1	18:C:66:ARG:NH1	2.40	0.51
24:3:309:CLA:H191	23:7:301:CHL:H43	1.91	0.51
7:8:131:VAL:HG12	7:8:135:MET:HE2	1.92	0.51
27:9:316:LHG:O3	27:9:316:LHG:O1	2.26	0.51
10:B:126:THR:HG21	10:B:358:TYR:HD1	1.76	0.51
17:L:68:GLY:O	17:L:71:ARG:HG3	2.10	0.51
7:4:238:VAL:HG22	7:4:243:LEU:HD21	1.93	0.51
4:3:168:GLN:HE22	24:3:314:CLA:C1A	2.23	0.51
9:A:60:ASP:O	9:A:67:HIS:NE2	2.36	0.50
10:B:545:LYS:NZ	12:E:18:SER:O	2.44	0.50
24:B:810:CLA:HHB	24:B:811:CLA:HHB	1.92	0.50
9:A:222:GLN:O	9:A:227:ILE:HG12	2.11	0.50
9:A:585:ARG:NH2	11:D:135:GLU:OE2	2.37	0.50
10:B:442:VAL:HG21	24:B:833:CLA:HAC2	1.91	0.50
10:B:559:CYS:SG	10:B:561:GLY:N	2.75	0.50
10:B:560:ASP:CG	18:C:66:ARG:HH12	2.19	0.50
7:4:205:MET:HB2	23:4:302:CHL:HMC	1.94	0.50
23:6:301:CHL:OBD	6:7:142:ARG:NH1	2.44	0.50
31:A:841:PQN:H28	24:F:303:CLA:HBC1	1.93	0.50
19:K:6:THR:HG23	19:K:7:PRO:HD3	1.93	0.50
7:4:238:VAL:HB	24:4:312:CLA:H11	1.94	0.50
1:0:238:ASP:N	1:0:238:ASP:OD1	2.44	0.50
3:2:72:ALA:HB1	3:2:78:LEU:HD13	1.92	0.50
4:3:209:PHE:O	4:3:212:MET:HG3	2.10	0.50
24:L:201:CLA:H51	24:L:202:CLA:H43	1.94	0.50
7:8:91:MET:SD	24:8:310:CLA:HAB	2.51	0.50
9:A:507:ALA:O	9:A:509:ALA:N	2.43	0.50
10:B:292:ARG:NH1	14:G:34:GLN:O	2.45	0.50
24:B:827:CLA:HMB2	24:B:834:CLA:HBA1	1.94	0.50
19:K:52:PRO:HG2	24:K:103:CLA:HBC2	1.94	0.50
24:4:310:CLA:H2A	24:4:310:CLA:HED2	1.92	0.50
4:3:245:ALA:HA	24:A:814:CLA:H61	1.94	0.50
5:6:114:ARG:HE	23:6:307:CHL:CMC	2.25	0.50
10:B:228:GLY:HA3	14:G:86:LEU:HD13	1.94	0.50
18:C:3:HIS:HD2	18:C:69:LEU:HA	1.76	0.50
3:2:91:TRP:CE2	23:2:306:CHL:HED2	2.47	0.50
3:2:209:ARG:HA	3:2:212:MET:HE3	1.93	0.50
3:2:244:THR:HG21	4:3:158:THR:OG1	2.10	0.50
6:7:107:TRP:CZ3	6:7:212:ALA:HB2	2.47	0.50
13:F:156:ARG:NH1	24:F:302:CLA:OBD	2.45	0.50
2:5:49:LEU:HD22	23:5:301:CHL:HED2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:29:THR:HG23	29:A:851:LMG:O4	2.11	0.50
10:B:721:TYR:HB2	24:B:805:CLA:HED3	1.93	0.50
4:3:109:PHE:CE1	24:3:308:CLA:HBC3	2.46	0.50
8:9:156:PRO:HG2	26:9:314:0UR:C30	2.42	0.50
9:A:37:PRO:HB2	9:A:53:TRP:HH2	1.77	0.50
10:B:422:LEU:HG	24:B:838:CLA:HBB1	1.94	0.50
11:D:154:PHE:CZ	11:D:167:HIS:HB2	2.47	0.50
7:4:105:ASN:O	7:4:105:ASN:ND2	2.42	0.50
4:3:166:ALA:HB1	25:3:316:8CT:C18	2.42	0.49
24:A:807:CLA:H2	24:A:827:CLA:H43	1.94	0.49
10:B:490:GLN:HA	10:B:494:LEU:HB3	1.93	0.49
9:A:310:PHE:HE1	24:A:820:CLA:HAB	1.78	0.49
10:B:347:MET:HE1	24:B:819:CLA:H13	1.94	0.49
24:B:817:CLA:H8	14:G:84:TYR:CE1	2.47	0.49
4:3:74:GLY:HA3	4:3:230:ILE:HG21	1.95	0.49
4:3:221:SER:O	4:3:225:MET:HG2	2.11	0.49
13:F:78:ILE:HD11	13:F:157:TYR:HB2	1.93	0.49
13:F:214:ALA:HB3	7:4:67:LEU:HD22	1.94	0.49
14:G:18:LEU:O	14:G:22:VAL:HB	2.12	0.49
14:G:18:LEU:HD23	14:G:22:VAL:HG21	1.93	0.49
18:C:17:CYS:SG	18:C:18:VAL:N	2.85	0.49
23:1:301:CHL:H42	24:B:841:CLA:HBB2	1.94	0.49
24:2:308:CLA:HAB	26:2:315:0UR:C13	2.42	0.49
5:6:203:THR:HG22	5:6:205:PHE:N	2.26	0.49
10:B:631:LEU:HD22	10:B:724:PHE:HA	1.94	0.49
24:B:804:CLA:HMB1	24:B:804:CLA:HBB1	1.94	0.49
11:D:99:PHE:CE1	22:H:67:LEU:HD21	2.47	0.49
6:7:144:TRP:NE1	24:7:316:CLA:OBD	2.32	0.49
24:A:813:CLA:H8	24:A:815:CLA:HAB	1.94	0.49
24:B:808:CLA:HBD	24:B:808:CLA:H122	1.93	0.49
24:B:824:CLA:HED3	24:B:824:CLA:H2A	1.92	0.49
2:1:106:VAL:HG23	2:1:107:TYR:CD1	2.48	0.49
24:3:315:CLA:HHD	24:3:315:CLA:HBC3	1.94	0.49
2:5:158:PHE:O	2:5:160:PRO:HD3	2.13	0.49
8:9:160:THR:O	8:9:161:SER:C	2.52	0.49
24:A:802:CLA:H93	24:A:807:CLA:H172	1.93	0.49
7:8:119:ASN:HA	23:8:307:CHL:HED2	1.94	0.49
10:B:422:LEU:HD13	10:B:532:LEU:HA	1.93	0.49
1:0:48:GLY:N	1:0:53:ASP:OD2	2.43	0.49
23:0:301:CHL:H52	8:9:127:VAL:HG21	1.93	0.49
3:2:77:MET:HE1	16:J:5:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:106:HIS:HB3	4:3:237:MET:HE3	1.94	0.49
24:B:806:CLA:CGA	24:B:806:CLA:H3A	2.42	0.49
24:B:811:CLA:O1A	24:B:828:CLA:HBD	2.12	0.49
11:D:77:ASN:O	22:H:56:ARG:NH1	2.46	0.49
3:2:141:MET:O	3:2:145:GLU:HB2	2.11	0.49
8:9:124:ILE:HG21	23:9:305:CHL:HED2	1.93	0.49
10:B:524:ALA:HB2	24:B:837:CLA:HMA1	1.95	0.49
23:0:301:CHL:HBB2	23:0:302:CHL:CHD	2.39	0.49
7:8:72:ASP:OD1	7:8:75:THR:OG1	2.23	0.49
9:A:131:ILE:HG21	10:B:446:PHE:HA	1.95	0.49
24:A:839:CLA:H101	24:A:839:CLA:H61	1.50	0.49
10:B:123:TRP:O	10:B:127:ILE:HG12	2.13	0.49
10:B:344:ILE:HG23	24:B:819:CLA:H61	1.93	0.49
2:1:31:ARG:NH1	2:1:41:ALA:HB2	2.28	0.48
24:1:311:CLA:NC	24:1:311:CLA:H43	2.28	0.48
9:A:221:HIS:CE1	9:A:225:LEU:HD12	2.48	0.48
24:A:829:CLA:H93	24:A:839:CLA:HED3	1.93	0.48
11:D:191:ILE:HG21	18:C:62:PHE:CD2	2.48	0.48
2:1:191:LEU:HD12	24:1:311:CLA:HAC2	1.94	0.48
9:A:658:GLN:HB3	9:A:751:ARG:HD2	1.95	0.48
24:A:836:CLA:H62	24:A:836:CLA:H41	1.66	0.48
3:2:244:THR:HG23	3:2:246:ALA:H	1.77	0.48
8:9:76:ALA:O	8:9:80:ASN:ND2	2.37	0.48
9:A:579:PRO:HB3	9:A:725:ILE:HB	1.94	0.48
24:A:839:CLA:H202	24:F:303:CLA:HBB1	1.93	0.48
10:B:197:VAL:O	10:B:201:GLU:HB2	2.12	0.48
2:1:36:LEU:HD13	23:4:315:CHL:HMA3	1.93	0.48
2:5:207:HIS:HA	2:5:214:ALA:HB3	1.96	0.48
7:8:191:ASP:N	7:8:191:ASP:OD1	2.46	0.48
9:A:85:GLN:HE21	24:A:804:CLA:HMB3	1.78	0.48
24:A:848:CLA:HHC	24:A:848:CLA:HBB1	1.94	0.48
17:L:141:LEU:HD23	22:H:96:LEU:HD13	1.96	0.48
23:0:306:CHL:HHC	23:0:306:CHL:HBB1	1.95	0.48
2:5:160:PRO:HD2	26:5:314:0UR:O40	2.13	0.48
23:6:323:CHL:H62	23:8:314:CHL:H2	1.96	0.48
9:A:443:ILE:HG13	9:A:561:TYR:HE1	1.79	0.48
10:B:93:ASP:OD1	10:B:95:HIS:ND1	2.41	0.48
24:B:817:CLA:HBC3	24:B:817:CLA:HHD	1.94	0.48
12:E:54:ASN:OD1	18:C:61:ASP:N	2.45	0.48
2:1:200:PRO:O	26:1:315:0UR:O39	2.32	0.48
2:5:159:ASP:OD1	26:5:314:0UR:O40	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:802:CLA:HBB2	24:A:810:CLA:H121	1.95	0.48
10:B:134:ASP:OD1	10:B:134:ASP:N	2.47	0.48
13:F:94:GLU:HG2	13:F:129:PHE:HB3	1.95	0.48
21:O:65:TRP:CH2	21:O:113:TRP:HA	2.48	0.48
21:O:127:GLY:O	24:O:206:CLA:CMA	2.61	0.48
2:1:165:LYS:HE3	2:1:167:ASN:HB2	1.94	0.48
24:A:848:CLA:H121	16:J:18:TRP:CD1	2.49	0.48
14:G:20:ARG:HG3	14:G:64:VAL:HG11	1.95	0.48
15:I:32:LYS:HD2	15:I:35:ILE:HG22	1.96	0.48
24:L:202:CLA:H143	24:L:202:CLA:H162	1.74	0.48
4:3:192:LEU:HD21	6:7:65:MET:HE3	1.95	0.48
5:6:64:TRP:CE2	23:6:307:CHL:HED2	2.48	0.48
9:A:695:ARG:NH1	9:A:722:ALA:O	2.47	0.48
10:B:571:SER:OG	10:B:574:ASP:OD2	2.32	0.48
13:F:199:ILE:O	16:J:11:ALA:N	2.47	0.48
7:4:145:ILE:HG21	23:4:315:CHL:HBA1	1.96	0.48
2:1:46:PRO:HD2	2:1:49:LEU:HD11	1.96	0.48
27:2:317:LHG:HC81	23:3:301:CHL:C1C	2.43	0.48
24:3:309:CLA:HBA2	24:3:309:CLA:H3A	1.50	0.48
5:6:114:ARG:CZ	5:6:125:VAL:HG12	2.44	0.48
5:6:114:ARG:NH2	5:6:125:VAL:HG12	2.28	0.48
24:7:308:CLA:H11	24:7:316:CLA:HBC2	1.95	0.48
8:9:95:GLU:HG3	8:9:101:THR:HA	1.96	0.48
8:9:143:THR:HB	8:9:145:MET:HE3	1.96	0.48
24:9:307:CLA:H62	24:9:307:CLA:H2	1.59	0.48
9:A:178:MET:HE1	24:A:812:CLA:H71	1.96	0.48
24:A:830:CLA:HAB	24:A:837:CLA:HBB2	1.95	0.48
24:B:806:CLA:HBC2	24:B:806:CLA:HHD	1.95	0.48
5:6:97:ILE:HG13	5:6:98:ILE:HD12	1.96	0.48
24:B:824:CLA:HHB	24:B:841:CLA:O1D	2.14	0.48
11:D:154:PHE:CE2	11:D:167:HIS:HB2	2.49	0.48
2:1:70:MET:HE2	24:B:841:CLA:HAB	1.95	0.47
27:1:317:LHG:HC91	25:4:316:8CT:C05	2.44	0.47
4:3:153:TRP:H	4:3:153:TRP:CD1	2.32	0.47
5:6:112:GLU:OE1	5:6:115:ARG:NH1	2.30	0.47
9:A:436:ILE:O	9:A:439:ARG:HG3	2.14	0.47
9:A:583:PRO:HD3	10:B:561:GLY:HA2	1.94	0.47
9:A:723:LEU:HD21	31:A:841:PQN:H151	1.95	0.47
11:D:102:ILE:HG23	11:D:129:LEU:HB3	1.95	0.47
24:0:310:CLA:O1A	24:0:310:CLA:H2A	2.13	0.47
24:3:306:CLA:HBC2	27:3:320:LHG:H251	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:86:HIS:HB3	7:8:205:MET:HE3	1.96	0.47
10:B:290:MET:HE1	24:B:820:CLA:CAD	2.44	0.47
1:0:58:PRO:O	1:0:241:ARG:NH1	2.38	0.47
2:1:114:TRP:CD1	2:1:119:MET:HG2	2.49	0.47
7:8:108:ILE:C	7:8:110:LEU:H	2.22	0.47
7:8:166:LYS:O	7:8:168:PRO:HD3	2.14	0.47
2:5:98:ASN:HB2	2:5:200:PRO:HD2	1.96	0.47
5:6:95:PHE:HB3	7:8:234:TRP:CG	2.50	0.47
7:8:144:GLU:HG3	7:8:147:ARG:HH12	1.79	0.47
8:9:155:ASP:O	8:9:156:PRO:C	2.58	0.47
24:B:832:CLA:H12	13:F:177:THR:HB	1.97	0.47
14:G:38:GLN:N	14:G:41:LEU:O	2.44	0.47
19:K:66:PHE:CE2	24:K:104:CLA:HAB	2.50	0.47
7:4:88:ARG:HA	7:4:91:MET:HE3	1.96	0.47
1:0:150:ASP:O	1:0:152:LEU:N	2.48	0.47
1:0:204:ILE:HD11	1:0:213:VAL:HG21	1.97	0.47
10:B:714:SER:HB2	34:B:849:DGD:HBH1	1.95	0.47
24:B:839:CLA:H122	24:B:840:CLA:H13	1.97	0.47
1:0:79:GLY:O	1:0:83:MET:HG3	2.14	0.47
3:2:229:PRO:O	26:2:315:0UR:O39	2.33	0.47
24:5:302:CLA:H42	7:4:166:LYS:HG3	1.97	0.47
6:7:210:LEU:HD12	24:7:312:CLA:HAC2	1.96	0.47
7:8:146:ARG:HD2	23:8:301:CHL:HED3	1.97	0.47
9:A:44:LEU:HD13	9:A:57:LEU:HA	1.97	0.47
1:0:180:GLN:HB3	1:0:191:ASN:ND2	2.30	0.47
24:1:303:CLA:H43	23:1:304:CHL:HBD	1.95	0.47
6:7:87:TRP:CE2	24:7:308:CLA:HBC3	2.50	0.47
8:9:145:MET:SD	8:9:153:PRO:HG3	2.55	0.47
9:A:34:TRP:HE1	24:A:810:CLA:CHB	2.26	0.47
24:A:807:CLA:H193	24:A:807:CLA:H162	1.74	0.47
24:A:825:CLA:H141	24:A:825:CLA:H161	1.70	0.47
24:A:825:CLA:H101	24:A:825:CLA:H62	1.60	0.47
10:B:15:ASP:HB3	10:B:20:ARG:HB2	1.97	0.47
10:B:283:LEU:HD22	24:B:818:CLA:HMC1	1.97	0.47
10:B:359:ALA:O	10:B:360:PHE:HB2	2.15	0.47
10:B:415:LYS:O	10:B:419:ILE:HG12	2.14	0.47
10:B:653:GLY:HA3	10:B:720:THR:HG23	1.95	0.47
13:F:93:ARG:NH2	13:F:142:ASP:O	2.42	0.47
1:0:102:GLU:HA	23:0:306:CHL:HED1	1.97	0.47
2:1:49:LEU:HD22	2:1:71:ILE:HD11	1.97	0.47
10:B:203:ARG:NH2	10:B:253:ALA:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:801:CLA:HBA2	14:G:50:ARG:HD3	1.97	0.47
14:G:81:VAL:O	14:G:85:ILE:HG12	2.15	0.47
17:L:10:ILE:HA	17:L:20:GLU:HG2	1.97	0.47
7:4:122:ALA:C	7:4:124:PRO:HD3	2.40	0.47
1:0:76:LEU:O	1:0:80:ARG:HG3	2.15	0.47
7:8:159:VAL:HG22	7:8:168:PRO:HD2	1.96	0.47
7:8:196:LYS:HD3	24:8:312:CLA:HBD	1.97	0.47
24:9:307:CLA:H141	24:9:307:CLA:H203	1.95	0.47
9:A:435:VAL:HA	9:A:438:HIS:CE1	2.50	0.47
24:A:805:CLA:H61	24:A:805:CLA:H2	1.67	0.47
24:A:831:CLA:H93	24:A:831:CLA:H62	1.70	0.47
10:B:84:ILE:HD13	22:H:145:ILE:HB	1.97	0.47
10:B:102:GLU:OE1	22:H:135:LYS:NZ	2.36	0.47
10:B:519:VAL:HG21	10:B:593:TYR:HB2	1.96	0.47
23:6:302:CHL:HBC1	27:6:322:LHG:H282	1.97	0.47
9:A:215:SER:OG	9:A:303:HIS:O	2.33	0.47
7:4:136:GLN:O	7:4:140:MET:HB2	2.15	0.47
24:4:304:CLA:H51	23:4:305:CHL:HBD	1.96	0.47
23:3:307:CHL:HBA1	25:3:323:8CT:C24	2.45	0.46
2:5:198:LYS:HE2	2:5:202:GLN:HG3	1.97	0.46
24:6:312:CLA:H101	27:6:322:LHG:H142	1.96	0.46
24:A:807:CLA:CHC	24:A:808:CLA:HMD2	2.45	0.46
2:1:91:GLN:HE22	2:1:96:PHE:HD2	1.62	0.46
2:1:148:MET:O	2:1:152:VAL:HG23	2.15	0.46
3:2:111:ASP:OD1	3:2:111:ASP:N	2.48	0.46
24:2:309:CLA:HED2	24:2:309:CLA:H2A	1.96	0.46
23:9:306:CHL:HBA1	23:9:306:CHL:H3A	1.64	0.46
9:A:302:HIS:CE1	9:A:306:ILE:HD13	2.50	0.46
9:A:589:CYS:HB2	10:B:667:TRP:HB3	1.97	0.46
24:B:819:CLA:H62	24:B:819:CLA:H41	1.57	0.46
24:B:823:CLA:HHC	24:B:841:CLA:HED1	1.97	0.46
16:J:24:SER:CB	24:J:103:CLA:HAB	2.45	0.46
18:C:25:VAL:HG21	18:C:48:CYS:HA	1.97	0.46
7:4:146:ARG:HA	23:4:315:CHL:HED3	1.97	0.46
24:0:313:CLA:HMA3	27:I:102:LHG:H241	1.97	0.46
3:2:206:LYS:NZ	27:2:317:LHG:O4	2.32	0.46
2:5:63:ASN:HB3	2:5:66:ASN:HB2	1.98	0.46
7:8:97:MET:O	7:8:100:PRO:HD2	2.15	0.46
9:A:366:GLY:HA2	9:A:403:GLY:HA2	1.96	0.46
27:A:842:LHG:O1	27:A:842:LHG:O3	2.28	0.46
24:B:809:CLA:H192	24:B:809:CLA:H161	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:810:CLA:HBC2	24:B:810:CLA:HHD	1.97	0.46
2:1:70:MET:HA	2:1:73:CYS:HG	1.81	0.46
4:3:215:LEU:HB2	24:3:309:CLA:HBA1	1.98	0.46
24:7:308:CLA:H42	24:7:316:CLA:HBC1	1.97	0.46
9:A:686:PHE:HZ	24:A:839:CLA:HBC2	1.79	0.46
10:B:382:MET:HE3	24:B:809:CLA:HMB1	1.96	0.46
21:O:127:GLY:C	24:O:206:CLA:HMA3	2.40	0.46
24:0:311:CLA:H121	27:0:317:LHG:H101	1.96	0.46
9:A:206:HIS:ND1	24:A:824:CLA:OBD	2.48	0.46
9:A:431:LEU:HD13	24:A:823:CLA:C1C	2.45	0.46
24:A:806:CLA:HBB1	24:A:806:CLA:HMB1	1.96	0.46
10:B:374:HIS:HB2	24:B:828:CLA:C1B	2.46	0.46
10:B:558:PRO:HB3	10:B:702:ILE:HB	1.97	0.46
24:B:809:CLA:HHB	24:B:830:CLA:HAB	1.97	0.46
24:B:834:CLA:HBC2	24:B:835:CLA:HAB	1.97	0.46
16:J:2:GLN:O	16:J:6:ILE:HG13	2.16	0.46
7:4:179:ILE:HG23	7:4:179:ILE:O	2.15	0.46
3:2:248:ASN:OD1	3:2:249:GLY:N	2.48	0.46
23:2:301:CHL:H93	23:2:301:CHL:H61	1.73	0.46
9:A:15:ILE:HG13	9:A:16:LYS:H	1.80	0.46
24:A:827:CLA:H41	24:A:827:CLA:H61	1.55	0.46
10:B:585:ASN:HB2	24:B:804:CLA:HBC2	1.98	0.46
14:G:11:SER:HB2	14:G:82:ALA:HB2	1.97	0.46
2:1:104:SER:HA	2:1:108:GLU:OE1	2.14	0.46
23:2:312:CHL:H12	23:3:305:CHL:H42	1.96	0.46
2:5:127:LEU:HD21	23:5:304:CHL:C4D	2.46	0.46
6:7:89:MET:HE3	6:7:198:GLY:N	2.30	0.46
24:9:308:CLA:HMB3	24:9:310:CLA:HAA1	1.98	0.46
9:A:361:ASN:O	9:A:365:PHE:HB2	2.15	0.46
1:0:192:LEU:O	1:0:196:ILE:HG12	2.15	0.46
23:1:301:CHL:H143	23:1:301:CHL:H162	1.72	0.46
4:3:189:PHE:N	4:3:193:GLU:OE1	2.39	0.46
23:6:301:CHL:H12	27:6:322:LHG:H131	1.97	0.46
7:8:55:ASP:OD1	7:8:55:ASP:N	2.47	0.46
7:8:144:GLU:HG3	7:8:147:ARG:NH1	2.30	0.46
17:L:38:ALA:O	17:L:48:ARG:NH2	2.48	0.46
23:1:304:CHL:HMB1	24:1:307:CLA:HBC2	1.97	0.46
4:3:169:PHE:O	4:3:173:ARG:HB2	2.15	0.46
24:6:303:CLA:H61	24:6:303:CLA:H41	1.58	0.46
24:7:304:CLA:H62	24:7:304:CLA:H41	1.68	0.46
24:A:805:CLA:H41	27:A:842:LHG:H271	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:4:88:ARG:HB3	24:4:309:CLA:CAC	2.46	0.46
1:0:150:ASP:OD2	1:0:154:MET:HB2	2.16	0.46
23:1:312:CHL:HAA2	7:4:135:MET:HE2	1.98	0.46
24:6:310:CLA:H2A	24:6:310:CLA:HED2	1.98	0.46
9:A:124:TRP:CD2	24:A:808:CLA:HED3	2.51	0.46
9:A:610:ILE:HD12	32:A:852:CL0:H53	1.98	0.46
24:A:830:CLA:HBA2	27:A:843:LHG:HC92	1.98	0.46
10:B:128:GLY:HA2	10:B:130:ARG:NH1	2.30	0.46
10:B:441:ASP:OD1	10:B:616:LEU:N	2.41	0.46
2:1:88:MET:HE1	2:1:186:PHE:CD1	2.50	0.45
2:5:127:LEU:HD11	23:5:304:CHL:C2D	2.45	0.45
24:7:308:CLA:H121	24:7:308:CLA:H162	1.41	0.45
21:O:122:THR:HG23	24:O:201:CLA:HBA2	1.98	0.45
24:4:310:CLA:H43	24:4:311:CLA:HMD2	1.97	0.45
3:2:236:HIS:CG	24:2:311:CLA:HAA2	2.50	0.45
4:3:218:THR:C	4:3:220:GLU:H	2.25	0.45
24:3:313:CLA:H3A	24:3:313:CLA:HBA2	1.57	0.45
2:5:69:ARG:NH2	24:5:302:CLA:O1D	2.48	0.45
24:7:308:CLA:H91	24:7:308:CLA:H111	1.67	0.45
24:7:312:CLA:H61	24:7:312:CLA:H92	1.73	0.45
8:9:95:GLU:CD	8:9:194:VAL:HG12	2.42	0.45
9:A:699:GLN:O	9:A:703:GLU:HG3	2.17	0.45
24:A:829:CLA:H42	27:A:842:LHG:H241	1.99	0.45
10:B:22:TRP:CG	10:B:704:GLN:HE22	2.34	0.45
10:B:101:VAL:O	10:B:105:THR:HG23	2.17	0.45
24:B:819:CLA:H3A	24:B:819:CLA:HBA2	1.48	0.45
7:4:114:GLY:O	7:4:116:GLU:N	2.49	0.45
24:0:303:CLA:H62	24:0:303:CLA:H41	1.57	0.45
8:9:157:LEU:O	8:9:158:GLY:C	2.59	0.45
9:A:484:LEU:H	9:A:535:THR:HG22	1.81	0.45
24:A:813:CLA:H62	24:A:813:CLA:H101	1.70	0.45
24:A:821:CLA:H12	24:K:104:CLA:HMB2	1.98	0.45
10:B:286:ILE:O	24:B:822:CLA:HBC1	2.16	0.45
24:B:811:CLA:H143	24:B:811:CLA:H161	1.75	0.45
24:B:831:CLA:HBB2	24:B:838:CLA:HMC1	1.97	0.45
24:B:834:CLA:H3A	24:B:834:CLA:HBA2	1.49	0.45
1:0:72:ARG:NH1	1:0:75:GLU:OE1	2.50	0.45
23:0:302:CHL:H161	23:0:302:CHL:H122	1.53	0.45
24:3:303:CLA:H2	24:3:303:CLA:H61	1.54	0.45
23:5:305:CHL:HHC	23:5:305:CHL:HBB1	1.97	0.45
5:6:47:ASN:OD1	5:6:47:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:808:CLA:H91	24:A:808:CLA:H111	1.67	0.45
24:B:809:CLA:HED1	24:B:830:CLA:H2	1.98	0.45
11:D:104:TRP:NE1	11:D:122:MET:SD	2.88	0.45
17:L:69:PRO:HG3	24:H:202:CLA:HBA2	1.99	0.45
23:4:308:CHL:H3A	23:4:308:CHL:HBA1	1.78	0.45
1:0:162:LYS:HD3	24:0:310:CLA:HBA1	1.99	0.45
23:2:301:CHL:H161	23:2:301:CHL:H122	1.45	0.45
23:7:301:CHL:HHC	23:7:301:CHL:HBB1	1.99	0.45
7:8:56:GLY:HA2	7:8:61:ASP:HB3	1.98	0.45
9:A:643:SER:OG	9:A:653:ASP:OD2	2.22	0.45
9:A:697:TYR:CE2	10:B:536:LYS:HD2	2.51	0.45
24:A:807:CLA:H3A	24:A:807:CLA:HBA2	1.38	0.45
24:A:812:CLA:H93	24:A:812:CLA:H111	1.73	0.45
24:A:838:CLA:H172	13:F:181:GLY:HA2	1.99	0.45
24:B:826:CLA:HMA1	25:B:847:8CT:C17	2.47	0.45
24:B:836:CLA:HBB1	24:B:836:CLA:HMB1	1.97	0.45
12:E:11:VAL:HB	12:E:61:VAL:HG13	1.98	0.45
18:C:3:HIS:HE1	18:C:76:SER:HB2	1.79	0.45
2:1:85:VAL:HG13	2:1:189:PHE:CE2	2.52	0.45
4:3:246:GLN:O	4:3:250:THR:OG1	2.27	0.45
23:7:307:CHL:CBB	24:7:314:CLA:HMC2	2.47	0.45
7:8:161:PRO:HB3	23:8:316:CHL:C1C	2.47	0.45
9:A:439:ARG:NH1	9:A:564:SER:O	2.49	0.45
10:B:430:GLY:HA2	10:B:525:LEU:HD22	1.98	0.45
24:B:832:CLA:H62	24:B:832:CLA:H2	1.70	0.45
17:L:6:VAL:HG13	21:O:50:TRP:HB2	1.97	0.45
7:4:116:GLU:CD	7:4:116:GLU:H	2.25	0.45
1:0:109:VAL:HG12	1:0:111:ILE:H	1.82	0.45
1:0:128:GLU:HG3	24:0:307:CLA:NB	2.32	0.45
2:1:72:GLU:HG3	2:1:152:VAL:HG22	1.98	0.45
23:2:301:CHL:H93	23:2:301:CHL:H111	1.70	0.45
9:A:705:ILE:HD13	24:A:838:CLA:HMD1	1.99	0.45
7:4:97:MET:HE1	7:4:208:THR:HG23	1.98	0.45
7:4:159:VAL:HG13	7:4:162:ILE:HB	1.99	0.45
4:3:168:GLN:NE2	24:3:314:CLA:O1D	2.50	0.45
24:6:304:CLA:HMB1	23:6:305:CHL:HBB1	1.98	0.45
7:8:103:LEU:HD13	7:8:111:PRO:HG2	1.99	0.45
24:9:307:CLA:H111	24:9:307:CLA:H142	1.63	0.45
9:A:703:GLU:CD	10:B:545:LYS:HB2	2.41	0.45
31:A:841:PQN:H141	24:A:848:CLA:HBB2	1.99	0.45
24:B:830:CLA:H42	34:B:849:DGD:HB42	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:219:ASN:ND2	24:1:311:CLA:OBD	2.50	0.45
3:2:113:PRO:HG3	3:2:121:VAL:HG21	1.99	0.45
27:6:322:LHG:O3	27:6:322:LHG:O1	2.29	0.45
6:7:240:GLY:O	6:7:264:GLN:N	2.49	0.45
23:7:302:CHL:H143	23:7:302:CHL:H162	1.79	0.45
9:A:594:TRP:NE1	24:A:829:CLA:HMD3	2.31	0.45
27:A:850:LHG:H242	27:A:850:LHG:HC61	1.76	0.45
10:B:134:ASP:OD2	10:B:208:ARG:NE	2.49	0.45
7:4:229:HIS:CG	24:4:312:CLA:HAA2	2.52	0.45
4:3:195:VAL:HG23	4:3:208:ALA:HB3	1.99	0.45
10:B:686:PRO:HD2	24:L:201:CLA:HBA1	1.99	0.45
24:B:804:CLA:H142	24:B:804:CLA:H112	1.76	0.45
24:B:817:CLA:H61	24:B:817:CLA:H41	1.77	0.45
7:4:217:VAL:HG11	7:4:241:ILE:HD13	1.98	0.45
9:A:33:LYS:HB2	24:A:810:CLA:HAA2	2.00	0.44
24:A:830:CLA:HAB	24:A:837:CLA:CBB	2.47	0.44
24:A:836:CLA:HBB1	24:A:837:CLA:CHD	2.47	0.44
24:A:840:CLA:H41	24:A:840:CLA:H62	1.59	0.44
29:A:854:LMG:H111	29:A:854:LMG:H142	1.72	0.44
10:B:86:PRO:HB3	10:B:121:TYR:CG	2.52	0.44
24:F:303:CLA:HBA1	24:F:303:CLA:H3A	1.60	0.44
2:5:130:ILE:HA	2:5:133:VAL:HG12	1.99	0.44
2:5:161:ALA:O	2:5:163:PHE:N	2.51	0.44
24:7:304:CLA:H71	23:7:305:CHL:HBD	1.98	0.44
9:A:295:TRP:HB2	9:A:298:ASP:OD2	2.17	0.44
10:B:174:ARG:HH11	24:B:808:CLA:H141	1.82	0.44
24:1:302:CLA:H62	24:1:302:CLA:H41	1.59	0.44
27:1:317:LHG:H151	27:1:317:LHG:H322	1.98	0.44
24:3:303:CLA:HBB1	24:3:303:CLA:HMB3	1.99	0.44
6:7:259:CYS:O	27:7:323:LHG:HC62	2.16	0.44
23:8:306:CHL:HBA1	25:8:317:8CT:C15	2.48	0.44
9:A:337:PRO:HB2	17:L:6:VAL:HG23	1.99	0.44
9:A:434:ARG:O	9:A:438:HIS:ND1	2.48	0.44
24:B:839:CLA:H2A	15:I:27:PHE:HE2	1.82	0.44
7:4:160:ASP:OD1	7:4:160:ASP:N	2.50	0.44
23:6:313:CHL:HAA2	6:7:131:PHE:HA	2.00	0.44
9:A:225:LEU:C	9:A:228:PRO:HD2	2.43	0.44
9:A:601:LEU:HB3	9:A:737:ILE:HD11	1.99	0.44
27:A:850:LHG:O3	27:A:850:LHG:O1	2.31	0.44
10:B:290:MET:CB	24:B:822:CLA:HBC3	2.45	0.44
10:B:347:MET:O	10:B:351:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:78:THR:HG23	11:D:126:PRO:HB2	1.98	0.44
7:4:58:ILE:HG22	7:4:59:PRO:HD2	2.00	0.44
7:4:190:VAL:HG12	7:4:194:LYS:HE3	1.98	0.44
7:4:222:PRO:O	26:4:317:0UR:O39	2.36	0.44
1:0:161:LEU:HD23	24:0:309:CLA:HED2	1.99	0.44
1:0:241:ARG:HH22	28:0:318:SQD:H5	1.83	0.44
24:3:306:CLA:H3A	24:3:306:CLA:HBA2	1.65	0.44
23:6:301:CHL:H142	23:6:301:CHL:H111	1.81	0.44
8:9:45:PRO:HG3	14:G:54:TYR:HE1	1.83	0.44
9:A:121:GLN:NE2	24:A:808:CLA:OBD	2.47	0.44
9:A:133:ASN:HB3	9:A:141:GLN:HB3	1.99	0.44
9:A:716:PRO:HG2	9:A:720:PRO:HD3	2.00	0.44
24:A:827:CLA:H93	24:A:827:CLA:H62	1.77	0.44
24:B:811:CLA:H91	24:B:811:CLA:H112	1.72	0.44
12:E:54:ASN:ND2	18:C:61:ASP:HB2	2.33	0.44
14:G:54:TYR:CG	14:G:55:VAL:N	2.85	0.44
16:J:26:ILE:HG21	25:J:104:8CT:C29	2.48	0.44
1:0:243:ILE:O	1:0:245:TRP:N	2.47	0.44
2:1:133:VAL:HG22	14:G:14:LEU:HD13	1.99	0.44
23:1:305:CHL:HHC	23:1:305:CHL:HBB1	1.99	0.44
3:2:135:MET:HB2	23:4:313:CHL:HED1	2.00	0.44
5:6:212:LEU:O	6:7:256:PRO:HD3	2.17	0.44
9:A:14:GLU:OE2	9:A:326:SER:OG	2.35	0.44
9:A:665:SER:O	9:A:671:SER:HA	2.17	0.44
10:B:128:GLY:O	10:B:208:ARG:NH2	2.51	0.44
10:B:340:SER:O	10:B:344:ILE:HG12	2.17	0.44
24:B:808:CLA:HBB1	24:B:808:CLA:HMB1	2.00	0.44
24:B:812:CLA:HBA2	24:B:812:CLA:H3A	1.87	0.44
24:B:836:CLA:H112	24:B:836:CLA:H91	1.64	0.44
27:I:102:LHG:H371	20:M:23:LEU:HD11	2.00	0.44
24:L:202:CLA:H3A	24:L:202:CLA:HBA2	1.65	0.44
7:4:98:LEU:O	7:4:102:LEU:N	2.43	0.44
7:4:98:LEU:HD13	7:4:211:PHE:HZ	1.82	0.44
1:0:74:ALA:O	1:0:78:ASN:ND2	2.37	0.44
8:9:213:VAL:HG11	27:B:852:LHG:H251	2.00	0.44
9:A:119:SER:HB2	9:A:136:VAL:HG11	1.99	0.44
9:A:536:SER:O	9:A:540:VAL:HG23	2.18	0.44
10:B:658:ALA:HB3	24:B:806:CLA:HBB2	1.99	0.44
17:L:3:GLN:OE1	21:O:131:ARG:HB2	2.18	0.44
7:4:137:PHE:CD2	23:4:308:CHL:HBB2	2.53	0.44
2:5:213:GLY:HA2	2:5:218:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:45:LEU:HB3	7:8:48:ALA:HB2	1.99	0.44
23:8:316:CHL:HHC	23:8:316:CHL:HBB1	2.00	0.44
9:A:401:TRP:CD1	24:A:827:CLA:HAB	2.53	0.44
9:A:519:ILE:HD13	9:A:632:VAL:HG21	2.00	0.44
10:B:290:MET:HE1	24:B:820:CLA:C3D	2.48	0.44
10:B:583:MET:HG2	24:B:826:CLA:HBC1	2.00	0.44
24:B:802:CLA:HMC1	24:B:838:CLA:HAC1	2.00	0.44
1:0:200:LEU:HD21	8:9:114:VAL:HG23	1.99	0.44
2:1:112:PRO:HG2	2:1:114:TRP:CZ2	2.53	0.44
8:9:212:ASN:ND2	24:9:311:CLA:OBD	2.51	0.44
9:A:29:THR:HG21	9:A:183:TRP:NE1	2.21	0.44
9:A:603:TRP:HE1	24:B:806:CLA:C1D	2.30	0.44
24:A:816:CLA:H41	24:A:816:CLA:H61	1.71	0.44
24:B:828:CLA:H3A	24:B:828:CLA:HBA2	1.39	0.44
17:L:28:ILE:HD12	17:L:28:ILE:H	1.83	0.44
7:4:171:ASN:HB2	7:4:178:GLY:HA2	1.99	0.44
24:6:310:CLA:HAB	6:7:158:VAL:HG12	2.00	0.43
8:9:121:LEU:HD12	8:9:121:LEU:HA	1.80	0.43
9:A:126:ILE:HG12	9:A:127:VAL:H	1.83	0.43
9:A:183:TRP:HB2	24:A:810:CLA:HMC2	2.00	0.43
9:A:272:LEU:O	19:K:79:LYS:NZ	2.47	0.43
32:A:852:CL0:H14	24:B:805:CLA:C1A	2.48	0.43
17:L:40:ARG:HD2	22:H:80:ARG:HH11	1.82	0.43
23:4:301:CHL:H41	23:4:301:CHL:H62	1.57	0.43
2:1:145:GLU:HB3	2:1:151:ARG:HG3	2.00	0.43
2:5:44:TYR:OH	2:5:59:GLY:HA2	2.18	0.43
24:7:317:CLA:HBA1	24:7:317:CLA:H3A	1.60	0.43
9:A:296:LEU:HD23	9:A:299:ILE:HD12	2.00	0.43
10:B:378:ILE:O	10:B:382:MET:HG3	2.18	0.43
10:B:582:TRP:O	10:B:586:THR:HG22	2.17	0.43
24:B:822:CLA:H143	14:G:81:VAL:HB	1.99	0.43
24:B:827:CLA:H202	24:B:827:CLA:H162	1.74	0.43
17:L:40:ARG:HD2	22:H:80:ARG:NH1	2.33	0.43
7:4:243:LEU:HD22	7:4:244:ALA:N	2.33	0.43
2:5:225:PHE:HD1	2:5:225:PHE:H	1.66	0.43
24:9:303:CLA:HED2	24:9:303:CLA:H12	1.99	0.43
23:9:312:CHL:H3A	23:9:312:CHL:HBA2	1.82	0.43
9:A:145:ILE:HD12	24:A:807:CLA:CAD	2.48	0.43
24:A:809:CLA:HBB2	24:A:812:CLA:HMA3	1.99	0.43
22:H:76:GLU:OE1	22:H:76:GLU:N	2.49	0.43
24:1:311:CLA:H111	24:1:311:CLA:H93	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:52:ARG:HA	4:3:52:ARG:HD3	1.80	0.43
2:5:191:LEU:HD12	24:5:311:CLA:HAC2	2.01	0.43
8:9:159:MET:HG3	24:9:308:CLA:O1A	2.18	0.43
9:A:458:PHE:O	9:A:462:ILE:HG12	2.18	0.43
24:A:813:CLA:H62	24:A:813:CLA:H41	1.75	0.43
10:B:275:HIS:HB3	24:B:818:CLA:HMB2	2.00	0.43
10:B:444:LEU:HD22	10:B:615:TYR:CZ	2.54	0.43
1:0:175:VAL:HG12	24:0:311:CLA:HAC1	2.01	0.43
4:3:189:PHE:CZ	23:3:307:CHL:HBB2	2.54	0.43
4:3:189:PHE:CE2	23:3:307:CHL:HBB2	2.53	0.43
2:5:42:PRO:HB2	2:5:44:TYR:CE2	2.53	0.43
2:5:158:PHE:HE1	23:5:306:CHL:HBA2	1.83	0.43
23:6:301:CHL:H92	23:6:301:CHL:H61	1.77	0.43
23:6:315:CHL:HHC	23:6:315:CHL:HBB1	2.00	0.43
27:7:323:LHG:H111	27:7:323:LHG:H142	1.85	0.43
7:8:222:PRO:O	26:8:318:0UR:O39	2.36	0.43
24:8:315:CLA:HBA1	24:8:315:CLA:H3A	1.24	0.43
8:9:77:GLU:HB2	24:9:302:CLA:C1B	2.48	0.43
8:9:145:MET:HE3	8:9:145:MET:HB2	1.62	0.43
8:9:152:PHE:CB	8:9:153:PRO:CD	2.95	0.43
9:A:18:VAL:HG21	9:A:319:THR:HB	1.98	0.43
24:A:838:CLA:H51	24:A:838:CLA:C4C	2.48	0.43
32:A:852:CL0:H15	24:B:804:CLA:CED	2.37	0.43
10:B:325:THR:HG21	10:B:403:ASN:OD1	2.17	0.43
10:B:378:ILE:HD13	24:B:829:CLA:CBB	2.49	0.43
10:B:652:PHE:O	10:B:656:VAL:HG23	2.19	0.43
2:1:114:TRP:HD1	2:1:118:GLY:O	2.01	0.43
27:3:324:LHG:H262	24:K:102:CLA:C1D	2.48	0.43
24:5:308:CLA:H102	24:5:310:CLA:HBC1	2.00	0.43
5:6:204:ILE:HD13	24:6:312:CLA:HMD3	2.00	0.43
8:9:61:LEU:O	24:B:813:CLA:HBA1	2.19	0.43
9:A:125:PRO:HA	9:A:130:GLU:HG3	2.01	0.43
9:A:661:GLN:O	9:A:665:SER:HB3	2.19	0.43
24:A:802:CLA:H193	24:B:804:CLA:H192	2.00	0.43
24:B:811:CLA:C1A	24:B:811:CLA:CGA	2.97	0.43
24:B:814:CLA:H162	24:B:814:CLA:H192	1.68	0.43
24:0:303:CLA:H142	24:0:303:CLA:H111	1.79	0.43
2:1:61:SER:OG	2:1:61:SER:O	2.33	0.43
9:A:291:ASN:HB3	9:A:383:PRO:HA	2.01	0.43
9:A:458:PHE:CE1	24:A:801:CLA:HHB	2.54	0.43
24:A:829:CLA:H41	24:A:829:CLA:H62	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:257:PHE:HZ	24:B:818:CLA:H71	1.83	0.43
10:B:282:VAL:HG21	24:B:817:CLA:HAB	2.01	0.43
10:B:451:LYS:HB3	24:B:833:CLA:HED3	2.00	0.43
24:B:830:CLA:H62	24:B:830:CLA:H41	1.87	0.43
11:D:156:ARG:HB2	11:D:166:LEU:HD11	2.01	0.43
13:F:222:ASN:HB3	7:4:75:THR:HG21	2.00	0.43
18:C:55:GLU:HB3	18:C:63:LEU:HD13	2.01	0.43
2:5:60:ILE:HB	23:5:301:CHL:O1A	2.19	0.43
7:8:172:ILE:HD13	7:8:172:ILE:HA	1.88	0.43
8:9:157:LEU:O	8:9:159:MET:HG2	2.19	0.43
9:A:302:HIS:HB2	24:A:817:CLA:CHB	2.48	0.43
9:A:343:HIS:HB3	9:A:346:LEU:HD12	2.00	0.43
24:A:828:CLA:H91	24:A:828:CLA:H111	1.69	0.43
24:B:806:CLA:H111	24:B:806:CLA:H142	1.64	0.43
24:B:814:CLA:H93	24:B:814:CLA:H61	1.87	0.43
13:F:135:SER:HB2	16:J:38:ILE:HD11	2.01	0.43
24:L:201:CLA:H121	24:L:201:CLA:H8	1.79	0.43
27:3:324:LHG:H311	24:K:102:CLA:C4B	2.49	0.43
24:5:313:CLA:HBA1	24:5:313:CLA:H3A	1.58	0.43
24:8:305:CLA:H141	24:8:305:CLA:H162	1.73	0.43
24:8:313:CLA:HMD2	24:8:315:CLA:HBC3	2.01	0.43
8:9:94:CYS:HB3	8:9:99:ILE:O	2.19	0.43
24:A:805:CLA:H62	24:A:805:CLA:H102	1.65	0.43
10:B:59:LEU:HD23	10:B:59:LEU:HA	1.89	0.43
24:B:802:CLA:H111	24:B:802:CLA:H142	1.82	0.43
24:B:811:CLA:H111	24:B:811:CLA:H142	1.77	0.43
24:B:825:CLA:H143	24:B:825:CLA:H161	1.80	0.43
24:B:837:CLA:H192	24:B:837:CLA:H161	1.82	0.43
17:L:23:VAL:O	17:L:29:VAL:HG11	2.18	0.43
24:1:311:CLA:H42	23:1:312:CHL:HMD1	2.01	0.43
3:2:178:TYR:HB3	24:2:308:CLA:HED2	2.01	0.43
4:3:76:TYR:HD2	23:3:302:CHL:HMD2	1.83	0.43
24:6:316:CLA:HBB1	24:6:316:CLA:HMB1	2.00	0.43
6:7:144:TRP:HB2	24:7:308:CLA:CMA	2.48	0.43
24:7:316:CLA:HBA2	24:7:316:CLA:CGD	2.49	0.43
7:8:181:ASP:OD1	26:8:318:0UR:O40	2.37	0.43
9:A:513:LEU:HB2	9:A:528:MET:HG3	1.99	0.43
9:A:697:TYR:HA	10:B:536:LYS:HZ2	1.83	0.43
24:A:853:CLA:H193	24:A:853:CLA:H162	1.83	0.43
14:G:41:LEU:HD12	14:G:45:GLU:HB3	2.01	0.43
7:4:193:LEU:HD13	24:4:309:CLA:O1A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:254:PRO:O	26:3:318:0UR:O39	2.37	0.42
2:5:85:VAL:HG13	2:5:189:PHE:CE2	2.53	0.42
23:6:323:CHL:HBB2	23:8:303:CHL:HBC2	2.01	0.42
7:8:149:GLN:CB	7:8:158:ASN:HD21	2.29	0.42
9:A:412:ALA:HB2	9:A:597:VAL:HG11	2.01	0.42
24:A:826:CLA:H2	24:A:826:CLA:H61	1.76	0.42
10:B:69:ALA:HB2	10:B:135:LEU:HB2	2.01	0.42
10:B:240:ILE:HA	10:B:263:PRO:HG2	2.00	0.42
10:B:616:LEU:HD23	10:B:616:LEU:HA	1.90	0.42
10:B:662:MET:HB2	24:B:806:CLA:C1C	2.49	0.42
29:O:210:LMG:H292	29:O:210:LMG:H142	2.01	0.42
3:2:185:ASP:OD1	26:2:315:0UR:O40	2.36	0.42
4:3:137:TRP:C	4:3:139:ARG:H	2.27	0.42
7:8:136:GLN:HG3	7:8:137:PHE:N	2.33	0.42
24:9:310:CLA:HHC	24:9:310:CLA:HBB1	2.01	0.42
9:A:120:ALA:N	9:A:145:ILE:HG12	2.34	0.42
9:A:316:MET:HE1	24:A:820:CLA:C3D	2.49	0.42
10:B:697:PRO:HB3	24:B:839:CLA:C1C	2.49	0.42
24:B:816:CLA:H142	24:B:816:CLA:H111	1.88	0.42
23:0:301:CHL:H43	24:0:311:CLA:H52	2.01	0.42
23:3:307:CHL:H91	23:3:307:CHL:H112	1.80	0.42
24:3:309:CLA:H62	24:3:309:CLA:H41	1.78	0.42
9:A:548:ILE:HD11	24:A:835:CLA:HBB1	2.02	0.42
27:A:842:LHG:H251	27:A:842:LHG:H281	1.87	0.42
27:A:843:LHG:HC32	24:O:201:CLA:CHC	2.49	0.42
24:A:853:CLA:HBA2	10:B:427:LEU:HD23	2.02	0.42
10:B:700:LEU:HD22	10:B:704:GLN:NE2	2.34	0.42
24:B:809:CLA:H43	34:B:849:DGD:HB51	2.01	0.42
15:I:4:ALA:O	15:I:7:PRO:HD2	2.20	0.42
9:A:195:TRP:CZ2	24:A:809:CLA:HMA1	2.54	0.42
9:A:330:ILE:O	9:A:334:HIS:ND1	2.52	0.42
9:A:364:LEU:HD21	24:A:820:CLA:H71	2.01	0.42
10:B:181:GLY:HA3	24:B:814:CLA:HBB1	2.00	0.42
10:B:276:HIS:HB2	24:B:818:CLA:CHB	2.50	0.42
24:B:823:CLA:H41	24:B:823:CLA:H62	1.55	0.42
14:G:59:LYS:HE3	14:G:59:LYS:HB3	1.76	0.42
2:1:31:ARG:NH2	2:1:33:GLY:O	2.39	0.42
24:2:311:CLA:H2	23:2:312:CHL:HMD1	2.01	0.42
4:3:92:GLY:O	4:3:95:ASN:ND2	2.52	0.42
23:6:308:CHL:H2	23:6:308:CHL:H62	1.73	0.42
6:7:142:ARG:HE	23:7:307:CHL:CMC	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:156:ASP:OD1	6:7:158:VAL:N	2.52	0.42
24:7:304:CLA:CMB	23:7:305:CHL:HBB1	2.49	0.42
9:A:481:THR:O	9:A:483:GLN:HG3	2.19	0.42
9:A:581:ASP:OD2	9:A:585:ARG:NH1	2.44	0.42
9:A:731:VAL:O	9:A:735:HIS:ND1	2.52	0.42
10:B:105:THR:OG1	22:H:137:GLY:HA2	2.19	0.42
21:O:125:GLN:NE2	24:O:201:CLA:HED2	2.34	0.42
1:0:162:LYS:O	1:0:166:ASN:ND2	2.26	0.42
1:0:169:LEU:HD13	24:0:309:CLA:HBC1	2.01	0.42
3:2:103:GLY:C	3:2:230:VAL:HG11	2.43	0.42
24:2:313:CLA:HBC1	4:3:161:PHE:HB2	2.02	0.42
4:3:168:GLN:HE22	24:3:314:CLA:CHA	2.31	0.42
4:3:270:ILE:HD13	24:3:312:CLA:H42	2.02	0.42
24:3:303:CLA:H42	24:A:809:CLA:H11	2.00	0.42
6:7:136:MET:HA	6:7:139:VAL:HG22	2.00	0.42
31:A:841:PQN:H222	24:A:848:CLA:C1B	2.50	0.42
10:B:397:ASP:HA	11:D:198:ILE:HD13	2.00	0.42
24:B:820:CLA:HBC2	24:B:824:CLA:H72	2.00	0.42
13:F:216:TRP:CG	13:F:217:PRO:HD3	2.54	0.42
13:F:232:LYS:HG3	13:F:234:GLU:OE1	2.20	0.42
21:O:55:PRO:HB3	24:O:209:CLA:OBD	2.20	0.42
24:H:201:CLA:HBA2	24:H:201:CLA:H3A	1.60	0.42
7:4:159:VAL:HG22	7:4:161:PRO:HD2	2.00	0.42
7:4:162:ILE:HD13	7:4:162:ILE:HA	1.87	0.42
1:0:212:GLU:H	1:0:212:GLU:HG3	1.54	0.42
24:1:308:CLA:H62	24:1:308:CLA:H41	1.68	0.42
4:3:249:LEU:O	4:3:277:VAL:HA	2.19	0.42
23:8:301:CHL:HBB1	23:8:301:CHL:CHC	2.47	0.42
9:A:310:PHE:CE1	24:A:820:CLA:HAB	2.55	0.42
24:B:808:CLA:HBA1	24:B:808:CLA:H3A	1.47	0.42
24:1:310:CLA:H61	24:1:310:CLA:H41	1.83	0.42
2:5:139:GLU:HG3	24:5:307:CLA:NB	2.34	0.42
23:5:301:CHL:HHD	23:8:301:CHL:HBB2	2.01	0.42
6:7:143:ARG:NH1	24:7:308:CLA:O1D	2.44	0.42
7:8:229:HIS:ND1	7:8:236:ASN:O	2.37	0.42
24:9:307:CLA:H111	24:9:307:CLA:H72	1.52	0.42
9:A:540:VAL:HG11	9:A:614:HIS:CG	2.54	0.42
9:A:729:ARG:NH2	33:B:803:SF4:S4	2.92	0.42
24:A:853:CLA:H143	24:A:853:CLA:H111	1.65	0.42
7:4:138:LEU:HB3	23:4:315:CHL:H43	2.02	0.42
2:1:63:ASN:HD22	10:B:311:PRO:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:80:TRP:CD1	24:1:307:CLA:HMD3	2.54	0.42
4:3:261:HIS:ND1	4:3:268:ASN:O	2.36	0.42
5:6:235:THR:HA	23:6:306:CHL:O1A	2.19	0.42
9:A:99:HIS:CE1	24:A:806:CLA:NA	2.88	0.42
9:A:719:GLN:NE2	12:E:19:TYR:OH	2.52	0.42
24:A:817:CLA:H161	24:A:817:CLA:H122	1.72	0.42
18:C:32:ASP:OD1	18:C:32:ASP:N	2.51	0.42
2:1:65:ALA:O	2:1:68:GLU:HG3	2.20	0.42
6:7:257:LEU:HA	23:7:306:CHL:O1A	2.20	0.42
7:8:146:ARG:NH1	23:8:301:CHL:OBD	2.52	0.42
24:A:805:CLA:H161	24:A:805:CLA:H192	1.69	0.42
24:A:818:CLA:H3A	24:A:818:CLA:HBA2	1.42	0.42
24:B:810:CLA:HMA1	24:B:811:CLA:CHB	2.49	0.42
2:1:82:MET:SD	24:1:308:CLA:HAB	2.60	0.41
7:8:167:LEU:HD23	7:8:169:ASP:H	1.85	0.41
8:9:193:PRO:O	26:9:314:0UR:O39	2.38	0.41
23:9:301:CHL:CGA	27:9:316:LHG:H142	2.50	0.41
9:A:225:LEU:HD11	24:A:813:CLA:C2D	2.50	0.41
9:A:681:HIS:HB3	24:B:804:CLA:HBD	2.02	0.41
24:A:840:CLA:H191	17:L:56:HIS:HD2	1.85	0.41
24:B:831:CLA:HBA2	24:B:831:CLA:H3A	1.34	0.41
18:C:66:ARG:HD3	18:C:66:ARG:HA	1.89	0.41
7:4:72:ASP:HB2	7:4:75:THR:OG1	2.20	0.41
24:0:313:CLA:HAB	15:I:21:ILE:CG2	2.49	0.41
24:7:309:CLA:H3A	24:7:309:CLA:HBA2	1.52	0.41
9:A:29:THR:HG23	29:A:851:LMG:HO4	1.85	0.41
9:A:117:LYS:HB2	9:A:136:VAL:HB	2.03	0.41
9:A:379:MET:SD	9:A:511:THR:HG22	2.60	0.41
24:A:824:CLA:H203	24:A:824:CLA:H162	1.75	0.41
10:B:175:LEU:HD21	24:B:820:CLA:HMA2	2.02	0.41
24:B:816:CLA:H51	24:B:816:CLA:H11	1.73	0.41
24:B:832:CLA:H3A	25:F:301:8CT:C20	2.49	0.41
19:K:2:PHE:O	19:K:5:SER:OG	2.34	0.41
4:3:108:ARG:NE	4:3:229:GLU:OE2	2.40	0.41
2:5:102:ALA:HB3	2:5:103:PRO:HD3	2.02	0.41
5:6:195:HIS:CG	24:6:312:CLA:HAA2	2.55	0.41
6:7:235:ILE:O	6:7:239:ILE:HG12	2.21	0.41
6:7:246:ASP:OD1	6:7:246:ASP:N	2.52	0.41
9:A:368:LEU:HB2	24:A:826:CLA:H41	2.03	0.41
27:A:850:LHG:H132	27:A:850:LHG:H101	1.87	0.41
24:B:813:CLA:H61	24:B:813:CLA:H41	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:818:CLA:H43	24:B:834:CLA:HED3	2.01	0.41
24:B:825:CLA:H152	24:B:825:CLA:H18	1.83	0.41
24:B:833:CLA:H92	16:J:25:LEU:HD21	2.02	0.41
14:G:5:SER:HA	24:G:102:CLA:OBD	2.20	0.41
21:O:125:GLN:HG3	24:O:201:CLA:HBD	2.01	0.41
23:0:301:CHL:H3A	23:0:301:CHL:HBA2	1.70	0.41
23:2:305:CHL:HBB1	23:2:305:CHL:CHC	2.48	0.41
24:2:309:CLA:H61	24:2:309:CLA:H92	1.62	0.41
5:6:164:LEU:HD23	5:6:164:LEU:HA	1.91	0.41
6:7:129:LEU:HD13	23:7:306:CHL:HBC3	2.02	0.41
7:8:137:PHE:CD2	23:8:309:CHL:HBB2	2.55	0.41
9:A:440:ASP:OD1	9:A:561:TYR:OH	2.29	0.41
24:A:809:CLA:H152	24:A:809:CLA:H111	1.85	0.41
24:A:810:CLA:H202	24:A:810:CLA:H162	1.77	0.41
10:B:90:ALA:HA	10:B:113:VAL:HG12	2.03	0.41
24:H:202:CLA:O1D	24:H:202:CLA:H2	2.20	0.41
1:0:148:PRO:O	1:0:150:ASP:N	2.54	0.41
23:0:301:CHL:H51	23:0:301:CHL:H12	1.78	0.41
24:0:313:CLA:HAB	15:I:21:ILE:HG21	2.02	0.41
27:3:324:LHG:HC61	19:K:2:PHE:CD2	2.55	0.41
5:6:72:ILE:HG21	5:6:188:PRO:HG2	2.03	0.41
7:8:161:PRO:HD2	7:8:164:GLY:O	2.20	0.41
8:9:61:LEU:HB3	24:B:813:CLA:HBA1	2.03	0.41
8:9:161:SER:OG	8:9:162:GLU:N	2.48	0.41
9:A:685:ALA:O	9:A:686:PHE:C	2.57	0.41
10:B:8:PHE:HB2	10:B:34:HIS:CG	2.56	0.41
10:B:432:HIS:ND1	29:J:105:LMG:H401	2.35	0.41
24:B:808:CLA:H62	24:B:814:CLA:H2	2.02	0.41
24:B:833:CLA:HMA2	29:J:105:LMG:H332	2.01	0.41
14:G:38:GLN:O	14:G:40:GLY:N	2.53	0.41
15:I:21:ILE:HD11	22:H:107:PHE:HD1	1.85	0.41
24:K:102:CLA:H61	24:K:102:CLA:H41	1.78	0.41
7:4:181:ASP:OD1	7:4:185:PHE:HB2	2.20	0.41
1:0:223:TRP:HB3	1:0:224:PRO:HD3	2.02	0.41
3:2:143:TRP:O	3:2:147:MET:HG3	2.20	0.41
23:6:301:CHL:H12	23:6:301:CHL:H51	1.85	0.41
8:9:82:ARG:HA	8:9:85:MET:HE3	2.03	0.41
24:A:818:CLA:CAD	24:A:828:CLA:H41	2.51	0.41
10:B:659:THR:O	10:B:662:MET:HB3	2.21	0.41
24:B:809:CLA:HBA1	24:B:809:CLA:H3A	1.83	0.41
11:D:137:CYS:O	11:D:141:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:147:LYS:HE3	11:D:147:LYS:HB2	1.90	0.41
24:0:313:CLA:HBA1	24:0:313:CLA:H3A	1.33	0.41
4:3:55:ASP:OD1	4:3:55:ASP:N	2.47	0.41
27:5:316:LHG:H132	27:5:316:LHG:H322	2.02	0.41
9:A:582:GLY:HA2	10:B:562:PRO:HD3	2.02	0.41
24:A:807:CLA:HBB1	24:A:808:CLA:O1A	2.21	0.41
24:A:812:CLA:H61	24:A:812:CLA:H41	1.87	0.41
24:A:817:CLA:HBA2	24:A:817:CLA:H3A	1.66	0.41
10:B:340:SER:CB	24:B:825:CLA:HMA3	2.51	0.41
24:B:817:CLA:C1D	24:B:818:CLA:HBB2	2.50	0.41
24:B:826:CLA:HMB3	24:B:827:CLA:H193	2.01	0.41
14:G:77:ILE:HD13	14:G:77:ILE:HA	1.92	0.41
21:O:53:ALA:HA	26:O:207:0UR:O40	2.21	0.41
7:4:169:ASP:OD1	23:4:307:CHL:HBC3	2.21	0.41
7:4:199:LYS:HE2	7:4:199:LYS:HB3	1.82	0.41
23:5:301:CHL:H143	23:5:301:CHL:H161	1.81	0.41
7:8:229:HIS:ND1	24:8:313:CLA:HAA2	2.36	0.41
9:A:27:THR:O	9:A:187:HIS:ND1	2.42	0.41
24:A:811:CLA:HED2	24:A:812:CLA:HAC1	2.03	0.41
24:A:853:CLA:HMD3	10:B:533:ILE:HG12	2.03	0.41
10:B:548:PRO:HD2	18:C:62:PHE:CE1	2.56	0.41
10:B:561:GLY:O	10:B:567:THR:OG1	2.38	0.41
24:B:802:CLA:H122	24:B:802:CLA:H161	1.89	0.41
24:B:802:CLA:H193	24:B:802:CLA:H162	1.91	0.41
24:B:807:CLA:C4A	24:B:807:CLA:HBA2	2.50	0.41
24:B:813:CLA:HHC	24:B:813:CLA:HBB1	2.03	0.41
24:B:827:CLA:H91	24:B:827:CLA:H112	1.82	0.41
22:H:76:GLU:CD	22:H:76:GLU:H	2.27	0.41
23:4:305:CHL:HBC2	23:4:306:CHL:HHD	2.01	0.41
24:0:308:CLA:H62	24:0:308:CLA:H41	1.61	0.41
24:0:311:CLA:H2	24:0:312:CLA:CMC	2.51	0.41
2:1:88:MET:HE1	2:1:186:PHE:HD1	1.85	0.41
2:1:183:MET:SD	23:1:301:CHL:HBB1	2.61	0.41
23:1:306:CHL:H43	23:1:306:CHL:H161	2.02	0.41
3:2:107:ARG:NH1	3:2:231:ASP:OD1	2.49	0.41
24:2:309:CLA:H91	24:2:309:CLA:H111	1.68	0.41
24:3:304:CLA:H172	23:7:302:CHL:H161	2.03	0.41
24:5:311:CLA:HBA2	24:5:311:CLA:H3A	1.80	0.41
24:6:304:CLA:CMB	23:6:305:CHL:HBB1	2.51	0.41
6:7:76:TRP:HB2	24:7:316:CLA:HAA1	2.03	0.41
6:7:124:ASN:O	6:7:125:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:7:305:CHL:HMB1	24:7:308:CLA:HBC2	2.03	0.41
23:7:307:CHL:H3A	23:7:307:CHL:HBA2	1.65	0.41
23:8:314:CHL:H41	23:8:314:CHL:H62	1.57	0.41
24:9:308:CLA:H92	24:9:308:CLA:H61	1.73	0.41
9:A:14:GLU:OE2	9:A:329:GLU:HG3	2.21	0.41
9:A:222:GLN:HA	9:A:226:SER:HB2	2.02	0.41
9:A:446:LEU:HA	9:A:449:VAL:HG12	2.03	0.41
9:A:752:ILE:HD12	9:A:752:ILE:HA	1.97	0.41
24:A:820:CLA:H62	24:A:820:CLA:H2	1.77	0.41
29:A:851:LMG:H131	29:A:851:LMG:H162	1.98	0.41
24:A:853:CLA:HMD1	10:B:578:LEU:HB3	2.03	0.41
29:A:854:LMG:H151	24:L:203:CLA:C1B	2.51	0.41
10:B:183:PHE:CE2	24:B:814:CLA:H72	2.55	0.41
24:B:809:CLA:HHB	24:B:830:CLA:CAB	2.51	0.41
24:B:817:CLA:CHD	24:B:818:CLA:HBB2	2.50	0.41
24:B:818:CLA:H3A	24:B:818:CLA:HBA2	1.27	0.41
15:I:5:TYR:O	15:I:8:SER:OG	2.38	0.41
23:4:301:CHL:H93	23:4:301:CHL:H61	1.63	0.41
24:0:311:CLA:C4C	24:0:311:CLA:H42	2.50	0.41
2:1:129:VAL:O	2:1:133:VAL:HG23	2.21	0.41
4:3:154:VAL:HG23	4:3:159:LEU:HG	2.03	0.41
23:6:308:CHL:HBB1	23:6:308:CHL:HHC	2.03	0.41
6:7:60:TYR:HB2	23:7:302:CHL:HMD3	2.03	0.41
9:A:379:MET:HG2	24:A:817:CLA:HAA2	2.03	0.41
9:A:423:ASP:OD2	9:A:425:THR:OG1	2.39	0.41
24:A:816:CLA:H12	24:A:816:CLA:C4D	2.51	0.41
10:B:157:LEU:HA	10:B:157:LEU:HD12	1.75	0.41
13:F:171:ILE:O	13:F:216:TRP:HZ2	2.04	0.41
5:6:72:ILE:HG13	26:6:321:0UR:C36	2.51	0.40
24:6:316:CLA:H151	6:7:129:LEU:HD11	2.02	0.40
6:7:190:LEU:HD23	6:7:190:LEU:HA	1.90	0.40
9:A:116:ILE:HD12	9:A:138:GLY:N	2.36	0.40
9:A:208:ALA:HB2	9:A:314:GLY:HA3	2.02	0.40
9:A:417:PHE:CD1	9:A:421:ASP:HB2	2.56	0.40
24:A:838:CLA:HBB2	13:F:181:GLY:HA3	2.02	0.40
10:B:352:MET:HE2	10:B:352:MET:HB3	1.87	0.40
24:B:833:CLA:HAA2	16:J:36:PRO:O	2.21	0.40
7:4:53:TRP:CE3	7:4:54:LEU:HD13	2.56	0.40
7:4:189:ASP:N	7:4:189:ASP:OD1	2.54	0.40
1:0:198:ASP:OD1	1:0:198:ASP:N	2.53	0.40
23:1:306:CHL:H61	23:1:306:CHL:H2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:311:CLA:H41	24:1:311:CLA:H61	1.46	0.40
4:3:81:PHE:CD2	24:A:811:CLA:H2	2.56	0.40
24:5:311:CLA:HMB1	23:5:312:CHL:HAC2	2.03	0.40
23:6:301:CHL:H111	23:6:301:CHL:H91	1.62	0.40
7:8:196:LYS:HD3	24:8:312:CLA:HAA2	2.03	0.40
23:8:308:CHL:H3A	23:8:308:CHL:HBA2	1.64	0.40
8:9:140:TRP:CD1	8:9:144:GLY:HA2	2.56	0.40
8:9:148:LEU:O	8:9:150:ASP:N	2.54	0.40
10:B:388:ALA:O	10:B:392:ILE:HG13	2.21	0.40
14:G:8:ILE:HD13	14:G:82:ALA:HB1	2.03	0.40
17:L:10:ILE:HB	17:L:18:MET:HB3	2.02	0.40
24:O:204:CLA:HBC2	26:O:207:0UR:C37	2.51	0.40
2:1:53:TYR:HB2	23:1:301:CHL:HMD3	2.03	0.40
29:3:321:LMG:O3	29:3:321:LMG:O6	2.40	0.40
5:6:21:PRO:HD2	23:6:301:CHL:O2D	2.21	0.40
24:6:310:CLA:H92	24:6:310:CLA:H61	1.90	0.40
9:A:126:ILE:HD12	16:J:27:ILE:HG23	2.03	0.40
9:A:325:HIS:HB3	9:A:330:ILE:HD11	2.02	0.40
24:A:812:CLA:H161	24:A:812:CLA:H122	1.83	0.40
24:A:817:CLA:H92	24:A:817:CLA:H62	1.90	0.40
10:B:35:ASP:OD1	10:B:36:SER:N	2.53	0.40
24:B:834:CLA:H61	24:B:834:CLA:H102	1.96	0.40
11:D:71:PRO:HA	11:D:72:PRO:HD3	1.99	0.40
14:G:62:ASP:OD2	14:G:64:VAL:HG12	2.22	0.40
17:L:96:CYS:HB3	25:L:204:8CT:C23	2.51	0.40
2:1:131:GLU:OE1	23:1:305:CHL:HMC	2.21	0.40
5:6:149:ALA:HB2	24:6:309:CLA:HBD	2.02	0.40
5:6:233:ILE:H	5:6:233:ILE:HG12	1.59	0.40
24:A:827:CLA:H72	25:A:847:8CT:C28	2.51	0.40
10:B:415:LYS:NZ	13:F:238:VAL:HG21	2.29	0.40
23:4:301:CHL:HBB1	23:4:301:CHL:CHC	2.45	0.40
1:0:147:MET:O	1:0:149:PHE:N	2.55	0.40
23:0:305:CHL:C1C	23:0:306:CHL:HBC3	2.51	0.40
24:5:303:CLA:C4A	24:5:303:CLA:HBA2	2.50	0.40
5:6:66:MET:HE2	5:6:167:ALA:HB2	2.04	0.40
8:9:125:GLU:O	8:9:129:MET:HB2	2.22	0.40
10:B:5:PHE:HB2	15:I:30:ILE:HA	2.04	0.40
10:B:126:THR:HG21	10:B:358:TYR:HA	2.03	0.40
10:B:418:ILE:HG23	24:B:838:CLA:HBB2	2.03	0.40
10:B:507:SER:HA	10:B:510:LEU:HD21	2.02	0.40
24:B:837:CLA:H193	13:F:171:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:216:TRP:CD1	13:F:217:PRO:HD3	2.57	0.40
14:G:28:ARG:NH2	14:G:70:ASP:OD2	2.43	0.40
23:4:301:CHL:H91	23:4:301:CHL:H112	1.60	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	0	211/245 (86%)	192 (91%)	17 (8%)	2 (1%)	14 31
2	1	193/226 (85%)	186 (96%)	6 (3%)	1 (0%)	24 45
2	5	193/226 (85%)	177 (92%)	15 (8%)	1 (0%)	24 45
3	2	214/256 (84%)	205 (96%)	9 (4%)	0	100 100
4	3	226/281 (80%)	219 (97%)	7 (3%)	0	100 100
5	6	227/267 (85%)	222 (98%)	5 (2%)	0	100 100
6	7	226/264 (86%)	212 (94%)	12 (5%)	2 (1%)	14 31
7	4	205/248 (83%)	176 (86%)	28 (14%)	1 (0%)	24 45
7	8	203/248 (82%)	187 (92%)	14 (7%)	2 (1%)	12 28
8	9	187/222 (84%)	168 (90%)	12 (6%)	7 (4%)	2 5
9	A	744/751 (99%)	711 (96%)	32 (4%)	1 (0%)	48 71
10	B	731/734 (100%)	707 (97%)	24 (3%)	0	100 100
11	D	140/198 (71%)	134 (96%)	6 (4%)	0	100 100
12	E	62/91 (68%)	60 (97%)	2 (3%)	0	100 100
13	F	163/236 (69%)	155 (95%)	8 (5%)	0	100 100
14	G	91/167 (54%)	85 (93%)	6 (7%)	0	100 100
15	I	33/36 (92%)	30 (91%)	3 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J	39/41 (95%)	39 (100%)	0	0	100	100
17	L	160/204 (78%)	157 (98%)	3 (2%)	0	100	100
18	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
19	K	78/123 (63%)	78 (100%)	0	0	100	100
20	M	29/32 (91%)	29 (100%)	0	0	100	100
21	O	90/137 (66%)	85 (94%)	5 (6%)	0	100	100
22	H	92/133 (69%)	82 (89%)	10 (11%)	0	100	100
All	All	4615/5447 (85%)	4371 (95%)	227 (5%)	17 (0%)	31	51

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	148	PRO
6	7	125	LEU
7	8	108	ILE
8	9	153	PRO
1	0	149	PHE
2	1	110	GLY
2	5	162	GLY
7	8	113	LYS
8	9	158	GLY
7	4	115	THR
8	9	161	SER
9	A	16	LYS
8	9	149	ASN
8	9	162	GLU
8	9	146	SER
8	9	156	PRO
6	7	243	VAL

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	0	167/194 (86%)	162 (97%)	5 (3%)	36 63
2	1	148/175 (85%)	139 (94%)	9 (6%)	17 37
2	5	149/175 (85%)	144 (97%)	5 (3%)	32 59
3	2	166/197 (84%)	163 (98%)	3 (2%)	51 76
4	3	186/225 (83%)	183 (98%)	3 (2%)	55 78
5	6	188/216 (87%)	181 (96%)	7 (4%)	30 56
6	7	181/209 (87%)	176 (97%)	5 (3%)	38 65
7	4	158/189 (84%)	133 (84%)	25 (16%)	2 6
7	8	159/189 (84%)	150 (94%)	9 (6%)	18 40
8	9	147/173 (85%)	136 (92%)	11 (8%)	12 28
9	A	609/614 (99%)	591 (97%)	18 (3%)	36 63
10	B	600/601 (100%)	586 (98%)	14 (2%)	44 71
11	D	119/162 (74%)	117 (98%)	2 (2%)	53 77
12	E	56/77 (73%)	54 (96%)	2 (4%)	31 57
13	F	129/180 (72%)	123 (95%)	6 (5%)	23 47
14	G	79/145 (54%)	71 (90%)	8 (10%)	7 16
15	I	27/28 (96%)	26 (96%)	1 (4%)	30 56
16	J	38/38 (100%)	36 (95%)	2 (5%)	20 43
17	L	124/157 (79%)	119 (96%)	5 (4%)	28 53
18	C	68/69 (99%)	66 (97%)	2 (3%)	37 64
19	K	58/94 (62%)	55 (95%)	3 (5%)	21 43
20	M	26/27 (96%)	26 (100%)	0	100 100
21	O	76/111 (68%)	75 (99%)	1 (1%)	61 81
22	H	69/103 (67%)	69 (100%)	0	100 100
All	All	3727/4348 (86%)	3581 (96%)	146 (4%)	30 54

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	57	ASP
1	0	145	SER
1	0	147	MET
1	0	206	THR
1	0	212	GLU
2	1	91	GLN

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Mol	Chain	Res	Type
2	1	106	VAL
2	1	111	SER
2	1	113	THR
2	1	122	THR
2	1	129	VAL
2	1	141	MET
2	1	176	ILE
2	1	187	VAL
3	2	83	GLN
3	2	123	ILE
3	2	145	GLU
4	3	219	GLU
4	3	270	ILE
4	3	277	VAL
2	5	127	LEU
2	5	152	VAL
2	5	173	LEU
2	5	187	VAL
2	5	225	PHE
5	6	72	ILE
5	6	86	ASP
5	6	125	VAL
5	6	172	LEU
5	6	209	VAL
5	6	220	CYS
5	6	233	ILE
6	7	67	LEU
6	7	107	TRP
6	7	181	PHE
6	7	235	ILE
6	7	253	VAL
7	8	94	LEU
7	8	99	VAL
7	8	110	LEU
7	8	136	GLN
7	8	140	MET
7	8	144	GLU
7	8	166	LYS
7	8	169	ASP
7	8	181	ASP
8	9	114	VAL
8	9	121	LEU

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Mol	Chain	Res	Type
8	9	145	MET
8	9	148	LEU
8	9	150	ASP
8	9	157	LEU
8	9	159	MET
8	9	160	THR
8	9	162	GLU
8	9	189	VAL
8	9	213	VAL
9	A	29	THR
9	A	43	THR
9	A	51	THR
9	A	102	ARG
9	A	126	ILE
9	A	130	GLU
9	A	216	LEU
9	A	254	LEU
9	A	379	MET
9	A	432	LEU
9	A	446	LEU
9	A	522	VAL
9	A	526	VAL
9	A	543	ILE
9	A	589	CYS
9	A	670	LEU
9	A	743	THR
9	A	755	VAL
10	B	95	HIS
10	B	96	PHE
10	B	157	LEU
10	B	175	LEU
10	B	283	LEU
10	B	407	VAL
10	B	444	LEU
10	B	458	VAL
10	B	518	LEU
10	B	568	CYS
10	B	641	ASN
10	B	698	VAL
10	B	720	THR
10	B	729	THR
11	D	177	VAL

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Mol	Chain	Res	Type
11	D	200	VAL
12	E	46	VAL
12	E	61	VAL
13	F	82	THR
13	F	94	GLU
13	F	129	PHE
13	F	159	HIS
13	F	232	LYS
13	F	236	ILE
14	G	8	ILE
14	G	14	LEU
14	G	42	THR
14	G	45	GLU
14	G	55	VAL
14	G	57	LEU
14	G	59	LYS
14	G	93	TYR
15	I	30	ILE
16	J	18	TRP
16	J	21	LEU
17	L	3	GLN
17	L	36	LEU
17	L	106	GLU
17	L	112	ILE
17	L	155	THR
18	C	11	CYS
18	C	49	VAL
19	K	6	THR
19	K	17	LEU
19	K	45	LEU
21	O	131	ARG
7	4	41	ARG
7	4	49	ASP
7	4	54	LEU
7	4	55	ASP
7	4	57	THR
7	4	58	ILE
7	4	102	LEU
7	4	105	ASN
7	4	108	ILE
7	4	113	LYS
7	4	139	LEU

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Mol	Chain	Res	Type
7	4	159	VAL
7	4	162	ILE
7	4	163	PHE
7	4	166	LYS
7	4	167	LEU
7	4	179	ILE
7	4	187	LYS
7	4	199	LYS
7	4	203	LEU
7	4	223	ILE
7	4	226	TRP
7	4	238	VAL
7	4	241	ILE
7	4	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	180	GLN
1	0	191	ASN
1	0	201	HIS
2	1	202	GLN
3	2	83	GLN
3	2	198	GLN
4	3	95	ASN
4	3	168	GLN
4	3	176	GLN
6	7	166	ASN
7	8	158	ASN
8	9	86	ASN
8	9	215	ASN
9	A	62	HIS
9	A	99	HIS
9	A	447	ASN
9	A	614	HIS
10	B	34	HIS
10	B	53	GLN
10	B	79	GLN
10	B	114	ASN
10	B	156	HIS
10	B	242	HIS
10	B	467	GLN

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Mol	Chain	Res	Type
10	B	603	GLN
10	B	608	GLN
13	F	95	ASN
17	L	8	GLN
17	L	35	ASN
18	C	3	HIS
21	O	79	ASN
21	O	125	GLN
21	O	129	ASN
22	H	134	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

352 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	$\#\|Z\| > 2$
24	CLA	G	101	14	54,58,73	1.31	9 (16%)	64,95,113	1.41	6 (9%)
23	CHL	1	306	-	60,74,74	3.22	19 (31%)	58,114,114	2.53	18 (31%)
34	DGD	B	849	-	57,57,67	0.88	2 (3%)	71,71,81	1.18	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LHG	7	324	-	38,38,48	1.27	6 (15%)	41,44,54	1.00	2 (4%)
24	CLA	9	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
23	CHL	7	302	6	58,72,74	3.14	19 (32%)	55,111,114	2.84	17 (30%)
24	CLA	7	309	-	63,67,73	1.20	9 (14%)	74,105,113	1.33	7 (9%)
25	8CT	3	317	-	40,41,41	4.79	23 (57%)	51,56,56	2.60	17 (33%)
24	CLA	A	819	9	59,63,73	1.24	9 (15%)	70,101,113	1.36	5 (7%)
24	CLA	A	837	9	60,64,73	1.24	9 (15%)	71,102,113	1.32	6 (8%)
24	CLA	3	312	4	59,63,73	1.24	9 (15%)	70,101,113	1.32	5 (7%)
24	CLA	5	310	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
24	CLA	8	310	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	7 (9%)
24	CLA	7	311	6	56,60,73	1.29	9 (16%)	65,97,113	1.38	6 (9%)
23	CHL	7	306	-	55,69,74	3.32	19 (34%)	51,107,114	2.73	18 (35%)
24	CLA	7	303	6	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
24	CLA	8	311	27	50,54,73	1.34	9 (18%)	59,90,113	1.35	4 (6%)
23	CHL	7	305	-	42,56,74	3.76	19 (45%)	36,92,114	3.29	17 (47%)
24	CLA	B	809	10	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
24	CLA	1	311	2	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
24	CLA	B	818	10	63,67,73	1.20	9 (14%)	74,105,113	1.36	7 (9%)
24	CLA	A	853	-	69,73,73	1.14	9 (13%)	82,113,113	1.35	9 (10%)
23	CHL	7	301	6	57,71,74	3.30	19 (33%)	54,110,114	2.66	18 (33%)
24	CLA	A	822	9	55,59,73	1.32	9 (16%)	64,96,113	1.39	6 (9%)
31	PQN	A	841	-	34,34,34	1.53	2 (5%)	43,45,45	1.31	5 (11%)
24	CLA	A	818	9	69,73,73	1.15	9 (13%)	82,113,113	1.31	9 (10%)
24	CLA	A	826	9	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
24	CLA	B	827	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
24	CLA	1	313	-	50,54,73	1.33	9 (18%)	59,90,113	1.41	4 (6%)
31	PQN	B	842	-	34,34,34	1.57	2 (5%)	43,45,45	1.13	3 (6%)
24	CLA	A	825	-	69,73,73	1.14	9 (13%)	82,113,113	1.28	7 (8%)
23	CHL	2	312	3	45,59,74	3.63	19 (42%)	40,96,114	3.06	17 (42%)
23	CHL	3	301	-	55,69,74	3.29	19 (34%)	52,108,114	2.88	19 (36%)
24	CLA	B	815	10	59,63,73	1.24	9 (15%)	70,101,113	1.36	8 (11%)
25	8CT	B	846	-	40,41,41	4.90	23 (57%)	51,56,56	3.31	22 (43%)
27	LHG	8	320	24	43,43,48	1.20	6 (13%)	46,49,54	0.94	2 (4%)
23	CHL	6	308	5	54,68,74	3.34	19 (35%)	50,106,114	2.76	17 (34%)
24	CLA	B	814	10	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	H	204	-	51,55,73	1.33	9 (17%)	60,91,113	1.43	5 (8%)
24	CLA	B	813	10	59,63,73	1.25	9 (15%)	70,101,113	1.34	5 (7%)
25	8CT	2	314	-	40,41,41	4.79	23 (57%)	51,56,56	3.05	19 (37%)
24	CLA	8	304	7	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
27	LHG	A	850	-	41,41,48	1.24	6 (14%)	44,47,54	1.04	3 (6%)
24	CLA	A	802	9	69,73,73	1.15	9 (13%)	82,113,113	1.31	7 (8%)
25	8CT	0	314	-	40,41,41	4.80	23 (57%)	51,56,56	2.82	18 (35%)
25	8CT	A	845	-	40,41,41	4.73	23 (57%)	51,56,56	3.14	20 (39%)
24	CLA	A	834	9	61,65,73	1.23	8 (13%)	72,103,113	1.37	5 (6%)
24	CLA	3	306	4	51,55,73	1.32	9 (17%)	60,91,113	1.40	5 (8%)
26	0UR	4	317	-	49,52,58	0.99	2 (4%)	58,71,77	2.19	21 (36%)
24	CLA	B	817	10	64,68,73	1.17	9 (14%)	76,107,113	1.45	9 (11%)
24	CLA	0	319	-	50,54,73	1.33	9 (18%)	59,90,113	1.39	4 (6%)
24	CLA	3	315	-	56,60,73	1.28	9 (16%)	65,97,113	1.48	7 (10%)
23	CHL	5	306	-	41,55,74	3.95	20 (48%)	35,91,114	3.04	16 (45%)
24	CLA	A	820	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
24	CLA	A	828	9	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
25	8CT	K	105	-	40,41,41	4.75	23 (57%)	51,56,56	3.31	23 (45%)
23	CHL	8	309	-	41,55,74	3.84	19 (46%)	35,91,114	3.20	17 (48%)
26	0UR	1	315	-	50,53,58	0.97	1 (2%)	59,72,77	1.76	17 (28%)
24	CLA	B	806	-	69,73,73	1.15	10 (14%)	82,113,113	1.34	7 (8%)
24	CLA	1	302	2	60,64,73	1.25	9 (15%)	71,102,113	1.39	5 (7%)
27	LHG	3	324	-	42,42,48	1.20	6 (14%)	45,47,54	1.06	4 (8%)
24	CLA	A	806	9	57,61,73	1.26	9 (15%)	65,97,113	1.43	8 (12%)
29	LMG	O	203	-	31,31,55	0.92	0	39,39,63	1.25	5 (12%)
25	8CT	4	316	-	40,41,41	4.77	23 (57%)	51,56,56	3.00	19 (37%)
27	LHG	3	322	-	35,35,48	1.31	6 (17%)	38,41,54	1.07	2 (5%)
23	CHL	5	305	-	42,56,74	3.95	18 (42%)	36,92,114	2.83	13 (36%)
25	8CT	B	843	-	40,41,41	4.88	23 (57%)	51,56,56	2.79	19 (37%)
23	CHL	6	302	5	58,72,74	3.15	18 (31%)	55,111,114	2.98	19 (34%)
24	CLA	5	303	-	56,60,73	1.29	7 (12%)	65,97,113	1.34	4 (6%)
24	CLA	A	812	9	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
24	CLA	A	824	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
24	CLA	4	303	7	49,53,73	1.36	9 (18%)	58,89,113	1.42	4 (6%)
24	CLA	6	314	-	49,53,73	1.35	9 (18%)	58,89,113	1.44	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	L	202	17	67,71,73	1.17	9 (13%)	79,110,113	1.32	5 (6%)
24	CLA	B	810	10	66,70,73	1.16	9 (13%)	78,109,113	1.32	7 (8%)
24	CLA	O	209	-	55,59,73	1.31	9 (16%)	64,96,113	1.33	5 (7%)
27	LHG	0	317	-	48,48,48	1.13	6 (12%)	51,54,54	0.94	2 (3%)
25	8CT	J	104	-	40,41,41	4.80	23 (57%)	51,56,56	3.45	22 (43%)
24	CLA	4	304	-	64,68,73	1.19	8 (12%)	76,107,113	1.27	5 (6%)
30	0IE	7	321	-	42,45,45	1.16	5 (11%)	51,63,63	1.49	11 (21%)
24	CLA	H	202	10	59,63,73	1.24	9 (15%)	70,101,113	1.36	8 (11%)
24	CLA	K	101	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	6 (7%)
24	CLA	B	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	4 (4%)
23	CHL	3	302	4	56,70,74	3.24	19 (33%)	53,109,114	2.86	19 (35%)
23	CHL	5	304	-	40,54,74	3.98	19 (47%)	34,90,114	3.21	15 (44%)
24	CLA	4	311	-	52,56,73	1.32	9 (17%)	61,92,113	1.41	5 (8%)
23	CHL	4	307	-	45,59,74	3.63	19 (42%)	40,96,114	3.19	17 (42%)
24	CLA	B	840	10	69,73,73	1.16	7 (10%)	82,113,113	1.30	5 (6%)
23	CHL	8	307	-	45,59,74	3.71	18 (40%)	40,96,114	3.02	19 (47%)
24	CLA	5	307	-	50,54,73	1.36	9 (18%)	59,90,113	1.36	4 (6%)
24	CLA	0	310	-	51,55,73	1.33	9 (17%)	60,91,113	1.46	5 (8%)
24	CLA	B	819	10	64,68,73	1.19	9 (14%)	76,107,113	1.32	7 (9%)
24	CLA	3	304	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	6 (7%)
26	0UR	2	315	-	49,52,58	1.02	2 (4%)	58,71,77	2.17	19 (32%)
24	CLA	3	314	4	50,54,73	1.34	9 (18%)	59,90,113	1.41	4 (6%)
25	8CT	B	848	-	40,41,41	4.81	23 (57%)	51,56,56	2.63	19 (37%)
24	CLA	4	314	7	49,53,73	1.35	9 (18%)	58,89,113	1.41	5 (8%)
26	0UR	1	316	-	50,53,58	1.01	1 (2%)	59,72,77	1.88	12 (20%)
23	CHL	3	307	-	60,74,74	3.06	19 (31%)	58,114,114	2.90	18 (31%)
24	CLA	F	302	13	51,55,73	1.34	9 (17%)	60,91,113	1.39	5 (8%)
27	LHG	B	852	-	37,37,48	1.29	6 (16%)	40,43,54	1.16	4 (10%)
24	CLA	5	311	2	60,64,73	1.24	9 (15%)	71,102,113	1.34	4 (5%)
24	CLA	6	309	5	62,66,73	1.22	9 (14%)	73,104,113	1.33	8 (10%)
25	8CT	J	101	-	40,41,41	4.75	23 (57%)	51,56,56	2.87	18 (35%)
24	CLA	5	308	-	64,68,73	1.21	9 (14%)	76,107,113	1.29	7 (9%)
24	CLA	5	309	27	49,53,73	1.37	9 (18%)	58,89,113	1.40	4 (6%)
23	CHL	6	306	-	45,59,74	3.61	19 (42%)	40,96,114	3.26	19 (47%)
25	8CT	L	207	-	40,41,41	4.80	23 (57%)	51,56,56	2.63	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	6	312	5	60,64,73	1.23	9 (15%)	71,102,113	1.33	5 (7%)
24	CLA	A	835	-	55,59,73	1.27	9 (16%)	64,96,113	1.42	8 (12%)
23	CHL	6	315	5	37,51,74	4.03	17 (45%)	30,86,114	3.31	14 (46%)
23	CHL	2	307	-	41,55,74	3.82	19 (46%)	35,91,114	3.10	15 (42%)
24	CLA	A	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
27	LHG	I	102	-	45,45,48	1.17	5 (11%)	48,51,54	0.98	3 (6%)
24	CLA	0	309	-	45,49,73	1.39	9 (20%)	54,84,113	1.47	5 (9%)
24	CLA	B	826	-	53,56,73	1.41	11 (20%)	63,89,113	2.42	11 (17%)
24	CLA	B	811	10	69,73,73	1.15	9 (13%)	82,113,113	1.35	7 (8%)
24	CLA	7	315	6	52,56,73	1.31	9 (17%)	61,92,113	1.41	5 (8%)
24	CLA	A	816	9	65,69,73	1.17	9 (13%)	77,108,113	1.35	6 (7%)
24	CLA	3	309	4	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
24	CLA	6	303	5	56,60,73	1.29	8 (14%)	65,97,113	1.38	5 (7%)
24	CLA	A	829	9	69,73,73	1.17	10 (14%)	82,113,113	1.42	9 (10%)
24	CLA	0	312	1	50,54,73	1.34	8 (16%)	59,90,113	1.36	4 (6%)
24	CLA	B	835	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	4 (6%)
23	CHL	8	301	2	46,60,74	3.74	19 (41%)	40,97,114	2.94	16 (40%)
24	CLA	9	310	8	56,60,73	1.29	9 (16%)	65,97,113	1.38	6 (9%)
26	0UR	5	314	-	49,52,58	0.97	1 (2%)	58,71,77	1.82	13 (22%)
25	8CT	A	847	-	40,41,41	4.70	23 (57%)	51,56,56	3.21	23 (45%)
23	CHL	1	301	-	58,72,74	3.19	19 (32%)	55,111,114	2.82	20 (36%)
23	CHL	6	301	5	55,69,74	3.30	19 (34%)	52,108,114	2.77	18 (34%)
24	CLA	A	808	9	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
24	CLA	6	311	5	52,56,73	1.33	9 (17%)	61,92,113	1.38	5 (8%)
29	LMG	9	317	-	55,55,55	0.70	1 (1%)	63,63,63	1.39	9 (14%)
24	CLA	B	837	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	7 (8%)
24	CLA	2	310	3	52,56,73	1.30	8 (15%)	61,92,113	1.45	6 (9%)
24	CLA	6	316	5	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
25	8CT	L	204	-	40,41,41	4.76	23 (57%)	51,56,56	3.02	19 (37%)
26	0UR	6	321	-	50,53,58	1.02	2 (4%)	59,72,77	1.75	13 (22%)
23	CHL	3	305	-	45,59,74	3.64	19 (42%)	40,96,114	3.14	17 (42%)
33	SF4	C	102	18	0,12,12	-	-	-		
23	CHL	2	304	-	37,51,74	3.93	18 (48%)	30,86,114	3.72	15 (50%)
24	CLA	A	838	9	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
24	CLA	6	318	-	55,59,73	1.30	9 (16%)	64,96,113	1.32	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CHL	0	301	1	46,60,74	3.61	19 (41%)	40,97,114	3.06	17 (42%)
24	CLA	0	307	-	64,68,73	1.21	9 (14%)	76,107,113	1.27	5 (6%)
24	CLA	A	827	9	69,73,73	1.14	9 (13%)	82,113,113	1.29	8 (9%)
23	CHL	0	306	-	42,56,74	3.89	18 (42%)	36,92,114	3.32	14 (38%)
24	CLA	3	311	4	50,54,73	1.35	9 (18%)	59,90,113	1.47	5 (8%)
24	CLA	K	102	19	57,61,73	1.25	9 (15%)	67,98,113	1.39	7 (10%)
27	LHG	1	318	-	42,42,48	1.22	6 (14%)	45,48,54	0.98	2 (4%)
24	CLA	1	309	27	67,71,73	1.17	9 (13%)	79,110,113	1.28	4 (5%)
23	CHL	5	312	2	41,55,74	4.04	18 (43%)	35,91,114	3.02	14 (40%)
23	CHL	8	308	-	45,59,74	3.66	19 (42%)	40,96,114	3.08	17 (42%)
23	CHL	0	305	-	45,59,74	3.74	18 (40%)	40,96,114	3.07	19 (47%)
24	CLA	B	838	10	51,55,73	1.30	8 (15%)	60,91,113	1.41	6 (10%)
24	CLA	L	206	-	51,55,73	1.34	9 (17%)	60,91,113	1.37	5 (8%)
27	LHG	5	316	24	36,36,48	1.29	6 (16%)	39,42,54	1.09	3 (7%)
25	8CT	B	845	-	40,41,41	4.76	23 (57%)	51,56,56	3.28	22 (43%)
24	CLA	A	814	9	69,73,73	1.15	9 (13%)	82,113,113	1.33	6 (7%)
24	CLA	9	304	-	55,59,73	1.29	8 (14%)	64,96,113	1.37	5 (7%)
27	LHG	3	320	-	35,35,48	1.32	6 (17%)	38,41,54	1.14	2 (5%)
32	CL0	A	852	9	58,73,73	2.15	13 (22%)	60,113,113	1.55	11 (18%)
24	CLA	1	303	-	56,60,73	1.28	9 (16%)	65,97,113	1.33	6 (9%)
23	CHL	4	306	-	42,56,74	3.84	19 (45%)	36,92,114	3.25	16 (44%)
24	CLA	G	102	14	49,53,73	1.36	9 (18%)	58,89,113	1.45	4 (6%)
23	CHL	4	315	2	48,62,74	3.55	19 (39%)	43,99,114	3.10	17 (39%)
24	CLA	B	841	27	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
26	0UR	2	316	-	48,51,58	1.01	1 (2%)	57,70,77	1.99	13 (22%)
24	CLA	0	311	1	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
27	LHG	6	322	24	36,36,48	1.29	5 (13%)	39,42,54	1.06	2 (5%)
24	CLA	B	804	-	69,73,73	1.14	9 (13%)	82,113,113	1.25	7 (8%)
24	CLA	6	310	27	64,68,73	1.21	9 (14%)	76,107,113	1.30	5 (6%)
24	CLA	B	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
24	CLA	F	303	-	49,53,73	1.36	9 (18%)	58,89,113	1.43	4 (6%)
23	CHL	6	323	7	55,69,74	3.35	19 (34%)	52,108,114	2.89	19 (36%)
25	8CT	3	323	-	40,41,41	4.76	23 (57%)	51,56,56	3.69	24 (47%)
26	0UR	0	316	-	50,53,58	0.98	1 (2%)	59,72,77	1.96	18 (30%)
26	0UR	O	207	-	50,53,58	0.99	2 (4%)	59,72,77	1.97	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	O	204	-	45,49,73	1.40	9 (20%)	54,84,113	1.51	5 (9%)
24	CLA	4	310	27	64,68,73	1.20	9 (14%)	76,107,113	1.29	5 (6%)
24	CLA	1	308	2	59,63,73	1.25	9 (15%)	70,101,113	1.31	6 (8%)
24	CLA	7	304	-	59,63,73	1.25	9 (15%)	70,101,113	1.36	7 (10%)
24	CLA	B	822	10	64,68,73	1.20	8 (12%)	76,107,113	1.34	5 (6%)
27	LHG	A	842	-	48,48,48	1.11	5 (10%)	51,54,54	1.00	3 (5%)
23	CHL	1	312	2	56,70,74	3.30	19 (33%)	53,109,114	2.70	17 (32%)
26	0UR	6	320	-	49,52,58	1.00	2 (4%)	58,71,77	1.92	15 (25%)
25	8CT	3	316	-	40,41,41	4.78	23 (57%)	51,56,56	3.09	18 (35%)
23	CHL	7	307	-	45,59,74	3.64	19 (42%)	40,96,114	2.86	16 (40%)
23	CHL	2	306	-	45,59,74	3.58	19 (42%)	40,96,114	3.44	19 (47%)
23	CHL	8	314	7	50,64,74	3.45	19 (38%)	46,102,114	2.94	17 (36%)
24	CLA	9	308	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	8 (10%)
24	CLA	7	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	5 (6%)
23	CHL	2	305	-	42,56,74	3.82	19 (45%)	36,92,114	3.23	16 (44%)
24	CLA	6	304	-	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
24	CLA	0	308	-	64,68,73	1.20	8 (12%)	76,107,113	1.32	7 (9%)
33	SF4	C	101	-	0,12,12	-	-	-		
23	CHL	4	313	7	45,59,74	3.63	19 (42%)	40,96,114	3.20	18 (45%)
25	8CT	7	318	-	40,41,41	4.73	23 (57%)	51,56,56	2.70	19 (37%)
23	CHL	6	307	-	45,59,74	3.62	19 (42%)	40,96,114	3.14	18 (45%)
24	CLA	A	848	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
24	CLA	A	836	9	65,69,73	1.18	9 (13%)	77,108,113	1.35	7 (9%)
23	CHL	0	302	1	58,72,74	3.20	19 (32%)	55,111,114	2.74	18 (32%)
25	8CT	9	313	-	40,41,41	4.80	23 (57%)	51,56,56	2.77	19 (37%)
26	0UR	3	318	-	49,52,58	1.03	1 (2%)	58,71,77	2.13	21 (36%)
23	CHL	5	301	2	58,72,74	3.18	19 (32%)	55,111,114	2.79	18 (32%)
24	CLA	2	313	3	49,53,73	1.37	9 (18%)	58,89,113	1.42	4 (6%)
25	8CT	6	324	-	40,41,41	4.84	23 (57%)	51,56,56	2.59	17 (33%)
24	CLA	0	304	-	56,60,73	1.30	9 (16%)	65,97,113	1.37	6 (9%)
24	CLA	J	103	16	46,50,73	1.38	9 (19%)	53,85,113	1.44	4 (7%)
25	8CT	O	202	-	40,41,41	4.73	23 (57%)	51,56,56	2.84	23 (45%)
33	SF4	B	803	-	0,12,12	-	-	-		
29	LMG	A	854	-	37,37,55	0.88	1 (2%)	45,45,63	1.26	4 (8%)
24	CLA	B	830	10	60,64,73	1.28	10 (16%)	71,102,113	1.44	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	O	201	27	56,60,73	1.27	9 (16%)	65,97,113	1.41	8 (12%)
24	CLA	A	832	9	69,73,73	1.14	9 (13%)	82,113,113	1.29	5 (6%)
24	CLA	O	205	21	41,46,73	1.48	9 (21%)	47,80,113	1.50	5 (10%)
24	CLA	H	203	22	51,55,73	1.33	9 (17%)	60,91,113	1.38	4 (6%)
24	CLA	9	309	27	45,49,73	1.40	9 (20%)	54,84,113	1.46	5 (9%)
23	CHL	8	303	7	58,72,74	3.18	19 (32%)	55,111,114	2.79	19 (34%)
24	CLA	B	802	10	69,73,73	1.15	9 (13%)	82,113,113	1.26	6 (7%)
24	CLA	B	816	10	64,68,73	1.19	9 (14%)	76,107,113	1.35	7 (9%)
25	8CT	O	208	-	40,41,41	4.79	23 (57%)	51,56,56	2.64	19 (37%)
24	CLA	2	309	27	64,68,73	1.19	9 (14%)	76,107,113	1.28	5 (6%)
25	8CT	B	844	-	40,41,41	4.85	23 (57%)	51,56,56	2.73	22 (43%)
24	CLA	A	840	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	6 (7%)
27	LHG	8	302	-	30,30,48	1.38	6 (20%)	33,36,54	1.12	2 (6%)
25	8CT	I	101	-	40,41,41	4.72	23 (57%)	51,56,56	2.84	18 (35%)
24	CLA	A	830	9	54,58,73	1.29	9 (16%)	64,95,113	1.44	6 (9%)
25	8CT	B	850	-	40,41,41	4.76	23 (57%)	51,56,56	2.52	17 (33%)
24	CLA	H	205	-	55,59,73	1.30	9 (16%)	64,96,113	1.38	6 (9%)
24	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
26	0UR	9	314	-	50,53,58	0.96	1 (2%)	59,72,77	1.76	16 (27%)
24	CLA	1	307	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
24	CLA	B	812	10	56,60,73	1.27	8 (14%)	65,97,113	1.41	7 (10%)
30	0IE	3	319	-	42,45,45	1.16	5 (11%)	51,63,63	1.51	11 (21%)
29	LMG	2	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.24	5 (11%)
24	CLA	3	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
25	8CT	B	847	-	40,41,41	4.75	23 (57%)	51,56,56	3.17	20 (39%)
24	CLA	B	808	10	69,73,73	1.15	9 (13%)	82,113,113	1.34	9 (10%)
26	0UR	5	315	-	50,53,58	0.98	1 (2%)	59,72,77	1.96	14 (23%)
27	LHG	7	323	-	37,37,48	1.22	6 (16%)	40,43,54	1.06	2 (5%)
23	CHL	9	312	8	41,55,74	3.85	18 (43%)	35,91,114	3.34	16 (45%)
24	CLA	A	815	-	49,53,73	1.39	9 (18%)	58,89,113	1.46	4 (6%)
25	8CT	1	314	-	40,41,41	4.83	23 (57%)	51,56,56	2.75	19 (37%)
29	LMG	M	101	-	42,42,55	0.79	0	50,50,63	1.31	7 (14%)
24	CLA	8	305	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
25	8CT	A	846	-	40,41,41	4.71	23 (57%)	51,56,56	3.07	21 (41%)
25	8CT	F	301	-	40,41,41	4.78	23 (57%)	51,56,56	2.63	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	2	303	-	64,68,73	1.20	9 (14%)	76,107,113	1.28	5 (6%)
24	CLA	A	821	-	53,57,73	1.29	9 (16%)	61,93,113	1.39	5 (8%)
23	CHL	6	313	5	46,60,74	3.62	19 (41%)	40,97,114	3.26	19 (47%)
24	CLA	6	317	-	50,54,73	1.34	9 (18%)	59,90,113	1.40	4 (6%)
29	LMG	3	321	-	36,36,55	0.86	0	44,44,63	1.26	5 (11%)
24	CLA	B	831	10	54,58,73	1.30	9 (16%)	64,95,113	1.39	5 (7%)
24	CLA	2	302	3	60,64,73	1.25	9 (15%)	71,102,113	1.35	5 (7%)
24	CLA	L	203	-	50,54,73	1.34	9 (18%)	59,90,113	1.38	4 (6%)
25	8CT	G	104	-	40,41,41	4.81	23 (57%)	51,56,56	3.09	20 (39%)
24	CLA	A	831	9	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
24	CLA	A	807	9	69,73,73	1.13	9 (13%)	82,113,113	1.29	6 (7%)
24	CLA	0	303	1	66,70,73	1.19	9 (13%)	78,109,113	1.27	4 (5%)
24	CLA	7	316	-	49,53,73	1.38	7 (14%)	58,89,113	1.47	5 (8%)
24	CLA	1	310	2	56,60,73	1.28	9 (16%)	65,97,113	1.40	6 (9%)
24	CLA	3	303	-	59,63,73	1.24	9 (15%)	70,101,113	1.35	8 (11%)
24	CLA	A	810	9	69,73,73	1.14	8 (11%)	82,113,113	1.26	4 (4%)
26	0UR	4	318	-	48,51,58	0.99	1 (2%)	57,70,77	1.73	13 (22%)
24	CLA	B	801	10	62,66,73	1.21	8 (12%)	73,104,113	1.38	7 (9%)
24	CLA	4	312	7	57,61,73	1.27	9 (15%)	67,98,113	1.35	4 (5%)
23	CHL	1	304	-	45,59,74	3.65	19 (42%)	40,96,114	3.26	17 (42%)
27	LHG	B	851	24	22,22,48	1.33	3 (13%)	25,28,54	1.08	1 (4%)
25	8CT	A	844	-	40,41,41	4.76	23 (57%)	51,56,56	2.93	19 (37%)
25	8CT	7	319	-	40,41,41	4.74	23 (57%)	51,56,56	2.77	20 (39%)
24	CLA	A	823	9	59,63,73	1.24	9 (15%)	70,101,113	1.32	5 (7%)
24	CLA	8	315	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	4 (6%)
24	CLA	B	805	10	69,73,73	1.14	9 (13%)	82,113,113	1.25	6 (7%)
24	CLA	B	834	10	65,69,73	1.19	9 (13%)	77,108,113	1.26	4 (5%)
24	CLA	B	821	10	54,58,73	1.28	9 (16%)	64,95,113	1.45	8 (12%)
29	LMG	A	851	-	36,36,55	0.90	1 (2%)	44,44,63	1.31	5 (11%)
27	LHG	7	322	24	29,29,48	1.41	6 (20%)	32,35,54	1.11	2 (6%)
29	LMG	J	105	-	46,46,55	0.88	2 (4%)	54,54,63	1.36	7 (12%)
24	CLA	8	312	7	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
24	CLA	5	313	2	50,54,73	1.36	9 (18%)	59,90,113	1.35	4 (6%)
24	CLA	G	103	14	50,54,73	1.35	8 (16%)	59,90,113	1.38	4 (6%)
24	CLA	A	813	9	61,65,73	1.22	8 (13%)	72,103,113	1.34	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LHG	1	317	24	48,48,48	1.14	5 (10%)	51,54,54	0.98	2 (3%)
23	CHL	7	313	6	41,55,74	3.90	19 (46%)	35,91,114	3.03	16 (45%)
23	CHL	9	301	8	41,55,74	3.85	19 (46%)	35,91,114	3.19	15 (42%)
24	CLA	3	310	-	66,70,73	1.18	9 (13%)	78,109,113	1.28	5 (6%)
24	CLA	K	104	19	54,58,73	1.30	9 (16%)	64,95,113	1.39	6 (9%)
25	8CT	A	849	-	40,41,41	4.78	23 (57%)	51,56,56	2.92	21 (41%)
24	CLA	A	803	9	59,63,73	1.22	9 (15%)	70,101,113	1.39	6 (8%)
24	CLA	K	103	19	50,54,73	1.35	9 (18%)	59,90,113	1.43	4 (6%)
24	CLA	A	839	9	69,73,73	1.14	9 (13%)	82,113,113	1.32	6 (7%)
26	0UR	8	319	-	50,53,58	0.99	1 (2%)	59,72,77	1.96	13 (22%)
24	CLA	7	312	6	59,63,73	1.25	9 (15%)	70,101,113	1.33	4 (5%)
24	CLA	2	308	3	64,68,73	1.19	9 (14%)	76,107,113	1.31	8 (10%)
25	8CT	F	304	-	40,41,41	4.77	23 (57%)	51,56,56	2.76	17 (33%)
27	LHG	2	317	24	31,31,48	1.38	5 (16%)	34,37,54	1.13	3 (8%)
26	0UR	8	318	-	49,52,58	0.97	1 (2%)	58,71,77	1.83	17 (29%)
24	CLA	A	804	9	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
27	LHG	A	843	24	26,26,48	1.29	4 (15%)	29,32,54	1.20	2 (6%)
24	CLA	9	303	8	52,56,73	1.32	8 (15%)	61,92,113	1.42	5 (8%)
24	CLA	B	820	-	60,64,73	1.24	9 (15%)	71,102,113	1.35	5 (7%)
23	CHL	4	302	7	47,61,74	3.53	19 (40%)	41,98,114	3.14	19 (46%)
24	CLA	7	317	6	64,68,73	1.19	9 (14%)	76,107,113	1.32	6 (7%)
24	CLA	B	824	10	64,68,73	1.21	9 (14%)	76,107,113	1.28	6 (7%)
27	LHG	9	316	24	45,45,48	1.18	6 (13%)	47,50,54	0.97	2 (4%)
26	0UR	0	315	-	50,53,58	0.96	1 (2%)	59,72,77	1.76	13 (22%)
24	CLA	B	836	10	64,68,73	1.20	9 (14%)	76,107,113	1.34	8 (10%)
24	CLA	7	310	27	41,45,73	1.44	8 (19%)	50,78,113	1.41	5 (10%)
24	CLA	A	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	4 (4%)
24	CLA	A	811	9	58,62,73	1.27	9 (15%)	68,99,113	1.32	6 (8%)
29	LMG	O	210	-	39,39,55	0.81	1 (2%)	47,47,63	1.27	5 (10%)
26	0UR	7	320	-	49,52,58	1.00	1 (2%)	58,71,77	2.14	18 (31%)
24	CLA	B	833	10	59,63,73	1.26	9 (15%)	70,101,113	1.37	8 (11%)
24	CLA	L	201	9	62,66,73	1.21	9 (14%)	73,104,113	1.37	7 (9%)
24	CLA	8	313	7	60,64,73	1.24	9 (15%)	71,102,113	1.33	4 (5%)
24	CLA	9	311	8	60,64,73	1.23	9 (15%)	71,102,113	1.32	5 (7%)
24	CLA	9	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	6	319	-	40,41,41	4.80	23 (57%)	51,56,56	3.46	21 (41%)
24	CLA	H	201	17	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
24	CLA	A	817	9	69,73,73	1.14	7 (10%)	82,113,113	1.32	9 (10%)
24	CLA	5	302	2	63,67,73	1.22	8 (12%)	74,105,113	1.35	5 (6%)
23	CHL	9	305	-	45,59,74	3.63	19 (42%)	40,96,114	3.17	17 (42%)
23	CHL	6	305	-	37,51,74	3.96	18 (48%)	30,86,114	3.57	14 (46%)
24	CLA	0	313	1	49,53,73	1.40	8 (16%)	58,89,113	1.46	4 (6%)
28	SQD	0	318	-	36,36,54	1.20	4 (11%)	43,44,65	1.46	6 (13%)
23	CHL	8	316	-	37,51,74	4.10	17 (45%)	30,86,114	3.27	13 (43%)
24	CLA	A	833	9	50,54,73	1.32	8 (16%)	59,90,113	1.43	4 (6%)
25	8CT	L	205	-	40,41,41	4.79	23 (57%)	51,56,56	2.83	19 (37%)
24	CLA	7	314	6	51,55,73	1.33	9 (17%)	60,91,113	1.42	5 (8%)
24	CLA	3	313	4	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
23	CHL	1	305	-	42,56,74	3.85	19 (45%)	36,92,114	2.98	17 (47%)
23	CHL	2	301	3	58,72,74	3.17	19 (32%)	55,111,114	2.79	20 (36%)
24	CLA	4	309	-	64,68,73	1.21	8 (12%)	76,107,113	1.23	6 (7%)
24	CLA	B	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
27	LHG	L	208	-	30,30,48	1.37	6 (20%)	33,36,54	1.15	2 (6%)
24	CLA	B	823	-	56,60,73	1.29	9 (16%)	65,97,113	3.60	8 (12%)
29	LMG	J	102	-	29,29,55	0.97	1 (3%)	37,37,63	1.28	4 (10%)
24	CLA	B	828	-	64,68,73	1.19	9 (14%)	76,107,113	1.27	5 (6%)
23	CHL	4	301	7	55,69,74	3.32	19 (34%)	52,108,114	2.92	17 (32%)
27	LHG	2	319	24	31,31,48	1.37	5 (16%)	34,37,54	1.16	3 (8%)
23	CHL	4	308	-	41,55,74	3.83	19 (46%)	35,91,114	3.17	16 (45%)
24	CLA	B	807	10	49,53,73	1.35	9 (18%)	58,89,113	1.51	7 (12%)
24	CLA	O	206	-	41,46,73	1.59	9 (21%)	51,81,113	1.53	7 (13%)
25	8CT	8	317	-	40,41,41	4.81	23 (57%)	51,56,56	2.76	19 (37%)
24	CLA	2	311	3	64,68,73	1.18	8 (12%)	76,107,113	1.34	6 (7%)
25	8CT	M	102	-	40,41,41	4.76	23 (57%)	51,56,56	2.90	19 (37%)
26	0UR	9	315	-	50,53,58	1.01	2 (4%)	59,72,77	1.87	17 (28%)
23	CHL	9	306	-	42,56,74	3.80	19 (45%)	36,92,114	3.36	16 (44%)
23	CHL	8	306	-	41,55,74	3.85	19 (46%)	35,91,114	3.20	16 (45%)
23	CHL	4	305	-	37,51,74	3.97	18 (48%)	30,86,114	3.63	14 (46%)
24	CLA	A	809	9	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	G	101	14	1/1/12/20	7/21/97/115	-
23	CHL	1	306	-	3/3/20/26	22/39/137/137	-
34	DGD	B	849	-	-	27/45/85/95	0/2/2/2
27	LHG	7	324	-	-	20/43/43/53	-
24	CLA	9	302	-	1/1/15/20	15/39/115/115	-
23	CHL	7	302	6	3/3/19/26	16/37/135/137	-
24	CLA	7	309	-	1/1/13/20	11/32/108/115	-
25	8CT	3	317	-	-	9/29/63/63	0/2/2/2
24	CLA	A	819	9	1/1/13/20	8/27/103/115	-
24	CLA	A	837	9	1/1/13/20	3/29/105/115	-
24	CLA	3	312	4	1/1/13/20	5/27/103/115	-
24	CLA	5	310	-	1/1/11/20	8/15/91/115	-
24	CLA	8	310	-	1/1/14/20	6/33/109/115	-
24	CLA	7	311	6	1/1/12/20	8/24/100/115	-
23	CHL	7	306	-	3/3/18/26	17/33/131/137	-
24	CLA	7	303	6	1/1/11/20	6/15/91/115	-
24	CLA	8	311	27	1/1/11/20	4/17/93/115	-
23	CHL	7	305	-	3/3/16/26	7/18/116/137	-
24	CLA	B	809	10	1/1/15/20	11/39/115/115	-
24	CLA	1	311	2	1/1/15/20	12/39/115/115	-
24	CLA	B	818	10	1/1/13/20	8/32/108/115	-
24	CLA	A	853	-	1/1/15/20	10/39/115/115	-
23	CHL	7	301	6	3/3/19/26	14/36/134/137	-
24	CLA	A	822	9	1/1/12/20	4/23/99/115	-
31	PQN	A	841	-	-	7/23/43/43	0/2/2/2
24	CLA	A	818	9	1/1/15/20	18/39/115/115	-
24	CLA	A	826	9	1/1/15/20	2/39/115/115	-
24	CLA	B	827	-	1/1/15/20	10/39/115/115	-
24	CLA	1	313	-	1/1/11/20	4/17/93/115	-
31	PQN	B	842	-	-	6/23/43/43	0/2/2/2
24	CLA	A	825	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	2	312	3	3/3/17/26	3/21/119/137	-
23	CHL	3	301	-	3/3/19/26	9/33/131/137	-
24	CLA	B	815	10	1/1/13/20	3/27/103/115	-
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
27	LHG	8	320	24	-	30/48/48/53	-
23	CHL	6	308	5	3/3/18/26	8/32/130/137	-
24	CLA	B	814	10	1/1/15/20	15/39/115/115	-
24	CLA	H	204	-	1/1/11/20	3/18/94/115	-
24	CLA	B	813	10	1/1/13/20	10/27/103/115	-
25	8CT	2	314	-	-	12/29/63/63	0/2/2/2
24	CLA	8	304	7	1/1/11/20	6/17/93/115	-
27	LHG	A	850	-	-	26/46/46/53	-
24	CLA	A	802	9	1/1/15/20	9/39/115/115	-
25	8CT	0	314	-	-	5/29/63/63	0/2/2/2
25	8CT	A	845	-	-	10/29/63/63	0/2/2/2
24	CLA	A	834	9	1/1/13/20	12/30/106/115	-
24	CLA	3	306	4	1/1/11/20	5/18/94/115	-
26	0UR	4	317	-	-	9/41/80/86	0/2/2/2
24	CLA	B	817	10	1/1/14/20	18/33/109/115	-
24	CLA	0	319	-	1/1/11/20	1/17/93/115	-
24	CLA	3	315	-	1/1/12/20	5/24/100/115	-
23	CHL	5	306	-	3/3/16/26	7/17/115/137	-
24	CLA	A	820	-	1/1/15/20	10/39/115/115	-
24	CLA	A	828	9	1/1/15/20	13/39/115/115	-
25	8CT	K	105	-	-	12/29/63/63	0/2/2/2
23	CHL	8	309	-	3/3/16/26	2/17/115/137	-
26	0UR	1	315	-	-	3/42/81/86	0/2/2/2
24	CLA	B	806	-	1/1/15/20	11/39/115/115	-
24	CLA	1	302	2	1/1/13/20	14/29/105/115	-
27	LHG	3	324	-	-	23/46/46/53	-
24	CLA	A	806	9	1/1/12/20	4/23/99/115	-
29	LMG	O	203	-	-	13/26/46/70	0/1/1/1
25	8CT	4	316	-	-	8/29/63/63	0/2/2/2
27	LHG	3	322	-	-	18/40/40/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	5	305	-	3/3/16/26	11/18/116/137	-
25	8CT	B	843	-	-	14/29/63/63	0/2/2/2
23	CHL	6	302	5	3/3/19/26	19/37/135/137	-
24	CLA	5	303	-	1/1/12/20	8/24/100/115	-
24	CLA	A	812	9	1/1/15/20	7/39/115/115	-
24	CLA	A	824	-	1/1/15/20	8/39/115/115	-
24	CLA	4	303	7	1/1/11/20	4/15/91/115	-
24	CLA	6	314	-	1/1/11/20	2/15/91/115	-
24	CLA	L	202	17	1/1/14/20	19/37/113/115	-
24	CLA	B	810	10	1/1/14/20	6/36/112/115	-
24	CLA	O	209	-	1/1/12/20	9/23/99/115	-
27	LHG	0	317	-	-	30/53/53/53	-
25	8CT	J	104	-	-	8/29/63/63	0/2/2/2
24	CLA	4	304	-	1/1/14/20	8/33/109/115	-
30	0IE	7	321	-	-	2/33/72/72	0/2/2/2
24	CLA	H	202	10	1/1/13/20	7/27/103/115	-
24	CLA	K	101	-	1/1/14/20	10/33/109/115	-
24	CLA	B	829	-	1/1/15/20	9/39/115/115	-
23	CHL	3	302	4	3/3/19/26	18/35/133/137	-
23	CHL	5	304	-	3/3/16/26	9/15/113/137	-
24	CLA	4	311	-	1/1/11/20	4/19/95/115	-
23	CHL	4	307	-	3/3/17/26	10/21/119/137	-
24	CLA	B	840	10	1/1/15/20	10/39/115/115	-
23	CHL	8	307	-	3/3/17/26	13/21/119/137	-
24	CLA	5	307	-	1/1/11/20	7/17/93/115	-
24	CLA	0	310	-	1/1/11/20	8/18/94/115	-
24	CLA	B	819	10	1/1/14/20	14/33/109/115	-
24	CLA	3	304	-	1/1/15/20	7/39/115/115	-
26	0UR	2	315	-	-	7/41/80/86	0/2/2/2
24	CLA	3	314	4	1/1/11/20	0/17/93/115	-
25	8CT	B	848	-	-	9/29/63/63	0/2/2/2
24	CLA	4	314	7	1/1/11/20	4/15/91/115	-
26	0UR	1	316	-	-	10/42/81/86	0/2/2/2
23	CHL	3	307	-	3/3/20/26	26/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	F	302	13	1/1/11/20	4/18/94/115	-
27	LHG	B	852	-	-	27/42/42/53	-
24	CLA	5	311	2	1/1/13/20	10/29/105/115	-
24	CLA	6	309	5	1/1/13/20	2/31/107/115	-
25	8CT	J	101	-	-	11/29/63/63	0/2/2/2
24	CLA	5	308	-	1/1/14/20	8/33/109/115	-
24	CLA	5	309	27	1/1/11/20	5/15/91/115	-
23	CHL	6	306	-	3/3/17/26	7/21/119/137	-
25	8CT	L	207	-	-	9/29/63/63	0/2/2/2
24	CLA	6	312	5	1/1/13/20	7/29/105/115	-
24	CLA	A	835	-	1/1/12/20	8/23/99/115	-
23	CHL	6	315	5	3/3/15/26	4/12/110/137	-
23	CHL	2	307	-	3/3/16/26	4/17/115/137	-
24	CLA	A	805	-	1/1/15/20	19/39/115/115	-
27	LHG	I	102	-	-	20/50/50/53	-
24	CLA	0	309	-	1/1/10/20	2/10/86/115	-
24	CLA	B	826	-	1/1/10/20	1/23/87/115	-
24	CLA	B	811	10	1/1/15/20	9/39/115/115	-
24	CLA	7	315	6	1/1/12/20	2/15/91/115	-
24	CLA	A	816	9	1/1/14/20	16/35/111/115	-
24	CLA	3	309	4	1/1/15/20	12/39/115/115	-
24	CLA	6	303	5	1/1/12/20	6/24/100/115	-
24	CLA	A	829	9	1/1/15/20	12/39/115/115	-
24	CLA	0	312	1	1/1/11/20	10/17/93/115	-
24	CLA	B	835	-	1/1/11/20	0/15/91/115	-
23	CHL	8	301	2	3/3/17/26	10/23/121/137	-
24	CLA	9	310	8	1/1/12/20	6/24/100/115	-
26	0UR	5	314	-	-	11/41/80/86	0/2/2/2
25	8CT	A	847	-	-	10/29/63/63	0/2/2/2
23	CHL	1	301	-	3/3/19/26	16/37/135/137	-
23	CHL	6	301	5	3/3/19/26	14/33/131/137	-
24	CLA	A	808	9	1/1/15/20	9/39/115/115	-
24	CLA	6	311	5	1/1/11/20	3/19/95/115	-
29	LMG	9	317	-	-	31/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	837	-	1/1/15/20	4/39/115/115	-
24	CLA	2	310	3	1/1/11/20	5/19/95/115	-
24	CLA	6	316	5	1/1/15/20	15/39/115/115	-
25	8CT	L	204	-	-	7/29/63/63	0/2/2/2
26	0UR	6	321	-	-	11/42/81/86	0/2/2/2
23	CHL	3	305	-	3/3/17/26	4/21/119/137	-
33	SF4	C	102	18	-	-	0/6/5/5
23	CHL	2	304	-	3/3/15/26	0/12/110/137	-
24	CLA	A	838	9	1/1/15/20	12/39/115/115	-
24	CLA	6	318	-	1/1/12/20	10/23/99/115	-
23	CHL	0	301	1	3/3/17/26	12/23/121/137	-
24	CLA	0	307	-	1/1/14/20	12/33/109/115	-
24	CLA	A	827	9	1/1/15/20	18/39/115/115	-
23	CHL	0	306	-	3/3/16/26	8/18/116/137	-
24	CLA	3	311	4	1/1/11/20	1/17/93/115	-
24	CLA	K	102	19	1/1/12/20	11/25/101/115	-
27	LHG	1	318	-	-	17/47/47/53	-
24	CLA	1	309	27	1/1/14/20	11/37/113/115	-
23	CHL	5	312	2	3/3/16/26	9/17/115/137	-
23	CHL	8	308	-	3/3/17/26	9/21/119/137	-
23	CHL	0	305	-	3/3/17/26	7/21/119/137	-
24	CLA	B	838	10	1/1/11/20	2/18/94/115	-
24	CLA	L	206	-	1/1/11/20	7/18/94/115	-
27	LHG	5	316	24	-	13/41/41/53	-
25	8CT	B	845	-	-	10/29/63/63	0/2/2/2
24	CLA	A	814	9	1/1/15/20	8/39/115/115	-
24	CLA	9	304	-	1/1/12/20	0/23/99/115	-
32	CL0	A	852	9	3/3/20/25	10/37/135/135	-
27	LHG	3	320	-	-	15/40/40/53	-
24	CLA	1	303	-	1/1/12/20	3/24/100/115	-
23	CHL	4	306	-	3/3/16/26	6/18/116/137	-
24	CLA	G	102	14	1/1/11/20	4/15/91/115	-
23	CHL	4	315	2	3/3/17/26	11/25/123/137	-
24	CLA	B	841	27	1/1/15/20	8/39/115/115	-
26	0UR	2	316	-	-	11/40/79/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	0	311	1	1/1/15/20	12/39/115/115	-
27	LHG	6	322	24	-	17/41/41/53	-
24	CLA	B	804	-	1/1/15/20	13/39/115/115	-
24	CLA	6	310	27	1/1/14/20	11/33/109/115	-
24	CLA	B	839	-	1/1/15/20	8/39/115/115	-
24	CLA	F	303	-	1/1/11/20	6/15/91/115	-
23	CHL	6	323	7	3/3/19/26	5/33/131/137	-
25	8CT	3	323	-	-	7/29/63/63	0/2/2/2
26	0UR	0	316	-	-	12/42/81/86	0/2/2/2
26	0UR	O	207	-	-	5/42/81/86	0/2/2/2
24	CLA	O	204	-	1/1/10/20	6/10/86/115	-
24	CLA	4	310	27	1/1/14/20	14/33/109/115	-
24	CLA	1	308	2	1/1/13/20	6/27/103/115	-
24	CLA	7	304	-	1/1/13/20	7/27/103/115	-
24	CLA	B	822	10	1/1/14/20	11/33/109/115	-
27	LHG	A	842	-	-	19/53/53/53	-
23	CHL	1	312	2	3/3/19/26	21/35/133/137	-
26	0UR	6	320	-	-	11/41/80/86	0/2/2/2
25	8CT	3	316	-	-	9/29/63/63	0/2/2/2
23	CHL	7	307	-	3/3/17/26	4/21/119/137	-
23	CHL	2	306	-	3/3/17/26	6/21/119/137	-
23	CHL	8	314	7	3/3/18/26	9/27/125/137	-
24	CLA	9	308	-	1/1/14/20	7/33/109/115	-
24	CLA	7	308	-	1/1/15/20	15/39/115/115	-
23	CHL	2	305	-	3/3/16/26	5/18/116/137	-
24	CLA	6	304	-	1/1/11/20	6/17/93/115	-
24	CLA	0	308	-	1/1/14/20	9/33/109/115	-
33	SF4	C	101	-	-	-	0/6/5/5
23	CHL	4	313	7	3/3/17/26	5/21/119/137	-
25	8CT	7	318	-	-	15/29/63/63	0/2/2/2
23	CHL	6	307	-	3/3/17/26	7/21/119/137	-
24	CLA	A	848	-	1/1/15/20	12/39/115/115	-
24	CLA	A	836	9	1/1/14/20	12/35/111/115	-
23	CHL	0	302	1	3/3/19/26	14/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	9	313	-	-	11/29/63/63	0/2/2/2
26	0UR	3	318	-	-	9/41/80/86	0/2/2/2
23	CHL	5	301	2	3/3/19/26	18/37/135/137	-
24	CLA	2	313	3	1/1/11/20	5/15/91/115	-
25	8CT	6	324	-	-	11/29/63/63	0/2/2/2
24	CLA	0	304	-	1/1/12/20	4/24/100/115	-
24	CLA	J	103	16	1/1/10/20	3/12/88/115	-
25	8CT	O	202	-	-	7/29/63/63	0/2/2/2
33	SF4	B	803	-	-	-	0/6/5/5
29	LMG	A	854	-	-	15/32/52/70	0/1/1/1
24	CLA	B	830	10	1/1/13/20	7/29/105/115	-
24	CLA	O	201	27	1/1/12/20	6/24/100/115	-
24	CLA	A	832	9	1/1/15/20	12/39/115/115	-
24	CLA	O	205	21	1/1/9/20	2/6/78/115	-
24	CLA	H	203	22	1/1/11/20	6/18/94/115	-
24	CLA	9	309	27	1/1/10/20	4/10/86/115	-
23	CHL	8	303	7	3/3/19/26	17/37/135/137	-
24	CLA	B	802	10	1/1/15/20	13/39/115/115	-
24	CLA	B	816	10	1/1/14/20	8/33/109/115	-
25	8CT	O	208	-	-	6/29/63/63	0/2/2/2
24	CLA	2	309	27	1/1/14/20	14/33/109/115	-
25	8CT	B	844	-	-	11/29/63/63	0/2/2/2
24	CLA	A	840	-	1/1/15/20	10/39/115/115	-
27	LHG	8	302	-	-	12/35/35/53	-
25	8CT	I	101	-	-	8/29/63/63	0/2/2/2
24	CLA	A	830	9	1/1/12/20	3/21/97/115	-
25	8CT	B	850	-	-	13/29/63/63	0/2/2/2
24	CLA	H	205	-	1/1/12/20	9/23/99/115	-
24	CLA	B	825	-	1/1/15/20	7/39/115/115	-
26	0UR	9	314	-	-	3/42/81/86	0/2/2/2
24	CLA	1	307	-	1/1/11/20	6/15/91/115	-
24	CLA	B	812	10	1/1/12/20	4/24/100/115	-
30	0IE	3	319	-	-	2/33/72/72	0/2/2/2
29	LMG	2	318	-	-	14/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	3	308	-	1/1/15/20	16/39/115/115	-
25	8CT	B	847	-	-	9/29/63/63	0/2/2/2
24	CLA	B	808	10	1/1/15/20	10/39/115/115	-
26	0UR	5	315	-	-	10/42/81/86	0/2/2/2
27	LHG	7	323	-	-	20/42/42/53	-
23	CHL	9	312	8	3/3/16/26	9/17/115/137	-
24	CLA	A	815	-	1/1/11/20	5/15/91/115	-
25	8CT	1	314	-	-	8/29/63/63	0/2/2/2
29	LMG	M	101	-	-	23/37/57/70	0/1/1/1
24	CLA	8	305	-	1/1/15/20	10/39/115/115	-
25	8CT	A	846	-	-	7/29/63/63	0/2/2/2
25	8CT	F	301	-	-	14/29/63/63	0/2/2/2
24	CLA	2	303	-	1/1/14/20	11/33/109/115	-
24	CLA	A	821	-	1/1/11/20	5/20/96/115	-
23	CHL	6	313	5	3/3/17/26	6/23/121/137	-
24	CLA	6	317	-	1/1/11/20	11/17/93/115	-
29	LMG	3	321	-	-	16/31/51/70	0/1/1/1
24	CLA	B	831	10	1/1/12/20	7/21/97/115	-
24	CLA	2	302	3	1/1/13/20	9/29/105/115	-
24	CLA	L	203	-	1/1/11/20	6/17/93/115	-
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
24	CLA	A	831	9	1/1/15/20	10/39/115/115	-
24	CLA	A	807	9	1/1/15/20	21/39/115/115	-
24	CLA	0	303	1	1/1/14/20	10/36/112/115	-
24	CLA	7	316	-	1/1/11/20	13/15/91/115	-
24	CLA	1	310	2	1/1/12/20	6/24/100/115	-
24	CLA	3	303	-	1/1/13/20	7/27/103/115	-
24	CLA	A	810	9	1/1/15/20	12/39/115/115	-
26	0UR	4	318	-	-	13/40/79/86	0/2/2/2
24	CLA	B	801	10	1/1/13/20	13/31/107/115	-
24	CLA	4	312	7	1/1/12/20	6/25/101/115	-
23	CHL	1	304	-	3/3/17/26	7/21/119/137	-
27	LHG	B	851	24	-	17/26/26/53	-
25	8CT	A	844	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	7	319	-	-	10/29/63/63	0/2/2/2
24	CLA	A	823	9	1/1/13/20	8/27/103/115	-
24	CLA	8	315	-	1/1/11/20	9/15/91/115	-
24	CLA	B	805	10	1/1/15/20	9/39/115/115	-
24	CLA	B	834	10	1/1/14/20	15/35/111/115	-
24	CLA	B	821	10	1/1/12/20	0/21/97/115	-
29	LMG	A	851	-	-	13/31/51/70	0/1/1/1
27	LHG	7	322	24	-	10/34/34/53	-
29	LMG	J	105	-	-	15/41/61/70	0/1/1/1
24	CLA	8	312	7	1/1/11/20	8/17/93/115	-
24	CLA	5	313	2	1/1/11/20	9/17/93/115	-
24	CLA	G	103	14	1/1/11/20	5/17/93/115	-
24	CLA	A	813	9	1/1/13/20	10/30/106/115	-
27	LHG	1	317	24	-	21/53/53/53	-
23	CHL	7	313	6	3/3/16/26	9/17/115/137	-
23	CHL	9	301	8	3/3/16/26	8/17/115/137	-
24	CLA	3	310	-	1/1/14/20	13/36/112/115	-
24	CLA	K	104	19	1/1/12/20	11/21/97/115	-
25	8CT	A	849	-	-	10/29/63/63	0/2/2/2
24	CLA	A	803	9	1/1/13/20	8/27/103/115	-
24	CLA	K	103	19	1/1/11/20	5/17/93/115	-
24	CLA	A	839	9	1/1/15/20	17/39/115/115	-
26	0UR	8	319	-	-	8/42/81/86	0/2/2/2
24	CLA	7	312	6	1/1/13/20	10/27/103/115	-
24	CLA	2	308	3	1/1/14/20	3/33/109/115	-
25	8CT	F	304	-	-	9/29/63/63	0/2/2/2
27	LHG	2	317	24	-	17/36/36/53	-
26	0UR	8	318	-	-	7/41/80/86	0/2/2/2
24	CLA	A	804	9	1/1/15/20	13/39/115/115	-
27	LHG	A	843	24	-	17/31/31/53	-
24	CLA	9	303	8	1/1/11/20	5/19/95/115	-
24	CLA	B	820	-	1/1/13/20	10/29/105/115	-
23	CHL	4	302	7	3/3/17/26	13/24/122/137	-
24	CLA	7	317	6	1/1/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	824	10	1/1/14/20	8/33/109/115	-
27	LHG	9	316	24	-	18/48/48/53	-
26	0UR	0	315	-	-	3/42/81/86	0/2/2/2
24	CLA	B	836	10	1/1/14/20	11/33/109/115	-
24	CLA	7	310	27	1/1/8/20	2/4/76/115	-
24	CLA	A	801	-	1/1/15/20	4/39/115/115	-
24	CLA	A	811	9	1/1/12/20	1/26/102/115	-
29	LMG	O	210	-	-	10/34/54/70	0/1/1/1
26	0UR	7	320	-	-	9/41/80/86	0/2/2/2
24	CLA	B	833	10	1/1/13/20	9/27/103/115	-
24	CLA	L	201	9	1/1/13/20	7/31/107/115	-
24	CLA	8	313	7	1/1/13/20	8/29/105/115	-
24	CLA	9	311	8	1/1/13/20	6/29/105/115	-
24	CLA	9	307	-	1/1/15/20	12/39/115/115	-
25	8CT	6	319	-	-	8/29/63/63	0/2/2/2
24	CLA	H	201	17	1/1/11/20	5/17/93/115	-
24	CLA	A	817	9	1/1/15/20	12/39/115/115	-
24	CLA	5	302	2	1/1/13/20	13/32/108/115	-
23	CHL	9	305	-	3/3/17/26	7/21/119/137	-
23	CHL	6	305	-	3/3/15/26	0/12/110/137	-
24	CLA	0	313	1	1/1/11/20	11/15/91/115	-
28	SQD	0	318	-	-	17/31/51/69	0/1/1/1
23	CHL	8	316	-	3/3/15/26	4/12/110/137	-
24	CLA	A	833	9	1/1/11/20	0/17/93/115	-
25	8CT	L	205	-	-	8/29/63/63	0/2/2/2
24	CLA	7	314	6	1/1/11/20	8/18/94/115	-
24	CLA	3	313	4	1/1/11/20	7/15/91/115	-
23	CHL	1	305	-	3/3/16/26	7/18/116/137	-
23	CHL	2	301	3	3/3/19/26	26/37/135/137	-
24	CLA	4	309	-	1/1/14/20	5/33/109/115	-
24	CLA	B	832	-	1/1/15/20	8/39/115/115	-
27	LHG	L	208	-	-	13/35/35/53	-
24	CLA	B	823	-	1/1/12/20	10/24/100/115	-
29	LMG	J	102	-	-	12/24/44/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	828	-	1/1/14/20	6/33/109/115	-
23	CHL	4	301	7	3/3/19/26	16/33/131/137	-
27	LHG	2	319	24	-	12/36/36/53	-
23	CHL	4	308	-	3/3/16/26	3/17/115/137	-
24	CLA	B	807	10	1/1/11/20	5/15/91/115	-
24	CLA	O	206	-	1/1/10/20	1/4/80/115	-
25	8CT	8	317	-	-	10/29/63/63	0/2/2/2
24	CLA	2	311	3	1/1/14/20	10/33/109/115	-
25	8CT	M	102	-	-	8/29/63/63	0/2/2/2
26	0UR	9	315	-	-	8/42/81/86	0/2/2/2
23	CHL	9	306	-	3/3/16/26	7/18/116/137	-
23	CHL	8	306	-	3/3/16/26	6/17/115/137	-
23	CHL	4	305	-	3/3/15/26	0/12/110/137	-
24	CLA	A	809	9	1/1/15/20	3/39/115/115	-

All (3884) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	104	8CT	C02-C03	14.90	1.59	1.34
25	B	844	8CT	C02-C03	14.87	1.59	1.34
25	6	324	8CT	C02-C03	14.86	1.59	1.34
25	A	844	8CT	C02-C03	14.78	1.59	1.34
25	G	104	8CT	C02-C03	14.77	1.59	1.34
25	F	301	8CT	C02-C03	14.75	1.59	1.34
25	B	848	8CT	C02-C03	14.74	1.59	1.34
25	F	304	8CT	C02-C03	14.73	1.59	1.34
25	A	846	8CT	C02-C03	14.71	1.59	1.34
25	1	314	8CT	C02-C03	14.69	1.59	1.34
25	O	208	8CT	C02-C03	14.68	1.59	1.34
25	6	319	8CT	C02-C03	14.66	1.59	1.34
25	M	102	8CT	C02-C03	14.63	1.59	1.34
25	8	317	8CT	C02-C03	14.63	1.59	1.34
25	L	207	8CT	C02-C03	14.62	1.59	1.34
25	3	323	8CT	C02-C03	14.61	1.59	1.34
25	B	843	8CT	C02-C03	14.60	1.59	1.34
25	A	845	8CT	C02-C03	14.59	1.59	1.34
25	B	847	8CT	C02-C03	14.58	1.59	1.34
25	A	849	8CT	C02-C03	14.57	1.58	1.34
25	K	105	8CT	C02-C03	14.57	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	314	8CT	C02-C03	14.56	1.58	1.34
25	L	205	8CT	C02-C03	14.55	1.58	1.34
25	O	202	8CT	C02-C03	14.54	1.58	1.34
25	I	101	8CT	C02-C03	14.53	1.58	1.34
25	7	319	8CT	C02-C03	14.51	1.58	1.34
25	B	846	8CT	C02-C03	14.50	1.58	1.34
25	3	316	8CT	C02-C03	14.50	1.58	1.34
25	B	850	8CT	C02-C03	14.49	1.58	1.34
25	L	204	8CT	C02-C03	14.48	1.58	1.34
25	0	314	8CT	C02-C03	14.46	1.58	1.34
25	9	313	8CT	C02-C03	14.45	1.58	1.34
25	B	845	8CT	C02-C03	14.42	1.58	1.34
25	3	317	8CT	C02-C03	14.42	1.58	1.34
25	4	316	8CT	C02-C03	14.42	1.58	1.34
25	J	101	8CT	C02-C03	14.35	1.58	1.34
25	B	843	8CT	C32-C31	14.33	1.60	1.32
25	7	318	8CT	C02-C03	14.32	1.58	1.34
25	A	847	8CT	C02-C03	14.32	1.58	1.34
25	B	846	8CT	C32-C31	14.32	1.59	1.32
25	1	314	8CT	C32-C31	14.31	1.59	1.32
25	3	317	8CT	C32-C31	14.31	1.59	1.32
25	6	324	8CT	C32-C31	14.31	1.59	1.32
25	7	318	8CT	C32-C31	14.30	1.59	1.32
25	F	301	8CT	C32-C31	14.29	1.59	1.32
25	9	313	8CT	C32-C31	14.28	1.59	1.32
25	6	319	8CT	C32-C31	14.27	1.59	1.32
25	L	205	8CT	C32-C31	14.25	1.59	1.32
25	O	208	8CT	C32-C31	14.24	1.59	1.32
25	8	317	8CT	C32-C31	14.19	1.59	1.32
25	L	207	8CT	C32-C31	14.17	1.59	1.32
25	7	319	8CT	C32-C31	14.17	1.59	1.32
25	B	850	8CT	C32-C31	14.16	1.59	1.32
25	B	848	8CT	C32-C31	14.16	1.59	1.32
25	F	304	8CT	C32-C31	14.10	1.59	1.32
25	0	314	8CT	C32-C31	14.07	1.59	1.32
25	A	844	8CT	C32-C31	14.07	1.59	1.32
25	L	204	8CT	C32-C31	14.06	1.59	1.32
25	3	316	8CT	C32-C31	14.04	1.59	1.32
25	B	847	8CT	C32-C31	14.04	1.59	1.32
25	G	104	8CT	C32-C31	14.03	1.59	1.32
25	J	101	8CT	C32-C31	14.02	1.59	1.32
25	O	202	8CT	C32-C31	14.01	1.59	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	323	8CT	C32-C31	14.01	1.59	1.32
25	A	847	8CT	C32-C31	13.97	1.59	1.32
25	M	102	8CT	C32-C31	13.96	1.59	1.32
25	J	104	8CT	C32-C31	13.96	1.59	1.32
25	B	844	8CT	C32-C31	13.95	1.59	1.32
25	A	846	8CT	C32-C31	13.93	1.59	1.32
25	A	849	8CT	C32-C31	13.93	1.59	1.32
25	B	845	8CT	C32-C31	13.92	1.59	1.32
25	A	845	8CT	C32-C31	13.92	1.59	1.32
25	I	101	8CT	C32-C31	13.90	1.59	1.32
25	2	314	8CT	C32-C31	13.89	1.59	1.32
25	K	105	8CT	C32-C31	13.86	1.59	1.32
25	4	316	8CT	C32-C31	13.81	1.59	1.32
23	5	312	CHL	C2C-C3C	11.43	1.47	1.36
23	0	306	CHL	C2C-C3C	11.39	1.47	1.36
23	5	305	CHL	C2C-C3C	11.31	1.47	1.36
23	5	306	CHL	C2C-C3C	11.08	1.47	1.36
23	8	301	CHL	C2C-C3C	11.05	1.47	1.36
23	8	316	CHL	C2C-C3C	10.85	1.46	1.36
23	0	305	CHL	C2C-C3C	10.78	1.46	1.36
23	5	304	CHL	C2C-C3C	10.73	1.46	1.36
23	6	323	CHL	C2C-C3C	10.70	1.46	1.36
23	1	306	CHL	C2C-C3C	10.66	1.46	1.36
23	1	305	CHL	C2C-C3C	10.64	1.46	1.36
23	9	312	CHL	C2C-C3C	10.64	1.46	1.36
23	7	313	CHL	C2C-C3C	10.64	1.46	1.36
23	7	301	CHL	C2C-C3C	10.63	1.46	1.36
23	7	306	CHL	C2C-C3C	10.62	1.46	1.36
23	6	315	CHL	C2C-C3C	10.59	1.46	1.36
23	8	309	CHL	C2C-C3C	10.57	1.46	1.36
23	8	307	CHL	C2C-C3C	10.57	1.46	1.36
23	3	301	CHL	C2C-C3C	10.56	1.46	1.36
23	4	308	CHL	C2C-C3C	10.56	1.46	1.36
23	2	307	CHL	C2C-C3C	10.52	1.46	1.36
23	2	305	CHL	C2C-C3C	10.50	1.46	1.36
23	9	306	CHL	C2C-C3C	10.49	1.46	1.36
23	4	306	CHL	C2C-C3C	10.49	1.46	1.36
23	0	301	CHL	C2C-C3C	10.48	1.46	1.36
23	8	306	CHL	C2C-C3C	10.47	1.46	1.36
23	4	315	CHL	C2C-C3C	10.47	1.46	1.36
23	9	301	CHL	C2C-C3C	10.47	1.46	1.36
23	6	301	CHL	C2C-C3C	10.41	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	312	CHL	C2C-C3C	10.41	1.46	1.36
23	6	313	CHL	C2C-C3C	10.41	1.46	1.36
23	4	301	CHL	C2C-C3C	10.40	1.46	1.36
23	2	312	CHL	C2C-C3C	10.36	1.46	1.36
23	6	308	CHL	C2C-C3C	10.36	1.46	1.36
23	1	304	CHL	C2C-C3C	10.35	1.46	1.36
23	8	314	CHL	C2C-C3C	10.35	1.46	1.36
23	4	313	CHL	C2C-C3C	10.33	1.46	1.36
23	4	307	CHL	C2C-C3C	10.29	1.46	1.36
23	6	305	CHL	C2C-C3C	10.27	1.46	1.36
23	4	305	CHL	C2C-C3C	10.24	1.46	1.36
23	6	306	CHL	C2C-C3C	10.23	1.46	1.36
23	8	308	CHL	C2C-C3C	10.22	1.46	1.36
23	2	304	CHL	C2C-C3C	10.21	1.46	1.36
23	3	305	CHL	C2C-C3C	10.20	1.46	1.36
23	6	307	CHL	C2C-C3C	10.18	1.46	1.36
23	9	305	CHL	C2C-C3C	10.18	1.46	1.36
23	0	302	CHL	C2C-C3C	10.11	1.46	1.36
23	4	302	CHL	C2C-C3C	10.08	1.46	1.36
23	7	305	CHL	C2C-C3C	10.05	1.46	1.36
23	3	307	CHL	C2C-C3C	10.01	1.46	1.36
23	3	302	CHL	C2C-C3C	9.99	1.46	1.36
23	5	301	CHL	C2C-C3C	9.98	1.46	1.36
23	7	307	CHL	C2C-C3C	9.98	1.46	1.36
23	6	302	CHL	C2C-C3C	9.95	1.46	1.36
23	7	302	CHL	C2C-C3C	9.91	1.46	1.36
23	1	301	CHL	C2C-C3C	9.88	1.45	1.36
23	2	301	CHL	C2C-C3C	9.88	1.45	1.36
23	2	306	CHL	C2C-C3C	9.87	1.45	1.36
23	8	303	CHL	C2C-C3C	9.79	1.45	1.36
25	O	202	8CT	C34-C35	-9.20	1.36	1.54
25	F	301	8CT	C34-C35	-9.07	1.37	1.54
25	B	848	8CT	C34-C35	-9.01	1.37	1.54
25	L	207	8CT	C34-C35	-8.98	1.37	1.54
25	B	846	8CT	C34-C35	-8.97	1.37	1.54
25	B	843	8CT	C34-C35	-8.93	1.37	1.54
25	3	317	8CT	C34-C35	-8.91	1.37	1.54
25	B	850	8CT	C34-C35	-8.91	1.37	1.54
25	A	847	8CT	C34-C35	-8.90	1.37	1.54
25	A	849	8CT	C34-C35	-8.88	1.37	1.54
25	6	324	8CT	C34-C35	-8.88	1.37	1.54
25	7	319	8CT	C34-C35	-8.84	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	314	8CT	C34-C35	-8.84	1.37	1.54
25	F	304	8CT	C34-C35	-8.82	1.37	1.54
25	O	208	8CT	C34-C35	-8.82	1.37	1.54
25	3	323	8CT	C34-C35	-8.82	1.37	1.54
25	J	104	8CT	C34-C35	-8.81	1.37	1.54
25	A	844	8CT	C34-C35	-8.81	1.37	1.54
25	6	319	8CT	C34-C35	-8.79	1.37	1.54
25	8	317	8CT	C34-C35	-8.79	1.37	1.54
25	A	845	8CT	C34-C35	-8.74	1.37	1.54
25	B	847	8CT	C34-C35	-8.74	1.37	1.54
25	M	102	8CT	C34-C35	-8.70	1.37	1.54
25	L	205	8CT	C34-C35	-8.70	1.37	1.54
25	L	204	8CT	C34-C35	-8.69	1.37	1.54
25	7	318	8CT	C34-C35	-8.69	1.37	1.54
25	9	313	8CT	C34-C35	-8.67	1.37	1.54
25	B	845	8CT	C34-C35	-8.64	1.37	1.54
25	B	844	8CT	C34-C35	-8.63	1.37	1.54
25	A	846	8CT	C34-C35	-8.58	1.38	1.54
25	I	101	8CT	C34-C35	-8.57	1.38	1.54
25	2	314	8CT	C34-C35	-8.54	1.38	1.54
25	K	105	8CT	C34-C35	-8.52	1.38	1.54
25	3	316	8CT	C34-C35	-8.52	1.38	1.54
23	8	316	CHL	C1B-C2B	8.51	1.49	1.39
23	5	306	CHL	C1B-C2B	8.46	1.49	1.39
25	J	101	8CT	C34-C35	-8.45	1.38	1.54
23	0	306	CHL	C1B-C2B	8.44	1.49	1.39
25	G	104	8CT	C34-C35	-8.40	1.38	1.54
23	6	313	CHL	C1B-C2B	8.40	1.49	1.39
23	5	312	CHL	C1B-C2B	8.31	1.49	1.39
25	0	314	8CT	C34-C35	-8.31	1.38	1.54
23	5	312	CHL	C1A-CHA	8.30	1.49	1.40
23	1	305	CHL	C1B-C2B	8.30	1.49	1.39
23	1	306	CHL	C1B-C2B	8.30	1.49	1.39
23	9	312	CHL	C1B-C2B	8.29	1.49	1.39
23	8	301	CHL	C3B-C4B	8.20	1.49	1.41
23	0	301	CHL	C1B-C2B	8.20	1.48	1.39
23	6	315	CHL	C1B-C2B	8.19	1.48	1.39
23	8	306	CHL	C1B-C2B	8.19	1.48	1.39
23	5	305	CHL	C1B-C2B	8.19	1.48	1.39
23	6	323	CHL	C1B-C2B	8.19	1.48	1.39
23	1	312	CHL	C1B-C2B	8.18	1.48	1.39
23	8	314	CHL	C1B-C2B	8.16	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	308	CHL	C1B-C2B	8.15	1.48	1.39
23	7	313	CHL	C1A-CHA	8.14	1.49	1.40
25	4	316	8CT	C34-C35	-8.13	1.38	1.54
23	2	307	CHL	C1B-C2B	8.13	1.48	1.39
23	6	301	CHL	C1B-C2B	8.13	1.48	1.39
23	7	313	CHL	C1B-C2B	8.12	1.48	1.39
23	8	309	CHL	C1B-C2B	8.12	1.48	1.39
23	4	308	CHL	C1B-C2B	8.12	1.48	1.39
23	5	304	CHL	C1B-C2B	8.11	1.48	1.39
23	4	307	CHL	C1B-C2B	8.11	1.48	1.39
23	8	307	CHL	C1B-C2B	8.11	1.48	1.39
23	6	306	CHL	C1B-C2B	8.09	1.48	1.39
23	8	308	CHL	C1B-C2B	8.08	1.48	1.39
23	0	306	CHL	C1A-CHA	8.08	1.49	1.40
23	4	313	CHL	C1B-C2B	8.07	1.48	1.39
23	1	306	CHL	C1A-CHA	8.06	1.49	1.40
23	0	302	CHL	C1B-C2B	8.04	1.48	1.39
23	2	312	CHL	C1B-C2B	8.04	1.48	1.39
23	7	305	CHL	C1B-C2B	8.03	1.48	1.39
23	9	301	CHL	C1A-CHA	8.02	1.49	1.40
23	6	305	CHL	C1B-C2B	8.02	1.48	1.39
23	6	302	CHL	C1B-C2B	8.00	1.48	1.39
23	4	305	CHL	C1B-C2B	8.00	1.48	1.39
23	4	306	CHL	C1B-C2B	8.00	1.48	1.39
23	5	301	CHL	C1B-C2B	7.99	1.48	1.39
23	7	307	CHL	C3B-C4B	7.99	1.49	1.41
23	9	306	CHL	C1B-C2B	7.99	1.48	1.39
23	9	301	CHL	C1B-C2B	7.98	1.48	1.39
23	4	306	CHL	C3B-C4B	7.96	1.49	1.41
23	1	301	CHL	C3B-C4B	7.96	1.49	1.41
23	1	305	CHL	C1A-CHA	7.95	1.49	1.40
23	2	305	CHL	C1B-C2B	7.95	1.48	1.39
23	8	301	CHL	C1B-C2B	7.95	1.48	1.39
23	6	307	CHL	C1B-C2B	7.94	1.48	1.39
23	3	305	CHL	C1B-C2B	7.94	1.48	1.39
23	7	301	CHL	C1B-C2B	7.92	1.48	1.39
23	0	305	CHL	C1B-C2B	7.91	1.48	1.39
23	0	305	CHL	C3B-C4B	7.91	1.49	1.41
23	3	305	CHL	C1A-CHA	7.89	1.49	1.40
23	2	306	CHL	C1B-C2B	7.89	1.48	1.39
23	2	301	CHL	C1B-C2B	7.89	1.48	1.39
23	4	315	CHL	C3B-C4B	7.88	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	301	CHL	C1B-C2B	7.87	1.48	1.39
23	2	304	CHL	C1B-C2B	7.86	1.48	1.39
23	8	308	CHL	C3B-C4B	7.86	1.49	1.41
23	9	305	CHL	C3B-C4B	7.84	1.49	1.41
23	2	312	CHL	C1A-CHA	7.84	1.48	1.40
23	7	307	CHL	C1A-CHA	7.84	1.48	1.40
23	8	306	CHL	C3B-C4B	7.83	1.49	1.41
23	4	307	CHL	C1A-CHA	7.82	1.48	1.40
23	3	301	CHL	C1B-C2B	7.79	1.48	1.39
23	4	302	CHL	C1B-C2B	7.79	1.48	1.39
23	5	304	CHL	C1A-CHA	7.79	1.48	1.40
23	6	323	CHL	C1A-CHA	7.78	1.48	1.40
23	2	305	CHL	C3B-C4B	7.78	1.49	1.41
23	8	307	CHL	C1A-CHA	7.77	1.48	1.40
23	7	301	CHL	C3B-C4B	7.76	1.48	1.41
23	7	306	CHL	C1B-C2B	7.75	1.48	1.39
23	4	315	CHL	C1B-C2B	7.75	1.48	1.39
23	4	301	CHL	C3B-C4B	7.74	1.48	1.41
23	4	305	CHL	C3B-C4B	7.74	1.48	1.41
23	1	301	CHL	C1B-C2B	7.74	1.48	1.39
23	5	305	CHL	C1A-CHA	7.73	1.48	1.40
23	1	312	CHL	C1A-CHA	7.72	1.48	1.40
23	6	323	CHL	C3B-C4B	7.72	1.48	1.41
23	6	315	CHL	C1A-CHA	7.70	1.48	1.40
23	5	305	CHL	C3B-C4B	7.70	1.48	1.41
23	3	302	CHL	C3B-C4B	7.70	1.48	1.41
31	B	842	PQN	C3-C2	7.69	1.49	1.35
23	8	316	CHL	C1A-CHA	7.69	1.48	1.40
23	8	303	CHL	C3B-C4B	7.68	1.48	1.41
23	7	302	CHL	C1B-C2B	7.68	1.48	1.39
23	2	306	CHL	C3B-C4B	7.67	1.48	1.41
23	7	307	CHL	C1B-C2B	7.67	1.48	1.39
23	7	306	CHL	C3B-C4B	7.67	1.48	1.41
23	1	304	CHL	C1B-C2B	7.66	1.48	1.39
23	0	301	CHL	C1A-CHA	7.65	1.48	1.40
23	4	305	CHL	C1A-CHA	7.65	1.48	1.40
23	3	307	CHL	C1B-C2B	7.64	1.48	1.39
23	6	308	CHL	C1A-CHA	7.64	1.48	1.40
23	7	301	CHL	C1A-CHA	7.64	1.48	1.40
32	A	852	CL0	C1B-C2B	7.63	1.48	1.39
23	5	306	CHL	C1A-CHA	7.62	1.48	1.40
23	8	314	CHL	C1A-CHA	7.62	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	316	CHL	C3B-C4B	7.61	1.48	1.41
23	0	302	CHL	C1A-CHA	7.61	1.48	1.40
23	7	305	CHL	C1A-CHA	7.61	1.48	1.40
23	3	302	CHL	C1B-C2B	7.61	1.48	1.39
23	6	305	CHL	C3B-C4B	7.59	1.48	1.41
23	6	306	CHL	C1A-CHA	7.58	1.48	1.40
23	5	304	CHL	C3B-C4B	7.58	1.48	1.41
23	2	307	CHL	C1A-CHA	7.58	1.48	1.40
23	4	306	CHL	C1A-CHA	7.57	1.48	1.40
23	2	304	CHL	C3B-C4B	7.57	1.48	1.41
23	8	308	CHL	C1A-CHA	7.57	1.48	1.40
23	8	303	CHL	C1B-C2B	7.56	1.48	1.39
23	6	313	CHL	C1A-CHA	7.56	1.48	1.40
23	9	305	CHL	C1B-C2B	7.55	1.48	1.39
23	0	305	CHL	C1A-CHA	7.54	1.48	1.40
23	5	312	CHL	C3B-C4B	7.54	1.48	1.41
23	9	306	CHL	C3B-C4B	7.54	1.48	1.41
23	1	306	CHL	C3B-C4B	7.54	1.48	1.41
23	6	307	CHL	C1A-CHA	7.53	1.48	1.40
23	8	307	CHL	C3B-C4B	7.53	1.48	1.41
23	7	313	CHL	C3B-C4B	7.52	1.48	1.41
23	8	309	CHL	C1A-CHA	7.50	1.48	1.40
23	4	308	CHL	C1A-CHA	7.50	1.48	1.40
23	1	304	CHL	C3B-C4B	7.48	1.48	1.41
23	9	306	CHL	C1A-CHA	7.47	1.48	1.40
23	4	313	CHL	C1A-CHA	7.46	1.48	1.40
23	5	306	CHL	C3B-C4B	7.46	1.48	1.41
23	1	305	CHL	C3B-C4B	7.46	1.48	1.41
23	6	305	CHL	C1A-CHA	7.44	1.48	1.40
23	8	301	CHL	C1A-CHA	7.43	1.48	1.40
23	0	306	CHL	C3B-C4B	7.43	1.48	1.41
23	4	315	CHL	C1A-CHA	7.43	1.48	1.40
23	8	306	CHL	C1A-CHA	7.42	1.48	1.40
23	1	312	CHL	C3B-C4B	7.41	1.48	1.41
23	1	304	CHL	C1A-CHA	7.39	1.48	1.40
23	5	301	CHL	C1A-CHA	7.39	1.48	1.40
23	2	301	CHL	C1A-CHA	7.39	1.48	1.40
23	4	307	CHL	C3B-C4B	7.39	1.48	1.41
23	6	315	CHL	C3B-C4B	7.39	1.48	1.41
23	9	301	CHL	C3B-C4B	7.37	1.48	1.41
23	4	301	CHL	C1A-CHA	7.37	1.48	1.40
23	2	305	CHL	C1A-CHA	7.36	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	312	CHL	C1A-CHA	7.36	1.48	1.40
23	0	301	CHL	C3B-C4B	7.36	1.48	1.41
23	2	304	CHL	C1A-CHA	7.35	1.48	1.40
23	9	305	CHL	C1A-CHA	7.35	1.48	1.40
31	A	841	PQN	C3-C2	7.35	1.48	1.35
23	6	307	CHL	C3B-C4B	7.33	1.48	1.41
23	7	302	CHL	C3B-C4B	7.33	1.48	1.41
23	4	302	CHL	C1A-CHA	7.33	1.48	1.40
23	4	302	CHL	C3B-C4B	7.32	1.48	1.41
23	1	301	CHL	C1A-CHA	7.32	1.48	1.40
23	7	305	CHL	C3B-C4B	7.30	1.48	1.41
23	3	307	CHL	C1A-CHA	7.30	1.48	1.40
23	2	306	CHL	C1A-CHA	7.29	1.48	1.40
23	6	301	CHL	C1A-CHA	7.29	1.48	1.40
23	6	308	CHL	C3B-C4B	7.28	1.48	1.41
23	6	302	CHL	C1A-CHA	7.28	1.48	1.40
32	A	852	CL0	C1D-C2D	7.26	1.47	1.39
23	3	305	CHL	C3B-C4B	7.25	1.48	1.41
23	9	312	CHL	C3B-C4B	7.25	1.48	1.41
23	2	312	CHL	C3B-C4B	7.25	1.48	1.41
23	2	301	CHL	C3B-C4B	7.23	1.48	1.41
23	2	307	CHL	C3B-C4B	7.23	1.48	1.41
23	8	309	CHL	C3B-C4B	7.21	1.48	1.41
23	4	313	CHL	C3B-C4B	7.20	1.48	1.41
23	3	301	CHL	C1A-CHA	7.19	1.48	1.40
23	5	301	CHL	C3B-C4B	7.17	1.48	1.41
23	7	302	CHL	C1A-CHA	7.15	1.48	1.40
23	0	302	CHL	C3B-C4B	7.15	1.48	1.41
23	6	301	CHL	C3B-C4B	7.14	1.48	1.41
23	3	301	CHL	C3B-C4B	7.13	1.48	1.41
23	8	303	CHL	C1A-CHA	7.11	1.48	1.40
23	7	306	CHL	C1A-CHA	7.11	1.48	1.40
23	6	302	CHL	C3B-C4B	7.11	1.48	1.41
23	8	314	CHL	C3B-C4B	7.10	1.48	1.41
23	6	313	CHL	C3B-C4B	7.06	1.48	1.41
23	6	306	CHL	C3B-C4B	7.02	1.48	1.41
25	J	104	8CT	C05-C06	-6.98	1.36	1.52
23	3	302	CHL	C1A-CHA	6.97	1.47	1.40
25	F	301	8CT	C05-C06	-6.96	1.36	1.52
25	B	848	8CT	C05-C06	-6.95	1.36	1.52
25	G	104	8CT	C05-C06	-6.95	1.36	1.52
25	B	846	8CT	C15-C16	6.93	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	304	8CT	C05-C06	-6.92	1.36	1.52
25	6	324	8CT	C05-C06	-6.90	1.36	1.52
23	4	308	CHL	C3B-C4B	6.90	1.48	1.41
25	M	102	8CT	C05-C06	-6.90	1.36	1.52
25	1	314	8CT	C05-C06	-6.89	1.36	1.52
25	B	847	8CT	C05-C06	-6.89	1.36	1.52
25	3	323	8CT	C05-C06	-6.88	1.36	1.52
25	A	846	8CT	C05-C06	-6.88	1.36	1.52
25	6	319	8CT	C05-C06	-6.88	1.36	1.52
25	3	316	8CT	C05-C06	-6.87	1.36	1.52
25	B	850	8CT	C05-C06	-6.87	1.36	1.52
25	8	317	8CT	C05-C06	-6.86	1.36	1.52
25	B	844	8CT	C15-C16	6.86	1.60	1.46
25	B	843	8CT	C05-C06	-6.86	1.36	1.52
25	A	849	8CT	C05-C06	-6.86	1.36	1.52
25	7	318	8CT	C05-C06	-6.85	1.36	1.52
25	7	319	8CT	C05-C06	-6.83	1.36	1.52
23	5	312	CHL	C1D-C2D	6.83	1.47	1.39
25	L	204	8CT	C05-C06	-6.81	1.36	1.52
25	I	101	8CT	C05-C06	-6.81	1.36	1.52
25	9	313	8CT	C05-C06	-6.81	1.36	1.52
25	O	208	8CT	C05-C06	-6.81	1.36	1.52
23	3	307	CHL	C3B-C4B	6.81	1.48	1.41
25	J	101	8CT	C05-C06	-6.79	1.36	1.52
25	B	844	8CT	C05-C06	-6.79	1.36	1.52
25	L	207	8CT	C05-C06	-6.78	1.36	1.52
25	B	845	8CT	C05-C06	-6.78	1.36	1.52
25	L	205	8CT	C05-C06	-6.78	1.36	1.52
25	4	316	8CT	C05-C06	-6.78	1.36	1.52
25	3	317	8CT	C05-C06	-6.77	1.36	1.52
25	A	845	8CT	C05-C06	-6.77	1.36	1.52
25	0	314	8CT	C05-C06	-6.77	1.36	1.52
25	A	844	8CT	C05-C06	-6.75	1.36	1.52
25	A	847	8CT	C05-C06	-6.74	1.36	1.52
25	B	843	8CT	C15-C16	6.74	1.60	1.46
23	5	306	CHL	C1D-C2D	6.73	1.47	1.39
25	B	846	8CT	C05-C06	-6.73	1.36	1.52
23	8	316	CHL	C1D-C2D	6.73	1.47	1.39
25	2	314	8CT	C05-C06	-6.72	1.36	1.52
23	5	305	CHL	C1D-C2D	6.71	1.47	1.39
25	K	105	8CT	C05-C06	-6.71	1.36	1.52
23	5	304	CHL	C1D-C2D	6.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	202	8CT	C05-C06	-6.63	1.36	1.52
25	B	845	8CT	C15-C16	6.61	1.60	1.46
23	8	306	CHL	C1D-C2D	6.58	1.47	1.39
23	6	315	CHL	C1D-C2D	6.54	1.47	1.39
23	0	305	CHL	C1D-C2D	6.51	1.46	1.39
23	9	312	CHL	C1D-C2D	6.46	1.46	1.39
25	2	314	8CT	C28-C26	6.46	1.59	1.46
25	4	316	8CT	C28-C26	6.45	1.59	1.46
25	A	847	8CT	C04-C03	-6.44	1.45	1.53
25	B	848	8CT	C15-C16	6.44	1.59	1.46
25	3	316	8CT	C15-C16	6.43	1.59	1.46
23	1	304	CHL	C1D-C2D	6.43	1.46	1.39
23	8	301	CHL	C1D-C2D	6.42	1.46	1.39
25	B	846	8CT	C28-C26	6.42	1.59	1.46
23	8	307	CHL	C1D-C2D	6.41	1.46	1.39
23	1	305	CHL	C1D-C2D	6.40	1.46	1.39
23	8	314	CHL	C1D-C2D	6.38	1.46	1.39
25	G	104	8CT	C15-C16	6.38	1.59	1.46
25	4	316	8CT	C15-C16	6.38	1.59	1.46
25	8	317	8CT	C15-C16	6.37	1.59	1.46
25	A	849	8CT	C15-C16	6.37	1.59	1.46
25	6	324	8CT	C15-C16	6.36	1.59	1.46
25	0	314	8CT	C28-C26	6.36	1.59	1.46
23	5	301	CHL	C1D-C2D	6.36	1.46	1.39
23	0	306	CHL	C1D-C2D	6.35	1.46	1.39
23	6	301	CHL	C1D-C2D	6.35	1.46	1.39
25	L	207	8CT	C15-C16	6.34	1.59	1.46
23	9	301	CHL	C1D-C2D	6.34	1.46	1.39
23	6	313	CHL	C1D-C2D	6.33	1.46	1.39
25	K	105	8CT	C15-C16	6.33	1.59	1.46
25	2	314	8CT	C15-C16	6.32	1.59	1.46
25	B	843	8CT	C28-C26	6.31	1.59	1.46
25	0	314	8CT	C15-C16	6.30	1.59	1.46
25	3	323	8CT	C15-C16	6.30	1.59	1.46
23	7	306	CHL	C1D-C2D	6.30	1.46	1.39
25	9	313	8CT	C15-C16	6.29	1.59	1.46
25	L	205	8CT	C15-C16	6.29	1.59	1.46
25	3	317	8CT	C15-C16	6.29	1.59	1.46
25	6	324	8CT	C28-C26	6.28	1.59	1.46
25	A	844	8CT	C15-C16	6.28	1.59	1.46
23	2	305	CHL	C1D-C2D	6.28	1.46	1.39
25	9	313	8CT	C28-C26	6.27	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	301	CHL	C1D-C2D	6.27	1.46	1.39
25	O	208	8CT	C15-C16	6.26	1.59	1.46
25	6	319	8CT	C15-C16	6.26	1.59	1.46
25	B	844	8CT	C23-C21	6.26	1.59	1.46
23	1	306	CHL	C1D-C2D	6.25	1.46	1.39
25	1	314	8CT	C15-C16	6.25	1.59	1.46
23	4	308	CHL	C1D-C2D	6.25	1.46	1.39
23	7	305	CHL	C1D-C2D	6.25	1.46	1.39
25	J	104	8CT	C15-C16	6.24	1.59	1.46
25	G	104	8CT	C28-C26	6.24	1.59	1.46
23	7	313	CHL	C1D-C2D	6.24	1.46	1.39
25	7	318	8CT	C04-C03	-6.23	1.45	1.53
23	4	306	CHL	C1D-C2D	6.23	1.46	1.39
25	F	304	8CT	C15-C16	6.22	1.59	1.46
25	1	314	8CT	C28-C26	6.22	1.59	1.46
25	A	845	8CT	C15-C16	6.21	1.59	1.46
23	3	301	CHL	C1D-C2D	6.21	1.46	1.39
23	8	303	CHL	C1D-C2D	6.21	1.46	1.39
23	7	301	CHL	C1D-C2D	6.21	1.46	1.39
25	F	301	8CT	C15-C16	6.20	1.59	1.46
25	I	101	8CT	C15-C16	6.20	1.59	1.46
23	8	309	CHL	C1D-C2D	6.20	1.46	1.39
25	A	849	8CT	C28-C26	6.19	1.59	1.46
23	3	302	CHL	C1D-C2D	6.19	1.46	1.39
25	B	847	8CT	C15-C16	6.19	1.59	1.46
25	8	317	8CT	C28-C26	6.18	1.59	1.46
23	9	306	CHL	C1D-C2D	6.18	1.46	1.39
23	4	315	CHL	C1D-C2D	6.18	1.46	1.39
23	4	302	CHL	C1D-C2D	6.17	1.46	1.39
23	2	304	CHL	C1D-C2D	6.17	1.46	1.39
25	M	102	8CT	C15-C16	6.17	1.59	1.46
25	J	101	8CT	C04-C03	-6.17	1.45	1.53
23	0	302	CHL	C1D-C2D	6.16	1.46	1.39
23	1	312	CHL	C1D-C2D	6.16	1.46	1.39
23	0	301	CHL	C1D-C2D	6.16	1.46	1.39
25	J	104	8CT	C28-C26	6.15	1.59	1.46
25	L	207	8CT	C28-C26	6.15	1.59	1.46
25	B	844	8CT	C28-C26	6.15	1.59	1.46
23	6	305	CHL	C1D-C2D	6.15	1.46	1.39
23	4	305	CHL	C1D-C2D	6.14	1.46	1.39
25	L	204	8CT	C15-C16	6.14	1.59	1.46
23	1	301	CHL	C1D-C2D	6.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	313	8CT	C04-C03	-6.13	1.45	1.53
25	A	845	8CT	C04-C03	-6.12	1.45	1.53
23	8	308	CHL	C1D-C2D	6.12	1.46	1.39
25	K	105	8CT	C28-C26	6.12	1.59	1.46
25	L	205	8CT	C28-C26	6.12	1.59	1.46
23	6	323	CHL	C1D-C2D	6.12	1.46	1.39
25	3	316	8CT	C28-C26	6.11	1.59	1.46
25	O	208	8CT	C28-C26	6.11	1.59	1.46
23	4	313	CHL	C1D-C2D	6.10	1.46	1.39
23	2	307	CHL	C1D-C2D	6.10	1.46	1.39
25	0	314	8CT	C04-C03	-6.10	1.46	1.53
25	F	304	8CT	C28-C26	6.09	1.59	1.46
25	B	850	8CT	C15-C16	6.09	1.59	1.46
25	3	317	8CT	C28-C26	6.09	1.59	1.46
23	9	305	CHL	C1D-C2D	6.08	1.46	1.39
25	B	845	8CT	C04-C03	-6.08	1.46	1.53
23	6	306	CHL	C1D-C2D	6.08	1.46	1.39
25	3	317	8CT	C04-C03	-6.08	1.46	1.53
23	2	301	CHL	C1D-C2D	6.07	1.46	1.39
25	A	846	8CT	C04-C03	-6.07	1.46	1.53
23	7	307	CHL	C1D-C2D	6.06	1.46	1.39
25	M	102	8CT	C28-C26	6.06	1.58	1.46
23	3	305	CHL	C1D-C2D	6.06	1.46	1.39
23	3	307	CHL	C1D-C2D	6.05	1.46	1.39
25	B	850	8CT	C04-C03	-6.05	1.46	1.53
25	J	101	8CT	C28-C26	6.05	1.58	1.46
25	I	101	8CT	C04-C03	-6.04	1.46	1.53
23	7	302	CHL	C1D-C2D	6.03	1.46	1.39
25	J	101	8CT	C15-C16	6.03	1.58	1.46
23	6	307	CHL	C1D-C2D	6.03	1.46	1.39
25	7	319	8CT	C15-C16	6.03	1.58	1.46
25	O	202	8CT	C04-C03	-6.02	1.46	1.53
25	B	843	8CT	C23-C21	6.02	1.58	1.46
25	6	319	8CT	C28-C26	6.01	1.58	1.46
25	B	850	8CT	C28-C26	6.00	1.58	1.46
25	B	846	8CT	C04-C03	-6.00	1.46	1.53
25	7	318	8CT	C15-C16	6.00	1.58	1.46
23	6	308	CHL	C1D-C2D	5.99	1.46	1.39
25	L	204	8CT	C28-C26	5.99	1.58	1.46
25	A	846	8CT	C15-C16	5.99	1.58	1.46
23	4	307	CHL	C1D-C2D	5.98	1.46	1.39
25	B	848	8CT	C28-C26	5.98	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	847	8CT	C15-C16	5.98	1.58	1.46
23	2	312	CHL	C1D-C2D	5.97	1.46	1.39
25	2	314	8CT	C23-C21	5.97	1.58	1.46
25	B	846	8CT	C23-C21	5.96	1.58	1.46
25	M	102	8CT	C04-C03	-5.96	1.46	1.53
25	F	301	8CT	C04-C03	-5.95	1.46	1.53
25	F	301	8CT	C28-C26	5.95	1.58	1.46
25	O	202	8CT	C15-C16	5.95	1.58	1.46
23	2	306	CHL	C1D-C2D	5.94	1.46	1.39
25	B	843	8CT	C04-C03	-5.94	1.46	1.53
25	7	319	8CT	C28-C26	5.93	1.58	1.46
25	4	316	8CT	C04-C03	-5.92	1.46	1.53
25	I	101	8CT	C28-C26	5.91	1.58	1.46
25	0	314	8CT	C23-C21	5.91	1.58	1.46
25	7	318	8CT	C28-C26	5.91	1.58	1.46
25	A	844	8CT	C28-C26	5.90	1.58	1.46
25	4	316	8CT	C23-C21	5.90	1.58	1.46
25	B	847	8CT	C28-C26	5.90	1.58	1.46
25	L	204	8CT	C04-C03	-5.90	1.46	1.53
25	L	205	8CT	C04-C03	-5.88	1.46	1.53
25	O	208	8CT	C04-C03	-5.88	1.46	1.53
25	3	323	8CT	C28-C26	5.88	1.58	1.46
25	A	844	8CT	C04-C03	-5.87	1.46	1.53
25	4	316	8CT	C34-C33	5.87	1.65	1.52
25	A	845	8CT	C28-C26	5.87	1.58	1.46
25	6	319	8CT	C23-C21	5.85	1.58	1.46
25	3	316	8CT	C04-C03	-5.85	1.46	1.53
25	A	846	8CT	C28-C26	5.83	1.58	1.46
25	A	849	8CT	C04-C03	-5.83	1.46	1.53
25	0	314	8CT	C34-C33	5.83	1.65	1.52
25	2	314	8CT	C04-C03	-5.83	1.46	1.53
23	6	302	CHL	C1D-C2D	5.83	1.46	1.39
25	G	104	8CT	C23-C21	5.83	1.58	1.46
25	O	202	8CT	C28-C26	5.82	1.58	1.46
25	J	104	8CT	C23-C21	5.82	1.58	1.46
25	1	314	8CT	C04-C03	-5.81	1.46	1.53
25	B	845	8CT	C28-C26	5.81	1.58	1.46
25	J	101	8CT	C34-C33	5.80	1.65	1.52
25	8	317	8CT	C04-C03	-5.80	1.46	1.53
25	2	314	8CT	C34-C33	5.80	1.65	1.52
25	A	849	8CT	C34-C33	5.79	1.65	1.52
25	9	313	8CT	C23-C21	5.78	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	319	8CT	C04-C03	-5.77	1.46	1.53
25	B	847	8CT	C04-C03	-5.77	1.46	1.53
25	B	844	8CT	C34-C33	5.77	1.65	1.52
25	I	101	8CT	C34-C33	5.76	1.65	1.52
25	L	205	8CT	C23-C21	5.76	1.58	1.46
25	3	316	8CT	C23-C21	5.76	1.58	1.46
25	B	845	8CT	C23-C21	5.75	1.58	1.46
25	3	316	8CT	C34-C33	5.75	1.65	1.52
32	A	852	CL0	C3B-C4B	5.75	1.47	1.41
25	6	324	8CT	C23-C21	5.74	1.58	1.46
25	A	849	8CT	C23-C21	5.74	1.58	1.46
25	7	319	8CT	C04-C03	-5.74	1.46	1.53
25	3	323	8CT	C04-C03	-5.74	1.46	1.53
25	9	313	8CT	C34-C33	5.74	1.65	1.52
25	F	304	8CT	C04-C03	-5.72	1.46	1.53
25	B	848	8CT	C23-C21	5.72	1.58	1.46
25	1	314	8CT	C23-C21	5.70	1.58	1.46
25	B	847	8CT	C23-C21	5.70	1.58	1.46
25	7	318	8CT	C34-C33	5.69	1.65	1.52
25	A	846	8CT	C34-C33	5.68	1.65	1.52
25	L	207	8CT	C04-C03	-5.67	1.46	1.53
25	A	847	8CT	C28-C26	5.67	1.58	1.46
25	J	104	8CT	C34-C33	5.65	1.65	1.52
25	8	317	8CT	C23-C21	5.65	1.58	1.46
25	B	844	8CT	C04-C03	-5.64	1.46	1.53
25	L	205	8CT	C34-C33	5.64	1.65	1.52
25	8	317	8CT	C34-C33	5.64	1.65	1.52
25	F	304	8CT	C23-C21	5.64	1.58	1.46
25	O	208	8CT	C34-C33	5.64	1.65	1.52
25	7	319	8CT	C23-C21	5.63	1.58	1.46
25	G	104	8CT	C04-C03	-5.63	1.46	1.53
25	L	207	8CT	C23-C21	5.63	1.58	1.46
25	K	105	8CT	C04-C03	-5.63	1.46	1.53
25	O	208	8CT	C23-C21	5.61	1.58	1.46
25	J	101	8CT	C23-C21	5.61	1.58	1.46
25	K	105	8CT	C23-C21	5.60	1.57	1.46
25	K	105	8CT	C34-C33	5.60	1.65	1.52
25	B	850	8CT	C23-C21	5.60	1.57	1.46
25	3	317	8CT	C23-C21	5.59	1.57	1.46
25	F	304	8CT	C34-C33	5.58	1.65	1.52
25	G	104	8CT	C34-C33	5.58	1.65	1.52
25	I	101	8CT	C23-C21	5.57	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	M	102	8CT	C34-C33	5.57	1.65	1.52
25	3	323	8CT	C23-C21	5.56	1.57	1.46
25	6	324	8CT	C34-C33	5.56	1.65	1.52
25	A	844	8CT	C34-C33	5.55	1.65	1.52
25	L	204	8CT	C23-C21	5.55	1.57	1.46
25	M	102	8CT	C23-C21	5.54	1.57	1.46
25	B	845	8CT	C34-C33	5.53	1.65	1.52
25	3	323	8CT	C34-C33	5.53	1.65	1.52
25	7	318	8CT	C23-C21	5.53	1.57	1.46
25	6	319	8CT	C34-C33	5.53	1.65	1.52
25	B	846	8CT	C34-C33	5.52	1.65	1.52
25	B	848	8CT	C34-C33	5.52	1.65	1.52
25	1	314	8CT	C34-C33	5.52	1.65	1.52
25	A	845	8CT	C34-C33	5.52	1.65	1.52
25	J	104	8CT	C04-C03	-5.51	1.46	1.53
25	B	850	8CT	C34-C33	5.51	1.65	1.52
25	L	204	8CT	C34-C33	5.50	1.65	1.52
25	6	324	8CT	C04-C03	-5.49	1.46	1.53
25	L	207	8CT	C34-C33	5.47	1.64	1.52
25	B	843	8CT	C34-C33	5.47	1.64	1.52
25	A	844	8CT	C23-C21	5.46	1.57	1.46
25	F	301	8CT	C34-C33	5.45	1.64	1.52
25	F	301	8CT	C23-C21	5.44	1.57	1.46
25	B	847	8CT	C34-C33	5.43	1.64	1.52
25	7	319	8CT	C34-C33	5.42	1.64	1.52
25	3	317	8CT	C34-C33	5.42	1.64	1.52
23	9	305	CHL	C3A-C2A	-5.38	1.50	1.54
25	O	202	8CT	C23-C21	5.37	1.57	1.46
23	3	302	CHL	C3A-C2A	-5.36	1.50	1.54
25	A	845	8CT	C23-C21	5.36	1.57	1.46
25	A	846	8CT	C23-C21	5.36	1.57	1.46
25	B	848	8CT	C04-C03	-5.36	1.46	1.53
25	A	847	8CT	C34-C33	5.36	1.64	1.52
23	5	301	CHL	C3A-C2A	-5.35	1.50	1.54
23	7	302	CHL	C3A-C2A	-5.35	1.50	1.54
23	4	315	CHL	C3A-C2A	-5.34	1.50	1.54
23	4	301	CHL	C3A-C2A	-5.33	1.50	1.54
23	8	301	CHL	CHC-C4B	5.32	1.48	1.39
23	1	304	CHL	C3A-C2A	-5.31	1.50	1.54
23	2	306	CHL	C3A-C2A	-5.30	1.50	1.54
25	O	202	8CT	C34-C33	5.30	1.64	1.52
23	3	307	CHL	C3A-C2A	-5.30	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	301	CHL	CHB-C4A	-5.27	1.32	1.38
23	3	301	CHL	C3A-C2A	-5.26	1.50	1.54
25	A	847	8CT	C23-C21	5.25	1.57	1.46
23	1	304	CHL	CHB-C4A	-5.25	1.32	1.38
23	8	303	CHL	CHB-C4A	-5.24	1.32	1.38
25	K	105	8CT	C05-C04	5.24	1.66	1.54
23	8	303	CHL	C3A-C2A	-5.22	1.50	1.54
23	4	313	CHL	C3A-C2A	-5.22	1.50	1.54
23	0	302	CHL	C3A-C2A	-5.22	1.50	1.54
23	6	305	CHL	C3A-C2A	-5.22	1.50	1.54
23	5	306	CHL	CHC-C4B	5.21	1.48	1.39
23	4	305	CHL	C3A-C2A	-5.21	1.50	1.54
23	5	312	CHL	C3D-C2D	5.21	1.48	1.39
23	9	305	CHL	CHB-C4A	-5.20	1.32	1.38
23	5	305	CHL	CHC-C4B	5.20	1.48	1.39
23	7	305	CHL	C3A-C2A	-5.20	1.50	1.54
23	5	312	CHL	CHC-C4B	5.19	1.48	1.39
25	O	202	8CT	C05-C04	5.19	1.66	1.54
23	0	302	CHL	CHB-C4A	-5.19	1.32	1.38
23	2	304	CHL	C3A-C2A	-5.18	1.50	1.54
23	3	302	CHL	CHB-C4A	-5.18	1.32	1.38
25	2	314	8CT	C05-C04	5.18	1.66	1.54
25	O	208	8CT	C05-C04	5.18	1.66	1.54
23	5	305	CHL	C3D-C2D	5.18	1.48	1.39
23	2	301	CHL	C3A-C2A	-5.18	1.50	1.54
25	L	204	8CT	C05-C04	5.17	1.65	1.54
25	L	207	8CT	C05-C04	5.16	1.65	1.54
23	7	307	CHL	CHC-C4B	5.15	1.48	1.39
23	3	305	CHL	C3A-C2A	-5.15	1.50	1.54
23	8	308	CHL	C3A-C2A	-5.15	1.50	1.54
23	1	312	CHL	C3A-C2A	-5.14	1.50	1.54
23	5	312	CHL	C3B-C2B	5.14	1.47	1.40
23	4	307	CHL	C3A-C2A	-5.13	1.50	1.54
23	2	304	CHL	CHB-C4A	-5.12	1.32	1.38
23	4	302	CHL	C3A-C2A	-5.12	1.50	1.54
23	4	306	CHL	CHB-C4A	-5.12	1.32	1.38
23	3	302	CHL	CHC-C4B	5.12	1.47	1.39
25	1	314	8CT	C05-C04	5.11	1.65	1.54
23	5	305	CHL	O2D-CGD	5.11	1.45	1.33
23	7	307	CHL	CHB-C4A	-5.10	1.32	1.38
23	2	305	CHL	CHB-C4A	-5.10	1.32	1.38
25	L	205	8CT	C05-C04	5.10	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	313	CHL	CHC-C4B	5.10	1.47	1.39
23	7	302	CHL	CHB-C4A	-5.10	1.32	1.38
25	9	313	8CT	C05-C04	5.10	1.65	1.54
23	4	302	CHL	CHB-C4A	-5.09	1.32	1.38
23	8	303	CHL	CHC-C4B	5.08	1.47	1.39
23	5	304	CHL	O2D-CGD	5.08	1.45	1.33
23	6	323	CHL	CHC-C4B	5.07	1.47	1.39
23	4	306	CHL	C3A-C2A	-5.07	1.50	1.54
23	1	301	CHL	C3A-C2A	-5.07	1.50	1.54
25	7	319	8CT	C05-C04	5.07	1.65	1.54
23	5	306	CHL	C3B-C2B	5.06	1.47	1.40
23	1	301	CHL	CHC-C4B	5.06	1.47	1.39
25	6	324	8CT	C05-C04	5.06	1.65	1.54
26	3	318	0UR	O44-C45	5.06	1.45	1.34
23	8	316	CHL	OBD-CAD	5.05	1.28	1.22
23	6	307	CHL	CHB-C4A	-5.05	1.32	1.38
23	0	305	CHL	O2D-CGD	5.05	1.45	1.33
23	5	312	CHL	CHD-C1D	5.05	1.47	1.39
23	0	305	CHL	CHC-C4B	5.05	1.47	1.39
23	3	301	CHL	CHB-C4A	-5.05	1.32	1.38
25	0	314	8CT	C05-C04	5.05	1.65	1.54
26	0	315	0UR	O44-C45	5.05	1.45	1.34
23	5	305	CHL	CHD-C1D	5.04	1.47	1.39
26	2	315	0UR	O44-C45	5.04	1.45	1.34
25	8	317	8CT	C05-C04	5.04	1.65	1.54
23	8	316	CHL	CHC-C4B	5.04	1.47	1.39
23	3	305	CHL	CHB-C4A	-5.03	1.32	1.38
23	6	306	CHL	C3A-C2A	-5.03	1.50	1.54
26	7	320	0UR	O44-C45	5.03	1.45	1.34
25	J	101	8CT	C05-C04	5.03	1.65	1.54
23	0	301	CHL	CHB-C4A	-5.03	1.32	1.38
23	4	315	CHL	CHB-C4A	-5.03	1.32	1.38
23	6	307	CHL	C3A-C2A	-5.03	1.50	1.54
23	8	314	CHL	C3A-C2A	-5.03	1.50	1.54
23	8	316	CHL	C3B-C2B	5.03	1.47	1.40
23	6	305	CHL	CHB-C4A	-5.03	1.32	1.38
23	8	316	CHL	O2D-CGD	5.02	1.45	1.33
25	3	323	8CT	C05-C04	5.02	1.65	1.54
23	6	315	CHL	O2D-CGD	5.02	1.45	1.33
26	O	207	0UR	O44-C45	5.02	1.45	1.34
23	7	306	CHL	CHB-C4A	-5.02	1.32	1.38
23	5	305	CHL	C3B-C2B	5.01	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	301	CHL	CHB-C4A	-5.01	1.32	1.38
23	4	301	CHL	CHB-C4A	-5.01	1.32	1.38
23	3	307	CHL	CHB-C4A	-5.01	1.32	1.38
25	B	847	8CT	C05-C04	5.01	1.65	1.54
23	8	306	CHL	O2D-CGD	5.01	1.45	1.33
23	5	305	CHL	OBD-CAD	5.01	1.28	1.22
23	6	302	CHL	CHB-C4A	-5.01	1.32	1.38
23	8	308	CHL	CHB-C4A	-5.00	1.32	1.38
25	B	844	8CT	C05-C04	5.00	1.65	1.54
25	B	846	8CT	C05-C04	5.00	1.65	1.54
23	1	304	CHL	O2D-CGD	5.00	1.45	1.33
23	9	312	CHL	O2D-CGD	5.00	1.45	1.33
23	8	314	CHL	O2D-CGD	5.00	1.45	1.33
25	G	104	8CT	C05-C04	5.00	1.65	1.54
23	7	301	CHL	C3A-C2A	-5.00	1.50	1.54
23	2	306	CHL	CHC-C4B	5.00	1.47	1.39
23	6	307	CHL	CHC-C4B	5.00	1.47	1.39
25	4	316	8CT	C05-C04	5.00	1.65	1.54
25	M	102	8CT	C05-C04	5.00	1.65	1.54
23	4	302	CHL	O2D-CGD	5.00	1.45	1.33
23	8	316	CHL	C3D-C2D	4.99	1.48	1.39
23	6	305	CHL	O2D-CGD	4.99	1.45	1.33
23	6	313	CHL	O2D-CGD	4.99	1.45	1.33
25	A	845	8CT	C05-C04	4.99	1.65	1.54
23	9	305	CHL	O2D-CGD	4.99	1.45	1.33
25	B	848	8CT	C05-C04	4.99	1.65	1.54
23	5	304	CHL	OBD-CAD	4.99	1.28	1.22
23	6	301	CHL	CHB-C4A	-4.99	1.32	1.38
23	4	307	CHL	CHB-C4A	-4.99	1.32	1.38
25	3	317	8CT	C05-C04	4.98	1.65	1.54
26	5	314	0UR	O44-C45	4.98	1.45	1.34
23	4	305	CHL	O2D-CGD	4.98	1.45	1.33
23	5	301	CHL	CHB-C4A	-4.98	1.32	1.38
23	7	305	CHL	CHC-C4B	4.97	1.47	1.39
23	6	315	CHL	CHC-C4B	4.97	1.47	1.39
23	1	312	CHL	O2D-CGD	4.97	1.45	1.33
23	2	301	CHL	CHC-C4B	4.97	1.47	1.39
25	B	843	8CT	C05-C04	4.97	1.65	1.54
23	4	305	CHL	CHB-C4A	-4.97	1.32	1.38
25	B	845	8CT	C05-C04	4.97	1.65	1.54
23	8	307	CHL	CHB-C4A	-4.97	1.32	1.38
23	9	305	CHL	CHC-C4B	4.97	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	316	8CT	C05-C04	4.97	1.65	1.54
23	4	306	CHL	CHC-C4B	4.96	1.47	1.39
23	5	312	CHL	O2D-CGD	4.96	1.45	1.33
23	0	305	CHL	OBD-CAD	4.96	1.28	1.22
23	5	304	CHL	CHC-C4B	4.96	1.47	1.39
23	0	301	CHL	O2D-CGD	4.96	1.45	1.33
25	6	319	8CT	C05-C04	4.96	1.65	1.54
23	2	306	CHL	CHB-C4A	-4.96	1.32	1.38
23	9	306	CHL	O2D-CGD	4.96	1.45	1.33
23	1	312	CHL	CHC-C4B	4.96	1.47	1.39
23	2	307	CHL	C3A-C2A	-4.96	1.50	1.54
23	7	301	CHL	O2D-CGD	4.96	1.45	1.33
23	6	306	CHL	CHB-C4A	-4.95	1.32	1.38
23	6	306	CHL	O2D-CGD	4.95	1.45	1.33
25	J	104	8CT	C05-C04	4.95	1.65	1.54
26	5	315	0UR	O44-C45	4.95	1.45	1.34
23	0	306	CHL	CHC-C4B	4.95	1.47	1.39
23	8	307	CHL	C3A-C2A	-4.95	1.50	1.54
23	7	313	CHL	O2D-CGD	4.95	1.45	1.33
23	4	313	CHL	CHB-C4A	-4.95	1.32	1.38
25	B	850	8CT	C05-C04	4.95	1.65	1.54
23	8	301	CHL	O2D-CGD	4.95	1.45	1.33
25	A	849	8CT	C05-C04	4.94	1.65	1.54
23	9	301	CHL	CHB-C4A	-4.94	1.32	1.38
23	7	307	CHL	O2D-CGD	4.94	1.45	1.33
23	7	301	CHL	CHC-C4B	4.94	1.47	1.39
23	1	306	CHL	O2D-CGD	4.94	1.45	1.33
23	3	301	CHL	CHC-C4B	4.94	1.47	1.39
23	8	309	CHL	CHC-C4B	4.93	1.47	1.39
23	4	306	CHL	O2D-CGD	4.93	1.45	1.33
26	9	314	0UR	O44-C45	4.93	1.45	1.34
23	9	301	CHL	O2D-CGD	4.93	1.45	1.33
23	6	307	CHL	O2D-CGD	4.93	1.45	1.33
23	2	312	CHL	O2D-CGD	4.93	1.45	1.33
23	5	306	CHL	O2D-CGD	4.93	1.45	1.33
23	3	305	CHL	O2D-CGD	4.93	1.45	1.33
23	1	306	CHL	CHC-C4B	4.93	1.47	1.39
23	0	302	CHL	O2D-CGD	4.93	1.45	1.33
26	0	316	0UR	O44-C45	4.92	1.45	1.34
23	5	304	CHL	C3D-C2D	4.92	1.48	1.39
23	1	305	CHL	CHC-C4B	4.92	1.47	1.39
23	9	306	CHL	CHC-C4B	4.92	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	318	0UR	O44-C45	4.92	1.45	1.34
23	3	302	CHL	O2D-CGD	4.92	1.45	1.33
23	7	305	CHL	O2D-CGD	4.92	1.45	1.33
23	8	301	CHL	C3D-C2D	4.92	1.48	1.39
23	9	306	CHL	CHB-C4A	-4.92	1.32	1.38
23	8	307	CHL	OBD-CAD	4.92	1.28	1.22
23	9	312	CHL	CHC-C4B	4.92	1.47	1.39
23	6	315	CHL	OBD-CAD	4.91	1.28	1.22
23	6	315	CHL	C3D-C2D	4.91	1.48	1.39
23	2	304	CHL	O2D-CGD	4.91	1.45	1.33
23	5	306	CHL	CHD-C1D	4.91	1.47	1.39
23	2	305	CHL	O2D-CGD	4.91	1.45	1.33
23	8	307	CHL	O2D-CGD	4.91	1.45	1.33
23	7	301	CHL	CHB-C4A	-4.91	1.32	1.38
23	4	306	CHL	OBD-CAD	4.90	1.28	1.22
26	2	316	0UR	O44-C45	4.90	1.45	1.34
25	I	101	8CT	C05-C04	4.90	1.65	1.54
23	0	302	CHL	OBD-CAD	4.90	1.28	1.22
26	8	319	0UR	O44-C45	4.90	1.45	1.34
23	4	307	CHL	O2D-CGD	4.90	1.45	1.33
23	2	306	CHL	O2D-CGD	4.90	1.45	1.33
23	2	312	CHL	CHC-C4B	4.90	1.47	1.39
23	8	303	CHL	O2D-CGD	4.90	1.45	1.33
23	6	313	CHL	C3A-C2A	-4.90	1.50	1.54
25	7	318	8CT	C05-C04	4.90	1.65	1.54
23	2	305	CHL	CHC-C4B	4.90	1.47	1.39
23	2	304	CHL	CHC-C4B	4.90	1.47	1.39
23	5	304	CHL	CHD-C1D	4.90	1.47	1.39
23	4	315	CHL	CHC-C4B	4.90	1.47	1.39
23	7	305	CHL	OBD-CAD	4.89	1.28	1.22
25	F	301	8CT	C05-C04	4.89	1.65	1.54
23	4	308	CHL	C3D-C2D	4.89	1.48	1.39
23	7	305	CHL	CHB-C4A	-4.89	1.32	1.38
23	3	305	CHL	CHC-C4B	4.89	1.47	1.39
23	4	308	CHL	CHC-C4B	4.89	1.47	1.39
23	1	301	CHL	O2D-CGD	4.89	1.45	1.33
23	7	306	CHL	O2D-CGD	4.89	1.45	1.33
23	9	306	CHL	C3D-C2D	4.89	1.48	1.39
23	0	306	CHL	C3B-C2B	4.89	1.47	1.40
23	0	306	CHL	OBD-CAD	4.89	1.28	1.22
23	4	302	CHL	CHC-C4B	4.89	1.47	1.39
23	2	312	CHL	C3A-C2A	-4.89	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	312	CHL	OBD-CAD	4.89	1.28	1.22
26	1	315	0UR	O44-C45	4.89	1.45	1.34
23	5	312	CHL	OBD-CAD	4.88	1.28	1.22
23	3	307	CHL	O2D-CGD	4.88	1.45	1.33
23	1	305	CHL	C3D-C2D	4.88	1.48	1.39
23	6	308	CHL	CHC-C4B	4.88	1.47	1.39
23	4	301	CHL	CHC-C4B	4.88	1.47	1.39
23	2	307	CHL	O2D-CGD	4.88	1.45	1.33
23	5	304	CHL	CHB-C4A	-4.88	1.32	1.38
23	5	306	CHL	C3D-C2D	4.88	1.48	1.39
23	7	302	CHL	CHC-C4B	4.88	1.47	1.39
23	2	305	CHL	C3A-C2A	-4.88	1.50	1.54
26	6	321	0UR	O44-C45	4.88	1.45	1.34
25	F	304	8CT	C05-C04	4.88	1.65	1.54
23	4	308	CHL	O2D-CGD	4.88	1.45	1.33
23	8	306	CHL	OBD-CAD	4.88	1.28	1.22
25	A	844	8CT	C05-C04	4.87	1.65	1.54
23	6	313	CHL	CHC-C4B	4.87	1.47	1.39
23	8	309	CHL	O2D-CGD	4.87	1.45	1.33
23	6	301	CHL	CHC-C4B	4.87	1.47	1.39
23	2	301	CHL	O2D-CGD	4.87	1.45	1.33
23	1	304	CHL	CHC-C4B	4.87	1.47	1.39
23	8	316	CHL	CHD-C1D	4.87	1.47	1.39
23	4	305	CHL	OBD-CAD	4.87	1.28	1.22
23	4	313	CHL	O2D-CGD	4.87	1.45	1.33
23	8	308	CHL	CHC-C4B	4.87	1.47	1.39
26	4	317	0UR	O44-C45	4.87	1.45	1.34
23	8	301	CHL	C3B-C2B	4.87	1.47	1.40
23	3	305	CHL	OBD-CAD	4.86	1.28	1.22
23	7	306	CHL	C3A-C2A	-4.86	1.50	1.54
23	7	306	CHL	C3D-C2D	4.86	1.47	1.39
23	4	305	CHL	CHC-C4B	4.86	1.47	1.39
23	6	323	CHL	CHB-C4A	-4.86	1.32	1.38
23	6	305	CHL	CHC-C4B	4.86	1.47	1.39
23	1	304	CHL	OBD-CAD	4.86	1.28	1.22
23	7	301	CHL	OBD-CAD	4.86	1.28	1.22
23	2	307	CHL	CHC-C4B	4.86	1.47	1.39
23	7	313	CHL	C3D-C2D	4.86	1.47	1.39
23	6	305	CHL	OBD-CAD	4.85	1.28	1.22
23	7	306	CHL	CHC-C4B	4.85	1.47	1.39
23	6	301	CHL	OBD-CAD	4.85	1.28	1.22
23	6	323	CHL	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	308	CHL	O2D-CGD	4.84	1.45	1.33
23	9	301	CHL	OBD-CAD	4.84	1.28	1.22
25	A	847	8CT	C05-C04	4.84	1.65	1.54
23	4	301	CHL	O2D-CGD	4.84	1.45	1.33
23	5	301	CHL	O2D-CGD	4.84	1.45	1.33
26	1	316	0UR	O44-C45	4.84	1.45	1.34
25	A	846	8CT	C05-C04	4.84	1.65	1.54
23	1	306	CHL	C3B-C2B	4.84	1.46	1.40
23	8	306	CHL	CHC-C4B	4.84	1.47	1.39
23	8	307	CHL	C3D-C2D	4.83	1.47	1.39
23	2	301	CHL	C3D-C2D	4.83	1.47	1.39
23	4	315	CHL	O2D-CGD	4.83	1.45	1.33
23	6	301	CHL	O2D-CGD	4.83	1.45	1.33
23	1	305	CHL	O2D-CGD	4.82	1.45	1.33
23	1	312	CHL	OBD-CAD	4.82	1.28	1.22
23	6	302	CHL	C3D-C2D	4.82	1.47	1.39
23	6	302	CHL	CHC-C4B	4.82	1.47	1.39
23	6	302	CHL	C3A-C2A	-4.82	1.50	1.54
23	8	301	CHL	OBD-CAD	4.82	1.28	1.22
23	1	305	CHL	OBD-CAD	4.82	1.28	1.22
23	4	313	CHL	OBD-CAD	4.81	1.28	1.22
23	6	315	CHL	C3B-C2B	4.81	1.46	1.40
23	6	301	CHL	C3D-C2D	4.81	1.47	1.39
23	2	312	CHL	CHB-C4A	-4.81	1.32	1.38
23	6	308	CHL	CHB-C4A	-4.81	1.32	1.38
23	6	308	CHL	O2D-CGD	4.81	1.45	1.33
23	5	304	CHL	C3B-C2B	4.81	1.46	1.40
23	5	301	CHL	CHC-C4B	4.81	1.47	1.39
23	2	305	CHL	C3D-C2D	4.80	1.47	1.39
23	6	301	CHL	C3A-C2A	-4.80	1.50	1.54
23	9	306	CHL	C3A-C2A	-4.80	1.50	1.54
26	9	315	0UR	O44-C45	4.80	1.45	1.34
23	8	309	CHL	C3D-C2D	4.80	1.47	1.39
23	4	313	CHL	C3D-C2D	4.80	1.47	1.39
23	6	302	CHL	OBD-CAD	4.79	1.28	1.22
23	0	306	CHL	O2D-CGD	4.79	1.45	1.33
23	0	301	CHL	C3A-C2A	-4.79	1.50	1.54
23	1	312	CHL	CHB-C4A	-4.79	1.32	1.38
23	2	307	CHL	CHB-C4A	-4.79	1.32	1.38
23	0	302	CHL	C3D-C2D	4.79	1.47	1.39
23	0	302	CHL	CHC-C4B	4.79	1.47	1.39
23	5	301	CHL	OBD-CAD	4.79	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	308	CHL	CHB-C4A	-4.78	1.32	1.38
23	1	306	CHL	CHB-C4A	-4.78	1.32	1.38
23	6	323	CHL	OBD-CAD	4.78	1.28	1.22
23	8	307	CHL	CHC-C4B	4.78	1.47	1.39
23	4	308	CHL	C3A-C2A	-4.78	1.50	1.54
23	1	305	CHL	C3B-C2B	4.78	1.46	1.40
23	6	308	CHL	C3D-C2D	4.78	1.47	1.39
23	1	306	CHL	C3A-C2A	-4.78	1.50	1.54
23	7	302	CHL	O2D-CGD	4.77	1.45	1.33
23	7	313	CHL	OBD-CAD	4.77	1.28	1.22
23	9	312	CHL	C3A-C2A	-4.77	1.50	1.54
23	5	305	CHL	CHB-C1B	4.77	1.47	1.39
23	2	305	CHL	OBD-CAD	4.77	1.28	1.22
23	8	316	CHL	CHB-C1B	4.77	1.47	1.39
23	0	301	CHL	CHC-C4B	4.77	1.47	1.39
23	1	301	CHL	C3D-C2D	4.77	1.47	1.39
23	4	301	CHL	OBD-CAD	4.76	1.28	1.22
23	6	308	CHL	OBD-CAD	4.76	1.28	1.22
26	4	318	0UR	O44-C45	4.76	1.45	1.34
23	0	305	CHL	C3A-C2A	-4.76	1.50	1.54
23	9	301	CHL	C3A-C2A	-4.76	1.50	1.54
23	0	305	CHL	C3D-C2D	4.76	1.47	1.39
23	2	304	CHL	OBD-CAD	4.76	1.28	1.22
23	3	301	CHL	O2D-CGD	4.75	1.44	1.33
26	6	320	0UR	O44-C45	4.75	1.45	1.34
23	2	307	CHL	C3D-C2D	4.75	1.47	1.39
23	1	301	CHL	OBD-CAD	4.75	1.28	1.22
23	6	313	CHL	OBD-CAD	4.75	1.28	1.22
23	8	314	CHL	OBD-CAD	4.75	1.28	1.22
23	0	306	CHL	C3D-C2D	4.75	1.47	1.39
23	4	302	CHL	OBD-CAD	4.75	1.28	1.22
23	9	306	CHL	OBD-CAD	4.75	1.28	1.22
23	4	308	CHL	C3B-C2B	4.75	1.46	1.40
23	9	301	CHL	CHC-C4B	4.74	1.47	1.39
23	1	305	CHL	CHB-C4A	-4.74	1.32	1.38
23	7	313	CHL	C3A-C2A	-4.74	1.50	1.54
23	3	302	CHL	C3D-C2D	4.74	1.47	1.39
23	6	323	CHL	C3D-C2D	4.74	1.47	1.39
23	8	303	CHL	C3D-C2D	4.74	1.47	1.39
23	8	309	CHL	CHB-C4A	-4.74	1.32	1.38
23	7	301	CHL	C3D-C2D	4.73	1.47	1.39
23	6	306	CHL	OBD-CAD	4.73	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	315	CHL	CHB-C4A	-4.73	1.32	1.38
23	4	313	CHL	CHC-C4B	4.73	1.47	1.39
23	3	305	CHL	C3D-C2D	4.72	1.47	1.39
23	3	301	CHL	C3D-C2D	4.72	1.47	1.39
23	8	301	CHL	CHB-C4A	-4.72	1.32	1.38
23	7	302	CHL	OBD-CAD	4.72	1.28	1.22
23	4	302	CHL	C3D-C2D	4.72	1.47	1.39
23	8	307	CHL	CHD-C1D	4.71	1.47	1.39
23	7	313	CHL	CHB-C4A	-4.71	1.32	1.38
23	9	312	CHL	C3D-C2D	4.71	1.47	1.39
23	0	305	CHL	CHD-C1D	4.71	1.47	1.39
23	6	313	CHL	CHB-C4A	-4.71	1.32	1.38
23	9	312	CHL	CHB-C4A	-4.71	1.32	1.38
23	9	301	CHL	C3D-C2D	4.71	1.47	1.39
25	B	848	8CT	C19-C20	4.71	1.57	1.43
23	8	301	CHL	CHD-C1D	4.71	1.47	1.39
23	6	305	CHL	C3D-C2D	4.71	1.47	1.39
23	6	306	CHL	CHC-C4B	4.70	1.47	1.39
23	8	306	CHL	C3D-C2D	4.70	1.47	1.39
23	3	307	CHL	CHC-C4B	4.70	1.47	1.39
23	3	302	CHL	OBD-CAD	4.70	1.28	1.22
23	2	305	CHL	C3B-C2B	4.70	1.46	1.40
23	0	305	CHL	CHB-C4A	-4.70	1.33	1.38
23	8	308	CHL	OBD-CAD	4.70	1.28	1.22
23	5	306	CHL	CHB-C1B	4.69	1.47	1.39
25	A	847	8CT	C06-C07	4.69	1.67	1.52
23	8	309	CHL	OBD-CAD	4.69	1.28	1.22
23	8	314	CHL	CHC-C4B	4.68	1.47	1.39
23	6	308	CHL	C3B-C2B	4.68	1.46	1.40
23	7	307	CHL	OBD-CAD	4.68	1.28	1.22
25	B	846	8CT	C06-C07	4.68	1.67	1.52
23	1	312	CHL	C3D-C2D	4.67	1.47	1.39
23	8	309	CHL	CHD-C1D	4.67	1.47	1.39
23	8	307	CHL	C3B-C2B	4.67	1.46	1.40
25	3	317	8CT	C06-C07	4.67	1.67	1.52
23	1	306	CHL	OBD-CAD	4.67	1.28	1.22
23	8	314	CHL	CHB-C4A	-4.67	1.33	1.38
23	9	305	CHL	C3D-C2D	4.67	1.47	1.39
23	1	312	CHL	C3B-C2B	4.66	1.46	1.40
23	1	305	CHL	CHD-C1D	4.66	1.47	1.39
23	4	307	CHL	OBD-CAD	4.66	1.28	1.22
23	4	306	CHL	C3D-C2D	4.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	7	313	CHL	C3B-C2B	4.66	1.46	1.40
23	7	306	CHL	CHD-C1D	4.65	1.47	1.39
23	6	307	CHL	OBD-CAD	4.65	1.28	1.22
23	2	312	CHL	OBD-CAD	4.65	1.28	1.22
23	8	306	CHL	C3A-C2A	-4.65	1.50	1.54
23	4	307	CHL	CHC-C4B	4.65	1.47	1.39
23	7	305	CHL	C3D-C2D	4.65	1.47	1.39
23	8	303	CHL	OBD-CAD	4.64	1.28	1.22
23	9	306	CHL	C3B-C2B	4.64	1.46	1.40
23	0	306	CHL	CHB-C1B	4.64	1.47	1.39
23	1	306	CHL	CHD-C1D	4.64	1.47	1.39
23	0	301	CHL	C3D-C2D	4.64	1.47	1.39
23	2	301	CHL	OBD-CAD	4.64	1.28	1.22
23	8	306	CHL	CHB-C4A	-4.64	1.33	1.38
23	5	306	CHL	OBD-CAD	4.64	1.28	1.22
23	4	308	CHL	CHD-C1D	4.63	1.47	1.39
23	4	315	CHL	C3D-C2D	4.63	1.47	1.39
23	6	323	CHL	C3B-C2B	4.63	1.46	1.40
25	K	105	8CT	C06-C07	4.62	1.67	1.52
23	3	301	CHL	OBD-CAD	4.62	1.28	1.22
23	0	301	CHL	OBD-CAD	4.62	1.28	1.22
23	7	307	CHL	C3D-C2D	4.62	1.47	1.39
23	3	307	CHL	OBD-CAD	4.62	1.28	1.22
23	6	315	CHL	CHD-C1D	4.62	1.47	1.39
25	B	845	8CT	C06-C07	4.62	1.67	1.52
25	0	314	8CT	C06-C07	4.61	1.67	1.52
23	4	305	CHL	C3D-C2D	4.61	1.47	1.39
23	5	312	CHL	CHB-C1B	4.61	1.47	1.39
23	4	315	CHL	OBD-CAD	4.61	1.28	1.22
25	J	101	8CT	C06-C07	4.61	1.66	1.52
23	8	314	CHL	C3D-C2D	4.61	1.47	1.39
23	9	301	CHL	C3B-C2B	4.61	1.46	1.40
25	A	845	8CT	C06-C07	4.61	1.66	1.52
25	O	202	8CT	C06-C07	4.60	1.66	1.52
25	A	844	8CT	C06-C07	4.60	1.66	1.52
23	8	309	CHL	C3A-C2A	-4.60	1.50	1.54
23	6	323	CHL	CHD-C1D	4.60	1.47	1.39
23	5	301	CHL	C3D-C2D	4.59	1.47	1.39
23	4	308	CHL	OBD-CAD	4.59	1.28	1.22
23	0	306	CHL	CHB-C4A	-4.59	1.33	1.38
31	A	841	PQN	C10-C5	4.59	1.48	1.40
25	7	318	8CT	C06-C07	4.59	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	312	CHL	C3B-C2B	4.59	1.46	1.40
23	6	302	CHL	O2D-CGD	4.59	1.44	1.33
23	8	306	CHL	CHD-C1D	4.58	1.47	1.39
23	6	306	CHL	C3D-C2D	4.58	1.47	1.39
25	L	207	8CT	C06-C07	4.58	1.66	1.52
23	2	312	CHL	C3B-C2B	4.58	1.46	1.40
25	B	844	8CT	C06-C07	4.58	1.66	1.52
23	6	308	CHL	C3A-C2A	-4.58	1.50	1.54
23	7	301	CHL	CHD-C1D	4.57	1.47	1.39
23	8	301	CHL	CHB-C1B	4.57	1.47	1.39
25	1	314	8CT	C19-C20	4.57	1.57	1.43
23	7	301	CHL	C3B-C2B	4.57	1.46	1.40
25	9	313	8CT	C06-C07	4.57	1.66	1.52
23	1	304	CHL	C3D-C2D	4.57	1.47	1.39
23	7	313	CHL	CHD-C1D	4.57	1.47	1.39
23	6	302	CHL	C3B-C2B	4.57	1.46	1.40
25	I	101	8CT	C06-C07	4.56	1.66	1.52
23	8	308	CHL	C3D-C2D	4.56	1.47	1.39
25	B	843	8CT	C19-C20	4.56	1.57	1.43
25	B	844	8CT	C19-C20	4.56	1.57	1.43
23	6	307	CHL	C3D-C2D	4.56	1.47	1.39
25	3	323	8CT	C19-C20	4.56	1.57	1.43
23	0	306	CHL	CHD-C1D	4.55	1.47	1.39
23	4	308	CHL	CHB-C1B	4.55	1.47	1.39
25	B	843	8CT	C06-C07	4.55	1.66	1.52
25	0	314	8CT	C19-C20	4.55	1.57	1.43
25	4	316	8CT	C06-C07	4.55	1.66	1.52
23	4	301	CHL	C3D-C2D	4.55	1.47	1.39
23	2	312	CHL	C3D-C2D	4.55	1.47	1.39
23	8	309	CHL	C3B-C2B	4.54	1.46	1.40
23	6	313	CHL	C3B-C2B	4.54	1.46	1.40
23	4	307	CHL	C3D-C2D	4.54	1.47	1.39
23	6	315	CHL	CHB-C1B	4.54	1.47	1.39
25	6	324	8CT	C19-C20	4.54	1.57	1.43
25	G	104	8CT	C19-C20	4.54	1.57	1.43
23	6	308	CHL	CHD-C1D	4.53	1.47	1.39
23	4	307	CHL	C3B-C2B	4.53	1.46	1.40
23	5	304	CHL	C3A-C2A	-4.53	1.50	1.54
25	O	208	8CT	C06-C07	4.53	1.66	1.52
25	7	319	8CT	C06-C07	4.53	1.66	1.52
23	9	305	CHL	OBD-CAD	4.53	1.28	1.22
25	3	316	8CT	C06-C07	4.53	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	1	305	CHL	CHB-C1B	4.53	1.47	1.39
23	4	301	CHL	CHD-C1D	4.53	1.47	1.39
31	B	842	PQN	C10-C5	4.52	1.48	1.40
23	6	308	CHL	CHB-C1B	4.52	1.46	1.39
25	B	845	8CT	C19-C20	4.52	1.57	1.43
23	1	304	CHL	CHD-C1D	4.52	1.46	1.39
23	2	307	CHL	OBD-CAD	4.52	1.28	1.22
23	4	306	CHL	C3B-C2B	4.52	1.46	1.40
23	2	305	CHL	CHD-C1D	4.52	1.46	1.39
23	6	323	CHL	C3A-C2A	-4.52	1.50	1.54
25	A	849	8CT	C06-C07	4.52	1.66	1.52
23	8	309	CHL	CHB-C1B	4.52	1.46	1.39
25	9	313	8CT	C19-C20	4.52	1.57	1.43
23	8	316	CHL	CHB-C4A	-4.52	1.33	1.38
23	5	304	CHL	O2A-CGA	4.51	1.45	1.30
25	L	204	8CT	C06-C07	4.51	1.66	1.52
25	B	847	8CT	C06-C07	4.51	1.66	1.52
23	9	312	CHL	CHB-C1B	4.51	1.46	1.39
23	5	305	CHL	CHB-C4A	-4.51	1.33	1.38
25	A	847	8CT	C19-C20	4.51	1.57	1.43
25	3	323	8CT	C06-C07	4.51	1.66	1.52
23	0	305	CHL	C3B-C2B	4.51	1.46	1.40
23	0	305	CHL	CHB-C1B	4.51	1.46	1.39
25	L	205	8CT	C06-C07	4.50	1.66	1.52
23	2	306	CHL	OBD-CAD	4.50	1.28	1.22
25	2	314	8CT	C06-C07	4.50	1.66	1.52
25	8	317	8CT	C06-C07	4.50	1.66	1.52
23	1	305	CHL	C3A-C2A	-4.50	1.50	1.54
23	7	307	CHL	C3A-C2A	-4.50	1.50	1.54
25	6	319	8CT	C19-C20	4.50	1.57	1.43
23	9	301	CHL	CHD-C1D	4.50	1.46	1.39
23	9	312	CHL	CHD-C1D	4.50	1.46	1.39
23	4	301	CHL	C3B-C2B	4.49	1.46	1.40
25	M	102	8CT	C06-C07	4.49	1.66	1.52
23	7	306	CHL	OBD-CAD	4.49	1.28	1.22
23	0	301	CHL	C3B-C2B	4.49	1.46	1.40
25	6	319	8CT	C06-C07	4.49	1.66	1.52
23	6	301	CHL	CHB-C1B	4.49	1.46	1.39
23	6	323	CHL	CHB-C1B	4.49	1.46	1.39
23	7	313	CHL	CHB-C1B	4.48	1.46	1.39
23	9	306	CHL	CHD-C1D	4.48	1.46	1.39
25	B	850	8CT	C06-C07	4.48	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	307	CHL	C3B-C2B	4.48	1.46	1.40
23	4	306	CHL	CHD-C1D	4.47	1.46	1.39
25	B	846	8CT	C19-C20	4.47	1.57	1.43
25	J	104	8CT	C06-C07	4.47	1.66	1.52
25	K	105	8CT	C19-C20	4.47	1.57	1.43
23	8	314	CHL	C3B-C2B	4.47	1.46	1.40
25	8	317	8CT	C19-C20	4.47	1.57	1.43
23	6	313	CHL	CHB-C1B	4.47	1.46	1.39
25	1	314	8CT	C06-C07	4.46	1.66	1.52
23	8	314	CHL	CHD-C1D	4.46	1.46	1.39
23	6	313	CHL	C3D-C2D	4.46	1.47	1.39
23	7	302	CHL	C3D-C2D	4.46	1.47	1.39
23	1	312	CHL	CHD-C1D	4.46	1.46	1.39
23	5	306	CHL	CHB-C4A	-4.45	1.33	1.38
25	F	301	8CT	C06-C07	4.45	1.66	1.52
25	O	208	8CT	C19-C20	4.45	1.57	1.43
23	6	305	CHL	C3B-C2B	4.44	1.46	1.40
23	4	313	CHL	C3B-C2B	4.44	1.46	1.40
25	G	104	8CT	C06-C07	4.44	1.66	1.52
23	1	306	CHL	CHB-C1B	4.44	1.46	1.39
25	A	846	8CT	C06-C07	4.44	1.66	1.52
25	J	104	8CT	C19-C20	4.44	1.56	1.43
25	L	205	8CT	C19-C20	4.43	1.56	1.43
25	B	848	8CT	C06-C07	4.43	1.66	1.52
25	A	849	8CT	C19-C20	4.43	1.56	1.43
25	F	301	8CT	C19-C20	4.43	1.56	1.43
25	6	324	8CT	C06-C07	4.43	1.66	1.52
23	7	307	CHL	CHD-C1D	4.43	1.46	1.39
25	F	304	8CT	C06-C07	4.43	1.66	1.52
25	L	207	8CT	C19-C20	4.43	1.56	1.43
25	M	102	8CT	C19-C20	4.43	1.56	1.43
25	3	316	8CT	C19-C20	4.43	1.56	1.43
23	8	306	CHL	CHB-C1B	4.42	1.46	1.39
25	B	846	8CT	C24-C25	4.42	1.56	1.43
23	5	312	CHL	CHD-C4C	4.42	1.47	1.39
23	6	301	CHL	CHD-C1D	4.42	1.46	1.39
23	6	305	CHL	CHD-C1D	4.42	1.46	1.39
23	2	306	CHL	C3D-C2D	4.42	1.47	1.39
25	B	847	8CT	C19-C20	4.41	1.56	1.43
23	1	306	CHL	C3D-C2D	4.41	1.47	1.39
23	8	308	CHL	C3B-C2B	4.41	1.46	1.40
25	L	204	8CT	C19-C20	4.41	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	305	CHL	CHD-C4C	4.41	1.47	1.39
25	3	317	8CT	C19-C20	4.41	1.56	1.43
23	6	315	CHL	C3A-C2A	-4.41	1.50	1.54
23	2	306	CHL	C3B-C2B	4.41	1.46	1.40
25	4	316	8CT	C19-C20	4.40	1.56	1.43
23	0	306	CHL	C3A-C2A	-4.40	1.50	1.54
23	3	301	CHL	C3B-C2B	4.40	1.46	1.40
23	4	302	CHL	CHD-C1D	4.40	1.46	1.39
23	6	306	CHL	CHD-C1D	4.40	1.46	1.39
23	5	304	CHL	CHB-C1B	4.39	1.46	1.39
25	A	844	8CT	C19-C20	4.39	1.56	1.43
23	5	312	CHL	CHB-C4A	-4.39	1.33	1.38
23	3	301	CHL	CHD-C1D	4.39	1.46	1.39
23	2	307	CHL	CHD-C1D	4.38	1.46	1.39
23	3	305	CHL	CHD-C1D	4.38	1.46	1.39
23	5	312	CHL	C3A-C2A	-4.37	1.50	1.54
25	J	101	8CT	C19-C20	4.37	1.56	1.43
25	B	850	8CT	C19-C20	4.37	1.56	1.43
23	8	308	CHL	CHB-C1B	4.37	1.46	1.39
23	6	301	CHL	C3B-C2B	4.37	1.46	1.40
25	7	319	8CT	C19-C20	4.36	1.56	1.43
25	B	843	8CT	C24-C25	4.36	1.56	1.43
25	I	101	8CT	C19-C20	4.36	1.56	1.43
23	4	306	CHL	O2A-CGA	4.36	1.46	1.33
25	F	304	8CT	C19-C20	4.35	1.56	1.43
23	4	305	CHL	CHD-C1D	4.35	1.46	1.39
23	3	307	CHL	C3D-C2D	4.35	1.47	1.39
23	7	305	CHL	C3B-C2B	4.35	1.46	1.40
23	0	302	CHL	CHD-C1D	4.35	1.46	1.39
23	5	305	CHL	O2A-CGA	4.35	1.46	1.33
23	2	304	CHL	CHD-C1D	4.34	1.46	1.39
23	8	308	CHL	CHD-C1D	4.34	1.46	1.39
23	7	306	CHL	CHB-C1B	4.34	1.46	1.39
25	A	845	8CT	C19-C20	4.34	1.56	1.43
23	9	306	CHL	CHB-C1B	4.34	1.46	1.39
23	5	301	CHL	O2A-CGA	4.34	1.46	1.33
23	3	301	CHL	O2A-CGA	4.34	1.46	1.33
23	0	301	CHL	CHD-C1D	4.34	1.46	1.39
23	2	307	CHL	CHB-C1B	4.34	1.46	1.39
23	2	301	CHL	CHD-C1D	4.33	1.46	1.39
23	6	306	CHL	C3B-C2B	4.33	1.46	1.40
23	6	306	CHL	O2A-CGA	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	305	CHL	CHD-C1D	4.33	1.46	1.39
23	4	315	CHL	C3B-C2B	4.33	1.46	1.40
25	2	314	8CT	C19-C20	4.33	1.56	1.43
23	0	301	CHL	O2A-CGA	4.33	1.46	1.33
23	2	305	CHL	CHB-C1B	4.33	1.46	1.39
23	2	305	CHL	O2A-CGA	4.33	1.46	1.33
23	8	316	CHL	CHD-C4C	4.32	1.47	1.39
23	7	305	CHL	CHD-C1D	4.32	1.46	1.39
23	4	315	CHL	CHD-C1D	4.32	1.46	1.39
25	4	316	8CT	C24-C25	4.32	1.56	1.43
23	1	304	CHL	O2A-CGA	4.32	1.45	1.33
23	1	305	CHL	O2A-CGA	4.32	1.45	1.33
25	2	314	8CT	C24-C25	4.32	1.56	1.43
23	4	305	CHL	C3B-C2B	4.31	1.46	1.40
23	2	304	CHL	C3B-C2B	4.31	1.46	1.40
23	9	305	CHL	O2A-CGA	4.31	1.45	1.33
23	8	301	CHL	CHD-C4C	4.31	1.47	1.39
23	7	301	CHL	O2A-CGA	4.31	1.45	1.33
23	6	313	CHL	CHD-C1D	4.31	1.46	1.39
23	8	307	CHL	O2A-CGA	4.31	1.45	1.33
23	2	312	CHL	CHD-C1D	4.30	1.46	1.39
23	6	307	CHL	CHD-C1D	4.30	1.46	1.39
23	6	308	CHL	O2A-CGA	4.30	1.45	1.33
23	3	307	CHL	O2A-CGA	4.30	1.45	1.33
23	7	305	CHL	O2A-CGA	4.29	1.45	1.33
23	8	306	CHL	C3B-C2B	4.29	1.46	1.40
23	9	301	CHL	CHB-C1B	4.29	1.46	1.39
23	0	306	CHL	O2A-CGA	4.29	1.45	1.33
23	6	307	CHL	C3B-C2B	4.29	1.46	1.40
23	1	312	CHL	CHB-C1B	4.29	1.46	1.39
23	7	301	CHL	CHB-C1B	4.28	1.46	1.39
23	9	305	CHL	C3B-C2B	4.28	1.46	1.40
25	7	318	8CT	C19-C20	4.28	1.56	1.43
23	3	305	CHL	O2A-CGA	4.28	1.45	1.33
23	8	314	CHL	O2A-CGA	4.28	1.45	1.33
23	0	305	CHL	O2A-CGA	4.27	1.45	1.33
23	8	301	CHL	C3A-C2A	-4.27	1.51	1.54
23	1	312	CHL	O2A-CGA	4.27	1.45	1.33
23	8	301	CHL	O2A-CGA	4.27	1.45	1.33
23	9	306	CHL	O2A-CGA	4.27	1.45	1.33
23	2	312	CHL	CHB-C1B	4.26	1.46	1.39
23	5	301	CHL	CHD-C1D	4.26	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	303	CHL	CHD-C1D	4.26	1.46	1.39
23	4	306	CHL	CHB-C1B	4.26	1.46	1.39
23	7	307	CHL	CHB-C1B	4.26	1.46	1.39
23	6	307	CHL	O2A-CGA	4.25	1.45	1.33
23	1	304	CHL	C3B-C2B	4.25	1.46	1.40
23	4	313	CHL	CHD-C1D	4.25	1.46	1.39
23	7	306	CHL	C3B-C2B	4.25	1.46	1.40
23	5	306	CHL	CHD-C4C	4.25	1.47	1.39
23	6	313	CHL	O2A-CGA	4.25	1.45	1.33
23	4	307	CHL	CHB-C1B	4.25	1.46	1.39
23	6	302	CHL	O2A-CGA	4.24	1.45	1.33
23	2	312	CHL	O2A-CGA	4.24	1.45	1.33
23	1	301	CHL	CHD-C1D	4.24	1.46	1.39
23	6	302	CHL	CHD-C1D	4.24	1.46	1.39
23	0	301	CHL	CHB-C1B	4.24	1.46	1.39
23	7	307	CHL	C3B-C2B	4.24	1.46	1.40
23	3	301	CHL	CHB-C1B	4.24	1.46	1.39
23	6	305	CHL	CHB-C1B	4.24	1.46	1.39
23	4	307	CHL	O2A-CGA	4.24	1.45	1.33
23	4	307	CHL	CHD-C1D	4.23	1.46	1.39
23	2	306	CHL	CHB-C1B	4.23	1.46	1.39
23	7	306	CHL	O2A-CGA	4.23	1.45	1.33
23	8	308	CHL	O2A-CGA	4.23	1.45	1.33
23	1	306	CHL	O2A-CGA	4.23	1.45	1.33
25	A	846	8CT	C19-C20	4.23	1.56	1.43
23	5	312	CHL	CHC-C1C	4.23	1.47	1.39
23	7	302	CHL	CHD-C1D	4.23	1.46	1.39
23	3	305	CHL	C3B-C2B	4.23	1.46	1.40
23	0	302	CHL	O2A-CGA	4.22	1.45	1.33
23	2	301	CHL	C3B-C2B	4.22	1.46	1.40
23	3	302	CHL	O2A-CGA	4.22	1.45	1.33
25	B	848	8CT	C24-C25	4.22	1.56	1.43
25	O	202	8CT	C19-C20	4.22	1.56	1.43
23	4	313	CHL	O2A-CGA	4.22	1.45	1.33
23	6	307	CHL	CHB-C1B	4.22	1.46	1.39
23	0	305	CHL	CHD-C4C	4.22	1.47	1.39
23	4	315	CHL	CHB-C1B	4.21	1.46	1.39
25	B	844	8CT	C24-C25	4.21	1.56	1.43
23	4	315	CHL	O2A-CGA	4.21	1.45	1.33
23	8	307	CHL	CHB-C1B	4.21	1.46	1.39
23	4	302	CHL	O2A-CGA	4.21	1.45	1.33
23	4	301	CHL	O2A-CGA	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	845	8CT	C24-C25	4.21	1.56	1.43
23	5	305	CHL	CHC-C1C	4.20	1.47	1.39
23	8	303	CHL	O2A-CGA	4.20	1.45	1.33
25	9	313	8CT	C24-C25	4.20	1.56	1.43
23	6	306	CHL	CHB-C1B	4.20	1.46	1.39
23	7	307	CHL	O2A-CGA	4.20	1.45	1.33
23	2	304	CHL	C3D-C2D	4.20	1.46	1.39
23	6	301	CHL	O2A-CGA	4.19	1.45	1.33
25	0	314	8CT	C24-C25	4.19	1.56	1.43
23	8	314	CHL	CHB-C1B	4.19	1.46	1.39
23	2	306	CHL	O2A-CGA	4.18	1.45	1.33
25	L	207	8CT	C24-C25	4.18	1.56	1.43
25	G	104	8CT	C24-C25	4.17	1.56	1.43
23	5	304	CHL	CHD-C4C	4.17	1.47	1.39
23	4	301	CHL	CHB-C1B	4.17	1.46	1.39
23	4	305	CHL	CHB-C1B	4.17	1.46	1.39
25	3	316	8CT	C24-C25	4.17	1.56	1.43
25	1	314	8CT	C24-C25	4.17	1.56	1.43
23	7	313	CHL	O2A-CGA	4.17	1.45	1.33
23	9	312	CHL	O2A-CGA	4.17	1.45	1.33
23	3	302	CHL	CHD-C1D	4.17	1.46	1.39
25	J	104	8CT	C24-C25	4.17	1.56	1.43
23	3	302	CHL	CHC-C1C	4.16	1.47	1.39
25	L	205	8CT	C24-C25	4.16	1.56	1.43
25	6	324	8CT	C24-C25	4.16	1.56	1.43
23	8	309	CHL	O2A-CGA	4.16	1.45	1.33
23	5	312	CHL	O2A-CGA	4.15	1.45	1.33
23	5	301	CHL	CHB-C1B	4.15	1.46	1.39
23	2	304	CHL	CHB-C1B	4.15	1.46	1.39
23	7	302	CHL	O2A-CGA	4.15	1.45	1.33
23	3	307	CHL	CHB-C1B	4.14	1.46	1.39
23	9	301	CHL	O2A-CGA	4.14	1.45	1.33
23	8	303	CHL	C3B-C2B	4.14	1.46	1.40
23	7	302	CHL	CHB-C1B	4.14	1.46	1.39
23	8	307	CHL	CHD-C4C	4.14	1.47	1.39
23	2	301	CHL	O2A-CGA	4.14	1.45	1.33
23	8	301	CHL	CHC-C1C	4.14	1.47	1.39
25	A	849	8CT	C24-C25	4.14	1.56	1.43
25	K	105	8CT	C24-C25	4.14	1.56	1.43
23	1	305	CHL	CHD-C4C	4.13	1.47	1.39
23	7	307	CHL	CHC-C1C	4.13	1.47	1.39
23	6	315	CHL	CHD-C4C	4.13	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	306	CHL	O2A-CGA	4.13	1.45	1.33
23	2	307	CHL	O2A-CGA	4.12	1.45	1.33
23	3	305	CHL	CHB-C1B	4.12	1.46	1.39
23	8	303	CHL	CHB-C1B	4.12	1.46	1.39
23	5	301	CHL	C3B-C2B	4.12	1.45	1.40
23	3	302	CHL	CHB-C1B	4.12	1.46	1.39
23	7	306	CHL	CHD-C4C	4.11	1.47	1.39
23	0	302	CHL	C3B-C2B	4.11	1.45	1.40
23	6	302	CHL	CHB-C1B	4.11	1.46	1.39
23	1	301	CHL	O2A-CGA	4.11	1.45	1.33
23	8	316	CHL	CHC-C1C	4.11	1.47	1.39
25	B	847	8CT	C24-C25	4.10	1.55	1.43
23	4	313	CHL	CHB-C1B	4.10	1.46	1.39
23	6	323	CHL	O2A-CGA	4.10	1.45	1.33
23	4	308	CHL	O2A-CGA	4.10	1.45	1.33
23	0	306	CHL	CHD-C4C	4.09	1.47	1.39
23	5	306	CHL	CHC-C1C	4.09	1.47	1.39
25	L	204	8CT	C24-C25	4.09	1.55	1.43
25	O	208	8CT	C24-C25	4.09	1.55	1.43
23	3	302	CHL	C3B-C2B	4.09	1.45	1.40
23	7	313	CHL	CHD-C4C	4.09	1.47	1.39
23	8	306	CHL	O2A-CGA	4.09	1.45	1.33
23	4	302	CHL	C3B-C2B	4.09	1.45	1.40
25	M	102	8CT	C24-C25	4.09	1.55	1.43
23	8	303	CHL	CHC-C1C	4.08	1.47	1.39
23	7	302	CHL	C3B-C2B	4.08	1.45	1.40
25	7	319	8CT	C24-C25	4.08	1.55	1.43
23	4	308	CHL	CHD-C4C	4.08	1.47	1.39
25	3	317	8CT	C24-C25	4.08	1.55	1.43
25	B	844	8CT	C14-C13	4.08	1.55	1.43
23	2	301	CHL	CHB-C1B	4.07	1.46	1.39
25	B	850	8CT	C24-C25	4.07	1.55	1.43
23	8	306	CHL	CHD-C4C	4.07	1.47	1.39
25	6	319	8CT	C24-C25	4.07	1.55	1.43
23	9	312	CHL	CHD-C4C	4.06	1.47	1.39
23	0	302	CHL	CHB-C1B	4.06	1.46	1.39
23	1	304	CHL	CHB-C1B	4.06	1.46	1.39
23	6	323	CHL	CHD-C4C	4.06	1.47	1.39
25	F	304	8CT	C24-C25	4.06	1.55	1.43
23	4	302	CHL	CHB-C1B	4.06	1.46	1.39
23	7	305	CHL	CHB-C1B	4.05	1.46	1.39
25	8	317	8CT	C24-C25	4.05	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	307	CHL	CHD-C1D	4.04	1.46	1.39
23	8	309	CHL	CHD-C4C	4.04	1.47	1.39
23	7	307	CHL	CHD-C4C	4.04	1.47	1.39
25	J	101	8CT	C24-C25	4.03	1.55	1.43
25	3	323	8CT	C24-C25	4.03	1.55	1.43
25	F	301	8CT	C24-C25	4.02	1.55	1.43
23	1	301	CHL	C3B-C2B	4.02	1.45	1.40
23	4	306	CHL	CHD-C4C	4.02	1.47	1.39
23	6	301	CHL	CHD-C4C	4.02	1.47	1.39
23	7	313	CHL	CHC-C1C	4.01	1.47	1.39
25	B	845	8CT	C14-C13	4.01	1.55	1.43
25	B	846	8CT	C28-C29	4.01	1.41	1.32
23	7	305	CHL	CHC-C1C	4.01	1.47	1.39
23	4	301	CHL	CHD-C4C	4.00	1.47	1.39
23	6	313	CHL	CHD-C4C	4.00	1.47	1.39
23	9	301	CHL	CHD-C4C	4.00	1.47	1.39
25	I	101	8CT	C24-C25	4.00	1.55	1.43
23	3	305	CHL	CHC-C1C	4.00	1.47	1.39
23	1	301	CHL	CHC-C1C	4.00	1.47	1.39
25	G	104	8CT	C14-C13	4.00	1.55	1.43
23	1	301	CHL	CHB-C1B	4.00	1.46	1.39
23	1	304	CHL	CHD-C4C	3.99	1.47	1.39
23	1	306	CHL	CHD-C4C	3.99	1.47	1.39
25	7	318	8CT	C24-C25	3.99	1.55	1.43
23	4	302	CHL	CHD-C4C	3.99	1.47	1.39
23	7	302	CHL	CHC-C1C	3.99	1.47	1.39
23	0	306	CHL	CHC-C1C	3.98	1.47	1.39
23	6	323	CHL	CHC-C1C	3.98	1.47	1.39
23	0	305	CHL	CHC-C1C	3.98	1.47	1.39
23	1	306	CHL	CHC-C1C	3.98	1.47	1.39
23	2	305	CHL	CHD-C4C	3.97	1.47	1.39
25	8	317	8CT	C14-C13	3.97	1.55	1.43
23	5	305	CHL	C3A-C2A	-3.97	1.51	1.54
25	A	844	8CT	C24-C25	3.97	1.55	1.43
23	6	315	CHL	CHC-C1C	3.97	1.47	1.39
23	2	306	CHL	CHD-C1D	3.97	1.46	1.39
34	B	849	DGD	O2G-C1B	3.97	1.45	1.34
23	6	308	CHL	CHD-C4C	3.96	1.47	1.39
23	6	307	CHL	CHC-C1C	3.96	1.47	1.39
23	4	315	CHL	CHD-C4C	3.96	1.47	1.39
23	7	301	CHL	CHD-C4C	3.96	1.47	1.39
23	2	301	CHL	CHD-C4C	3.95	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	314	CHL	CHD-C4C	3.95	1.46	1.39
23	3	301	CHL	CHD-C4C	3.95	1.46	1.39
25	B	843	8CT	C14-C13	3.94	1.55	1.43
23	1	312	CHL	CHD-C4C	3.94	1.46	1.39
23	2	304	CHL	CHD-C4C	3.94	1.46	1.39
23	5	306	CHL	C3A-C2A	-3.93	1.51	1.54
25	A	845	8CT	C24-C25	3.93	1.55	1.43
23	9	305	CHL	CHC-C1C	3.93	1.46	1.39
23	7	306	CHL	CHC-C1C	3.93	1.46	1.39
23	1	305	CHL	CHC-C1C	3.93	1.46	1.39
23	8	303	CHL	CHD-C4C	3.92	1.46	1.39
23	0	302	CHL	CHD-C4C	3.92	1.46	1.39
23	5	304	CHL	CHC-C1C	3.91	1.46	1.39
25	B	846	8CT	C14-C13	3.91	1.55	1.43
23	0	302	CHL	CHC-C1C	3.91	1.46	1.39
23	9	305	CHL	CHB-C1B	3.90	1.45	1.39
25	L	205	8CT	C14-C13	3.90	1.55	1.43
25	B	848	8CT	C14-C13	3.90	1.55	1.43
23	2	307	CHL	CHD-C4C	3.90	1.46	1.39
23	9	306	CHL	CHD-C4C	3.90	1.46	1.39
25	A	847	8CT	C24-C25	3.90	1.55	1.43
25	A	846	8CT	C24-C25	3.89	1.55	1.43
23	1	312	CHL	CHC-C1C	3.89	1.46	1.39
23	7	302	CHL	CHD-C4C	3.89	1.46	1.39
25	6	324	8CT	C14-C13	3.89	1.55	1.43
23	0	301	CHL	CHD-C4C	3.89	1.46	1.39
23	1	304	CHL	CHC-C1C	3.89	1.46	1.39
25	B	843	8CT	C28-C29	3.89	1.41	1.32
23	6	302	CHL	CHD-C4C	3.89	1.46	1.39
23	8	307	CHL	CHC-C1C	3.88	1.46	1.39
25	4	316	8CT	C14-C13	3.88	1.55	1.43
23	6	306	CHL	CHD-C4C	3.88	1.46	1.39
25	3	323	8CT	C28-C29	3.88	1.41	1.32
32	A	852	CL0	CMD-C2D	-3.88	1.43	1.51
23	3	302	CHL	CHD-C4C	3.88	1.46	1.39
23	6	308	CHL	CHC-C1C	3.87	1.46	1.39
23	4	305	CHL	CHD-C4C	3.87	1.46	1.39
23	5	301	CHL	CHD-C4C	3.87	1.46	1.39
23	1	301	CHL	CHD-C4C	3.87	1.46	1.39
25	6	319	8CT	C14-C13	3.87	1.55	1.43
25	K	105	8CT	C14-C13	3.87	1.55	1.43
25	O	202	8CT	C24-C25	3.86	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	309	CHL	CHC-C1C	3.86	1.46	1.39
23	7	301	CHL	CHC-C1C	3.86	1.46	1.39
23	6	305	CHL	CHD-C4C	3.86	1.46	1.39
23	6	302	CHL	CHC-C1C	3.86	1.46	1.39
25	3	323	8CT	C14-C13	3.86	1.55	1.43
23	3	305	CHL	CHD-C4C	3.85	1.46	1.39
23	4	313	CHL	CHD-C4C	3.85	1.46	1.39
23	3	307	CHL	C3B-C2B	3.85	1.45	1.40
23	7	305	CHL	CHD-C4C	3.85	1.46	1.39
23	8	308	CHL	CHD-C4C	3.85	1.46	1.39
23	7	306	CHL	CHA-CBD	-3.85	1.47	1.51
25	2	314	8CT	C14-C13	3.85	1.55	1.43
25	1	314	8CT	C14-C13	3.85	1.55	1.43
23	2	306	CHL	CHC-C1C	3.84	1.46	1.39
25	4	316	8CT	C28-C29	3.84	1.41	1.32
25	B	846	8CT	C30-C29	3.84	1.56	1.50
23	3	301	CHL	CHC-C1C	3.84	1.46	1.39
23	4	302	CHL	CHC-C1C	3.84	1.46	1.39
23	4	308	CHL	CHC-C1C	3.84	1.46	1.39
23	9	305	CHL	CHD-C4C	3.83	1.46	1.39
23	3	307	CHL	CHD-C4C	3.83	1.46	1.39
23	6	307	CHL	CHD-C4C	3.83	1.46	1.39
23	4	306	CHL	CHC-C1C	3.83	1.46	1.39
25	0	314	8CT	C14-C13	3.82	1.55	1.43
23	4	301	CHL	CHC-C1C	3.82	1.46	1.39
23	4	315	CHL	CHC-C1C	3.82	1.46	1.39
23	2	301	CHL	CHC-C1C	3.82	1.46	1.39
25	9	313	8CT	C14-C13	3.81	1.55	1.43
23	9	301	CHL	CHC-C1C	3.81	1.46	1.39
25	2	314	8CT	C28-C29	3.81	1.40	1.32
23	6	301	CHL	CHC-C1C	3.80	1.46	1.39
23	9	312	CHL	CHC-C1C	3.80	1.46	1.39
23	2	312	CHL	CHD-C4C	3.80	1.46	1.39
23	5	301	CHL	CHC-C1C	3.80	1.46	1.39
25	B	844	8CT	C28-C29	3.80	1.40	1.32
25	J	104	8CT	C14-C13	3.80	1.55	1.43
25	A	849	8CT	C14-C13	3.79	1.54	1.43
23	2	305	CHL	CHA-CBD	-3.79	1.47	1.51
23	8	308	CHL	CHC-C1C	3.79	1.46	1.39
23	3	302	CHL	CHA-CBD	-3.78	1.47	1.51
23	6	313	CHL	CHC-C1C	3.78	1.46	1.39
23	8	306	CHL	CHC-C1C	3.78	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	845	8CT	C14-C13	3.77	1.54	1.43
25	O	208	8CT	C14-C13	3.77	1.54	1.43
25	1	314	8CT	C28-C29	3.76	1.40	1.32
25	L	207	8CT	C14-C13	3.76	1.54	1.43
25	L	204	8CT	C14-C13	3.76	1.54	1.43
23	2	307	CHL	CHC-C1C	3.76	1.46	1.39
25	3	317	8CT	C14-C13	3.76	1.54	1.43
25	J	101	8CT	C14-C13	3.76	1.54	1.43
25	B	848	8CT	C28-C29	3.76	1.40	1.32
23	2	312	CHL	CHC-C1C	3.75	1.46	1.39
25	0	314	8CT	C28-C29	3.75	1.40	1.32
23	9	306	CHL	CHC-C1C	3.75	1.46	1.39
23	2	305	CHL	CHC-C1C	3.75	1.46	1.39
23	6	305	CHL	CHC-C1C	3.75	1.46	1.39
25	A	844	8CT	C14-C13	3.75	1.54	1.43
23	2	304	CHL	CHC-C1C	3.74	1.46	1.39
23	0	301	CHL	CHC-C1C	3.74	1.46	1.39
25	F	304	8CT	C14-C13	3.74	1.54	1.43
25	8	317	8CT	C11-C12	3.74	1.54	1.46
23	4	307	CHL	CHC-C1C	3.74	1.46	1.39
23	4	313	CHL	CHA-CBD	-3.74	1.47	1.51
23	8	316	CHL	C3A-C2A	-3.74	1.51	1.54
23	4	305	CHL	CHC-C1C	3.74	1.46	1.39
25	M	102	8CT	C14-C13	3.73	1.54	1.43
25	B	847	8CT	C14-C13	3.73	1.54	1.43
25	G	104	8CT	C28-C29	3.73	1.40	1.32
25	B	843	8CT	C11-C12	3.73	1.53	1.46
23	4	307	CHL	CHD-C4C	3.73	1.46	1.39
25	B	850	8CT	C14-C13	3.72	1.54	1.43
25	B	844	8CT	C11-C12	3.71	1.53	1.46
25	7	319	8CT	C14-C13	3.71	1.54	1.43
25	I	101	8CT	C14-C13	3.71	1.54	1.43
23	4	313	CHL	CHC-C1C	3.70	1.46	1.39
25	3	317	8CT	C28-C29	3.70	1.40	1.32
23	3	301	CHL	CHA-CBD	-3.70	1.47	1.51
25	B	845	8CT	C11-C12	3.70	1.53	1.46
25	F	301	8CT	C14-C13	3.70	1.54	1.43
25	A	849	8CT	C28-C29	3.69	1.40	1.32
23	9	306	CHL	CHA-CBD	-3.69	1.47	1.51
23	2	306	CHL	CHD-C4C	3.69	1.46	1.39
25	J	104	8CT	C28-C29	3.69	1.40	1.32
25	6	324	8CT	C11-C12	3.69	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	314	8CT	C11-C12	3.69	1.53	1.46
25	9	313	8CT	C28-C29	3.69	1.40	1.32
23	6	306	CHL	CHC-C1C	3.68	1.46	1.39
23	8	314	CHL	CHC-C1C	3.68	1.46	1.39
25	1	314	8CT	C11-C12	3.68	1.53	1.46
23	2	301	CHL	CHA-CBD	-3.68	1.47	1.51
23	8	303	CHL	CHA-CBD	-3.68	1.47	1.51
23	6	301	CHL	CHA-CBD	-3.68	1.47	1.51
25	B	846	8CT	C11-C12	3.67	1.53	1.46
25	6	319	8CT	C28-C29	3.67	1.40	1.32
25	4	316	8CT	C11-C12	3.67	1.53	1.46
25	7	318	8CT	C14-C13	3.66	1.54	1.43
23	4	302	CHL	CHA-CBD	-3.66	1.47	1.51
25	8	317	8CT	C28-C29	3.66	1.40	1.32
25	3	316	8CT	C11-C12	3.66	1.53	1.46
23	6	302	CHL	CHA-CBD	-3.66	1.47	1.51
34	B	849	DGD	O1G-C1A	3.65	1.44	1.33
23	7	301	CHL	CHA-CBD	-3.65	1.47	1.51
23	3	307	CHL	CHC-C1C	3.65	1.46	1.39
25	6	324	8CT	C28-C29	3.65	1.40	1.32
25	B	848	8CT	C11-C12	3.64	1.53	1.46
25	K	105	8CT	C11-C12	3.64	1.53	1.46
25	3	316	8CT	C28-C29	3.63	1.40	1.32
25	L	204	8CT	C28-C29	3.63	1.40	1.32
25	J	104	8CT	C11-C12	3.62	1.53	1.46
25	L	207	8CT	C28-C29	3.62	1.40	1.32
25	L	207	8CT	C11-C12	3.61	1.53	1.46
23	8	301	CHL	CHA-CBD	-3.61	1.47	1.51
25	J	101	8CT	C28-C29	3.61	1.40	1.32
25	M	102	8CT	C28-C29	3.61	1.40	1.32
23	4	315	CHL	CHA-CBD	-3.61	1.47	1.51
25	K	105	8CT	C28-C29	3.60	1.40	1.32
25	J	101	8CT	C11-C12	3.60	1.53	1.46
25	3	316	8CT	C14-C13	3.59	1.54	1.43
25	F	304	8CT	C28-C29	3.59	1.40	1.32
25	O	202	8CT	C14-C13	3.59	1.54	1.43
25	2	314	8CT	C11-C12	3.58	1.53	1.46
23	5	312	CHL	CHA-CBD	-3.58	1.47	1.51
25	L	205	8CT	C28-C29	3.58	1.40	1.32
25	A	846	8CT	C14-C13	3.58	1.54	1.43
25	G	104	8CT	C11-C12	3.58	1.53	1.46
23	1	301	CHL	CHA-CBD	-3.58	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	208	8CT	C28-C29	3.58	1.40	1.32
23	4	306	CHL	CHA-CBD	-3.57	1.47	1.51
23	4	308	CHL	CHA-CBD	-3.57	1.47	1.51
25	9	313	8CT	C11-C12	3.56	1.53	1.46
32	A	852	CL0	C3D-C4D	3.56	1.47	1.41
25	B	850	8CT	C28-C29	3.56	1.40	1.32
23	5	301	CHL	CHA-CBD	-3.55	1.47	1.51
25	A	847	8CT	C14-C13	3.55	1.54	1.43
24	5	310	CLA	C1D-ND	3.55	1.42	1.37
32	A	852	CL0	CBD-CGD	-3.53	1.48	1.52
24	0	313	CLA	C1D-ND	3.53	1.42	1.37
25	A	845	8CT	C11-C12	3.53	1.53	1.46
25	B	844	8CT	C01-C02	3.52	1.56	1.50
25	A	847	8CT	C28-C29	3.51	1.40	1.32
25	A	849	8CT	C11-C12	3.51	1.53	1.46
24	5	307	CLA	C1D-ND	3.51	1.42	1.37
25	O	208	8CT	C11-C12	3.51	1.53	1.46
25	A	846	8CT	C28-C29	3.51	1.40	1.32
25	7	319	8CT	C11-C12	3.50	1.53	1.46
25	B	847	8CT	C11-C12	3.50	1.53	1.46
24	O	206	CLA	C1D-ND	3.50	1.42	1.37
25	A	844	8CT	C11-C12	3.49	1.53	1.46
25	7	318	8CT	C28-C29	3.49	1.40	1.32
23	0	305	CHL	CHA-CBD	-3.49	1.47	1.51
24	5	303	CLA	C1D-ND	3.48	1.42	1.37
25	3	316	8CT	C30-C29	3.48	1.55	1.50
23	8	309	CHL	CHA-CBD	-3.48	1.47	1.51
23	7	302	CHL	CHA-CBD	-3.47	1.47	1.51
25	3	317	8CT	C11-C12	3.47	1.53	1.46
25	B	845	8CT	C28-C29	3.47	1.40	1.32
25	O	202	8CT	C01-C02	3.47	1.56	1.50
23	9	312	CHL	CHA-CBD	-3.46	1.47	1.51
25	L	205	8CT	C11-C12	3.46	1.53	1.46
24	1	307	CLA	C1D-ND	3.46	1.42	1.37
23	5	306	CHL	CHA-CBD	-3.46	1.47	1.51
25	A	845	8CT	C28-C29	3.46	1.40	1.32
25	G	104	8CT	C01-C02	3.46	1.56	1.50
25	L	204	8CT	C30-C29	3.45	1.55	1.50
24	B	826	CLA	C4D-ND	-3.45	1.33	1.37
25	L	204	8CT	C35-C30	3.44	1.66	1.56
23	6	315	CHL	CHA-CBD	-3.44	1.47	1.51
25	F	304	8CT	C11-C12	3.44	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	319	8CT	C11-C12	3.43	1.53	1.46
25	I	101	8CT	C28-C29	3.43	1.40	1.32
24	8	304	CLA	C1D-ND	3.43	1.42	1.37
25	F	301	8CT	C28-C29	3.43	1.40	1.32
24	5	311	CLA	C1D-ND	3.43	1.42	1.37
25	O	202	8CT	C11-C12	3.43	1.53	1.46
25	B	846	8CT	C35-C30	3.43	1.65	1.56
25	F	301	8CT	C11-C12	3.43	1.53	1.46
24	H	204	CLA	C1D-ND	3.42	1.42	1.37
25	A	844	8CT	C01-C02	3.42	1.56	1.50
25	4	316	8CT	C01-C02	3.42	1.56	1.50
25	7	319	8CT	C28-C29	3.41	1.40	1.32
25	B	847	8CT	C28-C29	3.41	1.40	1.32
25	3	317	8CT	C01-C02	3.41	1.56	1.50
25	J	101	8CT	C35-C30	3.41	1.65	1.56
24	0	308	CLA	C1D-ND	3.41	1.42	1.37
25	A	844	8CT	C28-C29	3.40	1.40	1.32
25	6	324	8CT	C01-C02	3.40	1.56	1.50
24	G	101	CLA	C1D-ND	3.40	1.42	1.37
25	7	318	8CT	C11-C12	3.40	1.53	1.46
23	3	307	CHL	CHA-CBD	-3.40	1.47	1.51
24	4	309	CLA	C1D-ND	3.40	1.42	1.37
25	B	850	8CT	C11-C12	3.40	1.53	1.46
24	G	103	CLA	C1D-ND	3.40	1.42	1.37
25	A	845	8CT	C01-C02	3.39	1.56	1.50
24	B	840	CLA	C1D-ND	3.39	1.42	1.37
25	K	105	8CT	C01-C02	3.39	1.56	1.50
25	G	104	8CT	C35-C30	3.38	1.65	1.56
23	2	304	CHL	CHA-CBD	-3.38	1.47	1.51
24	5	309	CLA	C1D-ND	3.38	1.42	1.37
25	A	847	8CT	C11-C12	3.38	1.53	1.46
25	I	101	8CT	C11-C12	3.38	1.53	1.46
24	J	103	CLA	C1D-ND	3.38	1.42	1.37
24	9	304	CLA	C1D-ND	3.38	1.42	1.37
23	2	307	CHL	CHA-CBD	-3.37	1.47	1.51
25	L	204	8CT	C11-C12	3.37	1.53	1.46
24	7	316	CLA	C1D-ND	3.37	1.42	1.37
24	L	206	CLA	C1D-ND	3.37	1.42	1.37
25	B	846	8CT	C01-C02	3.37	1.56	1.50
24	2	302	CLA	C1D-ND	3.36	1.42	1.37
24	8	310	CLA	C1D-ND	3.36	1.42	1.37
32	A	852	CL0	CMB-C2B	-3.36	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	0	302	CHL	CHA-CBD	-3.36	1.47	1.51
25	O	202	8CT	C28-C29	3.36	1.39	1.32
25	A	846	8CT	C01-C02	3.36	1.56	1.50
25	3	323	8CT	C11-C12	3.36	1.53	1.46
24	7	312	CLA	C1D-ND	3.35	1.42	1.37
24	8	315	CLA	C1D-ND	3.35	1.42	1.37
24	9	307	CLA	C1D-ND	3.35	1.42	1.37
24	B	822	CLA	C1D-ND	3.35	1.42	1.37
24	3	311	CLA	C1D-ND	3.35	1.42	1.37
24	4	310	CLA	C1D-ND	3.35	1.42	1.37
24	H	205	CLA	C1D-ND	3.35	1.42	1.37
24	O	209	CLA	C1D-ND	3.34	1.42	1.37
24	3	313	CLA	C1D-ND	3.34	1.42	1.37
25	3	316	8CT	C35-C30	3.34	1.65	1.56
25	M	102	8CT	C01-C02	3.34	1.56	1.50
24	8	311	CLA	C1D-ND	3.34	1.42	1.37
25	I	101	8CT	C01-C02	3.34	1.56	1.50
24	6	310	CLA	C1D-ND	3.34	1.42	1.37
24	0	307	CLA	C1D-ND	3.34	1.42	1.37
23	6	305	CHL	CHA-CBD	-3.34	1.47	1.51
25	L	204	8CT	C01-C02	3.34	1.56	1.50
24	A	802	CLA	C1D-ND	3.34	1.42	1.37
24	0	309	CLA	C1D-ND	3.33	1.42	1.37
24	A	834	CLA	C1D-ND	3.33	1.42	1.37
24	0	304	CLA	C1D-ND	3.33	1.42	1.37
25	3	317	8CT	C35-C30	3.33	1.65	1.56
24	1	309	CLA	C1D-ND	3.33	1.42	1.37
25	L	205	8CT	C01-C02	3.33	1.56	1.50
25	J	104	8CT	C01-C02	3.33	1.56	1.50
24	6	309	CLA	C1D-ND	3.32	1.42	1.37
25	7	318	8CT	C01-C02	3.32	1.56	1.50
25	4	316	8CT	C18-C17	3.32	1.53	1.43
24	1	310	CLA	C1D-ND	3.32	1.42	1.37
25	6	319	8CT	C35-C30	3.32	1.65	1.56
25	O	208	8CT	C01-C02	3.32	1.56	1.50
23	8	306	CHL	CHA-CBD	-3.32	1.47	1.51
24	5	313	CLA	C1D-ND	3.32	1.42	1.37
24	B	827	CLA	C1D-ND	3.32	1.42	1.37
24	8	313	CLA	C1D-ND	3.32	1.42	1.37
24	L	203	CLA	C1D-ND	3.32	1.42	1.37
23	4	301	CHL	CHA-CBD	-3.32	1.47	1.51
25	A	847	8CT	C35-C30	3.32	1.65	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	O	204	CLA	C1D-ND	3.31	1.42	1.37
24	9	309	CLA	C1D-ND	3.31	1.42	1.37
24	H	203	CLA	C1D-ND	3.31	1.42	1.37
25	2	314	8CT	C18-C17	3.31	1.53	1.43
24	K	104	CLA	C1D-ND	3.31	1.42	1.37
24	A	824	CLA	C1D-ND	3.31	1.42	1.37
23	9	305	CHL	CHA-CBD	-3.31	1.47	1.51
24	A	832	CLA	C1D-ND	3.31	1.42	1.37
24	B	832	CLA	C1D-ND	3.31	1.42	1.37
23	4	305	CHL	CHA-CBD	-3.31	1.47	1.51
24	A	823	CLA	C1D-ND	3.31	1.42	1.37
24	0	312	CLA	C1D-ND	3.31	1.42	1.37
24	5	302	CLA	C1D-ND	3.31	1.42	1.37
25	J	101	8CT	C30-C29	3.30	1.55	1.50
24	A	809	CLA	C1D-ND	3.30	1.42	1.37
25	A	846	8CT	C35-C30	3.30	1.65	1.56
24	7	310	CLA	C1D-ND	3.30	1.42	1.37
24	A	836	CLA	C1D-ND	3.30	1.42	1.37
24	7	317	CLA	C1D-ND	3.30	1.42	1.37
24	2	313	CLA	C1D-ND	3.30	1.42	1.37
24	7	304	CLA	C1D-ND	3.30	1.42	1.37
25	F	304	8CT	C01-C02	3.30	1.56	1.50
25	B	850	8CT	C01-C02	3.30	1.56	1.50
25	M	102	8CT	C11-C12	3.30	1.53	1.46
25	1	314	8CT	C35-C30	3.29	1.65	1.56
25	0	314	8CT	C01-C02	3.29	1.56	1.50
24	K	103	CLA	C1D-ND	3.29	1.42	1.37
24	9	310	CLA	C1D-ND	3.29	1.42	1.37
23	9	301	CHL	CHA-CBD	-3.29	1.47	1.51
23	4	307	CHL	CHA-CBD	-3.29	1.47	1.51
24	1	311	CLA	C1D-ND	3.29	1.42	1.37
25	B	847	8CT	C01-C02	3.28	1.56	1.50
24	3	304	CLA	C1D-ND	3.28	1.42	1.37
24	3	310	CLA	C1D-ND	3.28	1.42	1.37
24	B	833	CLA	C1D-ND	3.28	1.42	1.37
25	M	102	8CT	C35-C30	3.28	1.65	1.56
24	B	821	CLA	C1D-ND	3.28	1.42	1.37
24	F	302	CLA	C1D-ND	3.28	1.42	1.37
24	O	205	CLA	C1D-ND	3.28	1.42	1.37
24	A	813	CLA	C1D-ND	3.28	1.42	1.37
24	F	303	CLA	C1D-ND	3.28	1.42	1.37
24	0	311	CLA	C1D-ND	3.28	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	814	CLA	C1D-ND	3.28	1.42	1.37
24	2	310	CLA	C1D-ND	3.28	1.42	1.37
25	A	849	8CT	C01-C02	3.28	1.56	1.50
24	0	310	CLA	C1D-ND	3.28	1.42	1.37
24	6	318	CLA	C1D-ND	3.28	1.42	1.37
24	1	303	CLA	C1D-ND	3.28	1.42	1.37
24	7	314	CLA	C1D-ND	3.28	1.42	1.37
24	G	102	CLA	C1D-ND	3.28	1.42	1.37
25	L	207	8CT	C01-C02	3.27	1.56	1.50
27	7	322	LHG	C26-C25	-3.27	1.35	1.51
24	6	304	CLA	C1D-ND	3.27	1.42	1.37
24	A	831	CLA	C1D-ND	3.27	1.42	1.37
25	A	847	8CT	C01-C02	3.27	1.56	1.50
25	4	316	8CT	C35-C30	3.27	1.65	1.56
25	B	843	8CT	C30-C29	3.27	1.55	1.50
25	G	104	8CT	C30-C29	3.27	1.55	1.50
24	1	308	CLA	C1D-ND	3.27	1.42	1.37
24	3	306	CLA	C1D-ND	3.27	1.42	1.37
24	3	308	CLA	C1D-ND	3.27	1.42	1.37
24	B	835	CLA	C1D-ND	3.27	1.42	1.37
24	6	314	CLA	C1D-ND	3.27	1.42	1.37
25	L	207	8CT	C35-C30	3.27	1.65	1.56
25	B	843	8CT	C01-C02	3.27	1.56	1.50
24	B	825	CLA	C1D-ND	3.26	1.42	1.37
24	B	836	CLA	C1D-ND	3.26	1.42	1.37
25	G	104	8CT	C18-C17	3.26	1.53	1.43
24	B	816	CLA	C1D-ND	3.26	1.42	1.37
24	4	312	CLA	C1D-ND	3.26	1.42	1.37
24	O	201	CLA	C1D-ND	3.26	1.42	1.37
25	3	323	8CT	C18-C17	3.26	1.53	1.43
27	1	317	LHG	C26-C25	-3.26	1.35	1.51
23	7	305	CHL	CHA-CBD	-3.26	1.47	1.51
24	4	311	CLA	C1D-ND	3.26	1.42	1.37
25	6	324	8CT	C30-C29	3.26	1.55	1.50
27	3	320	LHG	C26-C25	-3.26	1.35	1.51
24	5	308	CLA	C1D-ND	3.26	1.42	1.37
24	7	311	CLA	C1D-ND	3.26	1.42	1.37
23	3	305	CHL	CHA-CBD	-3.26	1.47	1.51
25	1	314	8CT	C01-C02	3.25	1.56	1.50
24	B	801	CLA	C1D-ND	3.25	1.42	1.37
25	B	843	8CT	C35-C30	3.25	1.65	1.56
24	A	815	CLA	C1D-ND	3.25	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	306	CHL	CHA-CBD	-3.25	1.47	1.51
24	A	826	CLA	C1D-ND	3.25	1.42	1.37
23	5	305	CHL	CHA-CBD	-3.25	1.47	1.51
27	A	842	LHG	C26-C25	-3.25	1.35	1.51
24	7	303	CLA	C1D-ND	3.25	1.42	1.37
24	8	312	CLA	C1D-ND	3.25	1.42	1.37
25	J	101	8CT	C01-C02	3.25	1.56	1.50
23	5	304	CHL	CHA-CBD	-3.24	1.47	1.51
25	A	846	8CT	C11-C12	3.24	1.52	1.46
25	3	323	8CT	C01-C02	3.24	1.56	1.50
27	3	322	LHG	C26-C25	-3.24	1.35	1.51
24	9	308	CLA	C1D-ND	3.24	1.42	1.37
27	8	320	LHG	C26-C25	-3.24	1.35	1.51
25	6	324	8CT	C35-C30	3.24	1.65	1.56
25	B	848	8CT	C18-C17	3.24	1.53	1.43
27	2	317	LHG	C26-C25	-3.24	1.35	1.51
27	9	316	LHG	C26-C25	-3.24	1.35	1.51
24	9	302	CLA	C1D-ND	3.24	1.42	1.37
27	8	302	LHG	C26-C25	-3.24	1.35	1.51
25	B	848	8CT	C01-C02	3.24	1.56	1.50
24	4	314	CLA	C1D-ND	3.24	1.42	1.37
25	9	313	8CT	C01-C02	3.23	1.56	1.50
24	A	837	CLA	C1D-ND	3.23	1.42	1.37
27	5	316	LHG	C26-C25	-3.23	1.35	1.51
27	7	324	LHG	C26-C25	-3.23	1.35	1.51
24	3	303	CLA	C1D-ND	3.23	1.42	1.37
27	I	102	LHG	C26-C25	-3.23	1.35	1.51
24	9	311	CLA	C1D-ND	3.23	1.42	1.37
24	0	303	CLA	C1D-ND	3.23	1.42	1.37
25	B	845	8CT	C01-C02	3.23	1.56	1.50
24	B	820	CLA	C1D-ND	3.23	1.42	1.37
25	B	845	8CT	C18-C17	3.22	1.53	1.43
27	3	324	LHG	C26-C25	-3.22	1.35	1.51
24	1	302	CLA	C1D-ND	3.22	1.42	1.37
25	F	301	8CT	C01-C02	3.22	1.56	1.50
24	B	815	CLA	C1D-ND	3.22	1.42	1.37
24	4	303	CLA	C1D-ND	3.22	1.42	1.37
23	1	312	CHL	CHA-CBD	-3.22	1.47	1.51
27	6	322	LHG	C26-C25	-3.22	1.35	1.51
27	0	317	LHG	C26-C25	-3.22	1.35	1.51
24	6	317	CLA	C1D-ND	3.22	1.42	1.37
24	A	818	CLA	C1D-ND	3.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	316	CHL	CHA-CBD	-3.22	1.47	1.51
23	6	306	CHL	CHA-CBD	-3.22	1.47	1.51
27	1	318	LHG	C26-C25	-3.22	1.35	1.51
23	0	301	CHL	CHA-CBD	-3.22	1.47	1.51
25	0	314	8CT	C18-C17	3.21	1.53	1.43
24	2	308	CLA	C1D-ND	3.21	1.42	1.37
23	6	307	CHL	CHA-CBD	-3.21	1.47	1.51
25	0	314	8CT	C35-C30	3.21	1.65	1.56
27	B	852	LHG	C26-C25	-3.21	1.35	1.51
24	6	316	CLA	C1D-ND	3.21	1.42	1.37
25	3	323	8CT	C35-C30	3.21	1.65	1.56
27	L	208	LHG	C26-C25	-3.21	1.35	1.51
27	2	319	LHG	C26-C25	-3.21	1.35	1.51
25	2	314	8CT	C35-C30	3.21	1.65	1.56
24	B	841	CLA	C1D-ND	3.21	1.42	1.37
25	6	319	8CT	C01-C02	3.20	1.56	1.50
24	A	801	CLA	C1D-ND	3.20	1.42	1.37
24	A	807	CLA	C1D-ND	3.20	1.42	1.37
24	6	303	CLA	C1D-ND	3.20	1.42	1.37
24	A	817	CLA	C1D-ND	3.20	1.42	1.37
23	7	313	CHL	CHA-CBD	-3.20	1.47	1.51
23	8	308	CHL	CHA-CBD	-3.20	1.47	1.51
24	1	313	CLA	C1D-ND	3.20	1.42	1.37
24	L	202	CLA	C1D-ND	3.19	1.42	1.37
25	J	104	8CT	C18-C17	3.19	1.53	1.43
24	B	813	CLA	C1D-ND	3.19	1.42	1.37
24	8	305	CLA	C1D-ND	3.19	1.42	1.37
24	A	810	CLA	C1D-ND	3.19	1.42	1.37
24	7	309	CLA	C1D-ND	3.19	1.42	1.37
24	H	201	CLA	C1D-ND	3.19	1.42	1.37
25	3	316	8CT	C01-C02	3.19	1.56	1.50
25	6	319	8CT	C18-C17	3.19	1.53	1.43
24	7	315	CLA	C1D-ND	3.19	1.42	1.37
24	B	818	CLA	C1D-ND	3.19	1.42	1.37
24	3	314	CLA	C1D-ND	3.18	1.42	1.37
24	H	202	CLA	C1D-ND	3.18	1.42	1.37
24	B	808	CLA	C1D-ND	3.18	1.42	1.37
24	A	838	CLA	C1D-ND	3.18	1.42	1.37
24	B	811	CLA	C1D-ND	3.18	1.42	1.37
24	A	848	CLA	C1D-ND	3.18	1.42	1.37
23	6	308	CHL	CHA-CBD	-3.18	1.47	1.51
24	B	839	CLA	C1D-ND	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	850	LHG	C26-C25	-3.18	1.36	1.51
24	B	837	CLA	C1D-ND	3.18	1.42	1.37
24	4	304	CLA	C1D-ND	3.17	1.42	1.37
24	3	312	CLA	C1D-ND	3.17	1.42	1.37
24	9	303	CLA	C1D-ND	3.17	1.42	1.37
24	2	303	CLA	C1D-ND	3.17	1.42	1.37
24	7	308	CLA	C1D-ND	3.17	1.42	1.37
25	6	324	8CT	C18-C17	3.17	1.53	1.43
25	J	104	8CT	C30-C29	3.17	1.55	1.50
24	B	807	CLA	C1D-ND	3.17	1.42	1.37
25	9	313	8CT	C18-C17	3.17	1.53	1.43
25	2	314	8CT	C07-C02	-3.17	1.45	1.51
24	3	309	CLA	C1D-ND	3.17	1.42	1.37
25	B	847	8CT	C35-C30	3.17	1.65	1.56
24	A	827	CLA	C1D-ND	3.17	1.42	1.37
25	7	319	8CT	C01-C02	3.16	1.56	1.50
28	0	318	SQD	O48-C23	3.16	1.42	1.33
25	1	314	8CT	C18-C17	3.16	1.53	1.43
25	B	847	8CT	C07-C02	-3.16	1.45	1.51
25	I	101	8CT	C35-C30	3.16	1.65	1.56
25	B	844	8CT	C10-C03	3.16	1.55	1.45
25	L	205	8CT	C18-C17	3.16	1.53	1.43
24	B	829	CLA	C1D-ND	3.16	1.42	1.37
24	A	820	CLA	C1D-ND	3.16	1.42	1.37
25	7	319	8CT	C35-C30	3.16	1.65	1.56
24	A	811	CLA	C1D-ND	3.15	1.42	1.37
24	B	838	CLA	C1D-ND	3.15	1.42	1.37
25	B	843	8CT	C10-C03	3.15	1.55	1.45
24	B	819	CLA	C1D-ND	3.15	1.42	1.37
24	B	812	CLA	C1D-ND	3.15	1.42	1.37
24	2	309	CLA	C1D-ND	3.14	1.42	1.37
25	4	316	8CT	C10-C03	3.14	1.55	1.45
24	B	802	CLA	C1D-ND	3.14	1.42	1.37
25	K	105	8CT	C35-C30	3.14	1.65	1.56
24	A	819	CLA	C1D-ND	3.14	1.42	1.37
25	A	844	8CT	C35-C30	3.14	1.65	1.56
25	8	317	8CT	C35-C30	3.14	1.65	1.56
25	K	105	8CT	C18-C17	3.14	1.52	1.43
24	6	311	CLA	C1D-ND	3.14	1.42	1.37
24	B	828	CLA	C1D-ND	3.14	1.42	1.37
24	2	311	CLA	C1D-ND	3.14	1.42	1.37
24	6	312	CLA	C1D-ND	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	834	CLA	C1D-ND	3.13	1.42	1.37
25	L	207	8CT	C18-C17	3.13	1.52	1.43
25	J	104	8CT	C10-C03	3.13	1.55	1.45
23	1	304	CHL	CHA-CBD	-3.13	1.48	1.51
24	A	805	CLA	C1D-ND	3.13	1.42	1.37
25	L	205	8CT	C35-C30	3.12	1.65	1.56
24	A	821	CLA	C1D-ND	3.12	1.42	1.37
25	B	846	8CT	C18-C17	3.12	1.52	1.43
24	A	839	CLA	C1D-ND	3.12	1.42	1.37
24	0	319	CLA	C1D-ND	3.12	1.42	1.37
23	6	313	CHL	CHA-CBD	-3.12	1.48	1.51
23	1	305	CHL	CHA-CBD	-3.12	1.48	1.51
24	B	823	CLA	C1D-ND	3.12	1.42	1.37
25	F	304	8CT	C35-C30	3.11	1.65	1.56
24	A	812	CLA	C1D-ND	3.11	1.41	1.37
25	8	317	8CT	C18-C17	3.11	1.52	1.43
25	B	845	8CT	C10-C03	3.11	1.55	1.45
25	A	845	8CT	C35-C30	3.11	1.65	1.56
24	B	804	CLA	C1D-ND	3.11	1.41	1.37
24	A	804	CLA	C1D-ND	3.11	1.41	1.37
25	2	314	8CT	C01-C02	3.10	1.55	1.50
23	8	314	CHL	CHA-CBD	-3.10	1.48	1.51
24	O	206	CLA	CAB-C3B	-3.10	1.44	1.50
25	A	849	8CT	C18-C17	3.10	1.52	1.43
25	2	314	8CT	C10-C03	3.10	1.55	1.45
25	B	848	8CT	C35-C30	3.10	1.65	1.56
25	M	102	8CT	C18-C17	3.10	1.52	1.43
24	9	310	CLA	C4B-NB	3.10	1.41	1.37
24	A	806	CLA	C1D-ND	3.10	1.41	1.37
24	B	809	CLA	C1D-ND	3.10	1.41	1.37
25	6	324	8CT	C10-C03	3.10	1.55	1.45
25	L	204	8CT	C07-C02	-3.10	1.45	1.51
24	A	830	CLA	C1D-ND	3.10	1.41	1.37
25	B	850	8CT	C07-C02	-3.10	1.45	1.51
24	K	102	CLA	C1D-ND	3.10	1.41	1.37
25	O	202	8CT	C35-C30	3.09	1.65	1.56
24	B	824	CLA	C1D-ND	3.09	1.41	1.37
25	B	844	8CT	C18-C17	3.09	1.52	1.43
25	L	205	8CT	C07-C02	-3.09	1.45	1.51
24	3	315	CLA	C1D-ND	3.09	1.41	1.37
24	O	206	CLA	C4B-NB	3.09	1.41	1.37
25	B	848	8CT	C10-C03	3.09	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	304	8CT	C18-C17	3.09	1.52	1.43
24	6	311	CLA	C4B-NB	3.09	1.41	1.37
24	A	840	CLA	C1D-ND	3.09	1.41	1.37
24	A	822	CLA	C1D-ND	3.08	1.41	1.37
23	2	312	CHL	CHA-CBD	-3.08	1.48	1.51
25	O	208	8CT	C18-C17	3.08	1.52	1.43
24	A	829	CLA	C1D-ND	3.07	1.41	1.37
25	3	316	8CT	C10-C03	3.07	1.55	1.45
25	8	317	8CT	C10-C03	3.07	1.55	1.45
25	B	843	8CT	C18-C17	3.07	1.52	1.43
25	4	316	8CT	C07-C02	-3.07	1.45	1.51
25	B	846	8CT	C10-C03	3.07	1.55	1.45
24	A	808	CLA	C1D-ND	3.06	1.41	1.37
25	8	317	8CT	C01-C02	3.06	1.55	1.50
25	0	314	8CT	C10-C03	3.06	1.55	1.45
23	6	323	CHL	CHA-CBD	-3.06	1.48	1.51
24	K	101	CLA	C1D-ND	3.06	1.41	1.37
25	3	316	8CT	C07-C02	-3.06	1.45	1.51
25	A	845	8CT	C10-C03	3.06	1.55	1.45
25	A	844	8CT	C18-C17	3.06	1.52	1.43
24	8	312	CLA	C4B-NB	3.06	1.41	1.37
25	1	314	8CT	C30-C29	3.05	1.54	1.50
24	B	814	CLA	C1D-ND	3.05	1.41	1.37
24	B	830	CLA	CMB-C2B	-3.05	1.44	1.50
24	L	201	CLA	C1D-ND	3.05	1.41	1.37
24	A	835	CLA	C1D-ND	3.05	1.41	1.37
24	B	826	CLA	C1D-ND	3.05	1.41	1.37
25	3	317	8CT	C18-C17	3.05	1.52	1.43
25	B	850	8CT	C18-C17	3.05	1.52	1.43
25	K	105	8CT	C10-C03	3.04	1.55	1.45
25	J	101	8CT	C18-C17	3.04	1.52	1.43
25	B	850	8CT	C35-C30	3.04	1.64	1.56
25	3	317	8CT	C10-C03	3.04	1.55	1.45
25	3	317	8CT	C30-C29	3.03	1.54	1.50
24	B	817	CLA	C1D-ND	3.03	1.41	1.37
25	B	848	8CT	C07-C02	-3.03	1.45	1.51
23	7	307	CHL	CHA-CBD	-3.03	1.48	1.51
25	3	316	8CT	C18-C17	3.03	1.52	1.43
25	I	101	8CT	C18-C17	3.03	1.52	1.43
24	O	209	CLA	C4B-NB	3.03	1.41	1.37
25	B	847	8CT	C30-C29	3.03	1.54	1.50
24	0	313	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	816	CLA	C1D-ND	3.02	1.41	1.37
25	J	101	8CT	C10-C03	3.02	1.55	1.45
25	7	319	8CT	C18-C17	3.02	1.52	1.43
25	B	847	8CT	C18-C17	3.02	1.52	1.43
25	1	314	8CT	C10-C03	3.02	1.55	1.45
24	A	803	CLA	C1D-ND	3.02	1.41	1.37
24	A	828	CLA	C1D-ND	3.02	1.41	1.37
25	F	301	8CT	C07-C02	-3.02	1.45	1.51
25	A	846	8CT	C07-C02	-3.02	1.45	1.51
25	F	301	8CT	C18-C17	3.02	1.52	1.43
25	M	102	8CT	C07-C02	-3.02	1.45	1.51
25	9	313	8CT	C35-C30	3.02	1.64	1.56
25	A	849	8CT	C10-C03	3.01	1.55	1.45
25	L	204	8CT	C18-C17	3.01	1.52	1.43
25	L	207	8CT	C10-C03	3.01	1.55	1.45
24	6	304	CLA	C4B-NB	3.01	1.41	1.37
25	A	845	8CT	C18-C17	3.01	1.52	1.43
25	O	208	8CT	C10-C03	3.01	1.55	1.45
25	7	318	8CT	C10-C03	3.01	1.55	1.45
24	A	815	CLA	C4B-NB	3.01	1.41	1.37
25	8	317	8CT	C30-C29	3.01	1.54	1.50
24	A	833	CLA	C1D-ND	3.00	1.41	1.37
23	8	307	CHL	CHA-CBD	-3.00	1.48	1.51
25	G	104	8CT	C07-C02	-3.00	1.45	1.51
24	5	313	CLA	C4B-NB	3.00	1.41	1.37
24	A	825	CLA	C1D-ND	3.00	1.41	1.37
25	K	105	8CT	C07-C02	-3.00	1.45	1.51
24	A	829	CLA	CMB-C2B	-3.00	1.44	1.50
24	K	101	CLA	C4B-NB	3.00	1.41	1.37
25	A	844	8CT	C07-C02	-3.00	1.45	1.51
25	B	844	8CT	C35-C30	3.00	1.64	1.56
25	B	843	8CT	C07-C02	-2.99	1.45	1.51
25	A	844	8CT	C10-C03	2.99	1.55	1.45
25	G	104	8CT	C10-C03	2.99	1.55	1.45
25	9	313	8CT	C07-C02	-2.99	1.45	1.51
24	A	804	CLA	C4B-NB	2.98	1.41	1.37
25	L	205	8CT	C10-C03	2.98	1.55	1.45
25	8	317	8CT	C07-C02	-2.98	1.45	1.51
24	H	205	CLA	C4B-NB	2.98	1.41	1.37
24	L	206	CLA	C4B-NB	2.98	1.41	1.37
25	L	207	8CT	C07-C02	-2.98	1.45	1.51
25	6	319	8CT	C10-C03	2.97	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	202	8CT	C07-C02	-2.97	1.45	1.51
25	3	323	8CT	C10-C03	2.97	1.55	1.45
25	F	304	8CT	C10-C03	2.97	1.55	1.45
25	9	313	8CT	C10-C03	2.97	1.55	1.45
24	B	831	CLA	C1D-ND	2.97	1.41	1.37
25	6	319	8CT	C07-C02	-2.97	1.45	1.51
24	B	830	CLA	C1D-ND	2.96	1.41	1.37
25	A	849	8CT	C07-C02	-2.96	1.45	1.51
25	1	314	8CT	C07-C02	-2.96	1.45	1.51
25	6	324	8CT	C07-C02	-2.95	1.45	1.51
24	5	308	CLA	C4B-NB	2.95	1.41	1.37
24	8	305	CLA	C4B-NB	2.95	1.41	1.37
24	B	805	CLA	C1D-ND	2.95	1.41	1.37
25	B	847	8CT	C10-C03	2.95	1.55	1.45
24	B	810	CLA	C1D-ND	2.95	1.41	1.37
25	A	847	8CT	C07-C02	-2.95	1.45	1.51
25	O	208	8CT	C07-C02	-2.95	1.45	1.51
24	O	204	CLA	C4B-NB	2.94	1.41	1.37
25	B	845	8CT	C35-C30	2.94	1.64	1.56
25	K	105	8CT	C30-C29	2.94	1.54	1.50
24	F	302	CLA	C4B-NB	2.94	1.41	1.37
25	J	104	8CT	C07-C02	-2.94	1.45	1.51
25	O	208	8CT	C35-C30	2.94	1.64	1.56
25	O	202	8CT	C10-C03	2.93	1.55	1.45
25	J	101	8CT	C07-C02	-2.93	1.45	1.51
24	9	309	CLA	C4B-NB	2.93	1.41	1.37
25	A	846	8CT	C30-C29	2.93	1.54	1.50
25	A	847	8CT	C18-C17	2.93	1.52	1.43
25	L	204	8CT	C10-C03	2.93	1.55	1.45
24	B	806	CLA	C1D-ND	2.93	1.41	1.37
25	7	318	8CT	C18-C17	2.93	1.52	1.43
24	7	310	CLA	C4B-NB	2.92	1.41	1.37
24	A	822	CLA	C4B-NB	2.92	1.41	1.37
25	A	849	8CT	C30-C29	2.92	1.54	1.50
25	J	104	8CT	C35-C30	2.92	1.64	1.56
25	7	319	8CT	C10-C03	2.92	1.55	1.45
25	I	101	8CT	C10-C03	2.92	1.55	1.45
25	A	849	8CT	C35-C30	2.92	1.64	1.56
25	M	102	8CT	C10-C03	2.92	1.55	1.45
25	3	317	8CT	C07-C02	-2.92	1.45	1.51
24	5	307	CLA	C4B-NB	2.92	1.41	1.37
25	F	304	8CT	C30-C29	2.91	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	303	CLA	C4B-NB	2.91	1.41	1.37
24	6	310	CLA	C4B-NB	2.91	1.41	1.37
24	1	302	CLA	C4B-NB	2.91	1.41	1.37
25	B	845	8CT	C07-C02	-2.91	1.45	1.51
25	3	323	8CT	C07-C02	-2.91	1.45	1.51
25	I	101	8CT	C07-C02	-2.91	1.45	1.51
24	B	829	CLA	C4B-NB	2.91	1.41	1.37
25	F	304	8CT	C07-C02	-2.90	1.45	1.51
25	B	850	8CT	C10-C03	2.90	1.55	1.45
24	0	307	CLA	C4B-NB	2.90	1.41	1.37
25	O	202	8CT	C18-C17	2.90	1.52	1.43
24	5	303	CLA	C4B-NB	2.90	1.41	1.37
24	G	101	CLA	C4B-NB	2.90	1.41	1.37
25	A	845	8CT	C07-C02	-2.90	1.45	1.51
23	1	306	CHL	CHA-CBD	-2.90	1.48	1.51
24	B	822	CLA	C4B-NB	2.90	1.41	1.37
24	2	313	CLA	C4B-NB	2.89	1.41	1.37
24	4	309	CLA	C4B-NB	2.89	1.41	1.37
25	7	319	8CT	C07-C02	-2.89	1.45	1.51
24	7	314	CLA	C4B-NB	2.89	1.41	1.37
25	F	301	8CT	C10-C03	2.89	1.54	1.45
28	0	318	SQD	O47-C7	2.88	1.42	1.34
25	A	846	8CT	C18-C17	2.88	1.52	1.43
24	6	318	CLA	C4B-NB	2.88	1.41	1.37
24	5	302	CLA	C4B-NB	2.88	1.41	1.37
24	A	811	CLA	C4B-NB	2.88	1.41	1.37
24	8	304	CLA	C4B-NB	2.88	1.41	1.37
24	H	203	CLA	C4B-NB	2.88	1.41	1.37
24	0	303	CLA	C4B-NB	2.87	1.41	1.37
24	A	848	CLA	C4B-NB	2.87	1.41	1.37
24	0	319	CLA	C4B-NB	2.87	1.41	1.37
24	3	313	CLA	C4B-NB	2.87	1.41	1.37
25	L	207	8CT	C30-C29	2.87	1.54	1.50
24	6	317	CLA	C4B-NB	2.86	1.41	1.37
24	7	312	CLA	C4B-NB	2.86	1.41	1.37
24	8	313	CLA	C4B-NB	2.86	1.41	1.37
24	7	316	CLA	C4B-NB	2.86	1.41	1.37
24	A	809	CLA	C4B-NB	2.85	1.41	1.37
25	0	314	8CT	C07-C02	-2.85	1.45	1.51
24	0	304	CLA	C4B-NB	2.85	1.41	1.37
24	1	307	CLA	C4B-NB	2.85	1.41	1.37
25	F	301	8CT	C35-C30	2.85	1.64	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	103	CLA	C4B-NB	2.85	1.41	1.37
24	1	303	CLA	C4B-NB	2.84	1.41	1.37
32	A	852	CL0	C1A-CHA	-2.84	1.36	1.40
24	B	802	CLA	C4B-NB	2.84	1.41	1.37
25	7	318	8CT	C07-C02	-2.84	1.45	1.51
24	B	835	CLA	C4B-NB	2.83	1.41	1.37
24	B	823	CLA	C4B-NB	2.83	1.41	1.37
25	B	850	8CT	C30-C29	2.83	1.54	1.50
24	5	309	CLA	C4B-NB	2.83	1.41	1.37
25	7	318	8CT	C35-C30	2.83	1.64	1.56
25	A	847	8CT	C10-C03	2.83	1.54	1.45
25	B	844	8CT	C30-C29	2.83	1.54	1.50
24	A	853	CLA	C1D-ND	2.83	1.41	1.37
24	3	312	CLA	C4B-NB	2.83	1.41	1.37
25	0	314	8CT	C30-C29	2.82	1.54	1.50
25	B	846	8CT	C07-C02	-2.82	1.45	1.51
24	H	201	CLA	C4B-NB	2.81	1.41	1.37
25	A	846	8CT	C10-C03	2.81	1.54	1.45
24	A	801	CLA	C4B-NB	2.81	1.41	1.37
24	B	809	CLA	C4B-NB	2.81	1.41	1.37
24	B	824	CLA	C4B-NB	2.81	1.41	1.37
24	B	813	CLA	C4B-NB	2.81	1.41	1.37
24	9	302	CLA	C4B-NB	2.80	1.41	1.37
24	K	104	CLA	C4B-NB	2.80	1.41	1.37
24	9	304	CLA	C4B-NB	2.80	1.41	1.37
24	A	805	CLA	C4B-NB	2.80	1.41	1.37
25	6	319	8CT	C30-C29	2.79	1.54	1.50
24	5	310	CLA	C4B-NB	2.79	1.41	1.37
24	B	833	CLA	C4B-NB	2.79	1.41	1.37
24	0	311	CLA	C4B-NB	2.79	1.41	1.37
24	2	303	CLA	C4B-NB	2.79	1.41	1.37
24	3	315	CLA	C4B-NB	2.79	1.41	1.37
24	B	834	CLA	C4B-NB	2.78	1.41	1.37
24	6	303	CLA	C4B-NB	2.78	1.41	1.37
24	0	309	CLA	C4B-NB	2.78	1.41	1.37
25	B	848	8CT	C30-C29	2.78	1.54	1.50
24	7	311	CLA	C4B-NB	2.77	1.41	1.37
24	3	314	CLA	C4B-NB	2.77	1.41	1.37
24	3	311	CLA	C4B-NB	2.77	1.41	1.37
24	7	303	CLA	C4B-NB	2.77	1.41	1.37
24	5	311	CLA	C4B-NB	2.77	1.41	1.37
24	4	310	CLA	C4B-NB	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	303	CLA	C4B-NB	2.76	1.41	1.37
24	B	825	CLA	C4B-NB	2.76	1.41	1.37
24	5	303	CLA	C1B-C2B	2.76	1.49	1.43
25	9	313	8CT	C30-C29	2.76	1.54	1.50
24	B	832	CLA	C4B-NB	2.76	1.41	1.37
24	O	205	CLA	C4B-NB	2.76	1.41	1.37
25	L	205	8CT	C30-C29	2.76	1.54	1.50
24	A	840	CLA	C4B-NB	2.76	1.41	1.37
24	2	309	CLA	C4B-NB	2.76	1.41	1.37
24	1	313	CLA	C4B-NB	2.76	1.41	1.37
24	B	837	CLA	C4B-NB	2.75	1.41	1.37
24	B	841	CLA	C4B-NB	2.75	1.41	1.37
24	J	103	CLA	C4B-NB	2.75	1.41	1.37
24	6	312	CLA	C4B-NB	2.75	1.41	1.37
24	3	306	CLA	C4B-NB	2.75	1.41	1.37
24	L	203	CLA	C4B-NB	2.75	1.41	1.37
24	A	819	CLA	C4B-NB	2.75	1.41	1.37
24	0	308	CLA	C4B-NB	2.75	1.41	1.37
24	6	314	CLA	C4B-NB	2.74	1.41	1.37
24	7	316	CLA	C1B-C2B	2.74	1.49	1.43
25	B	844	8CT	C07-C02	-2.74	1.45	1.51
24	H	204	CLA	C4B-NB	2.74	1.41	1.37
24	A	825	CLA	C4B-NB	2.74	1.41	1.37
24	A	837	CLA	C4B-NB	2.74	1.41	1.37
24	B	805	CLA	C1B-C2B	2.74	1.49	1.43
24	0	312	CLA	C4B-NB	2.74	1.41	1.37
24	4	311	CLA	C4B-NB	2.73	1.41	1.37
24	1	310	CLA	C4B-NB	2.73	1.41	1.37
30	3	319	0IE	C13-C12	-2.73	1.40	1.46
24	H	204	CLA	C1B-C2B	2.73	1.49	1.43
24	8	311	CLA	C4B-NB	2.73	1.41	1.37
24	L	202	CLA	C4B-NB	2.73	1.41	1.37
24	O	206	CLA	C1B-C2B	2.73	1.49	1.43
24	3	310	CLA	C4B-NB	2.72	1.41	1.37
30	7	321	0IE	C13-C12	-2.72	1.40	1.46
24	B	816	CLA	C4B-NB	2.72	1.41	1.37
24	4	312	CLA	C4B-NB	2.72	1.41	1.37
24	B	808	CLA	C4B-NB	2.72	1.41	1.37
25	A	845	8CT	C30-C29	2.72	1.54	1.50
32	A	852	CL0	MG-NB	-2.72	2.00	2.05
24	2	302	CLA	C4B-NB	2.71	1.41	1.37
24	B	821	CLA	C4B-NB	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	828	CLA	C4B-NB	2.71	1.41	1.37
24	7	308	CLA	C4B-NB	2.71	1.41	1.37
24	A	813	CLA	C4B-NB	2.71	1.41	1.37
24	A	821	CLA	C4B-NB	2.71	1.41	1.37
24	G	102	CLA	C4B-NB	2.71	1.41	1.37
24	7	304	CLA	C4B-NB	2.70	1.41	1.37
24	1	309	CLA	C4B-NB	2.70	1.41	1.37
24	K	103	CLA	C4B-NB	2.70	1.41	1.37
24	8	310	CLA	C4B-NB	2.69	1.41	1.37
24	F	303	CLA	C4B-NB	2.69	1.41	1.37
32	A	852	CL0	CHC-C4B	-2.69	1.35	1.39
24	3	303	CLA	C4B-NB	2.69	1.41	1.37
24	4	314	CLA	C4B-NB	2.69	1.41	1.37
24	O	206	CLA	C4B-C3B	2.69	1.49	1.43
24	B	805	CLA	C4B-NB	2.69	1.41	1.37
24	7	315	CLA	C4B-NB	2.69	1.41	1.37
24	B	826	CLA	C4B-NB	2.69	1.41	1.37
24	A	834	CLA	C4B-NB	2.69	1.41	1.37
24	0	310	CLA	C4B-NB	2.68	1.41	1.37
24	B	812	CLA	C4B-NB	2.68	1.41	1.37
24	9	311	CLA	C4B-NB	2.68	1.41	1.37
24	B	820	CLA	C4B-NB	2.68	1.41	1.37
24	8	315	CLA	C4B-NB	2.68	1.41	1.37
25	M	102	8CT	C30-C29	2.68	1.54	1.50
25	F	301	8CT	C30-C29	2.67	1.54	1.50
24	B	831	CLA	C4B-NB	2.67	1.41	1.37
24	4	304	CLA	C4B-NB	2.67	1.41	1.37
24	1	309	CLA	C1B-C2B	2.67	1.49	1.43
27	1	317	LHG	O8-C6	-2.67	1.39	1.45
24	B	821	CLA	C1B-C2B	2.67	1.49	1.43
25	O	208	8CT	C30-C29	2.67	1.54	1.50
24	H	201	CLA	C1B-C2B	2.67	1.49	1.43
24	9	308	CLA	C4B-NB	2.67	1.41	1.37
24	5	307	CLA	C1B-C2B	2.67	1.49	1.43
24	O	201	CLA	C4B-NB	2.66	1.41	1.37
30	3	319	0IE	C17-C16	-2.66	1.40	1.46
25	A	844	8CT	C30-C29	2.66	1.54	1.50
24	B	830	CLA	C4B-NB	2.66	1.41	1.37
24	1	308	CLA	C4B-NB	2.66	1.41	1.37
23	0	306	CHL	CHA-CBD	-2.66	1.48	1.51
24	B	840	CLA	C4B-NB	2.66	1.41	1.37
24	L	203	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	314	CLA	C1B-C2B	2.66	1.49	1.43
24	A	833	CLA	C4B-NB	2.66	1.41	1.37
24	B	838	CLA	C4B-NB	2.66	1.41	1.37
24	0	313	CLA	C1B-C2B	2.65	1.49	1.43
24	B	814	CLA	C4B-NB	2.65	1.41	1.37
24	G	102	CLA	C1B-C2B	2.65	1.49	1.43
24	1	311	CLA	C4B-NB	2.65	1.41	1.37
24	6	314	CLA	C1B-C2B	2.65	1.49	1.43
24	9	307	CLA	C4B-NB	2.65	1.41	1.37
24	B	811	CLA	C4B-NB	2.65	1.41	1.37
24	5	313	CLA	C1B-C2B	2.65	1.49	1.43
24	B	839	CLA	C4B-NB	2.65	1.41	1.37
24	9	307	CLA	C1B-C2B	2.65	1.49	1.43
24	4	304	CLA	C1B-C2B	2.65	1.49	1.43
24	6	303	CLA	C1B-C2B	2.64	1.49	1.43
24	7	309	CLA	C4B-NB	2.64	1.41	1.37
24	5	309	CLA	C1B-C2B	2.64	1.49	1.43
24	A	816	CLA	C4B-NB	2.64	1.41	1.37
24	6	309	CLA	C4B-NB	2.64	1.41	1.37
24	8	315	CLA	C1B-C2B	2.64	1.49	1.43
24	0	312	CLA	C1B-C2B	2.63	1.49	1.43
24	7	317	CLA	C4B-NB	2.63	1.41	1.37
24	0	319	CLA	C1B-C2B	2.63	1.49	1.43
24	0	304	CLA	C1B-C2B	2.63	1.49	1.43
24	K	102	CLA	C4B-NB	2.63	1.41	1.37
24	A	810	CLA	C4B-NB	2.63	1.41	1.37
24	5	311	CLA	C1B-C2B	2.62	1.49	1.43
24	A	839	CLA	C4B-NB	2.62	1.41	1.37
30	7	321	0IE	C17-C16	-2.62	1.40	1.46
24	A	802	CLA	C4B-NB	2.62	1.41	1.37
24	A	830	CLA	C4B-NB	2.62	1.41	1.37
24	0	311	CLA	C1B-C2B	2.62	1.49	1.43
24	A	853	CLA	C4B-NB	2.62	1.41	1.37
24	L	201	CLA	C4B-NB	2.62	1.41	1.37
24	K	103	CLA	C1B-C2B	2.62	1.49	1.43
24	3	315	CLA	C1B-C2B	2.62	1.49	1.43
24	5	310	CLA	C1B-C2B	2.62	1.49	1.43
24	A	818	CLA	C4B-NB	2.62	1.41	1.37
24	B	815	CLA	C4B-NB	2.62	1.41	1.37
24	A	831	CLA	C4B-NB	2.61	1.41	1.37
24	B	807	CLA	C4B-NB	2.61	1.41	1.37
24	3	304	CLA	C4B-NB	2.61	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	305	CLA	C1B-C2B	2.61	1.49	1.43
24	B	804	CLA	C4B-NB	2.61	1.41	1.37
24	3	308	CLA	C4B-NB	2.61	1.41	1.37
24	A	824	CLA	C4B-NB	2.61	1.41	1.37
24	B	819	CLA	C4B-NB	2.61	1.41	1.37
27	7	323	LHG	O7-C5	-2.61	1.40	1.46
24	5	302	CLA	C1B-C2B	2.61	1.49	1.43
24	A	820	CLA	C4B-NB	2.61	1.41	1.37
24	0	308	CLA	C1B-C2B	2.60	1.49	1.43
24	6	318	CLA	C1B-C2B	2.60	1.49	1.43
32	A	852	CL0	CAC-C3C	-2.60	1.47	1.51
24	2	308	CLA	C4B-NB	2.60	1.41	1.37
24	B	817	CLA	C4B-NB	2.60	1.41	1.37
24	L	206	CLA	C1B-C2B	2.60	1.49	1.43
24	A	808	CLA	C4B-NB	2.60	1.41	1.37
24	A	832	CLA	C4B-NB	2.60	1.41	1.37
24	A	828	CLA	C4B-NB	2.59	1.41	1.37
24	1	307	CLA	C1B-C2B	2.59	1.49	1.43
24	3	308	CLA	C1B-C2B	2.59	1.49	1.43
24	2	310	CLA	C1B-C2B	2.59	1.49	1.43
24	O	205	CLA	C1B-C2B	2.59	1.49	1.43
24	2	310	CLA	C4B-NB	2.59	1.41	1.37
24	9	302	CLA	C1B-C2B	2.59	1.49	1.43
24	B	835	CLA	C1B-C2B	2.59	1.49	1.43
24	A	806	CLA	C4B-NB	2.59	1.41	1.37
24	7	311	CLA	C1B-C2B	2.59	1.49	1.43
27	B	851	LHG	O8-C6	-2.59	1.39	1.45
24	A	836	CLA	C4B-NB	2.59	1.41	1.37
24	3	306	CLA	C1B-C2B	2.59	1.49	1.43
24	3	309	CLA	C4B-NB	2.59	1.41	1.37
24	A	803	CLA	C4B-NB	2.59	1.41	1.37
24	A	821	CLA	C1B-C2B	2.59	1.49	1.43
24	A	836	CLA	C1B-C2B	2.59	1.49	1.43
24	B	840	CLA	C1B-C2B	2.58	1.49	1.43
24	0	309	CLA	C1B-C2B	2.58	1.49	1.43
24	A	826	CLA	C4B-NB	2.58	1.41	1.37
24	A	827	CLA	C4B-NB	2.58	1.41	1.37
24	1	311	CLA	C1B-C2B	2.58	1.49	1.43
24	2	303	CLA	C1B-C2B	2.58	1.49	1.43
24	B	801	CLA	C4B-NB	2.58	1.41	1.37
24	B	810	CLA	C4B-NB	2.58	1.41	1.37
24	H	202	CLA	C4B-NB	2.58	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	310	CLA	C1B-C2B	2.58	1.49	1.43
24	B	806	CLA	C4B-NB	2.58	1.41	1.37
24	B	818	CLA	C4B-NB	2.58	1.41	1.37
24	4	311	CLA	C1B-C2B	2.57	1.49	1.43
32	A	852	CL0	MG-ND	-2.57	2.00	2.05
24	B	830	CLA	CMD-C2D	-2.57	1.45	1.50
24	1	313	CLA	C1B-C2B	2.57	1.49	1.43
24	4	314	CLA	C1B-C2B	2.57	1.49	1.43
24	O	204	CLA	C1B-C2B	2.57	1.49	1.43
24	2	311	CLA	C4B-NB	2.57	1.41	1.37
24	7	315	CLA	C1B-C2B	2.57	1.49	1.43
24	A	829	CLA	C4B-NB	2.57	1.41	1.37
24	1	310	CLA	C1B-C2B	2.57	1.49	1.43
24	A	838	CLA	C4B-NB	2.57	1.41	1.37
24	0	303	CLA	C1B-C2B	2.57	1.49	1.43
27	7	323	LHG	C26-C25	-2.57	1.35	1.51
24	A	833	CLA	C1B-C2B	2.57	1.49	1.43
24	H	203	CLA	C1B-C2B	2.57	1.49	1.43
24	3	313	CLA	C1B-C2B	2.56	1.49	1.43
24	B	838	CLA	C1B-C2B	2.56	1.49	1.43
24	G	101	CLA	C1B-C2B	2.56	1.49	1.43
24	4	312	CLA	C1B-C2B	2.56	1.49	1.43
24	6	317	CLA	C1B-C2B	2.56	1.49	1.43
27	A	843	LHG	O8-C6	-2.56	1.39	1.45
24	6	310	CLA	C1B-C2B	2.56	1.49	1.43
24	B	830	CLA	MG-NB	-2.56	2.00	2.05
24	8	304	CLA	C1B-C2B	2.56	1.49	1.43
24	A	823	CLA	C4B-NB	2.56	1.41	1.37
24	2	311	CLA	C1B-C2B	2.55	1.49	1.43
24	2	313	CLA	C1B-C2B	2.55	1.49	1.43
24	8	312	CLA	C1B-C2B	2.55	1.49	1.43
24	9	304	CLA	C1B-C2B	2.55	1.49	1.43
24	4	310	CLA	C1B-C2B	2.55	1.49	1.43
24	A	816	CLA	C1B-C2B	2.55	1.49	1.43
27	2	319	LHG	O7-C5	-2.55	1.40	1.46
24	B	810	CLA	C1B-C2B	2.55	1.49	1.43
24	K	102	CLA	C1B-C2B	2.55	1.49	1.43
24	A	809	CLA	C3B-C4B	2.54	1.50	1.42
27	3	324	LHG	O8-C6	-2.54	1.39	1.45
24	6	309	CLA	C1B-C2B	2.54	1.49	1.43
24	J	103	CLA	C1B-C2B	2.54	1.49	1.43
24	H	205	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	817	CLA	C1B-C2B	2.54	1.49	1.43
24	6	316	CLA	C4B-NB	2.54	1.41	1.37
24	B	834	CLA	C1B-C2B	2.54	1.49	1.43
24	A	815	CLA	C1B-C2B	2.54	1.49	1.43
24	8	311	CLA	C1B-C2B	2.53	1.49	1.43
24	A	807	CLA	C1B-C2B	2.53	1.49	1.43
24	9	309	CLA	C1B-C2B	2.53	1.49	1.43
24	A	817	CLA	C4B-NB	2.53	1.41	1.37
24	F	302	CLA	C1B-C2B	2.53	1.49	1.43
24	8	313	CLA	C1B-C2B	2.53	1.49	1.43
24	H	202	CLA	C1B-C2B	2.53	1.49	1.43
30	7	321	0IE	C6-C7	-2.53	1.40	1.46
24	9	308	CLA	C1B-C2B	2.53	1.49	1.43
24	A	812	CLA	C4B-NB	2.53	1.41	1.37
24	A	813	CLA	C1B-C2B	2.53	1.49	1.43
24	A	827	CLA	C1B-C2B	2.53	1.49	1.43
24	A	835	CLA	C4B-NB	2.53	1.41	1.37
24	3	310	CLA	C1B-C2B	2.52	1.49	1.43
24	B	808	CLA	C1B-C2B	2.52	1.49	1.43
25	7	319	8CT	C30-C29	2.52	1.54	1.50
24	1	303	CLA	C1B-C2B	2.52	1.49	1.43
24	7	308	CLA	C1B-C2B	2.52	1.49	1.43
24	6	304	CLA	CMB-C2B	-2.52	1.45	1.50
24	A	848	CLA	C3B-C4B	2.52	1.50	1.42
24	A	828	CLA	C1B-C2B	2.52	1.49	1.43
24	3	311	CLA	C1B-C2B	2.51	1.49	1.43
24	4	309	CLA	C1B-C2B	2.51	1.49	1.43
24	A	838	CLA	C1B-C2B	2.51	1.49	1.43
24	B	831	CLA	CMD-C2D	-2.51	1.45	1.50
27	2	317	LHG	O8-C6	-2.51	1.39	1.45
27	1	317	LHG	O7-C5	-2.51	1.40	1.46
27	1	318	LHG	O8-C6	-2.51	1.39	1.45
24	A	825	CLA	C1B-C2B	2.51	1.49	1.43
24	A	808	CLA	C1B-C2B	2.51	1.49	1.43
24	L	202	CLA	C1B-C2B	2.51	1.49	1.43
25	3	323	8CT	C30-C29	2.51	1.54	1.50
24	7	304	CLA	C1B-C2B	2.51	1.49	1.43
27	A	842	LHG	O7-C5	-2.50	1.40	1.46
24	B	823	CLA	C1B-C2B	2.50	1.49	1.43
27	A	842	LHG	O8-C6	-2.50	1.39	1.45
24	7	317	CLA	C1B-C2B	2.50	1.49	1.43
27	5	316	LHG	O8-C6	-2.50	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	304	CLA	C1B-C2B	2.50	1.49	1.43
24	B	837	CLA	C1B-C2B	2.50	1.49	1.43
24	K	104	CLA	C1B-C2B	2.50	1.49	1.43
27	2	317	LHG	O7-C5	-2.50	1.40	1.46
24	7	312	CLA	C1B-C2B	2.50	1.49	1.43
24	B	836	CLA	C4B-NB	2.50	1.41	1.37
24	6	311	CLA	C1B-C2B	2.50	1.49	1.43
24	9	311	CLA	C1B-C2B	2.50	1.49	1.43
24	2	302	CLA	C1B-C2B	2.50	1.49	1.43
27	0	317	LHG	O7-C5	-2.49	1.40	1.46
24	0	307	CLA	C1B-C2B	2.49	1.49	1.43
24	B	827	CLA	C1B-C2B	2.49	1.49	1.43
24	2	309	CLA	C1B-C2B	2.49	1.49	1.43
25	A	847	8CT	C33-C32	-2.49	1.43	1.50
27	A	843	LHG	O7-C5	-2.49	1.40	1.46
24	0	310	CLA	C1B-C2B	2.49	1.49	1.43
24	G	103	CLA	C1B-C2B	2.49	1.49	1.43
24	A	814	CLA	C4B-NB	2.49	1.41	1.37
24	6	312	CLA	C1B-C2B	2.49	1.49	1.43
24	A	810	CLA	C1B-C2B	2.49	1.49	1.43
24	O	201	CLA	C1B-C2B	2.49	1.49	1.43
24	B	813	CLA	C3B-C4B	2.49	1.50	1.42
24	A	804	CLA	C3B-C4B	2.49	1.50	1.42
25	I	101	8CT	C30-C29	2.49	1.54	1.50
25	O	202	8CT	C30-C29	2.49	1.54	1.50
30	3	319	0IE	C6-C7	-2.48	1.40	1.46
24	A	840	CLA	C1B-C2B	2.48	1.49	1.43
24	B	824	CLA	C1B-C2B	2.48	1.49	1.43
25	4	316	8CT	C30-C29	2.48	1.54	1.50
24	A	834	CLA	C1B-C2B	2.48	1.49	1.43
24	B	804	CLA	C1B-C2B	2.48	1.48	1.43
24	A	839	CLA	C1B-C2B	2.48	1.48	1.43
24	B	826	CLA	C4D-CHA	2.48	1.43	1.39
24	B	811	CLA	C1B-C2B	2.48	1.48	1.43
24	2	308	CLA	C1B-C2B	2.48	1.48	1.43
24	B	833	CLA	C1B-C2B	2.47	1.48	1.43
24	B	841	CLA	C1B-C2B	2.47	1.48	1.43
27	0	317	LHG	O8-C6	-2.47	1.39	1.45
27	7	322	LHG	O8-C6	-2.47	1.39	1.45
24	3	303	CLA	C1B-C2B	2.47	1.48	1.43
23	6	313	CHL	CBD-CGD	-2.47	1.49	1.52
24	B	816	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	825	CLA	C1B-C2B	2.47	1.48	1.43
24	B	827	CLA	C4B-NB	2.47	1.41	1.37
24	3	312	CLA	C1B-C2B	2.47	1.48	1.43
24	A	822	CLA	C1B-C2B	2.47	1.48	1.43
24	A	835	CLA	C1B-C2B	2.46	1.48	1.43
29	J	105	LMG	O7-C8	-2.46	1.40	1.46
24	9	310	CLA	C3B-C4B	2.46	1.49	1.42
24	B	832	CLA	C1B-C2B	2.46	1.48	1.43
24	B	829	CLA	C3B-C4B	2.46	1.49	1.42
24	A	832	CLA	C1B-C2B	2.46	1.48	1.43
24	K	101	CLA	C1B-C2B	2.46	1.48	1.43
24	O	209	CLA	C1B-C2B	2.46	1.48	1.43
24	4	303	CLA	C1B-C2B	2.46	1.48	1.43
24	A	819	CLA	C1B-C2B	2.46	1.48	1.43
27	2	319	LHG	O8-C6	-2.46	1.39	1.45
27	7	324	LHG	O8-C6	-2.46	1.39	1.45
24	1	308	CLA	C1B-C2B	2.46	1.48	1.43
24	B	840	CLA	CMB-C2B	-2.46	1.45	1.50
24	7	303	CLA	C1B-C2B	2.46	1.48	1.43
24	B	820	CLA	CMB-C2B	-2.46	1.45	1.50
27	9	316	LHG	O8-C6	-2.45	1.39	1.45
24	A	824	CLA	C1B-C2B	2.45	1.48	1.43
24	A	818	CLA	MG-NB	-2.45	2.00	2.05
24	A	802	CLA	C1B-C2B	2.45	1.48	1.43
24	2	303	CLA	CMB-C2B	-2.45	1.45	1.50
24	6	304	CLA	C1B-C2B	2.45	1.48	1.43
24	B	817	CLA	C1B-C2B	2.45	1.48	1.43
24	A	815	CLA	CMB-C2B	-2.45	1.45	1.50
24	6	311	CLA	C3B-C4B	2.45	1.49	1.42
24	A	801	CLA	C1B-C2B	2.45	1.48	1.43
27	3	322	LHG	O7-C5	-2.44	1.40	1.46
24	1	302	CLA	C1B-C2B	2.44	1.48	1.43
24	B	812	CLA	C1B-C2B	2.44	1.48	1.43
24	B	802	CLA	C1B-C2B	2.44	1.48	1.43
24	B	814	CLA	C1B-C2B	2.44	1.48	1.43
24	B	819	CLA	C1B-C2B	2.44	1.48	1.43
25	2	314	8CT	C30-C29	2.44	1.54	1.50
27	6	322	LHG	O8-C6	-2.44	1.39	1.45
24	B	815	CLA	C1B-C2B	2.44	1.48	1.43
27	7	323	LHG	O8-C6	-2.44	1.39	1.45
24	B	836	CLA	C1B-C2B	2.44	1.48	1.43
24	F	303	CLA	C1B-C2B	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	I	102	LHG	O7-C5	-2.43	1.40	1.46
24	B	818	CLA	C1B-C2B	2.43	1.48	1.43
24	B	801	CLA	C1B-C2B	2.43	1.48	1.43
24	A	814	CLA	C1B-C2B	2.43	1.48	1.43
27	7	322	LHG	O7-C5	-2.43	1.40	1.46
24	A	835	CLA	MG-NB	-2.43	2.01	2.05
24	A	822	CLA	CMB-C2B	-2.43	1.45	1.50
24	A	807	CLA	C4B-NB	2.43	1.41	1.37
27	B	852	LHG	O8-C23	2.43	1.40	1.33
24	9	303	CLA	C1B-C2B	2.42	1.48	1.43
24	A	823	CLA	C1B-C2B	2.42	1.48	1.43
24	A	808	CLA	MG-NB	-2.42	2.01	2.05
24	B	812	CLA	CMB-C2B	-2.42	1.45	1.50
24	A	817	CLA	MG-NB	-2.42	2.01	2.05
27	3	320	LHG	O7-C5	-2.42	1.40	1.46
24	A	840	CLA	CMD-C2D	-2.42	1.45	1.50
24	9	310	CLA	C1B-C2B	2.42	1.48	1.43
27	8	320	LHG	O8-C6	-2.42	1.39	1.45
24	7	309	CLA	C1B-C2B	2.42	1.48	1.43
24	8	310	CLA	C1B-C2B	2.42	1.48	1.43
24	B	826	CLA	C1B-C2B	2.42	1.48	1.43
27	8	320	LHG	O7-C5	-2.42	1.40	1.46
24	B	831	CLA	MG-NB	-2.42	2.01	2.05
24	B	828	CLA	C1B-C2B	2.42	1.48	1.43
24	A	831	CLA	C1B-C2B	2.41	1.48	1.43
27	A	850	LHG	O8-C6	-2.41	1.39	1.45
23	3	301	CHL	CBD-CGD	-2.41	1.49	1.52
24	2	313	CLA	CMD-C2D	-2.41	1.45	1.50
27	3	324	LHG	O7-C5	-2.41	1.40	1.46
24	A	803	CLA	C1B-C2B	2.41	1.48	1.43
24	A	805	CLA	C1B-C2B	2.41	1.48	1.43
24	A	830	CLA	C1B-C2B	2.41	1.48	1.43
24	B	822	CLA	C1B-C2B	2.41	1.48	1.43
25	O	202	8CT	C33-C32	-2.41	1.43	1.50
24	A	829	CLA	MG-NB	-2.41	2.01	2.05
24	A	853	CLA	MG-NB	-2.41	2.01	2.05
24	A	822	CLA	CMD-C2D	-2.41	1.45	1.50
24	B	823	CLA	CMD-C2D	-2.40	1.45	1.50
24	B	809	CLA	C1B-C2B	2.40	1.48	1.43
24	A	840	CLA	MG-NB	-2.40	2.01	2.05
24	3	314	CLA	C1B-C2B	2.40	1.48	1.43
24	4	309	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	829	CLA	CMD-C2D	-2.40	1.45	1.50
24	A	820	CLA	MG-NB	-2.40	2.01	2.05
27	L	208	LHG	O7-C5	-2.40	1.41	1.46
24	5	307	CLA	C3B-C4B	2.40	1.49	1.42
27	3	322	LHG	O8-C6	-2.40	1.39	1.45
24	A	812	CLA	C1B-C2B	2.40	1.48	1.43
24	B	831	CLA	C1B-C2B	2.39	1.48	1.43
24	A	826	CLA	C1B-C2B	2.39	1.48	1.43
24	H	202	CLA	MG-NB	-2.39	2.01	2.05
24	A	811	CLA	C3B-C4B	2.39	1.49	1.42
24	B	813	CLA	C1B-C2B	2.39	1.48	1.43
27	1	318	LHG	O7-C5	-2.39	1.41	1.46
24	B	836	CLA	MG-NB	-2.39	2.01	2.05
24	A	837	CLA	C1B-C2B	2.39	1.48	1.43
24	B	839	CLA	C1B-C2B	2.38	1.48	1.43
25	K	105	8CT	C33-C32	-2.38	1.43	1.50
27	3	320	LHG	O8-C6	-2.38	1.39	1.45
24	0	307	CLA	C3B-C4B	2.38	1.49	1.42
27	B	852	LHG	O7-C5	-2.38	1.41	1.46
24	B	824	CLA	CMD-C2D	-2.38	1.45	1.50
24	A	837	CLA	C3B-C4B	2.38	1.49	1.42
27	A	850	LHG	O7-C7	2.38	1.41	1.34
25	B	845	8CT	C30-C29	2.38	1.54	1.50
24	A	820	CLA	C1B-C2B	2.38	1.48	1.43
24	B	806	CLA	C1B-C2B	2.38	1.48	1.43
25	J	104	8CT	C33-C32	-2.38	1.43	1.50
24	2	302	CLA	CMB-C2B	-2.38	1.45	1.50
24	B	819	CLA	MG-NB	-2.38	2.01	2.05
24	6	316	CLA	C1B-C2B	2.37	1.48	1.43
25	7	318	8CT	C30-C29	2.37	1.53	1.50
29	2	318	LMG	O7-C8	-2.37	1.41	1.46
25	7	319	8CT	C33-C32	-2.37	1.43	1.50
24	A	840	CLA	CMB-C2B	-2.37	1.45	1.50
27	8	302	LHG	O7-C5	-2.37	1.41	1.46
24	7	317	CLA	MG-NB	-2.37	2.01	2.05
24	B	807	CLA	C3B-C4B	2.37	1.49	1.42
24	1	302	CLA	C3B-C4B	2.37	1.49	1.42
24	A	831	CLA	MG-NB	-2.37	2.01	2.05
24	A	828	CLA	CMD-C2D	-2.37	1.45	1.50
24	L	201	CLA	MG-NB	-2.37	2.01	2.05
27	9	316	LHG	O7-C5	-2.37	1.41	1.46
24	6	303	CLA	CMB-C2B	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	804	CLA	CMC-C2C	-2.36	1.45	1.50
24	A	818	CLA	CMB-C2B	-2.36	1.45	1.50
24	F	303	CLA	MG-NB	-2.36	2.01	2.05
24	3	309	CLA	C3B-C4B	2.36	1.49	1.42
24	9	311	CLA	MG-NB	-2.36	2.01	2.05
24	B	818	CLA	MG-NB	-2.36	2.01	2.05
24	O	206	CLA	CHC-C1C	2.36	1.43	1.38
24	2	310	CLA	MG-NB	-2.36	2.01	2.05
24	A	826	CLA	CMC-C2C	-2.36	1.45	1.50
24	A	806	CLA	CMB-C2B	-2.36	1.45	1.50
27	5	316	LHG	O7-C5	-2.35	1.41	1.46
24	A	824	CLA	MG-NB	-2.35	2.01	2.05
27	6	322	LHG	O7-C5	-2.35	1.41	1.46
24	B	841	CLA	MG-NB	-2.35	2.01	2.05
24	A	804	CLA	C1B-C2B	2.35	1.48	1.43
24	B	838	CLA	MG-NB	-2.35	2.01	2.05
25	3	323	8CT	C33-C32	-2.35	1.44	1.50
27	L	208	LHG	O8-C6	-2.35	1.39	1.45
24	O	209	CLA	C3B-C4B	2.35	1.49	1.42
24	5	313	CLA	C3B-C4B	2.35	1.49	1.42
24	A	836	CLA	MG-NB	-2.35	2.01	2.05
24	A	848	CLA	CMD-C2D	-2.35	1.46	1.50
24	6	303	CLA	MG-NB	-2.35	2.01	2.05
24	A	826	CLA	MG-NB	-2.34	2.01	2.05
24	A	806	CLA	MG-NB	-2.34	2.01	2.05
24	9	309	CLA	C3B-C4B	2.34	1.49	1.42
24	4	309	CLA	CHC-C1C	2.34	1.43	1.38
24	A	806	CLA	C1B-C2B	2.34	1.48	1.43
27	I	102	LHG	O8-C6	-2.34	1.39	1.45
24	B	831	CLA	CMB-C2B	-2.34	1.46	1.50
24	B	827	CLA	MG-NB	-2.34	2.01	2.05
24	O	205	CLA	MG-NB	-2.34	2.01	2.05
24	B	806	CLA	CHC-C1C	2.34	1.43	1.38
24	5	308	CLA	C3B-C4B	2.34	1.49	1.42
24	8	312	CLA	C3B-C4B	2.34	1.49	1.42
25	4	316	8CT	C33-C32	-2.34	1.44	1.50
24	A	804	CLA	CHC-C1C	2.34	1.43	1.38
25	L	207	8CT	C33-C32	-2.34	1.44	1.50
27	B	852	LHG	O8-C6	-2.34	1.39	1.45
24	B	807	CLA	C1B-C2B	2.34	1.48	1.43
24	3	303	CLA	CMD-C2D	-2.34	1.46	1.50
24	A	853	CLA	CMB-C2B	-2.34	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	805	CLA	CMD-C2D	-2.34	1.46	1.50
24	B	820	CLA	MG-NB	-2.34	2.01	2.05
23	8	309	CHL	CBD-CGD	-2.34	1.49	1.52
24	A	838	CLA	MG-NB	-2.34	2.01	2.05
24	4	303	CLA	MG-NB	-2.34	2.01	2.05
24	A	808	CLA	CMD-C2D	-2.33	1.46	1.50
24	B	810	CLA	MG-NB	-2.33	2.01	2.05
25	F	304	8CT	C33-C32	-2.33	1.44	1.50
25	G	104	8CT	C33-C32	-2.33	1.44	1.50
25	L	204	8CT	C33-C32	-2.33	1.44	1.50
24	3	308	CLA	CMD-C2D	-2.33	1.46	1.50
24	A	805	CLA	MG-NB	-2.33	2.01	2.05
24	5	308	CLA	C1B-C2B	2.33	1.48	1.43
27	B	851	LHG	O7-C7	2.33	1.40	1.34
27	3	320	LHG	O8-C23	2.33	1.40	1.33
27	L	208	LHG	O8-C23	2.33	1.40	1.33
24	1	308	CLA	C3B-C4B	2.33	1.49	1.42
25	B	848	8CT	C33-C32	-2.33	1.44	1.50
27	8	302	LHG	O8-C6	-2.33	1.40	1.45
24	L	202	CLA	MG-NB	-2.33	2.01	2.05
24	A	830	CLA	CMB-C2B	-2.32	1.46	1.50
24	B	811	CLA	CMD-C2D	-2.32	1.46	1.50
25	M	102	8CT	C33-C32	-2.32	1.44	1.50
24	3	314	CLA	MG-NB	-2.32	2.01	2.05
23	2	305	CHL	CBD-CGD	-2.32	1.49	1.52
25	B	847	8CT	C33-C32	-2.32	1.44	1.50
32	A	852	CL0	C3B-C2B	-2.32	1.37	1.40
24	4	312	CLA	MG-NB	-2.32	2.01	2.05
24	A	830	CLA	MG-NB	-2.32	2.01	2.05
24	7	303	CLA	CMD-C2D	-2.32	1.46	1.50
24	A	809	CLA	CMB-C2B	-2.32	1.46	1.50
24	H	205	CLA	C3B-C4B	2.32	1.49	1.42
27	A	850	LHG	O8-C23	2.32	1.40	1.33
24	A	803	CLA	C3B-C4B	2.32	1.49	1.42
23	5	301	CHL	CBD-CGD	-2.32	1.49	1.52
24	7	309	CLA	MG-NB	-2.32	2.01	2.05
24	B	818	CLA	CMC-C2C	-2.32	1.46	1.50
24	L	201	CLA	C1B-C2B	2.32	1.48	1.43
24	L	206	CLA	C3B-C4B	2.32	1.49	1.42
24	7	303	CLA	MG-NB	-2.32	2.01	2.05
24	A	828	CLA	MG-NB	-2.32	2.01	2.05
25	2	314	8CT	C33-C32	-2.32	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	809	CLA	C1B-C2B	2.32	1.48	1.43
24	5	308	CLA	MG-NB	-2.32	2.01	2.05
24	B	819	CLA	CMB-C2B	-2.32	1.46	1.50
24	3	312	CLA	CMB-C2B	-2.32	1.46	1.50
24	B	832	CLA	MG-NB	-2.32	2.01	2.05
24	B	820	CLA	C1B-C2B	2.32	1.48	1.43
24	B	827	CLA	CMC-C2C	-2.31	1.46	1.50
25	A	847	8CT	C30-C29	2.31	1.53	1.50
24	2	309	CLA	MG-NB	-2.31	2.01	2.05
27	5	316	LHG	O7-C7	2.31	1.40	1.34
24	A	801	CLA	CMD-C2D	-2.31	1.46	1.50
24	F	302	CLA	C3B-C4B	2.31	1.49	1.42
24	B	812	CLA	MG-NB	-2.31	2.01	2.05
24	0	303	CLA	C3B-C4B	2.31	1.49	1.42
24	0	303	CLA	CMD-C2D	-2.31	1.46	1.50
24	A	825	CLA	CMD-C2D	-2.31	1.46	1.50
24	A	814	CLA	MG-NB	-2.31	2.01	2.05
25	3	317	8CT	C33-C32	-2.31	1.44	1.50
24	7	304	CLA	CMB-C2B	-2.31	1.46	1.50
24	K	102	CLA	MG-NB	-2.31	2.01	2.05
23	7	305	CHL	CBD-CGD	-2.31	1.49	1.52
24	2	308	CLA	CMC-C2C	-2.31	1.46	1.50
24	A	815	CLA	CMD-C2D	-2.31	1.46	1.50
24	B	822	CLA	C3B-C4B	2.31	1.49	1.42
24	6	317	CLA	C3B-C4B	2.31	1.49	1.42
24	7	315	CLA	MG-NB	-2.31	2.01	2.05
24	B	829	CLA	CMB-C2B	-2.31	1.46	1.50
24	K	101	CLA	C3B-C4B	2.31	1.49	1.42
24	6	314	CLA	MG-NB	-2.31	2.01	2.05
24	7	304	CLA	MG-NB	-2.31	2.01	2.05
24	6	312	CLA	MG-NB	-2.31	2.01	2.05
27	7	324	LHG	O7-C7	2.31	1.40	1.34
24	A	811	CLA	C1B-C2B	2.30	1.48	1.43
24	A	811	CLA	CMB-C2B	-2.30	1.46	1.50
24	B	815	CLA	CMD-C2D	-2.30	1.46	1.50
24	B	839	CLA	MG-NB	-2.30	2.01	2.05
24	9	308	CLA	C3B-C4B	2.30	1.49	1.42
24	B	823	CLA	CMB-C2B	-2.30	1.46	1.50
24	6	310	CLA	C3B-C4B	2.30	1.49	1.42
24	6	316	CLA	MG-NB	-2.30	2.01	2.05
24	A	822	CLA	MG-NB	-2.30	2.01	2.05
24	B	824	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	820	CLA	CMD-C2D	-2.30	1.46	1.50
24	7	312	CLA	C3B-C4B	2.30	1.49	1.42
23	8	301	CHL	CBD-CGD	-2.30	1.49	1.52
24	H	203	CLA	C3B-C4B	2.30	1.49	1.42
24	A	848	CLA	C1B-C2B	2.30	1.48	1.43
24	2	302	CLA	CMC-C2C	-2.30	1.46	1.50
25	A	844	8CT	C33-C32	-2.30	1.44	1.50
24	A	812	CLA	C3B-C4B	2.30	1.49	1.42
24	2	310	CLA	CMC-C2C	-2.29	1.46	1.50
24	A	839	CLA	CMB-C2B	-2.29	1.46	1.50
25	6	319	8CT	C33-C32	-2.29	1.44	1.50
24	A	802	CLA	MG-NB	-2.29	2.01	2.05
24	O	201	CLA	MG-NB	-2.29	2.01	2.05
24	B	829	CLA	C1B-C2B	2.29	1.48	1.43
24	7	317	CLA	CMB-C2B	-2.29	1.46	1.50
24	7	314	CLA	C3B-C4B	2.29	1.49	1.42
24	3	309	CLA	MG-NB	-2.29	2.01	2.05
24	A	823	CLA	MG-NB	-2.29	2.01	2.05
27	8	320	LHG	O8-C23	2.29	1.40	1.33
24	3	306	CLA	C3B-C4B	2.29	1.49	1.42
24	8	312	CLA	CHC-C1C	2.29	1.43	1.38
24	3	312	CLA	MG-NB	-2.29	2.01	2.05
23	6	307	CHL	CBD-CGD	-2.29	1.49	1.52
23	9	301	CHL	CBD-CGD	-2.29	1.49	1.52
27	8	302	LHG	O8-C23	2.29	1.40	1.33
24	2	303	CLA	MG-NB	-2.29	2.01	2.05
24	B	814	CLA	C3B-C4B	2.29	1.49	1.42
24	A	832	CLA	MG-NB	-2.29	2.01	2.05
24	4	311	CLA	CMD-C2D	-2.29	1.46	1.50
24	8	310	CLA	C3B-C4B	2.29	1.49	1.42
24	B	808	CLA	CMD-C2D	-2.29	1.46	1.50
24	8	313	CLA	C3B-C4B	2.29	1.49	1.42
27	3	320	LHG	O7-C7	2.29	1.40	1.34
24	9	303	CLA	MG-NB	-2.29	2.01	2.05
27	3	324	LHG	O8-C23	2.29	1.40	1.33
24	3	308	CLA	MG-NB	-2.29	2.01	2.05
24	A	816	CLA	MG-NB	-2.29	2.01	2.05
24	B	833	CLA	CMB-C2B	-2.29	1.46	1.50
24	B	814	CLA	MG-NB	-2.29	2.01	2.05
27	8	320	LHG	O7-C7	2.29	1.40	1.34
27	7	324	LHG	O7-C5	-2.29	1.41	1.46
24	8	310	CLA	MG-NB	-2.29	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	308	CHL	CBD-CGD	-2.29	1.49	1.52
24	0	311	CLA	C3B-C4B	2.29	1.49	1.42
27	7	322	LHG	O8-C23	2.29	1.40	1.33
23	8	303	CHL	CBD-CGD	-2.28	1.49	1.52
24	A	804	CLA	CMB-C2B	-2.28	1.46	1.50
24	0	309	CLA	MG-NB	-2.28	2.01	2.05
24	A	807	CLA	MG-NB	-2.28	2.01	2.05
24	A	839	CLA	MG-NB	-2.28	2.01	2.05
24	K	104	CLA	MG-NB	-2.28	2.01	2.05
24	0	313	CLA	C3B-C4B	2.28	1.49	1.42
24	3	304	CLA	CMB-C2B	-2.28	1.46	1.50
24	9	303	CLA	CMD-C2D	-2.28	1.46	1.50
23	7	306	CHL	CBD-CGD	-2.28	1.49	1.52
24	A	853	CLA	CHC-C1C	2.28	1.43	1.38
24	B	809	CLA	MG-NB	-2.28	2.01	2.05
24	7	303	CLA	C3B-C4B	2.28	1.49	1.42
24	4	310	CLA	CMC-C2C	-2.28	1.46	1.50
24	6	317	CLA	MG-NB	-2.28	2.01	2.05
24	A	822	CLA	C3B-C4B	2.28	1.49	1.42
23	7	302	CHL	CBD-CGD	-2.28	1.49	1.52
24	A	834	CLA	MG-NB	-2.28	2.01	2.05
24	B	806	CLA	CMC-C2C	-2.28	1.46	1.50
24	A	811	CLA	CHC-C1C	2.28	1.43	1.38
24	K	103	CLA	MG-NB	-2.28	2.01	2.05
24	2	309	CLA	C3B-C4B	2.28	1.49	1.42
24	0	308	CLA	C3B-C4B	2.28	1.49	1.42
24	B	806	CLA	MG-NB	-2.28	2.01	2.05
24	0	307	CLA	CMB-C2B	-2.28	1.46	1.50
27	7	323	LHG	O8-C23	2.28	1.40	1.33
24	B	826	CLA	MG-NB	-2.28	2.01	2.05
24	A	830	CLA	CMD-C2D	-2.28	1.46	1.50
24	3	309	CLA	CHC-C1C	2.28	1.43	1.38
24	J	103	CLA	C3B-C4B	2.28	1.49	1.42
24	1	313	CLA	MG-NB	-2.28	2.01	2.05
24	A	813	CLA	MG-NB	-2.28	2.01	2.05
24	B	839	CLA	CMD-C2D	-2.28	1.46	1.50
24	8	311	CLA	C3B-C4B	2.28	1.49	1.42
24	B	802	CLA	MG-NB	-2.28	2.01	2.05
27	L	208	LHG	O7-C7	2.28	1.40	1.34
24	1	302	CLA	CMD-C2D	-2.28	1.46	1.50
24	2	311	CLA	MG-NB	-2.28	2.01	2.05
24	A	839	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	804	CLA	CMD-C2D	-2.27	1.46	1.50
24	A	853	CLA	C3B-C4B	2.27	1.49	1.42
24	B	840	CLA	CMD-C2D	-2.27	1.46	1.50
24	1	303	CLA	C3B-C4B	2.27	1.49	1.42
24	B	809	CLA	C3B-C4B	2.27	1.49	1.42
24	A	811	CLA	MG-NB	-2.27	2.01	2.05
24	0	308	CLA	CHC-C1C	2.27	1.43	1.38
24	B	824	CLA	C3B-C4B	2.27	1.49	1.42
24	A	810	CLA	CMD-C2D	-2.27	1.46	1.50
24	B	815	CLA	C3B-C4B	2.27	1.49	1.42
24	5	313	CLA	CHC-C1C	2.27	1.43	1.38
24	B	841	CLA	C3B-C4B	2.27	1.49	1.42
24	B	833	CLA	MG-NB	-2.27	2.01	2.05
24	A	818	CLA	C3B-C4B	2.27	1.49	1.42
24	0	319	CLA	MG-NB	-2.27	2.01	2.05
24	B	829	CLA	CHC-C1C	2.27	1.43	1.38
24	6	318	CLA	CMD-C2D	-2.27	1.46	1.50
24	A	840	CLA	CMC-C2C	-2.27	1.46	1.50
24	A	853	CLA	CMD-C2D	-2.27	1.46	1.50
24	A	811	CLA	CMD-C2D	-2.27	1.46	1.50
24	B	814	CLA	CMC-C2C	-2.27	1.46	1.50
24	0	309	CLA	C3B-C4B	2.27	1.49	1.42
24	8	304	CLA	C3B-C4B	2.27	1.49	1.42
24	A	834	CLA	C3B-C4B	2.27	1.49	1.42
24	B	834	CLA	CMD-C2D	-2.27	1.46	1.50
24	7	309	CLA	C3B-C4B	2.27	1.49	1.42
23	2	307	CHL	CBD-CGD	-2.26	1.49	1.52
24	4	310	CLA	C3B-C4B	2.26	1.49	1.42
24	L	203	CLA	MG-NB	-2.26	2.01	2.05
24	2	303	CLA	CMD-C2D	-2.26	1.46	1.50
24	0	304	CLA	MG-NB	-2.26	2.01	2.05
24	8	304	CLA	CMB-C2B	-2.26	1.46	1.50
24	K	101	CLA	MG-NB	-2.26	2.01	2.05
24	7	310	CLA	C3B-C4B	2.26	1.49	1.42
24	8	305	CLA	C3B-C4B	2.26	1.49	1.42
24	K	101	CLA	CMD-C2D	-2.26	1.46	1.50
24	5	303	CLA	C3B-C4B	2.26	1.49	1.42
24	B	806	CLA	C3B-C4B	2.26	1.49	1.42
24	9	303	CLA	C3B-C4B	2.26	1.49	1.42
24	O	205	CLA	C3B-C4B	2.26	1.49	1.42
24	5	313	CLA	CMD-C2D	-2.26	1.46	1.50
24	7	314	CLA	CMC-C2C	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	314	CLA	C3B-C4B	2.26	1.49	1.42
24	A	825	CLA	MG-NB	-2.26	2.01	2.05
24	2	308	CLA	CHC-C1C	2.26	1.43	1.38
24	A	806	CLA	C3B-C4B	2.26	1.49	1.42
23	6	308	CHL	CBD-CGD	-2.26	1.49	1.52
24	G	103	CLA	C3B-C4B	2.26	1.49	1.42
24	2	308	CLA	MG-NB	-2.26	2.01	2.05
24	A	834	CLA	CMB-C2B	-2.26	1.46	1.50
24	0	304	CLA	CMB-C2B	-2.26	1.46	1.50
24	A	812	CLA	CMB-C2B	-2.26	1.46	1.50
24	A	812	CLA	CMC-C2C	-2.26	1.46	1.50
24	A	825	CLA	C3B-C4B	2.26	1.49	1.42
24	B	841	CLA	CHC-C1C	2.26	1.43	1.38
24	3	310	CLA	CMB-C2B	-2.26	1.46	1.50
24	0	308	CLA	MG-NB	-2.26	2.01	2.05
27	7	322	LHG	O7-C7	2.26	1.40	1.34
24	5	302	CLA	MG-NB	-2.26	2.01	2.05
25	B	844	8CT	C33-C32	-2.26	1.44	1.50
24	A	812	CLA	MG-NB	-2.26	2.01	2.05
24	O	204	CLA	MG-NB	-2.26	2.01	2.05
24	A	801	CLA	CMB-C2B	-2.26	1.46	1.50
24	3	310	CLA	MG-NB	-2.26	2.01	2.05
24	O	205	CLA	CHC-C1C	2.26	1.43	1.38
24	1	308	CLA	CHC-C1C	2.26	1.43	1.38
24	9	303	CLA	CMB-C2B	-2.25	1.46	1.50
25	B	845	8CT	C33-C32	-2.25	1.44	1.50
24	A	833	CLA	MG-NB	-2.25	2.01	2.05
23	4	315	CHL	CBD-CGD	-2.25	1.49	1.52
24	6	304	CLA	MG-NB	-2.25	2.01	2.05
24	A	827	CLA	MG-NB	-2.25	2.01	2.05
24	9	310	CLA	CHC-C1C	2.25	1.43	1.38
24	4	310	CLA	MG-NB	-2.25	2.01	2.05
24	1	311	CLA	CMD-C2D	-2.25	1.46	1.50
24	6	303	CLA	CMC-C2C	-2.25	1.46	1.50
24	G	102	CLA	MG-NB	-2.25	2.01	2.05
24	G	101	CLA	CHC-C1C	2.25	1.43	1.38
25	A	846	8CT	C33-C32	-2.25	1.44	1.50
24	6	309	CLA	C3B-C4B	2.25	1.49	1.42
24	A	833	CLA	CMB-C2B	-2.25	1.46	1.50
24	3	303	CLA	MG-NB	-2.25	2.01	2.05
24	B	824	CLA	CHC-C1C	2.25	1.43	1.38
25	B	846	8CT	C33-C32	-2.25	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	324	LHG	O8-C23	2.25	1.39	1.33
24	5	308	CLA	CMB-C2B	-2.25	1.46	1.50
24	O	209	CLA	CHC-C1C	2.25	1.43	1.38
24	G	103	CLA	MG-NB	-2.25	2.01	2.05
27	I	102	LHG	O8-C23	2.25	1.39	1.33
24	B	828	CLA	MG-NB	-2.25	2.01	2.05
24	G	101	CLA	MG-NB	-2.25	2.01	2.05
24	H	201	CLA	MG-NB	-2.25	2.01	2.05
27	1	318	LHG	O8-C23	2.25	1.39	1.33
24	3	314	CLA	CMD-C2D	-2.25	1.46	1.50
24	B	834	CLA	CMB-C2B	-2.25	1.46	1.50
24	9	308	CLA	CHC-C1C	2.25	1.43	1.38
24	A	819	CLA	CMD-C2D	-2.25	1.46	1.50
24	7	308	CLA	MG-NB	-2.25	2.01	2.05
24	4	311	CLA	MG-NB	-2.25	2.01	2.05
24	1	310	CLA	C3B-C4B	2.25	1.49	1.42
24	0	307	CLA	MG-NB	-2.25	2.01	2.05
24	A	801	CLA	MG-NB	-2.25	2.01	2.05
24	B	811	CLA	CMB-C2B	-2.25	1.46	1.50
24	B	826	CLA	C3B-C4B	2.25	1.49	1.42
24	5	308	CLA	CHC-C1C	2.25	1.43	1.38
24	7	308	CLA	CMD-C2D	-2.25	1.46	1.50
24	H	201	CLA	CMD-C2D	-2.25	1.46	1.50
24	7	311	CLA	CMB-C2B	-2.25	1.46	1.50
24	4	311	CLA	CMC-C2C	-2.25	1.46	1.50
24	8	312	CLA	MG-NB	-2.25	2.01	2.05
24	5	302	CLA	CMD-C2D	-2.25	1.46	1.50
24	A	826	CLA	CMD-C2D	-2.25	1.46	1.50
24	K	102	CLA	CMD-C2D	-2.25	1.46	1.50
24	3	313	CLA	C3B-C4B	2.25	1.49	1.42
27	8	302	LHG	O7-C7	2.25	1.40	1.34
24	0	303	CLA	MG-NB	-2.25	2.01	2.05
24	5	309	CLA	MG-NB	-2.25	2.01	2.05
24	A	809	CLA	CHC-C1C	2.24	1.43	1.38
24	3	309	CLA	CMB-C2B	-2.24	1.46	1.50
24	3	313	CLA	MG-NB	-2.24	2.01	2.05
27	9	316	LHG	O7-C7	2.24	1.40	1.34
27	A	850	LHG	O7-C5	-2.24	1.41	1.46
24	9	304	CLA	MG-NB	-2.24	2.01	2.05
24	A	810	CLA	CMB-C2B	-2.24	1.46	1.50
23	3	302	CHL	CBD-CGD	-2.24	1.49	1.52
24	O	204	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	316	LHG	O8-C23	2.24	1.39	1.33
23	2	306	CHL	CBD-CGD	-2.24	1.49	1.52
24	B	833	CLA	CHC-C1C	2.24	1.43	1.38
24	0	310	CLA	CMB-C2B	-2.24	1.46	1.50
24	6	312	CLA	CMD-C2D	-2.24	1.46	1.50
24	A	802	CLA	CMD-C2D	-2.24	1.46	1.50
24	5	310	CLA	MG-NB	-2.24	2.01	2.05
24	B	811	CLA	CMC-C2C	-2.24	1.46	1.50
24	4	303	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	825	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	832	CLA	CMB-C2B	-2.24	1.46	1.50
24	3	312	CLA	C3B-C4B	2.24	1.49	1.42
24	7	311	CLA	C3B-C4B	2.24	1.49	1.42
24	A	831	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	823	CLA	MG-NB	-2.24	2.01	2.05
24	A	805	CLA	CMD-C2D	-2.24	1.46	1.50
24	B	811	CLA	MG-NB	-2.24	2.01	2.05
24	A	826	CLA	C3B-C4B	2.24	1.49	1.42
24	2	302	CLA	MG-NB	-2.24	2.01	2.05
24	7	312	CLA	MG-NB	-2.24	2.01	2.05
24	B	808	CLA	MG-NB	-2.24	2.01	2.05
24	7	311	CLA	CMC-C2C	-2.24	1.46	1.50
24	A	816	CLA	CMD-C2D	-2.24	1.46	1.50
24	A	805	CLA	C3B-C4B	2.24	1.49	1.42
24	B	825	CLA	C3B-C4B	2.24	1.49	1.42
27	A	843	LHG	O7-C7	2.24	1.40	1.34
24	6	318	CLA	MG-NB	-2.24	2.01	2.05
24	B	804	CLA	CHC-C1C	2.24	1.43	1.38
24	4	314	CLA	MG-NB	-2.24	2.01	2.05
24	1	303	CLA	MG-NB	-2.24	2.01	2.05
24	1	307	CLA	C3B-C4B	2.24	1.49	1.42
24	A	833	CLA	CMD-C2D	-2.23	1.46	1.50
24	3	310	CLA	C3B-C4B	2.23	1.49	1.42
23	2	304	CHL	CBD-CGD	-2.23	1.49	1.52
27	6	322	LHG	O7-C7	2.23	1.40	1.34
24	A	805	CLA	CHC-C1C	2.23	1.43	1.38
24	2	302	CLA	C3B-C4B	2.23	1.49	1.42
24	B	801	CLA	MG-NB	-2.23	2.01	2.05
24	A	839	CLA	CMD-C2D	-2.23	1.46	1.50
24	2	313	CLA	C3B-C4B	2.23	1.49	1.42
24	7	310	CLA	MG-NB	-2.23	2.01	2.05
24	A	813	CLA	CMB-C2B	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	833	CLA	CMC-C2C	-2.23	1.46	1.50
24	K	104	CLA	C3B-C4B	2.23	1.49	1.42
24	A	831	CLA	CMB-C2B	-2.23	1.46	1.50
24	B	810	CLA	CMD-C2D	-2.23	1.46	1.50
24	K	101	CLA	CHC-C1C	2.23	1.43	1.38
24	0	312	CLA	MG-NB	-2.23	2.01	2.05
24	B	805	CLA	MG-NB	-2.23	2.01	2.05
24	B	835	CLA	MG-NB	-2.23	2.01	2.05
24	7	304	CLA	CMD-C2D	-2.23	1.46	1.50
24	K	103	CLA	CMD-C2D	-2.23	1.46	1.50
25	A	845	8CT	C33-C32	-2.23	1.44	1.50
24	A	834	CLA	CMD-C2D	-2.23	1.46	1.50
24	B	814	CLA	CMD-C2D	-2.23	1.46	1.50
24	B	837	CLA	C3B-C4B	2.23	1.49	1.42
24	8	310	CLA	CMD-C2D	-2.23	1.46	1.50
24	A	814	CLA	CMD-C2D	-2.23	1.46	1.50
24	A	837	CLA	CMB-C2B	-2.23	1.46	1.50
24	0	319	CLA	C3B-C4B	2.23	1.49	1.42
23	7	307	CHL	CBD-CGD	-2.23	1.49	1.52
24	G	102	CLA	C3B-C4B	2.23	1.49	1.42
24	B	826	CLA	CHC-C1C	2.23	1.42	1.38
24	B	801	CLA	CMD-C2D	-2.23	1.46	1.50
24	F	303	CLA	C3B-C4B	2.23	1.49	1.42
24	5	311	CLA	MG-NB	-2.23	2.01	2.05
24	6	311	CLA	CMD-C2D	-2.23	1.46	1.50
23	4	305	CHL	CBD-CGD	-2.22	1.49	1.52
24	B	826	CLA	C3D-C4D	2.22	1.47	1.42
24	G	102	CLA	CMD-C2D	-2.22	1.46	1.50
24	A	848	CLA	MG-NB	-2.22	2.01	2.05
24	B	825	CLA	MG-NB	-2.22	2.01	2.05
24	9	311	CLA	CHC-C1C	2.22	1.42	1.38
24	7	309	CLA	CMD-C2D	-2.22	1.46	1.50
24	A	823	CLA	CMB-C2B	-2.22	1.46	1.50
24	B	807	CLA	CHC-C1C	2.22	1.42	1.38
27	6	322	LHG	O8-C23	2.22	1.39	1.33
24	B	809	CLA	CMB-C2B	-2.22	1.46	1.50
24	B	836	CLA	CMD-C2D	-2.22	1.46	1.50
24	6	310	CLA	MG-NB	-2.22	2.01	2.05
24	B	804	CLA	MG-NB	-2.22	2.01	2.05
24	5	307	CLA	CMD-C2D	-2.22	1.46	1.50
24	9	307	CLA	CMB-C2B	-2.22	1.46	1.50
24	A	820	CLA	CMB-C2B	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	303	CLA	CMB-C2B	-2.22	1.46	1.50
27	3	322	LHG	O7-C7	2.22	1.40	1.34
24	B	807	CLA	MG-NB	-2.22	2.01	2.05
24	B	838	CLA	CMD-C2D	-2.22	1.46	1.50
24	3	304	CLA	MG-NB	-2.22	2.01	2.05
24	4	304	CLA	MG-NB	-2.22	2.01	2.05
24	8	315	CLA	CMD-C2D	-2.22	1.46	1.50
24	1	308	CLA	MG-NB	-2.22	2.01	2.05
25	8	317	8CT	C33-C32	-2.22	1.44	1.50
24	2	308	CLA	C3B-C4B	2.22	1.49	1.42
24	A	802	CLA	C3B-C4B	2.22	1.49	1.42
24	B	829	CLA	MG-NB	-2.22	2.01	2.05
24	A	836	CLA	CMD-C2D	-2.22	1.46	1.50
24	6	304	CLA	C3B-C4B	2.22	1.49	1.42
24	3	308	CLA	CMB-C2B	-2.22	1.46	1.50
24	B	834	CLA	MG-NB	-2.22	2.01	2.05
24	6	309	CLA	MG-NB	-2.22	2.01	2.05
24	A	821	CLA	MG-NB	-2.22	2.01	2.05
24	6	309	CLA	CMD-C2D	-2.22	1.46	1.50
24	G	101	CLA	CMC-C2C	-2.22	1.46	1.50
24	8	315	CLA	C3B-C4B	2.22	1.49	1.42
24	J	103	CLA	CHC-C1C	2.22	1.42	1.38
23	7	313	CHL	CBD-CGD	-2.22	1.49	1.52
24	3	310	CLA	CMD-C2D	-2.22	1.46	1.50
25	B	850	8CT	C33-C32	-2.22	1.44	1.50
24	1	311	CLA	MG-NB	-2.22	2.01	2.05
24	3	309	CLA	CMD-C2D	-2.22	1.46	1.50
24	A	802	CLA	CMC-C2C	-2.22	1.46	1.50
24	K	104	CLA	CMB-C2B	-2.22	1.46	1.50
24	A	803	CLA	CHC-C1C	2.22	1.42	1.38
24	A	825	CLA	CHC-C1C	2.22	1.42	1.38
24	6	311	CLA	CMC-C2C	-2.22	1.46	1.50
24	A	829	CLA	CMD-C2D	-2.22	1.46	1.50
24	1	303	CLA	CHC-C1C	2.22	1.42	1.38
24	4	304	CLA	C3B-C4B	2.22	1.49	1.42
24	B	815	CLA	MG-NB	-2.22	2.01	2.05
24	B	816	CLA	CMC-C2C	-2.22	1.46	1.50
24	B	824	CLA	CMB-C2B	-2.22	1.46	1.50
24	F	302	CLA	CHC-C1C	2.22	1.42	1.38
24	3	315	CLA	MG-NB	-2.21	2.01	2.05
24	A	829	CLA	CMC-C2C	-2.21	1.46	1.50
24	3	311	CLA	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	314	CLA	C3B-C4B	2.21	1.49	1.42
24	5	311	CLA	CMC-C2C	-2.21	1.46	1.50
24	1	302	CLA	MG-NB	-2.21	2.01	2.05
24	2	313	CLA	MG-NB	-2.21	2.01	2.05
24	A	819	CLA	MG-NB	-2.21	2.01	2.05
25	I	101	8CT	C33-C32	-2.21	1.44	1.50
27	9	316	LHG	O8-C23	2.21	1.39	1.33
24	A	821	CLA	CMD-C2D	-2.21	1.46	1.50
24	0	310	CLA	MG-NB	-2.21	2.01	2.05
24	9	309	CLA	MG-NB	-2.21	2.01	2.05
24	O	205	CLA	CMD-C2D	-2.21	1.46	1.50
24	H	204	CLA	CMB-C2B	-2.21	1.46	1.50
24	B	837	CLA	MG-NB	-2.21	2.01	2.05
24	0	309	CLA	CHC-C1C	2.21	1.42	1.38
24	B	825	CLA	CHC-C1C	2.21	1.42	1.38
24	L	202	CLA	C3B-C4B	2.21	1.49	1.42
24	B	813	CLA	CMB-C2B	-2.21	1.46	1.50
24	9	302	CLA	MG-NB	-2.21	2.01	2.05
24	H	205	CLA	CHC-C1C	2.21	1.42	1.38
24	7	304	CLA	C3B-C4B	2.21	1.49	1.42
24	B	828	CLA	C3B-C4B	2.21	1.49	1.42
24	3	313	CLA	CMD-C2D	-2.21	1.46	1.50
24	6	316	CLA	C3B-C4B	2.21	1.49	1.42
24	A	804	CLA	CMD-C2D	-2.21	1.46	1.50
24	A	848	CLA	CMB-C2B	-2.21	1.46	1.50
24	B	818	CLA	CMB-C2B	-2.21	1.46	1.50
27	B	852	LHG	O7-C7	2.21	1.40	1.34
24	B	802	CLA	CMB-C2B	-2.21	1.46	1.50
24	L	201	CLA	CMB-C2B	-2.21	1.46	1.50
24	8	311	CLA	MG-NB	-2.21	2.01	2.05
24	B	815	CLA	CHC-C1C	2.21	1.42	1.38
24	A	827	CLA	CHC-C1C	2.21	1.42	1.38
24	A	824	CLA	C3B-C4B	2.21	1.49	1.42
24	A	817	CLA	CMD-C2D	-2.21	1.46	1.50
24	0	313	CLA	CMB-C2B	-2.21	1.46	1.50
24	A	837	CLA	CMD-C2D	-2.21	1.46	1.50
24	3	311	CLA	CMD-C2D	-2.21	1.46	1.50
24	9	302	CLA	C3B-C4B	2.21	1.49	1.42
24	5	309	CLA	C3B-C4B	2.21	1.49	1.42
24	K	102	CLA	C3B-C4B	2.21	1.49	1.42
24	5	313	CLA	MG-NB	-2.21	2.01	2.05
24	B	840	CLA	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	302	CLA	CHC-C1C	2.21	1.42	1.38
24	A	815	CLA	C3B-C4B	2.21	1.49	1.42
24	A	828	CLA	C3B-C4B	2.21	1.49	1.42
24	B	839	CLA	C3B-C4B	2.21	1.49	1.42
24	3	304	CLA	CMD-C2D	-2.21	1.46	1.50
24	6	303	CLA	CMD-C2D	-2.21	1.46	1.50
24	A	828	CLA	CMB-C2B	-2.21	1.46	1.50
24	B	809	CLA	CMD-C2D	-2.21	1.46	1.50
24	B	837	CLA	CMB-C2B	-2.21	1.46	1.50
24	G	101	CLA	C3B-C4B	2.21	1.49	1.42
24	B	806	CLA	CMD-C2D	-2.21	1.46	1.50
27	1	318	LHG	O7-C7	2.20	1.40	1.34
24	3	311	CLA	CMC-C2C	-2.20	1.46	1.50
24	9	308	CLA	MG-NB	-2.20	2.01	2.05
23	3	307	CHL	CBD-CGD	-2.20	1.49	1.52
24	9	310	CLA	CMB-C2B	-2.20	1.46	1.50
24	B	832	CLA	C3B-C4B	2.20	1.49	1.42
24	7	303	CLA	CMB-C2B	-2.20	1.46	1.50
24	A	818	CLA	CMD-C2D	-2.20	1.46	1.50
24	A	824	CLA	CMD-C2D	-2.20	1.46	1.50
27	I	102	LHG	O7-C7	2.20	1.40	1.34
27	0	317	LHG	O8-C23	2.20	1.39	1.33
24	A	820	CLA	C3B-C4B	2.20	1.49	1.42
24	2	308	CLA	CMD-C2D	-2.20	1.46	1.50
24	7	312	CLA	CMB-C2B	-2.20	1.46	1.50
24	A	802	CLA	CHC-C1C	2.20	1.42	1.38
24	A	812	CLA	CHC-C1C	2.20	1.42	1.38
24	B	834	CLA	C3B-C4B	2.20	1.49	1.42
23	1	305	CHL	CBD-CGD	-2.20	1.49	1.52
24	B	836	CLA	CHC-C1C	2.20	1.42	1.38
24	3	304	CLA	CMC-C2C	-2.20	1.46	1.50
23	1	306	CHL	CBD-CGD	-2.20	1.49	1.52
23	4	301	CHL	CBD-CGD	-2.20	1.49	1.52
24	1	310	CLA	MG-NB	-2.20	2.01	2.05
24	8	312	CLA	CMD-C2D	-2.20	1.46	1.50
24	A	817	CLA	CMB-C2B	-2.20	1.46	1.50
24	2	302	CLA	CMD-C2D	-2.20	1.46	1.50
24	B	801	CLA	CMB-C2B	-2.20	1.46	1.50
24	B	813	CLA	CMD-C2D	-2.20	1.46	1.50
24	4	312	CLA	CMB-C2B	-2.20	1.46	1.50
24	4	303	CLA	C3B-C4B	2.20	1.49	1.42
24	A	835	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	201	CLA	CMB-C2B	-2.20	1.46	1.50
24	8	304	CLA	MG-NB	-2.20	2.01	2.05
24	B	817	CLA	MG-NB	-2.20	2.01	2.05
24	A	827	CLA	C3B-C4B	2.20	1.49	1.42
24	9	302	CLA	CMD-C2D	-2.20	1.46	1.50
24	A	838	CLA	CMB-C2B	-2.20	1.46	1.50
24	B	839	CLA	CMB-C2B	-2.20	1.46	1.50
24	7	309	CLA	CHC-C1C	2.20	1.42	1.38
24	1	313	CLA	C3B-C4B	2.20	1.49	1.42
24	B	821	CLA	CMD-C2D	-2.20	1.46	1.50
24	3	310	CLA	CHC-C1C	2.20	1.42	1.38
25	L	205	8CT	C33-C32	-2.20	1.44	1.50
24	0	307	CLA	CMD-C2D	-2.20	1.46	1.50
24	4	312	CLA	CMD-C2D	-2.20	1.46	1.50
24	O	201	CLA	C3B-C4B	2.20	1.49	1.42
24	B	808	CLA	C3B-C4B	2.20	1.49	1.42
24	4	311	CLA	C3B-C4B	2.20	1.49	1.42
24	A	802	CLA	CMB-C2B	-2.20	1.46	1.50
24	A	809	CLA	CMD-C2D	-2.20	1.46	1.50
24	1	313	CLA	CMD-C2D	-2.20	1.46	1.50
24	8	313	CLA	CMB-C2B	-2.20	1.46	1.50
24	F	302	CLA	CMB-C2B	-2.20	1.46	1.50
24	B	802	CLA	C3B-C4B	2.20	1.49	1.42
24	3	309	CLA	C1B-C2B	2.20	1.48	1.43
24	1	310	CLA	CMC-C2C	-2.19	1.46	1.50
24	7	311	CLA	CMD-C2D	-2.19	1.46	1.50
29	A	854	LMG	O7-C8	-2.19	1.41	1.46
24	J	103	CLA	MG-NB	-2.19	2.01	2.05
24	1	307	CLA	CMB-C2B	-2.19	1.46	1.50
24	8	305	CLA	MG-NB	-2.19	2.01	2.05
24	G	103	CLA	CHC-C1C	2.19	1.42	1.38
24	B	816	CLA	MG-NB	-2.19	2.01	2.05
24	1	308	CLA	CMB-C2B	-2.19	1.46	1.50
24	B	837	CLA	CMD-C2D	-2.19	1.46	1.50
24	H	205	CLA	MG-NB	-2.19	2.01	2.05
27	3	324	LHG	O7-C7	2.19	1.40	1.34
24	B	833	CLA	C3B-C4B	2.19	1.49	1.42
25	B	843	8CT	C33-C32	-2.19	1.44	1.50
24	7	309	CLA	CMB-C2B	-2.19	1.46	1.50
23	8	314	CHL	CBD-CGD	-2.19	1.49	1.52
24	8	313	CLA	MG-NB	-2.19	2.01	2.05
24	A	823	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	807	CLA	CMB-C2B	-2.19	1.46	1.50
23	0	301	CHL	CBD-CGD	-2.19	1.49	1.52
24	1	303	CLA	CMB-C2B	-2.19	1.46	1.50
24	A	814	CLA	CMC-C2C	-2.19	1.46	1.50
24	A	824	CLA	CMB-C2B	-2.19	1.46	1.50
24	F	303	CLA	CMD-C2D	-2.19	1.46	1.50
24	B	811	CLA	C3B-C4B	2.19	1.49	1.42
27	2	319	LHG	O8-C23	2.19	1.39	1.33
27	3	322	LHG	O8-C23	2.19	1.39	1.33
24	9	304	CLA	CMB-C2B	-2.19	1.46	1.50
24	B	832	CLA	CMD-C2D	-2.19	1.46	1.50
24	7	310	CLA	CHC-C1C	2.19	1.42	1.38
24	A	826	CLA	CHC-C1C	2.19	1.42	1.38
24	H	203	CLA	CHC-C1C	2.19	1.42	1.38
24	A	835	CLA	CMD-C2D	-2.19	1.46	1.50
24	K	103	CLA	CMB-C2B	-2.19	1.46	1.50
24	0	311	CLA	CMB-C2B	-2.19	1.46	1.50
24	A	813	CLA	CMD-C2D	-2.19	1.46	1.50
24	6	309	CLA	CHC-C1C	2.19	1.42	1.38
25	1	314	8CT	C33-C32	-2.19	1.44	1.50
25	6	324	8CT	C33-C32	-2.19	1.44	1.50
25	F	301	8CT	C33-C32	-2.19	1.44	1.50
25	A	849	8CT	C33-C32	-2.19	1.44	1.50
24	B	813	CLA	MG-NB	-2.19	2.01	2.05
24	1	309	CLA	CMD-C2D	-2.19	1.46	1.50
24	B	828	CLA	CMD-C2D	-2.19	1.46	1.50
24	A	821	CLA	C3B-C4B	2.19	1.49	1.42
24	1	310	CLA	CHC-C1C	2.19	1.42	1.38
24	A	816	CLA	C3B-C4B	2.19	1.49	1.42
24	6	310	CLA	CMB-C2B	-2.19	1.46	1.50
24	L	201	CLA	C3B-C4B	2.19	1.49	1.42
24	L	201	CLA	CHC-C1C	2.19	1.42	1.38
24	2	311	CLA	CMD-C2D	-2.19	1.46	1.50
24	B	816	CLA	CMB-C2B	-2.19	1.46	1.50
24	3	311	CLA	C3B-C4B	2.19	1.49	1.42
24	A	808	CLA	CMB-C2B	-2.19	1.46	1.50
27	0	317	LHG	O7-C7	2.18	1.40	1.34
24	A	832	CLA	C3B-C4B	2.18	1.49	1.42
24	3	303	CLA	CMB-C2B	-2.18	1.46	1.50
27	2	317	LHG	O7-C7	2.18	1.40	1.34
27	2	319	LHG	O7-C7	2.18	1.40	1.34
24	6	311	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	4	313	CHL	CBD-CGD	-2.18	1.49	1.52
24	H	205	CLA	CMB-C2B	-2.18	1.46	1.50
24	7	311	CLA	MG-NB	-2.18	2.01	2.05
24	K	103	CLA	C3B-C4B	2.18	1.49	1.42
24	B	814	CLA	CHC-C1C	2.18	1.42	1.38
24	L	203	CLA	C3B-C4B	2.18	1.49	1.42
24	A	805	CLA	CMB-C2B	-2.18	1.46	1.50
24	A	819	CLA	CMB-C2B	-2.18	1.46	1.50
24	4	314	CLA	CMD-C2D	-2.18	1.46	1.50
24	H	201	CLA	C3B-C4B	2.18	1.49	1.42
24	B	819	CLA	CMD-C2D	-2.18	1.46	1.50
24	4	310	CLA	CMB-C2B	-2.18	1.46	1.50
24	6	318	CLA	C3B-C4B	2.18	1.49	1.42
24	B	804	CLA	C3B-C4B	2.18	1.49	1.42
24	F	302	CLA	MG-NB	-2.18	2.01	2.05
24	B	822	CLA	CMB-C2B	-2.18	1.46	1.50
24	B	827	CLA	CMD-C2D	-2.18	1.46	1.50
24	L	203	CLA	CHC-C1C	2.18	1.42	1.38
24	B	827	CLA	CMB-C2B	-2.18	1.46	1.50
24	7	315	CLA	CMB-C2B	-2.18	1.46	1.50
24	H	204	CLA	MG-NB	-2.18	2.01	2.05
24	0	312	CLA	CMB-C2B	-2.18	1.46	1.50
24	7	309	CLA	CMC-C2C	-2.18	1.46	1.50
24	A	823	CLA	CHC-C1C	2.18	1.42	1.38
24	5	310	CLA	C3B-C4B	2.18	1.49	1.42
24	A	830	CLA	C3B-C4B	2.18	1.49	1.42
23	4	307	CHL	CBD-CGD	-2.18	1.49	1.52
24	0	310	CLA	CMC-C2C	-2.18	1.46	1.50
24	B	820	CLA	C3B-C4B	2.18	1.49	1.42
27	1	317	LHG	O8-C23	2.18	1.39	1.33
24	1	311	CLA	CMC-C2C	-2.18	1.46	1.50
24	5	302	CLA	CMB-C2B	-2.18	1.46	1.50
24	O	209	CLA	CMD-C2D	-2.18	1.46	1.50
24	A	828	CLA	CHC-C1C	2.18	1.42	1.38
24	6	311	CLA	CMB-C2B	-2.18	1.46	1.50
24	9	307	CLA	CMC-C2C	-2.18	1.46	1.50
24	0	304	CLA	CMD-C2D	-2.18	1.46	1.50
24	2	309	CLA	CHC-C1C	2.18	1.42	1.38
24	L	206	CLA	CHC-C1C	2.18	1.42	1.38
24	1	309	CLA	MG-NB	-2.18	2.01	2.05
24	8	310	CLA	CMB-C2B	-2.17	1.46	1.50
24	5	311	CLA	C3B-C4B	2.17	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	9	305	CHL	CBD-CGD	-2.17	1.49	1.52
24	1	311	CLA	C3B-C4B	2.17	1.49	1.42
25	J	101	8CT	C33-C32	-2.17	1.44	1.50
24	B	807	CLA	CMD-C2D	-2.17	1.46	1.50
24	9	304	CLA	CMD-C2D	-2.17	1.46	1.50
24	H	202	CLA	CMD-C2D	-2.17	1.46	1.50
24	B	802	CLA	CHC-C1C	2.17	1.42	1.38
24	B	809	CLA	CHC-C1C	2.17	1.42	1.38
24	A	814	CLA	CMB-C2B	-2.17	1.46	1.50
24	7	308	CLA	CMB-C2B	-2.17	1.46	1.50
24	9	307	CLA	CMD-C2D	-2.17	1.46	1.50
24	3	306	CLA	CHC-C1C	2.17	1.42	1.38
24	7	317	CLA	CMC-C2C	-2.17	1.46	1.50
24	B	816	CLA	CMD-C2D	-2.17	1.46	1.50
24	G	103	CLA	CMB-C2B	-2.17	1.46	1.50
24	6	317	CLA	CHC-C1C	2.17	1.42	1.38
24	B	838	CLA	CMB-C2B	-2.17	1.46	1.50
24	A	830	CLA	CHC-C1C	2.17	1.42	1.38
24	L	202	CLA	CHC-C1C	2.17	1.42	1.38
24	B	807	CLA	CMB-C2B	-2.17	1.46	1.50
24	4	304	CLA	CMB-C2B	-2.17	1.46	1.50
24	B	823	CLA	C3B-C4B	2.17	1.49	1.42
24	0	303	CLA	CMB-C2B	-2.17	1.46	1.50
24	3	312	CLA	CMD-C2D	-2.17	1.46	1.50
24	8	313	CLA	CMC-C2C	-2.17	1.46	1.50
24	8	315	CLA	MG-NB	-2.17	2.01	2.05
24	A	837	CLA	MG-NB	-2.17	2.01	2.05
24	B	817	CLA	C3B-C4B	2.17	1.49	1.42
24	A	831	CLA	C3B-C4B	2.17	1.49	1.42
24	5	308	CLA	CMD-C2D	-2.17	1.46	1.50
24	6	314	CLA	CMD-C2D	-2.17	1.46	1.50
24	7	312	CLA	CMD-C2D	-2.17	1.46	1.50
24	A	807	CLA	CMD-C2D	-2.17	1.46	1.50
24	0	307	CLA	CHC-C1C	2.17	1.42	1.38
24	B	828	CLA	CHC-C1C	2.17	1.42	1.38
24	1	309	CLA	CMB-C2B	-2.17	1.46	1.50
27	A	842	LHG	O8-C23	2.17	1.39	1.33
25	0	314	8CT	C33-C32	-2.17	1.44	1.50
23	6	301	CHL	CBD-CGD	-2.17	1.49	1.52
24	3	311	CLA	CMB-C2B	-2.17	1.46	1.50
24	8	311	CLA	CMD-C2D	-2.17	1.46	1.50
24	F	302	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	312	CLA	C3B-C4B	2.16	1.49	1.42
24	A	848	CLA	CHC-C1C	2.16	1.42	1.38
24	1	311	CLA	CMB-C2B	-2.16	1.46	1.50
24	A	832	CLA	CMD-C2D	-2.16	1.46	1.50
24	7	310	CLA	CMB-C2B	-2.16	1.46	1.50
24	4	304	CLA	CMC-C2C	-2.16	1.46	1.50
24	A	809	CLA	MG-NB	-2.16	2.01	2.05
24	2	309	CLA	CMB-C2B	-2.16	1.46	1.50
24	B	837	CLA	CHC-C1C	2.16	1.42	1.38
24	9	304	CLA	C3B-C4B	2.16	1.49	1.42
24	B	816	CLA	C3B-C4B	2.16	1.49	1.42
24	1	310	CLA	CMB-C2B	-2.16	1.46	1.50
24	8	313	CLA	CHC-C1C	2.16	1.42	1.38
24	A	853	CLA	CMC-C2C	-2.16	1.46	1.50
24	4	303	CLA	CMB-C2B	-2.16	1.46	1.50
23	6	306	CHL	CBD-CGD	-2.16	1.49	1.52
24	A	810	CLA	MG-NB	-2.16	2.01	2.05
24	B	808	CLA	CHC-C1C	2.16	1.42	1.38
24	A	801	CLA	CMC-C2C	-2.16	1.46	1.50
24	B	836	CLA	CMB-C2B	-2.16	1.46	1.50
24	L	202	CLA	CMD-C2D	-2.16	1.46	1.50
24	9	311	CLA	C3B-C4B	2.16	1.49	1.42
24	B	817	CLA	CHC-C1C	2.16	1.42	1.38
24	4	310	CLA	CMD-C2D	-2.16	1.46	1.50
24	3	306	CLA	CMB-C2B	-2.16	1.46	1.50
27	B	852	LHG	P-O6	2.16	1.67	1.59
24	9	309	CLA	CHC-C1C	2.16	1.42	1.38
24	1	310	CLA	CMD-C2D	-2.16	1.46	1.50
24	H	203	CLA	MG-NB	-2.16	2.01	2.05
24	4	303	CLA	CHC-C1C	2.16	1.42	1.38
23	0	302	CHL	CBD-CGD	-2.16	1.49	1.52
24	B	805	CLA	CMC-C2C	-2.16	1.46	1.50
24	3	314	CLA	CMB-C2B	-2.16	1.46	1.50
24	9	310	CLA	CMD-C2D	-2.16	1.46	1.50
24	K	101	CLA	CMB-C2B	-2.16	1.46	1.50
24	8	305	CLA	CHC-C1C	2.16	1.42	1.38
24	3	315	CLA	CMD-C2D	-2.16	1.46	1.50
24	B	801	CLA	CHC-C1C	2.16	1.42	1.38
24	B	818	CLA	CHC-C1C	2.16	1.42	1.38
24	3	314	CLA	CHC-C1C	2.16	1.42	1.38
24	8	311	CLA	CHC-C1C	2.16	1.42	1.38
24	1	308	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	837	CLA	CHC-C1C	2.16	1.42	1.38
23	4	308	CHL	CBD-CGD	-2.16	1.49	1.52
24	A	836	CLA	CMB-C2B	-2.16	1.46	1.50
24	L	206	CLA	CMB-C2B	-2.16	1.46	1.50
24	8	311	CLA	CMB-C2B	-2.15	1.46	1.50
24	A	818	CLA	C1B-C2B	2.15	1.48	1.43
24	1	309	CLA	C3B-C4B	2.15	1.49	1.42
24	A	819	CLA	C3B-C4B	2.15	1.49	1.42
27	2	317	LHG	O8-C23	2.15	1.39	1.33
24	0	308	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	838	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	827	CLA	C3B-C4B	2.15	1.49	1.42
24	7	316	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	817	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	831	CLA	CHC-C1C	2.15	1.42	1.38
24	A	820	CLA	CHC-C1C	2.15	1.42	1.38
24	6	312	CLA	CMB-C2B	-2.15	1.46	1.50
24	9	307	CLA	MG-NB	-2.15	2.01	2.05
24	0	310	CLA	C3B-C4B	2.15	1.49	1.42
24	9	307	CLA	C3B-C4B	2.15	1.49	1.42
23	4	302	CHL	CBD-CGD	-2.15	1.49	1.52
24	0	319	CLA	CMC-C2C	-2.15	1.46	1.50
24	5	311	CLA	CMD-C2D	-2.15	1.46	1.50
24	6	318	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	821	CLA	MG-NB	-2.15	2.01	2.05
24	B	834	CLA	CHC-C1C	2.15	1.42	1.38
24	O	209	CLA	MG-NB	-2.15	2.01	2.05
24	A	825	CLA	CMB-C2B	-2.15	1.46	1.50
27	3	320	LHG	P-O6	2.15	1.67	1.59
24	A	827	CLA	CMC-C2C	-2.15	1.46	1.50
24	0	312	CLA	C3B-C4B	2.15	1.49	1.42
24	B	835	CLA	C3B-C4B	2.15	1.49	1.42
24	A	812	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	827	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	832	CLA	CMB-C2B	-2.15	1.46	1.50
24	8	304	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	803	CLA	CMB-C2B	-2.15	1.46	1.50
24	3	306	CLA	MG-NB	-2.15	2.01	2.05
24	0	310	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	830	CLA	CMC-C2C	-2.15	1.46	1.50
24	9	308	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	821	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	306	CHL	CBD-CGD	-2.15	1.49	1.52
24	0	304	CLA	C3B-C4B	2.15	1.49	1.42
24	0	311	CLA	CMD-C2D	-2.15	1.46	1.50
24	K	103	CLA	CMC-C2C	-2.15	1.46	1.50
24	3	306	CLA	CMD-C2D	-2.15	1.46	1.50
24	A	829	CLA	C1B-C2B	2.15	1.48	1.43
23	2	312	CHL	CBD-CGD	-2.15	1.49	1.52
24	B	840	CLA	C3B-C4B	2.15	1.49	1.42
24	8	305	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	813	CLA	CHC-C1C	2.15	1.42	1.38
24	B	822	CLA	CHC-C1C	2.15	1.42	1.38
24	1	302	CLA	CMC-C2C	-2.15	1.46	1.50
24	B	809	CLA	CMC-C2C	-2.15	1.46	1.50
24	B	801	CLA	C3B-C4B	2.15	1.49	1.42
24	B	836	CLA	C3B-C4B	2.15	1.49	1.42
24	B	812	CLA	CMD-C2D	-2.14	1.46	1.50
24	B	822	CLA	MG-NB	-2.14	2.01	2.05
24	A	806	CLA	CMD-C2D	-2.14	1.46	1.50
24	2	308	CLA	CMB-C2B	-2.14	1.46	1.50
27	A	843	LHG	O8-C23	2.14	1.39	1.33
24	B	835	CLA	CHC-C1C	2.14	1.42	1.38
24	A	823	CLA	CMD-C2D	-2.14	1.46	1.50
24	H	204	CLA	CMD-C2D	-2.14	1.46	1.50
24	8	315	CLA	CHC-C1C	2.14	1.42	1.38
24	3	303	CLA	C3B-C4B	2.14	1.49	1.42
24	7	317	CLA	CMD-C2D	-2.14	1.46	1.50
24	A	816	CLA	CMC-C2C	-2.14	1.46	1.50
24	3	304	CLA	C3B-C4B	2.14	1.49	1.42
24	B	818	CLA	CMD-C2D	-2.14	1.46	1.50
24	3	312	CLA	CHC-C1C	2.14	1.42	1.38
23	7	301	CHL	CBD-CGD	-2.14	1.49	1.52
24	L	206	CLA	MG-NB	-2.14	2.01	2.05
23	1	301	CHL	CBD-CGD	-2.14	1.49	1.52
24	9	302	CLA	CMB-C2B	-2.14	1.46	1.50
24	B	805	CLA	CMB-C2B	-2.14	1.46	1.50
24	B	818	CLA	C3B-C4B	2.14	1.49	1.42
26	9	315	0UR	C23-C1	-2.14	1.50	1.53
24	0	319	CLA	CMD-C2D	-2.14	1.46	1.50
24	7	308	CLA	CMC-C2C	-2.14	1.46	1.50
24	7	314	CLA	CMB-C2B	-2.14	1.46	1.50
24	O	205	CLA	CMB-C2B	-2.14	1.46	1.50
24	2	309	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	303	CLA	CHC-C1C	2.14	1.42	1.38
24	4	314	CLA	CHC-C1C	2.14	1.42	1.38
29	9	317	LMG	O8-C9	-2.14	1.40	1.45
24	2	310	CLA	CMD-C2D	-2.14	1.46	1.50
24	3	315	CLA	CMB-C2B	-2.14	1.46	1.50
24	4	311	CLA	CHC-C1C	2.14	1.42	1.38
24	B	806	CLA	CMB-C2B	-2.14	1.46	1.50
24	A	810	CLA	CMC-C2C	-2.14	1.46	1.50
24	A	811	CLA	CMC-C2C	-2.14	1.46	1.50
24	O	201	CLA	CMC-C2C	-2.14	1.46	1.50
24	5	303	CLA	MG-NB	-2.14	2.01	2.05
29	O	210	LMG	O7-C8	-2.14	1.41	1.46
24	B	835	CLA	CMD-C2D	-2.14	1.46	1.50
24	B	810	CLA	CMB-C2B	-2.14	1.46	1.50
24	6	318	CLA	CHC-C1C	2.14	1.42	1.38
24	L	206	CLA	CMD-C2D	-2.14	1.46	1.50
24	H	204	CLA	C3B-C4B	2.14	1.49	1.42
24	A	815	CLA	MG-NB	-2.14	2.01	2.05
24	B	810	CLA	CMC-C2C	-2.13	1.46	1.50
24	7	316	CLA	CMD-C2D	-2.13	1.46	1.50
24	5	309	CLA	CHC-C1C	2.13	1.42	1.38
24	B	810	CLA	CHC-C1C	2.13	1.42	1.38
27	1	317	LHG	O7-C7	2.13	1.40	1.34
24	8	312	CLA	CMC-C2C	-2.13	1.46	1.50
24	A	823	CLA	CMC-C2C	-2.13	1.46	1.50
23	9	306	CHL	CBD-CGD	-2.13	1.49	1.52
24	A	824	CLA	CHC-C1C	2.13	1.42	1.38
24	3	313	CLA	CHC-C1C	2.13	1.42	1.38
24	A	813	CLA	CMC-C2C	-2.13	1.46	1.50
27	A	842	LHG	O7-C7	2.13	1.40	1.34
24	3	315	CLA	C3B-C4B	2.13	1.49	1.42
24	A	829	CLA	C1B-NB	-2.13	1.35	1.37
24	B	821	CLA	C3B-C4B	2.13	1.49	1.42
24	A	839	CLA	CMC-C2C	-2.13	1.46	1.50
24	B	841	CLA	CMD-C2D	-2.13	1.46	1.50
24	G	101	CLA	CMD-C2D	-2.13	1.46	1.50
24	B	826	CLA	CMB-C2B	-2.13	1.46	1.50
24	O	201	CLA	CMD-C2D	-2.13	1.46	1.50
24	A	816	CLA	CHC-C1C	2.13	1.42	1.38
24	B	808	CLA	CMC-C2C	-2.13	1.46	1.50
24	8	310	CLA	CHC-C1C	2.13	1.42	1.38
24	5	302	CLA	C3B-C4B	2.13	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	802	CLA	CMD-C2D	-2.13	1.46	1.50
24	0	311	CLA	MG-NB	-2.13	2.01	2.05
24	1	313	CLA	CMB-C2B	-2.13	1.46	1.50
24	A	839	CLA	CHC-C1C	2.13	1.42	1.38
24	0	312	CLA	CMD-C2D	-2.13	1.46	1.50
24	1	302	CLA	CMB-C2B	-2.13	1.46	1.50
24	7	308	CLA	CHC-C1C	2.13	1.42	1.38
25	O	208	8CT	C33-C32	-2.13	1.44	1.50
24	J	103	CLA	CMD-C2D	-2.13	1.46	1.50
24	4	312	CLA	CMC-C2C	-2.13	1.46	1.50
24	3	303	CLA	CHC-C1C	2.13	1.42	1.38
24	O	204	CLA	CHC-C1C	2.13	1.42	1.38
24	B	832	CLA	CMC-C2C	-2.13	1.46	1.50
25	3	316	8CT	C33-C32	-2.13	1.44	1.50
24	B	832	CLA	CHC-C1C	2.13	1.42	1.38
24	6	316	CLA	CHC-C1C	2.13	1.42	1.38
24	G	102	CLA	CHC-C1C	2.13	1.42	1.38
24	0	309	CLA	CMD-C2D	-2.12	1.46	1.50
24	3	311	CLA	CHC-C1C	2.12	1.42	1.38
24	6	304	CLA	CMD-C2D	-2.12	1.46	1.50
24	6	316	CLA	CMB-C2B	-2.12	1.46	1.50
24	9	311	CLA	CMD-C2D	-2.12	1.46	1.50
24	B	824	CLA	CMC-C2C	-2.12	1.46	1.50
24	H	203	CLA	CMC-C2C	-2.12	1.46	1.50
24	A	804	CLA	MG-NB	-2.12	2.01	2.05
24	2	311	CLA	CMB-C2B	-2.12	1.46	1.50
24	6	309	CLA	CMB-C2B	-2.12	1.46	1.50
24	A	814	CLA	C3B-C4B	2.12	1.48	1.42
24	9	310	CLA	MG-NB	-2.12	2.01	2.05
24	2	311	CLA	C3B-C4B	2.12	1.48	1.42
24	A	836	CLA	CHC-C1C	2.12	1.42	1.38
24	1	307	CLA	CMD-C2D	-2.12	1.46	1.50
24	2	313	CLA	CMB-C2B	-2.12	1.46	1.50
24	B	804	CLA	CMB-C2B	-2.12	1.46	1.50
24	0	311	CLA	CHC-C1C	2.12	1.42	1.38
24	A	806	CLA	CHC-C1C	2.12	1.42	1.38
24	A	836	CLA	C3B-C4B	2.12	1.48	1.42
24	3	313	CLA	CMB-C2B	-2.12	1.46	1.50
24	K	104	CLA	CMD-C2D	-2.12	1.46	1.50
24	A	803	CLA	MG-NB	-2.12	2.01	2.05
23	4	306	CHL	CBD-CGD	-2.12	1.49	1.52
24	6	317	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	851	LHG	O7-C5	-2.12	1.41	1.46
24	6	316	CLA	CMD-C2D	-2.12	1.46	1.50
24	H	202	CLA	CMB-C2B	-2.12	1.46	1.50
24	B	830	CLA	MG-ND	-2.12	2.01	2.05
27	3	324	LHG	P-O6	2.12	1.67	1.59
24	J	103	CLA	CMB-C2B	-2.12	1.46	1.50
24	L	201	CLA	CMD-C2D	-2.12	1.46	1.50
27	8	302	LHG	P-O6	2.12	1.67	1.59
24	3	312	CLA	CMC-C2C	-2.12	1.46	1.50
24	7	317	CLA	C3B-C4B	2.12	1.48	1.42
24	A	808	CLA	CHC-C1C	2.12	1.42	1.38
24	1	303	CLA	CMD-C2D	-2.12	1.46	1.50
24	8	310	CLA	CMC-C2C	-2.12	1.46	1.50
24	B	822	CLA	CMD-C2D	-2.12	1.46	1.50
24	B	825	CLA	CMB-C2B	-2.12	1.46	1.50
24	F	302	CLA	CMD-C2D	-2.12	1.46	1.50
24	O	201	CLA	CMB-C2B	-2.12	1.46	1.50
24	O	204	CLA	CMD-C2D	-2.12	1.46	1.50
24	5	310	CLA	CMD-C2D	-2.12	1.46	1.50
24	K	104	CLA	CHC-C1C	2.12	1.42	1.38
24	6	317	CLA	CMD-C2D	-2.12	1.46	1.50
24	B	833	CLA	CMD-C2D	-2.12	1.46	1.50
24	5	311	CLA	CHC-C1C	2.12	1.42	1.38
24	B	841	CLA	CMB-C2B	-2.12	1.46	1.50
24	B	820	CLA	CMD-C2D	-2.12	1.46	1.50
24	3	309	CLA	CMC-C2C	-2.11	1.46	1.50
24	5	309	CLA	CMD-C2D	-2.11	1.46	1.50
24	1	308	CLA	CMC-C2C	-2.11	1.46	1.50
24	7	310	CLA	CMD-C2D	-2.11	1.46	1.50
24	7	312	CLA	CHC-C1C	2.11	1.42	1.38
24	B	820	CLA	CHC-C1C	2.11	1.42	1.38
24	B	815	CLA	CMC-C2C	-2.11	1.46	1.50
24	0	309	CLA	CMB-C2B	-2.11	1.46	1.50
24	4	309	CLA	CMB-C2B	-2.11	1.46	1.50
24	0	304	CLA	CHC-C1C	2.11	1.42	1.38
27	7	323	LHG	P-O6	2.11	1.67	1.59
24	3	308	CLA	C3B-C4B	2.11	1.48	1.42
24	A	836	CLA	CMC-C2C	-2.11	1.46	1.50
24	H	201	CLA	CHC-C1C	2.11	1.42	1.38
24	8	304	CLA	CMC-C2C	-2.11	1.46	1.50
24	9	310	CLA	CMC-C2C	-2.11	1.46	1.50
24	A	838	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	315	CLA	C3B-C4B	2.11	1.48	1.42
24	B	814	CLA	CMB-C2B	-2.11	1.46	1.50
24	B	823	CLA	CHC-C1C	2.11	1.42	1.38
24	4	311	CLA	CMB-C2B	-2.11	1.46	1.50
24	0	313	CLA	CHC-C1C	2.11	1.42	1.38
24	9	309	CLA	CMB-C2B	-2.11	1.46	1.50
24	B	835	CLA	CMB-C2B	-2.11	1.46	1.50
24	4	303	CLA	CMC-C2C	-2.11	1.46	1.50
24	4	310	CLA	CHC-C1C	2.11	1.42	1.38
24	5	309	CLA	CMB-C2B	-2.11	1.46	1.50
24	A	803	CLA	CMD-C2D	-2.11	1.46	1.50
24	A	835	CLA	C3B-C4B	2.11	1.48	1.42
24	6	310	CLA	CMD-C2D	-2.11	1.46	1.50
24	A	826	CLA	CMB-C2B	-2.11	1.46	1.50
24	K	102	CLA	CMB-C2B	-2.11	1.46	1.50
24	A	833	CLA	C3B-C4B	2.11	1.48	1.42
24	1	313	CLA	CHC-C1C	2.11	1.42	1.38
24	B	816	CLA	CHC-C1C	2.11	1.42	1.38
24	H	202	CLA	C3B-C4B	2.11	1.48	1.42
24	H	202	CLA	CHC-C1C	2.11	1.42	1.38
24	L	203	CLA	CMB-C2B	-2.11	1.46	1.50
24	7	308	CLA	C3B-C4B	2.11	1.48	1.42
24	A	838	CLA	C3B-C4B	2.11	1.48	1.42
24	2	303	CLA	CMC-C2C	-2.11	1.46	1.50
24	4	312	CLA	C3B-C4B	2.11	1.48	1.42
24	F	303	CLA	CHC-C1C	2.11	1.42	1.38
24	B	823	CLA	CMC-C2C	-2.11	1.46	1.50
24	H	205	CLA	CMD-C2D	-2.11	1.46	1.50
27	A	850	LHG	P-O6	2.11	1.67	1.59
24	K	102	CLA	CHC-C1C	2.10	1.42	1.38
24	6	311	CLA	MG-NB	-2.10	2.01	2.05
24	A	808	CLA	C3B-C4B	2.10	1.48	1.42
24	6	310	CLA	CHC-C1C	2.10	1.42	1.38
24	A	819	CLA	CHC-C1C	2.10	1.42	1.38
24	B	817	CLA	CMB-C2B	-2.10	1.46	1.50
24	B	828	CLA	CMC-C2C	-2.10	1.46	1.50
27	7	323	LHG	O7-C7	2.10	1.40	1.34
24	2	303	CLA	C3B-C4B	2.10	1.48	1.42
24	7	311	CLA	CHC-C1C	2.10	1.42	1.38
24	2	310	CLA	C3B-C4B	2.10	1.48	1.42
24	B	812	CLA	C3B-C4B	2.10	1.48	1.42
24	B	819	CLA	C3B-C4B	2.10	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	312	CLA	CMB-C2B	-2.10	1.46	1.50
24	9	309	CLA	CMD-C2D	-2.10	1.46	1.50
24	5	303	CLA	CHC-C1C	2.10	1.42	1.38
24	K	103	CLA	CHC-C1C	2.10	1.42	1.38
24	7	315	CLA	CMD-C2D	-2.10	1.46	1.50
24	A	805	CLA	CMC-C2C	-2.10	1.46	1.50
24	A	831	CLA	CMC-C2C	-2.10	1.46	1.50
24	B	828	CLA	CMB-C2B	-2.10	1.46	1.50
24	9	304	CLA	CHC-C1C	2.10	1.42	1.38
24	B	834	CLA	CMC-C2C	-2.10	1.46	1.50
24	7	314	CLA	CMD-C2D	-2.10	1.46	1.50
24	A	810	CLA	C3B-C4B	2.10	1.48	1.42
24	7	316	CLA	MG-NB	-2.10	2.01	2.05
24	1	309	CLA	CHC-C1C	2.10	1.42	1.38
24	G	103	CLA	CMD-C2D	-2.10	1.46	1.50
24	A	834	CLA	CHC-C1C	2.10	1.42	1.38
27	3	322	LHG	P-O6	2.10	1.67	1.59
24	3	303	CLA	CMC-C2C	-2.10	1.46	1.50
24	6	314	CLA	CMB-C2B	-2.10	1.46	1.50
24	B	839	CLA	CHC-C1C	2.10	1.42	1.38
24	8	305	CLA	CMD-C2D	-2.10	1.46	1.50
23	6	323	CHL	CBD-CGD	-2.10	1.49	1.52
24	5	310	CLA	CMB-C2B	-2.10	1.46	1.50
24	A	835	CLA	CHC-C1C	2.10	1.42	1.38
24	F	303	CLA	CMC-C2C	-2.09	1.46	1.50
24	A	833	CLA	CMC-C2C	-2.09	1.46	1.50
24	B	802	CLA	CMC-C2C	-2.09	1.46	1.50
24	B	826	CLA	CMC-C2C	-2.09	1.46	1.50
24	7	314	CLA	CHC-C1C	2.09	1.42	1.38
24	B	807	CLA	CMC-C2C	-2.09	1.46	1.50
24	A	806	CLA	CMC-C2C	-2.09	1.46	1.50
24	L	203	CLA	CMC-C2C	-2.09	1.46	1.50
24	0	313	CLA	MG-NB	-2.09	2.01	2.05
24	3	314	CLA	CMC-C2C	-2.09	1.46	1.50
24	A	817	CLA	CMC-C2C	-2.09	1.46	1.50
27	L	208	LHG	P-O6	2.09	1.67	1.59
24	A	807	CLA	C3B-C4B	2.09	1.48	1.42
24	L	202	CLA	CMB-C2B	-2.09	1.46	1.50
24	H	204	CLA	CHC-C1C	2.09	1.42	1.38
24	A	818	CLA	CMC-C2C	-2.09	1.46	1.50
24	1	302	CLA	CHC-C1C	2.09	1.42	1.38
30	7	321	0IE	C8-C7	2.09	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	306	CHL	CBD-CGD	-2.09	1.49	1.52
24	9	311	CLA	CMB-C2B	-2.09	1.46	1.50
24	6	312	CLA	CHC-C1C	2.09	1.42	1.38
24	7	303	CLA	CMC-C2C	-2.09	1.46	1.50
24	A	821	CLA	CHC-C1C	2.09	1.42	1.38
24	A	808	CLA	CMC-C2C	-2.09	1.46	1.50
24	B	830	CLA	C1B-NB	-2.09	1.35	1.37
24	B	829	CLA	CMC-C2C	-2.09	1.46	1.50
24	B	836	CLA	CMC-C2C	-2.09	1.46	1.50
24	6	312	CLA	CMC-C2C	-2.09	1.46	1.50
24	A	825	CLA	CMC-C2C	-2.09	1.46	1.50
27	7	324	LHG	P-O6	2.09	1.67	1.59
24	A	840	CLA	C3B-C4B	2.09	1.48	1.42
24	A	815	CLA	CMC-C2C	-2.09	1.46	1.50
24	0	319	CLA	CMB-C2B	-2.09	1.46	1.50
24	9	308	CLA	CMB-C2B	-2.09	1.46	1.50
24	2	313	CLA	CMC-C2C	-2.09	1.46	1.50
24	B	810	CLA	C3B-C4B	2.09	1.48	1.42
24	A	820	CLA	CMC-C2C	-2.09	1.46	1.50
24	H	204	CLA	CMC-C2C	-2.09	1.46	1.50
24	4	314	CLA	CMB-C2B	-2.09	1.46	1.50
24	7	316	CLA	C3B-C4B	2.09	1.48	1.42
24	8	313	CLA	CMD-C2D	-2.09	1.46	1.50
24	A	832	CLA	CHC-C1C	2.08	1.42	1.38
24	0	313	CLA	CMD-C2D	-2.08	1.46	1.50
24	L	202	CLA	CMC-C2C	-2.08	1.46	1.50
24	2	309	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	809	CLA	CMC-C2C	-2.08	1.46	1.50
24	B	835	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	840	CLA	CHC-C1C	2.08	1.42	1.38
24	9	303	CLA	CMC-C2C	-2.08	1.46	1.50
24	4	309	CLA	MG-NB	-2.08	2.01	2.05
24	1	309	CLA	CMC-C2C	-2.08	1.46	1.50
24	1	311	CLA	CHC-C1C	2.08	1.42	1.38
24	B	808	CLA	CMB-C2B	-2.08	1.46	1.50
24	H	203	CLA	CMB-C2B	-2.08	1.46	1.50
25	7	318	8CT	C33-C32	-2.08	1.44	1.50
24	B	825	CLA	CMC-C2C	-2.08	1.46	1.50
24	6	314	CLA	C3B-C4B	2.08	1.48	1.42
24	A	819	CLA	CMC-C2C	-2.08	1.46	1.50
24	8	311	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	821	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	0	310	CLA	CHC-C1C	2.08	1.42	1.38
24	A	818	CLA	CHC-C1C	2.08	1.42	1.38
24	0	304	CLA	CMC-C2C	-2.08	1.46	1.50
24	A	837	CLA	CMC-C2C	-2.08	1.46	1.50
24	5	303	CLA	CMD-C2D	-2.08	1.46	1.50
24	B	812	CLA	CMC-C2C	-2.08	1.46	1.50
24	O	209	CLA	CMB-C2B	-2.08	1.46	1.50
24	3	315	CLA	CMC-C2C	-2.08	1.46	1.50
24	5	307	CLA	CMB-C2B	-2.08	1.46	1.50
24	L	201	CLA	CMC-C2C	-2.08	1.46	1.50
24	L	203	CLA	CMD-C2D	-2.07	1.46	1.50
24	O	201	CLA	CHC-C1C	2.07	1.42	1.38
24	7	304	CLA	CMC-C2C	-2.07	1.46	1.50
24	A	822	CLA	CMC-C2C	-2.07	1.46	1.50
24	H	203	CLA	CMD-C2D	-2.07	1.46	1.50
24	0	308	CLA	CMC-C2C	-2.07	1.46	1.50
24	2	311	CLA	CMC-C2C	-2.07	1.46	1.50
24	A	813	CLA	C3B-C4B	2.07	1.48	1.42
24	4	304	CLA	CMD-C2D	-2.07	1.46	1.50
24	6	316	CLA	CMC-C2C	-2.07	1.46	1.50
24	A	824	CLA	CMC-C2C	-2.07	1.46	1.50
24	B	838	CLA	CMC-C2C	-2.07	1.46	1.50
24	9	309	CLA	CMC-C2C	-2.07	1.46	1.50
24	A	803	CLA	CMC-C2C	-2.07	1.46	1.50
24	O	204	CLA	CMB-C2B	-2.07	1.46	1.50
24	5	302	CLA	CHC-C1C	2.07	1.42	1.38
24	A	822	CLA	CHC-C1C	2.07	1.42	1.38
26	O	207	0UR	C29-C28	-2.07	1.52	1.54
24	1	307	CLA	MG-NB	-2.07	2.01	2.05
24	5	311	CLA	CMB-C2B	-2.07	1.46	1.50
24	0	303	CLA	CHC-C1C	2.07	1.42	1.38
24	7	315	CLA	CMC-C2C	-2.07	1.46	1.50
24	2	313	CLA	CHC-C1C	2.07	1.42	1.38
24	7	315	CLA	CHC-C1C	2.07	1.42	1.38
30	3	319	0IE	C11-C12	2.07	1.40	1.35
24	8	304	CLA	CHC-C1C	2.07	1.42	1.38
24	8	315	CLA	CMB-C2B	-2.07	1.46	1.50
24	B	831	CLA	CMC-C2C	-2.07	1.46	1.50
24	2	310	CLA	CMB-C2B	-2.07	1.46	1.50
24	6	309	CLA	CMC-C2C	-2.07	1.46	1.50
24	A	830	CLA	CMC-C2C	-2.07	1.46	1.50
24	O	206	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	321	0IE	C11-C12	2.07	1.40	1.35
24	B	813	CLA	CMC-C2C	-2.07	1.46	1.50
24	B	817	CLA	CMC-C2C	-2.07	1.46	1.50
24	9	302	CLA	CMC-C2C	-2.06	1.46	1.50
24	B	811	CLA	CHC-C1C	2.06	1.42	1.38
24	A	816	CLA	CMB-C2B	-2.06	1.46	1.50
24	O	206	CLA	MG-NB	-2.06	2.01	2.05
30	3	319	0IE	C8-C7	2.06	1.40	1.35
24	0	312	CLA	CHC-C1C	2.06	1.42	1.38
26	6	320	0UR	C29-C28	-2.06	1.52	1.54
24	A	829	CLA	MG-ND	-2.06	2.01	2.05
29	J	105	LMG	O6-C5	-2.06	1.39	1.44
24	B	805	CLA	C3B-C4B	2.06	1.48	1.42
24	6	304	CLA	CMC-C2C	-2.06	1.46	1.50
24	7	314	CLA	MG-NB	-2.06	2.01	2.05
24	A	828	CLA	CMC-C2C	-2.06	1.46	1.50
24	J	103	CLA	CMC-C2C	-2.06	1.46	1.50
23	1	304	CHL	CBD-CGD	-2.06	1.49	1.52
24	6	304	CLA	CHC-C1C	2.06	1.42	1.38
24	A	838	CLA	CHC-C1C	2.06	1.42	1.38
24	B	831	CLA	C3B-C4B	2.06	1.48	1.42
24	A	807	CLA	CHC-C1C	2.05	1.42	1.38
24	A	835	CLA	CMC-C2C	-2.05	1.46	1.50
24	B	838	CLA	CHC-C1C	2.05	1.42	1.38
24	A	853	CLA	C1B-C2B	2.05	1.47	1.43
24	5	313	CLA	CMB-C2B	-2.05	1.46	1.50
24	K	102	CLA	CMC-C2C	-2.05	1.46	1.50
24	1	307	CLA	CHC-C1C	2.05	1.42	1.38
24	O	206	CLA	CMD-C2D	-2.05	1.46	1.50
24	6	314	CLA	CMC-C2C	-2.05	1.46	1.50
23	6	305	CHL	CBD-CGD	-2.05	1.49	1.52
24	3	313	CLA	CMC-C2C	-2.05	1.46	1.50
27	1	318	LHG	P-O6	2.05	1.67	1.59
24	5	307	CLA	MG-NB	-2.05	2.01	2.05
24	G	101	CLA	CMB-C2B	-2.05	1.46	1.50
24	A	815	CLA	CHC-C1C	2.05	1.42	1.38
24	B	805	CLA	CHC-C1C	2.05	1.42	1.38
24	G	102	CLA	CMB-C2B	-2.05	1.46	1.50
24	A	827	CLA	CMB-C2B	-2.05	1.46	1.50
24	6	314	CLA	CHC-C1C	2.05	1.42	1.38
24	5	307	CLA	CMC-C2C	-2.05	1.46	1.50
24	B	839	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	310	CLA	CHC-C1C	2.05	1.42	1.38
24	A	831	CLA	CHC-C1C	2.05	1.42	1.38
24	B	830	CLA	C3B-C4B	2.04	1.48	1.42
24	A	832	CLA	CMC-C2C	-2.04	1.46	1.50
24	H	201	CLA	CMC-C2C	-2.04	1.46	1.50
24	B	821	CLA	CMB-C2B	-2.04	1.46	1.50
29	J	102	LMG	O4-C4	-2.04	1.37	1.43
24	A	801	CLA	C3B-C4B	2.04	1.48	1.42
24	3	308	CLA	CHC-C1C	2.04	1.42	1.38
24	B	819	CLA	CMC-C2C	-2.04	1.46	1.50
27	9	316	LHG	P-O6	2.04	1.67	1.59
24	O	209	CLA	CMC-C2C	-2.04	1.46	1.50
24	1	303	CLA	CMC-C2C	-2.04	1.46	1.50
23	3	305	CHL	CBD-CGD	-2.04	1.49	1.52
24	6	317	CLA	CMC-C2C	-2.04	1.46	1.50
24	A	807	CLA	CMC-C2C	-2.04	1.46	1.50
24	9	308	CLA	CMC-C2C	-2.04	1.46	1.50
24	5	307	CLA	CHC-C1C	2.04	1.42	1.38
24	A	801	CLA	CHC-C1C	2.04	1.42	1.38
24	9	311	CLA	CMC-C2C	-2.04	1.46	1.50
24	A	829	CLA	C3B-C4B	2.04	1.48	1.42
24	0	311	CLA	CMC-C2C	-2.04	1.46	1.50
24	3	306	CLA	CMC-C2C	-2.04	1.46	1.50
24	5	309	CLA	CMC-C2C	-2.04	1.46	1.50
24	O	205	CLA	CMC-C2C	-2.03	1.46	1.50
24	6	310	CLA	CMC-C2C	-2.03	1.46	1.50
24	O	204	CLA	CMC-C2C	-2.03	1.46	1.50
24	H	202	CLA	CMC-C2C	-2.03	1.46	1.50
23	2	301	CHL	CBD-CGD	-2.03	1.49	1.52
24	7	304	CLA	CHC-C1C	2.03	1.42	1.38
24	4	309	CLA	CMD-C2D	-2.03	1.46	1.50
24	2	302	CLA	CHC-C1C	2.03	1.42	1.38
24	B	827	CLA	CHC-C1C	2.03	1.42	1.38
24	4	312	CLA	CHC-C1C	2.03	1.42	1.38
24	B	820	CLA	CMC-C2C	-2.03	1.46	1.50
24	3	315	CLA	CHC-C1C	2.03	1.42	1.38
24	3	304	CLA	CHC-C1C	2.03	1.42	1.38
24	B	806	CLA	MG-ND	-2.03	2.01	2.05
24	B	815	CLA	CMB-C2B	-2.03	1.46	1.50
26	2	315	0UR	C29-C28	-2.03	1.52	1.54
24	0	303	CLA	CMC-C2C	-2.03	1.46	1.50
24	0	309	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	313	8CT	C33-C32	-2.03	1.44	1.50
24	B	819	CLA	CHC-C1C	2.03	1.42	1.38
23	5	304	CHL	CBD-CGD	-2.03	1.50	1.52
24	B	830	CLA	C1B-C2B	2.03	1.47	1.43
24	8	315	CLA	CMC-C2C	-2.02	1.46	1.50
24	6	303	CLA	C3B-C4B	2.02	1.48	1.42
26	6	321	0UR	C19-C18	2.02	1.53	1.50
27	0	317	LHG	P-O6	2.02	1.67	1.59
27	7	322	LHG	P-O6	2.02	1.67	1.59
24	6	318	CLA	CMC-C2C	-2.02	1.46	1.50
24	7	312	CLA	CMC-C2C	-2.02	1.46	1.50
24	K	101	CLA	CMC-C2C	-2.02	1.46	1.50
24	3	308	CLA	CMC-C2C	-2.02	1.46	1.50
24	H	205	CLA	CMC-C2C	-2.02	1.46	1.50
24	B	821	CLA	CHC-C1C	2.02	1.42	1.38
23	1	312	CHL	CBD-CGD	-2.02	1.50	1.52
24	0	319	CLA	CHC-C1C	2.02	1.42	1.38
24	3	310	CLA	CMC-C2C	-2.01	1.46	1.50
24	G	102	CLA	CMC-C2C	-2.01	1.46	1.50
28	0	318	SQD	O2-C2	-2.01	1.38	1.43
24	2	303	CLA	CHC-C1C	2.01	1.42	1.38
24	7	317	CLA	CHC-C1C	2.01	1.42	1.38
24	5	313	CLA	CMC-C2C	-2.01	1.46	1.50
24	B	837	CLA	CMC-C2C	-2.01	1.46	1.50
24	L	206	CLA	CMC-C2C	-2.01	1.46	1.50
24	0	307	CLA	CMC-C2C	-2.01	1.46	1.50
24	1	307	CLA	CMC-C2C	-2.01	1.46	1.50
24	1	313	CLA	CMC-C2C	-2.01	1.46	1.50
24	9	307	CLA	CHC-C1C	2.01	1.42	1.38
24	5	308	CLA	CMC-C2C	-2.01	1.46	1.50
23	5	306	CHL	CMC-C2C	2.01	1.49	1.44
27	5	316	LHG	P-O6	2.01	1.67	1.59
24	A	814	CLA	CHC-C1C	2.01	1.42	1.38
29	A	851	LMG	O7-C8	-2.01	1.41	1.46
26	4	317	0UR	C29-C28	-2.01	1.52	1.54
24	4	314	CLA	CMC-C2C	-2.01	1.46	1.50
27	8	320	LHG	P-O6	2.00	1.67	1.59
28	0	318	SQD	O3-C3	-2.00	1.38	1.43
24	B	804	CLA	CMC-C2C	-2.00	1.46	1.50
24	B	821	CLA	CMC-C2C	-2.00	1.46	1.50
24	K	104	CLA	CMC-C2C	-2.00	1.46	1.50

All (3319) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	823	CLA	O2A-CGA-O1A	-19.95	73.72	123.63
24	B	823	CLA	O2A-CGA-CBA	15.01	157.60	111.83
25	K	105	8CT	C33-C32-C31	-11.86	113.51	124.83
25	G	104	8CT	C33-C32-C31	-11.78	113.58	124.83
24	B	826	CLA	CHA-C4D-ND	11.50	135.06	125.22
23	0	306	CHL	O2D-CGD-CBD	11.25	123.31	110.95
25	A	846	8CT	C33-C32-C31	-11.21	114.13	124.83
25	M	102	8CT	C33-C32-C31	-11.04	114.29	124.83
25	A	845	8CT	C33-C32-C31	-10.80	114.52	124.83
25	J	104	8CT	C33-C32-C31	-10.74	114.58	124.83
25	3	323	8CT	C33-C32-C31	-10.72	114.59	124.83
23	6	323	CHL	O2D-CGD-CBD	10.69	122.70	110.95
25	B	844	8CT	C33-C32-C31	-10.67	114.65	124.83
25	B	845	8CT	C33-C32-C31	-10.65	114.66	124.83
25	J	101	8CT	C33-C32-C31	-10.63	114.69	124.83
25	3	316	8CT	C33-C32-C31	-10.37	114.93	124.83
25	A	844	8CT	C33-C32-C31	-10.37	114.94	124.83
25	2	314	8CT	C33-C32-C31	-10.24	115.06	124.83
25	6	319	8CT	C14-C13-C12	-10.24	112.92	127.28
25	J	104	8CT	C18-C17-C16	-10.22	112.94	127.28
24	B	823	CLA	O1A-CGA-CBA	-10.19	83.94	123.78
25	B	847	8CT	C33-C32-C31	-10.09	115.20	124.83
23	6	302	CHL	O2D-CGD-CBD	10.05	121.99	110.95
25	0	314	8CT	C33-C32-C31	-10.00	115.29	124.83
25	L	204	8CT	C33-C32-C31	-9.90	115.38	124.83
25	A	847	8CT	C33-C32-C31	-9.86	115.42	124.83
25	4	316	8CT	C33-C32-C31	-9.84	115.44	124.83
23	6	306	CHL	C1B-CHB-C4A	9.83	127.65	121.32
25	8	317	8CT	C33-C32-C31	-9.81	115.46	124.83
25	I	101	8CT	C33-C32-C31	-9.80	115.47	124.83
25	3	323	8CT	C14-C13-C12	-9.76	113.59	127.28
25	A	849	8CT	C33-C32-C31	-9.75	115.53	124.83
23	9	306	CHL	O2D-CGD-CBD	9.74	121.65	110.95
25	3	316	8CT	C14-C13-C12	-9.65	113.74	127.28
23	2	306	CHL	C1B-CHB-C4A	9.63	127.52	121.32
25	3	323	8CT	C10-C11-C12	-9.45	112.25	126.23
23	2	304	CHL	C1B-CHB-C4A	9.42	127.38	121.32
23	4	313	CHL	O2D-CGD-CBD	9.41	121.28	110.95
23	6	301	CHL	O2D-CGD-CBD	9.39	121.26	110.95
23	9	305	CHL	C1B-CHB-C4A	9.37	127.35	121.32
23	4	301	CHL	O2D-CGD-CBD	9.33	121.19	110.95
23	1	301	CHL	C1B-CHB-C4A	9.29	127.30	121.32
23	5	301	CHL	C1B-CHB-C4A	9.25	127.27	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	307	CHL	C1B-CHB-C4A	9.23	127.26	121.32
23	1	304	CHL	C1B-CHB-C4A	9.22	127.25	121.32
23	3	302	CHL	C1B-CHB-C4A	9.21	127.25	121.32
25	F	304	8CT	C33-C32-C31	-9.20	116.05	124.83
23	5	312	CHL	O2D-CGD-CBD	9.19	121.05	110.95
23	7	301	CHL	O2D-CGD-CBD	9.17	121.02	110.95
23	7	302	CHL	C1B-CHB-C4A	9.17	127.22	121.32
25	7	319	8CT	C33-C32-C31	-9.15	116.09	124.83
25	J	104	8CT	C10-C11-C12	-9.15	112.70	126.23
23	2	305	CHL	O2D-CGD-CBD	9.12	120.96	110.95
23	7	306	CHL	O2D-CGD-CBD	9.10	120.95	110.95
23	9	312	CHL	O2D-CGD-CBD	9.07	120.92	110.95
23	8	303	CHL	C1B-CHB-C4A	9.04	127.14	121.32
23	0	305	CHL	O2D-CGD-CBD	9.00	120.83	110.95
25	B	848	8CT	C33-C32-C31	-8.99	116.25	124.83
23	6	302	CHL	C1B-CHB-C4A	8.97	127.10	121.32
23	4	305	CHL	O2D-CGD-CBD	8.93	120.76	110.95
23	4	305	CHL	C1B-CHB-C4A	8.93	127.07	121.32
23	4	308	CHL	O2D-CGD-CBD	8.87	120.70	110.95
25	6	319	8CT	C18-C17-C16	-8.85	114.87	127.28
23	3	301	CHL	O2D-CGD-CBD	8.84	120.66	110.95
23	9	301	CHL	O2D-CGD-CBD	8.82	120.64	110.95
23	5	304	CHL	O2D-CGD-CBD	8.81	120.63	110.95
24	B	826	CLA	CBD-CHA-C1A	8.79	130.49	118.85
23	8	307	CHL	O2D-CGD-CBD	8.79	120.60	110.95
25	L	207	8CT	C33-C32-C31	-8.78	116.44	124.83
23	3	305	CHL	O2D-CGD-CBD	8.78	120.59	110.95
25	6	319	8CT	C10-C11-C12	-8.77	113.26	126.23
23	7	313	CHL	O2D-CGD-CBD	8.76	120.57	110.95
23	2	301	CHL	O2D-CGD-CBD	8.75	120.56	110.95
23	2	301	CHL	C1B-CHB-C4A	8.75	126.95	121.32
23	7	302	CHL	O2D-CGD-CBD	8.74	120.55	110.95
23	6	305	CHL	C1B-CHB-C4A	8.72	126.93	121.32
23	4	306	CHL	O2D-CGD-CBD	8.66	120.46	110.95
23	4	301	CHL	C1B-CHB-C4A	8.64	126.88	121.32
23	4	315	CHL	C1B-CHB-C4A	8.62	126.87	121.32
23	7	305	CHL	C1B-CHB-C4A	8.62	126.87	121.32
23	1	312	CHL	O2D-CGD-CBD	8.61	120.41	110.95
25	L	205	8CT	C33-C32-C31	-8.61	116.61	124.83
25	9	313	8CT	C33-C32-C31	-8.60	116.62	124.83
23	8	316	CHL	O2D-CGD-CBD	8.59	120.39	110.95
25	O	202	8CT	C33-C32-C31	-8.53	116.69	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	0	302	CHL	O2D-CGD-CBD	8.52	120.30	110.95
23	8	314	CHL	O2D-CGD-CBD	8.50	120.29	110.95
25	6	319	8CT	C33-C32-C31	-8.49	116.72	124.83
23	4	315	CHL	O2D-CGD-CBD	8.48	120.26	110.95
25	B	846	8CT	C33-C32-C31	-8.46	116.75	124.83
23	4	302	CHL	C1B-CHB-C4A	8.45	126.76	121.32
25	B	846	8CT	C24-C25-C26	-8.44	115.45	127.28
23	8	301	CHL	O2D-CGD-CBD	8.42	120.20	110.95
25	7	318	8CT	C33-C32-C31	-8.39	116.82	124.83
23	2	304	CHL	O2D-CGD-CBD	8.39	120.17	110.95
23	6	305	CHL	O2D-CGD-CBD	8.38	120.16	110.95
23	5	301	CHL	O2D-CGD-CBD	8.36	120.13	110.95
23	6	315	CHL	O2D-CGD-CBD	8.35	120.12	110.95
23	8	309	CHL	O2D-CGD-CBD	8.33	120.10	110.95
23	3	302	CHL	O2D-CGD-CBD	8.33	120.10	110.95
23	4	313	CHL	C1B-CHB-C4A	8.31	126.67	121.32
23	7	305	CHL	O2D-CGD-CBD	8.31	120.08	110.95
23	1	305	CHL	O2D-CGD-CBD	8.29	120.06	110.95
23	3	301	CHL	C1B-CHB-C4A	8.28	126.65	121.32
23	1	304	CHL	O2D-CGD-CBD	8.28	120.04	110.95
23	6	313	CHL	O2D-CGD-CBD	8.26	120.02	110.95
25	B	846	8CT	C10-C11-C12	-8.25	114.02	126.23
23	2	306	CHL	CHA-C1A-C2A	-8.23	113.98	133.31
23	6	313	CHL	C1B-CHB-C4A	8.20	126.60	121.32
23	7	302	CHL	CHA-C1A-C2A	-8.16	114.15	133.31
25	O	208	8CT	C33-C32-C31	-8.15	117.05	124.83
23	2	304	CHL	CHA-C1A-C2A	-8.15	114.18	133.31
23	3	302	CHL	CHA-C1A-C2A	-8.13	114.23	133.31
23	8	306	CHL	O2D-CGD-CBD	8.10	119.84	110.95
23	3	307	CHL	CHA-C1A-C2A	-8.10	114.30	133.31
25	B	850	8CT	C33-C32-C31	-8.10	117.10	124.83
23	9	305	CHL	CHA-C1A-C2A	-8.09	114.32	133.31
23	8	303	CHL	CHA-C1A-C2A	-8.08	114.33	133.31
25	K	105	8CT	C14-C13-C12	-8.08	115.94	127.28
23	3	307	CHL	O2D-CGD-CBD	8.07	119.82	110.95
23	1	304	CHL	CHA-C1A-C2A	-8.07	114.36	133.31
23	6	308	CHL	O2D-CGD-CBD	8.04	119.78	110.95
23	1	301	CHL	CHA-C1A-C2A	-8.02	114.47	133.31
23	6	306	CHL	CHA-C1A-C2A	-8.02	114.47	133.31
23	5	301	CHL	CHA-C1A-C2A	-8.02	114.47	133.31
23	4	302	CHL	O2D-CGD-CBD	8.01	119.75	110.95
23	6	305	CHL	CHA-C1A-C2A	-7.99	114.54	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2	301	CHL	CHA-C1A-C2A	-7.99	114.55	133.31
23	4	313	CHL	CHA-C1A-C2A	-7.99	114.55	133.31
23	8	306	CHL	CHA-C1A-C2A	-7.95	114.65	133.31
23	6	302	CHL	CHA-C1A-C2A	-7.95	114.65	133.31
25	A	847	8CT	C19-C18-C17	-7.95	107.26	123.52
25	G	104	8CT	C18-C17-C16	-7.93	116.15	127.28
25	L	205	8CT	C14-C13-C12	-7.92	116.17	127.28
23	1	301	CHL	O2D-CGD-CBD	7.92	119.65	110.95
25	B	845	8CT	C19-C18-C17	-7.90	107.36	123.52
23	9	305	CHL	O2D-CGD-CBD	7.88	119.60	110.95
23	8	314	CHL	CHA-C1A-C2A	-7.87	114.82	133.31
23	4	302	CHL	CHA-C1A-C2A	-7.87	114.83	133.31
23	4	306	CHL	CHA-C1A-C2A	-7.85	114.89	133.31
23	6	313	CHL	CHA-C1A-C2A	-7.84	114.90	133.31
23	4	305	CHL	CHA-C1A-C2A	-7.84	114.91	133.31
23	4	315	CHL	CHA-C1A-C2A	-7.83	114.92	133.31
23	9	312	CHL	CHA-C1A-C2A	-7.83	114.93	133.31
23	7	305	CHL	CHA-C1A-C2A	-7.83	114.94	133.31
23	4	307	CHL	C1B-CHB-C4A	7.81	126.35	121.32
23	4	307	CHL	CHA-C1A-C2A	-7.80	114.98	133.31
23	0	302	CHL	C1B-CHB-C4A	7.79	126.34	121.32
23	3	301	CHL	CHA-C1A-C2A	-7.79	115.02	133.31
23	2	305	CHL	CHA-C1A-C2A	-7.78	115.04	133.31
23	5	306	CHL	O2D-CGD-CBD	7.78	119.50	110.95
23	8	303	CHL	O2D-CGD-CBD	7.77	119.48	110.95
23	2	307	CHL	C1B-CHB-C4A	7.76	126.31	121.32
23	0	302	CHL	CHA-C1A-C2A	-7.76	115.09	133.31
25	B	846	8CT	C04-C03-C02	-7.76	112.04	122.64
23	5	305	CHL	O2D-CGD-CBD	7.75	119.47	110.95
23	2	307	CHL	CHA-C1A-C2A	-7.75	115.10	133.31
23	4	301	CHL	CHA-C1A-C2A	-7.75	115.11	133.31
23	6	301	CHL	CHA-C1A-C2A	-7.74	115.13	133.31
25	K	105	8CT	C18-C17-C16	-7.73	116.44	127.28
23	6	307	CHL	O2D-CGD-CBD	7.73	119.44	110.95
23	0	301	CHL	CHA-C1A-C2A	-7.72	115.19	133.31
23	6	306	CHL	O2D-CGD-CBD	7.71	119.42	110.95
23	8	308	CHL	CHA-C1A-C2A	-7.71	115.21	133.31
23	1	306	CHL	O2D-CGD-CBD	7.70	119.41	110.95
25	1	314	8CT	C33-C32-C31	-7.69	117.48	124.83
23	2	312	CHL	O2D-CGD-CBD	7.67	119.37	110.95
23	6	307	CHL	CHA-C1A-C2A	-7.67	115.31	133.31
23	4	306	CHL	C1B-CHB-C4A	7.64	126.24	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	849	8CT	C24-C25-C26	-7.64	116.56	127.28
23	4	307	CHL	O2D-CGD-CBD	7.64	119.34	110.95
23	9	306	CHL	CHA-C1A-C2A	-7.62	115.41	133.31
23	8	309	CHL	CHA-C1A-C2A	-7.60	115.45	133.31
25	B	843	8CT	C18-C17-C16	-7.56	116.68	127.28
23	3	305	CHL	CHA-C1A-C2A	-7.54	115.60	133.31
25	6	324	8CT	C33-C32-C31	-7.53	117.64	124.83
25	A	846	8CT	C10-C11-C12	-7.53	115.10	126.23
23	1	312	CHL	CHA-C1A-C2A	-7.52	115.65	133.31
23	2	312	CHL	CHA-C1A-C2A	-7.51	115.68	133.31
25	3	323	8CT	C29-C28-C26	-7.50	110.19	126.32
23	9	312	CHL	C1B-CHB-C4A	7.50	126.15	121.32
23	8	308	CHL	O2D-CGD-CBD	7.50	119.19	110.95
23	6	308	CHL	CHA-C1A-C2A	-7.49	115.71	133.31
25	6	319	8CT	C24-C25-C26	-7.48	116.78	127.28
23	8	314	CHL	C1B-CHB-C4A	7.46	126.12	121.32
23	7	306	CHL	CHA-C1A-C2A	-7.46	115.79	133.31
25	A	845	8CT	C30-C29-C28	-7.46	112.97	124.58
23	5	304	CHL	CHA-C1A-C2A	-7.46	115.80	133.31
23	0	306	CHL	CHA-C1A-C2A	-7.46	115.80	133.31
23	0	305	CHL	CHA-C1A-C2A	-7.44	115.83	133.31
25	4	316	8CT	C30-C31-C32	-7.44	112.31	121.47
25	3	317	8CT	C33-C32-C31	-7.42	117.75	124.83
25	3	323	8CT	C18-C17-C16	-7.41	116.88	127.28
23	7	301	CHL	CHA-C1A-C2A	-7.41	115.91	133.31
23	9	301	CHL	CHA-C1A-C2A	-7.39	115.96	133.31
23	2	306	CHL	O2D-CGD-CBD	7.38	119.06	110.95
23	4	308	CHL	CHA-C1A-C2A	-7.37	115.99	133.31
23	8	307	CHL	CHA-C1A-C2A	-7.37	116.00	133.31
25	F	301	8CT	C33-C32-C31	-7.36	117.80	124.83
23	8	308	CHL	C1B-CHB-C4A	7.33	126.04	121.32
23	6	315	CHL	CHA-C1A-C2A	-7.30	116.16	133.31
25	B	847	8CT	C30-C31-C32	-7.29	112.50	121.47
23	0	301	CHL	C1B-CHB-C4A	7.29	126.01	121.32
25	3	316	8CT	C30-C31-C32	-7.27	112.53	121.47
23	6	323	CHL	CHA-C1A-C2A	-7.24	116.32	133.31
25	B	847	8CT	C14-C13-C12	-7.23	117.14	127.28
23	9	306	CHL	C1B-CHB-C4A	7.19	125.95	121.32
23	5	306	CHL	CHA-C1A-C2A	-7.18	116.46	133.31
23	2	307	CHL	O2D-CGD-CBD	7.15	118.81	110.95
25	J	101	8CT	C30-C31-C32	-7.14	112.68	121.47
23	1	306	CHL	CHA-C1A-C2A	-7.13	116.56	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	7	307	CHL	O2D-CGD-CBD	7.09	118.74	110.95
24	3	304	CLA	C4A-NA-C1A	7.09	109.91	106.68
23	1	305	CHL	CHA-C1A-C2A	-7.09	116.67	133.31
24	7	316	CLA	C4A-NA-C1A	7.06	109.90	106.68
23	7	307	CHL	CHA-C1A-C2A	-7.06	116.73	133.31
23	8	301	CHL	CHA-C1A-C2A	-7.04	116.77	133.31
24	H	204	CLA	C4A-NA-C1A	7.04	109.89	106.68
23	3	307	CHL	OBD-CAD-CBD	7.03	136.15	125.82
24	3	311	CLA	C4A-NA-C1A	6.97	109.86	106.68
24	B	821	CLA	C4A-NA-C1A	6.97	109.86	106.68
23	8	316	CHL	CHA-C1A-C2A	-6.96	116.96	133.31
24	A	815	CLA	C4A-NA-C1A	6.96	109.86	106.68
23	2	306	CHL	OBD-CAD-CBD	6.96	136.04	125.82
24	B	832	CLA	C4A-NA-C1A	6.96	109.85	106.68
25	O	208	8CT	C14-C13-C12	-6.95	117.53	127.28
24	B	835	CLA	C4A-NA-C1A	6.95	109.85	106.68
23	7	313	CHL	CHA-C1A-C2A	-6.94	117.01	133.31
25	B	843	8CT	C19-C20-C21	-6.94	117.55	127.28
25	L	207	8CT	C10-C11-C12	-6.94	115.97	126.23
23	8	306	CHL	C1B-CHB-C4A	6.93	125.78	121.32
23	5	305	CHL	CHA-C1A-C2A	-6.92	117.05	133.31
23	0	301	CHL	O2D-CGD-CBD	6.92	118.55	110.95
24	9	307	CLA	C4A-NA-C1A	6.91	109.83	106.68
25	A	849	8CT	C14-C13-C12	-6.90	117.61	127.28
24	5	302	CLA	C4A-NA-C1A	6.90	109.83	106.68
24	2	310	CLA	C4A-NA-C1A	6.89	109.82	106.68
25	B	843	8CT	C33-C32-C31	-6.89	118.25	124.83
25	A	844	8CT	C14-C13-C12	-6.88	117.63	127.28
25	A	847	8CT	C04-C03-C02	-6.87	113.25	122.64
24	A	836	CLA	C4A-NA-C1A	6.87	109.81	106.68
26	2	316	0UR	C14-C15-C16	-6.86	117.66	127.28
24	B	837	CLA	C4A-NA-C1A	6.85	109.80	106.68
24	A	816	CLA	C4A-NA-C1A	6.84	109.80	106.68
25	L	204	8CT	C30-C31-C32	-6.83	113.06	121.47
24	B	817	CLA	C4A-NA-C1A	6.83	109.80	106.68
24	A	833	CLA	C4A-NA-C1A	6.83	109.79	106.68
24	1	310	CLA	C4A-NA-C1A	6.82	109.79	106.68
23	8	309	CHL	C1B-CHB-C4A	6.82	125.71	121.32
24	5	311	CLA	C4A-NA-C1A	6.81	109.79	106.68
24	9	303	CLA	C4A-NA-C1A	6.81	109.79	106.68
24	0	310	CLA	C4A-NA-C1A	6.80	109.78	106.68
24	A	819	CLA	C4A-NA-C1A	6.79	109.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	807	CLA	C4A-NA-C1A	6.79	109.78	106.68
25	G	104	8CT	C10-C11-C12	-6.79	116.19	126.23
24	B	840	CLA	C4A-NA-C1A	6.79	109.78	106.68
24	1	309	CLA	C4A-NA-C1A	6.78	109.77	106.68
24	O	201	CLA	C4A-NA-C1A	6.77	109.77	106.68
25	2	314	8CT	C30-C31-C32	-6.77	113.14	121.47
24	B	808	CLA	C4A-NA-C1A	6.77	109.77	106.68
24	A	807	CLA	C4A-NA-C1A	6.76	109.77	106.68
24	1	302	CLA	C4A-NA-C1A	6.76	109.76	106.68
24	B	827	CLA	C4A-NA-C1A	6.76	109.76	106.68
24	A	829	CLA	C4A-NA-C1A	6.76	109.76	106.68
24	L	202	CLA	C4A-NA-C1A	6.76	109.76	106.68
24	A	808	CLA	C4A-NA-C1A	6.75	109.76	106.68
24	6	303	CLA	C4A-NA-C1A	6.74	109.76	106.68
24	A	803	CLA	C4A-NA-C1A	6.74	109.76	106.68
25	A	845	8CT	C30-C31-C32	-6.74	113.17	121.47
24	B	816	CLA	C4A-NA-C1A	6.74	109.75	106.68
23	3	305	CHL	C1B-CHB-C4A	6.73	125.65	121.32
24	7	314	CLA	C4A-NA-C1A	6.73	109.75	106.68
24	1	311	CLA	C4A-NA-C1A	6.72	109.75	106.68
24	3	308	CLA	C4A-NA-C1A	6.71	109.74	106.68
24	3	315	CLA	C4A-NA-C1A	6.71	109.74	106.68
24	7	309	CLA	C4A-NA-C1A	6.71	109.74	106.68
24	B	810	CLA	C4A-NA-C1A	6.70	109.74	106.68
24	B	838	CLA	C4A-NA-C1A	6.70	109.74	106.68
24	A	826	CLA	C4A-NA-C1A	6.69	109.73	106.68
25	A	845	8CT	C18-C17-C16	-6.69	117.90	127.28
24	7	311	CLA	C4A-NA-C1A	6.68	109.73	106.68
24	B	811	CLA	C4A-NA-C1A	6.67	109.72	106.68
25	2	314	8CT	C18-C17-C16	-6.67	117.92	127.28
24	0	319	CLA	C4A-NA-C1A	6.66	109.72	106.68
26	2	315	0UR	C4-C3-C2	-6.65	114.37	120.16
24	A	832	CLA	C4A-NA-C1A	6.65	109.71	106.68
24	2	302	CLA	C4A-NA-C1A	6.64	109.71	106.68
24	8	313	CLA	C4A-NA-C1A	6.63	109.70	106.68
24	B	818	CLA	C4A-NA-C1A	6.63	109.70	106.68
24	0	308	CLA	C4A-NA-C1A	6.61	109.69	106.68
23	2	305	CHL	C1B-CHB-C4A	6.61	125.57	121.32
24	B	822	CLA	C4A-NA-C1A	6.59	109.69	106.68
24	K	103	CLA	C4A-NA-C1A	6.59	109.69	106.68
24	A	814	CLA	C4A-NA-C1A	6.59	109.68	106.68
24	A	817	CLA	C4A-NA-C1A	6.59	109.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	316	8CT	C18-C17-C16	-6.58	118.04	127.28
24	7	304	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	4	310	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	6	304	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	B	812	CLA	C4A-NA-C1A	6.58	109.68	106.68
24	2	311	CLA	C4A-NA-C1A	6.58	109.68	106.68
23	5	312	CHL	C4D-ND-C1D	6.57	110.21	105.22
25	A	845	8CT	C14-C13-C12	-6.57	118.07	127.28
24	B	806	CLA	C4A-NA-C1A	6.57	109.67	106.68
24	1	307	CLA	C4A-NA-C1A	6.56	109.67	106.68
24	H	201	CLA	C4A-NA-C1A	6.55	109.67	106.68
24	A	839	CLA	C4A-NA-C1A	6.55	109.67	106.68
24	A	838	CLA	C4A-NA-C1A	6.54	109.66	106.68
24	G	102	CLA	C4A-NA-C1A	6.54	109.66	106.68
24	G	101	CLA	C4A-NA-C1A	6.54	109.66	106.68
24	8	315	CLA	C4A-NA-C1A	6.53	109.66	106.68
24	6	314	CLA	C4A-NA-C1A	6.53	109.66	106.68
24	7	315	CLA	C4A-NA-C1A	6.53	109.66	106.68
24	5	310	CLA	C4A-NA-C1A	6.53	109.66	106.68
24	6	311	CLA	C4A-NA-C1A	6.52	109.66	106.68
24	H	205	CLA	C4A-NA-C1A	6.52	109.66	106.68
24	A	830	CLA	C4A-NA-C1A	6.52	109.65	106.68
24	7	317	CLA	C4A-NA-C1A	6.51	109.65	106.68
24	A	813	CLA	C4A-NA-C1A	6.51	109.65	106.68
23	6	301	CHL	C1B-CHB-C4A	6.50	125.51	121.32
24	7	308	CLA	C4A-NA-C1A	6.50	109.65	106.68
24	0	311	CLA	C4A-NA-C1A	6.50	109.64	106.68
24	9	308	CLA	C4A-NA-C1A	6.50	109.64	106.68
24	A	840	CLA	C4A-NA-C1A	6.50	109.64	106.68
24	6	318	CLA	C4A-NA-C1A	6.49	109.64	106.68
24	A	810	CLA	C4A-NA-C1A	6.49	109.64	106.68
24	4	312	CLA	C4A-NA-C1A	6.49	109.64	106.68
24	B	823	CLA	C4A-NA-C1A	6.48	109.64	106.68
24	A	822	CLA	C4A-NA-C1A	6.47	109.63	106.68
24	4	311	CLA	C4A-NA-C1A	6.47	109.63	106.68
24	J	103	CLA	C4A-NA-C1A	6.46	109.63	106.68
23	9	301	CHL	C1B-CHB-C4A	6.46	125.48	121.32
24	B	805	CLA	C4A-NA-C1A	6.45	109.62	106.68
24	B	815	CLA	C4A-NA-C1A	6.45	109.62	106.68
24	0	304	CLA	C4A-NA-C1A	6.45	109.62	106.68
25	M	102	8CT	C10-C11-C12	-6.45	116.70	126.23
24	3	306	CLA	C4A-NA-C1A	6.45	109.62	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	310	CLA	C4A-NA-C1A	6.45	109.62	106.68
24	B	825	CLA	C4A-NA-C1A	6.44	109.62	106.68
24	A	834	CLA	C4A-NA-C1A	6.44	109.62	106.68
24	0	313	CLA	C4A-NA-C1A	6.43	109.61	106.68
24	F	302	CLA	C4A-NA-C1A	6.43	109.61	106.68
24	5	303	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	H	203	CLA	C4A-NA-C1A	6.42	109.61	106.68
25	F	304	8CT	C14-C13-C12	-6.41	118.29	127.28
24	0	303	CLA	C4A-NA-C1A	6.40	109.60	106.68
25	B	846	8CT	C19-C20-C21	-6.40	118.31	127.28
24	6	317	CLA	C4A-NA-C1A	6.39	109.60	106.68
26	5	315	0UR	C14-C15-C16	-6.39	118.31	127.28
24	A	821	CLA	C4A-NA-C1A	6.39	109.59	106.68
24	6	312	CLA	C4A-NA-C1A	6.38	109.59	106.68
23	3	307	CHL	OBD-CAD-C3D	-6.38	117.94	127.89
24	A	828	CLA	C4A-NA-C1A	6.38	109.59	106.68
24	B	833	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	A	844	8CT	C30-C29-C28	-6.38	114.65	124.58
24	5	309	CLA	C4A-NA-C1A	6.38	109.59	106.68
24	B	834	CLA	C4A-NA-C1A	6.37	109.59	106.68
25	F	301	8CT	C18-C17-C16	-6.37	118.35	127.28
24	7	303	CLA	C4A-NA-C1A	6.37	109.58	106.68
24	8	304	CLA	C4A-NA-C1A	6.36	109.58	106.68
24	9	311	CLA	C4A-NA-C1A	6.35	109.58	106.68
24	3	310	CLA	C4A-NA-C1A	6.35	109.58	106.68
24	1	313	CLA	C4A-NA-C1A	6.35	109.58	106.68
24	A	804	CLA	C4A-NA-C1A	6.35	109.57	106.68
25	F	301	8CT	C14-C13-C12	-6.34	118.38	127.28
24	O	204	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	1	314	8CT	C24-C25-C26	-6.34	118.39	127.28
24	6	310	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	O	208	8CT	C10-C11-C12	-6.34	116.86	126.23
24	0	307	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	6	319	8CT	C01-C02-C03	-6.33	117.58	124.48
24	K	104	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	O	202	8CT	C30-C29-C28	-6.33	114.73	124.58
24	B	819	CLA	C4A-NA-C1A	6.32	109.56	106.68
25	1	314	8CT	C18-C17-C16	-6.32	118.41	127.28
24	2	303	CLA	C4A-NA-C1A	6.32	109.56	106.68
24	A	827	CLA	C4A-NA-C1A	6.32	109.56	106.68
24	B	802	CLA	C4A-NA-C1A	6.32	109.56	106.68
24	O	206	CLA	C4A-NA-C1A	6.32	109.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	302	CLA	C4A-NA-C1A	6.32	109.56	106.68
24	B	814	CLA	C4A-NA-C1A	6.32	109.56	106.68
24	A	802	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	A	831	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	B	836	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	B	839	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	L	201	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	7	312	CLA	C4A-NA-C1A	6.30	109.56	106.68
24	8	310	CLA	C4A-NA-C1A	6.30	109.55	106.68
24	B	828	CLA	C4A-NA-C1A	6.30	109.55	106.68
24	A	805	CLA	C4A-NA-C1A	6.29	109.55	106.68
24	9	304	CLA	C4A-NA-C1A	6.29	109.55	106.68
23	5	312	CHL	CHA-C1A-C2A	-6.29	118.55	133.31
24	1	308	CLA	C4A-NA-C1A	6.29	109.55	106.68
26	3	318	0UR	C4-C3-C2	-6.29	114.69	120.16
24	B	801	CLA	C4A-NA-C1A	6.28	109.55	106.68
24	B	820	CLA	C4A-NA-C1A	6.28	109.54	106.68
24	5	313	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	K	101	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	B	809	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	2	309	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	2	313	CLA	C4A-NA-C1A	6.27	109.54	106.68
24	6	309	CLA	C4A-NA-C1A	6.26	109.54	106.68
24	8	312	CLA	C4A-NA-C1A	6.26	109.54	106.68
24	A	806	CLA	C4A-NA-C1A	6.26	109.53	106.68
24	K	102	CLA	C4A-NA-C1A	6.26	109.53	106.68
23	6	307	CHL	OBD-CAD-CBD	6.26	135.01	125.82
24	L	206	CLA	C4A-NA-C1A	6.26	109.53	106.68
25	6	324	8CT	C30-C29-C28	-6.25	114.85	124.58
24	B	831	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	3	303	CLA	C4A-NA-C1A	6.24	109.53	106.68
25	B	848	8CT	C10-C11-C12	-6.24	117.01	126.23
24	L	203	CLA	C4A-NA-C1A	6.23	109.52	106.68
24	1	303	CLA	C4A-NA-C1A	6.22	109.52	106.68
24	9	309	CLA	C4A-NA-C1A	6.22	109.52	106.68
24	4	314	CLA	C4A-NA-C1A	6.22	109.52	106.68
25	A	844	8CT	C18-C17-C16	-6.22	118.55	127.28
26	7	320	0UR	C4-C3-C2	-6.22	114.75	120.16
24	5	307	CLA	C4A-NA-C1A	6.22	109.52	106.68
24	G	103	CLA	C4A-NA-C1A	6.22	109.52	106.68
24	3	312	CLA	C4A-NA-C1A	6.21	109.51	106.68
24	A	809	CLA	C4A-NA-C1A	6.20	109.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	309	CLA	C4A-NA-C1A	6.20	109.51	106.68
24	H	202	CLA	C4A-NA-C1A	6.19	109.50	106.68
23	6	308	CHL	C1B-CHB-C4A	6.18	125.30	121.32
25	A	846	8CT	C18-C17-C16	-6.18	118.61	127.28
23	2	306	CHL	OBD-CAD-C3D	-6.18	118.25	127.89
24	A	835	CLA	C4A-NA-C1A	6.18	109.50	106.68
24	B	813	CLA	C4A-NA-C1A	6.17	109.50	106.68
24	7	310	CLA	C4A-NA-C1A	6.17	109.49	106.68
24	A	825	CLA	C4A-NA-C1A	6.16	109.49	106.68
25	2	314	8CT	C07-C02-C03	-6.16	114.38	122.70
24	2	308	CLA	C4A-NA-C1A	6.16	109.49	106.68
24	A	812	CLA	C4A-NA-C1A	6.15	109.49	106.68
25	B	843	8CT	C14-C13-C12	-6.15	118.65	127.28
25	9	313	8CT	C19-C20-C21	-6.15	118.66	127.28
24	4	303	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	F	301	8CT	C10-C11-C12	-6.14	117.15	126.23
24	O	209	CLA	C4A-NA-C1A	6.14	109.48	106.68
23	2	312	CHL	C1B-CHB-C4A	6.13	125.27	121.32
25	O	202	8CT	C04-C03-C02	-6.13	114.26	122.64
23	5	305	CHL	C4D-ND-C1D	6.13	109.87	105.22
25	B	847	8CT	C35-C30-C29	-6.12	105.78	112.83
23	4	307	CHL	OBD-CAD-CBD	6.11	134.79	125.82
24	0	312	CLA	C4A-NA-C1A	6.10	109.46	106.68
23	8	316	CHL	C4D-ND-C1D	6.09	109.84	105.22
23	5	306	CHL	C4D-ND-C1D	6.08	109.83	105.22
24	3	314	CLA	C4A-NA-C1A	6.08	109.45	106.68
24	F	303	CLA	C4A-NA-C1A	6.07	109.45	106.68
24	3	313	CLA	C4A-NA-C1A	6.07	109.45	106.68
24	A	837	CLA	C4A-NA-C1A	6.06	109.45	106.68
25	9	313	8CT	C10-C11-C12	-6.06	117.27	126.23
25	7	318	8CT	C35-C30-C29	-6.06	105.86	112.83
24	3	309	CLA	C4A-NA-C1A	6.05	109.44	106.68
24	A	820	CLA	C4A-NA-C1A	6.05	109.44	106.68
24	A	824	CLA	C4A-NA-C1A	6.05	109.44	106.68
24	4	304	CLA	C4A-NA-C1A	6.04	109.44	106.68
24	A	848	CLA	C4A-NA-C1A	6.03	109.43	106.68
24	A	823	CLA	C4A-NA-C1A	6.02	109.43	106.68
24	6	316	CLA	C4A-NA-C1A	6.02	109.43	106.68
23	8	307	CHL	C1B-CHB-C4A	6.02	125.19	121.32
24	A	818	CLA	C4A-NA-C1A	6.02	109.42	106.68
24	B	824	CLA	C4A-NA-C1A	6.01	109.42	106.68
26	0	316	0UR	C4-C3-C2	-6.00	114.93	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	314	8CT	C14-C13-C12	-5.99	118.88	127.28
25	L	204	8CT	C24-C25-C26	-5.98	118.89	127.28
24	8	311	CLA	C4A-NA-C1A	5.97	109.40	106.68
25	3	323	8CT	C19-C20-C21	-5.97	118.90	127.28
24	8	305	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	F	304	8CT	C18-C17-C16	-5.96	118.92	127.28
23	6	323	CHL	C1A-CHA-C4D	-5.95	109.06	118.98
25	A	847	8CT	C29-C28-C26	-5.95	113.53	126.32
25	A	847	8CT	C07-C02-C03	-5.93	114.69	122.70
25	A	846	8CT	C30-C31-C32	-5.92	114.18	121.47
25	M	102	8CT	C14-C13-C12	-5.92	118.98	127.28
25	J	101	8CT	C19-C20-C21	-5.92	118.98	127.28
23	6	307	CHL	C1A-CHA-C4D	-5.91	109.13	118.98
26	4	317	0UR	C43-C3-C4	-5.90	118.07	125.03
23	0	306	CHL	C1A-CHA-C4D	-5.89	109.15	118.98
24	O	205	CLA	C4A-NA-C1A	5.89	109.37	106.68
24	A	811	CLA	C4A-NA-C1A	5.88	109.36	106.68
23	0	305	CHL	C1B-CHB-C4A	5.88	125.10	121.32
25	F	304	8CT	C19-C20-C21	-5.88	119.04	127.28
24	B	841	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	0	314	8CT	C19-C20-C21	-5.85	119.07	127.28
24	B	829	CLA	C4A-NA-C1A	5.85	109.35	106.68
24	A	853	CLA	C4A-NA-C1A	5.85	109.35	106.68
25	B	847	8CT	C24-C25-C26	-5.84	119.09	127.28
25	F	304	8CT	C24-C25-C26	-5.84	119.09	127.28
25	1	314	8CT	C19-C20-C21	-5.83	119.10	127.28
23	2	304	CHL	C1A-CHA-C4D	-5.82	109.27	118.98
25	L	205	8CT	C18-C17-C16	-5.82	119.12	127.28
24	A	801	CLA	C4A-NA-C1A	5.81	109.33	106.68
23	2	312	CHL	C1A-CHA-C4D	-5.81	109.29	118.98
26	4	317	0UR	C4-C3-C2	-5.81	115.10	120.16
23	8	316	CHL	C1A-CHA-C4D	-5.81	109.30	118.98
23	1	306	CHL	C1A-CHA-C4D	-5.79	109.32	118.98
26	8	319	0UR	C14-C15-C16	-5.79	119.16	127.28
24	B	826	CLA	C4A-NA-C1A	5.78	109.32	106.68
23	4	308	CHL	C4D-ND-C1D	5.77	109.60	105.22
25	B	847	8CT	C18-C17-C16	-5.77	119.19	127.28
23	6	313	CHL	C1A-CHA-C4D	-5.76	109.38	118.98
24	B	830	CLA	C4A-NA-C1A	5.75	109.30	106.68
23	6	307	CHL	C1B-CHB-C4A	5.74	125.01	121.32
23	2	306	CHL	C1A-CHA-C4D	-5.74	109.41	118.98
25	2	314	8CT	C01-C02-C03	-5.73	118.23	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1	304	CHL	C1A-CHA-C4D	-5.73	109.43	118.98
23	9	312	CHL	C1A-CHA-C4D	-5.72	109.44	118.98
23	7	307	CHL	C1A-CHA-C4D	-5.72	109.44	118.98
24	4	309	CLA	C4A-NA-C1A	5.70	109.28	106.68
25	3	317	8CT	C24-C25-C26	-5.70	119.28	127.28
23	0	305	CHL	C1A-CHA-C4D	-5.69	109.48	118.98
23	8	314	CHL	C1A-CHA-C4D	-5.69	109.49	118.98
24	5	308	CLA	C4A-NA-C1A	5.69	109.27	106.68
25	L	204	8CT	C18-C17-C16	-5.68	119.31	127.28
23	3	307	CHL	C1A-CHA-C4D	-5.68	109.50	118.98
25	B	845	8CT	C04-C03-C02	-5.67	114.89	122.64
23	7	313	CHL	C1A-CHA-C4D	-5.67	109.52	118.98
23	6	307	CHL	OBD-CAD-C3D	-5.67	119.05	127.89
23	6	308	CHL	C1A-CHA-C4D	-5.67	109.53	118.98
23	1	305	CHL	C4D-ND-C1D	5.66	109.52	105.22
23	8	306	CHL	C1A-CHA-C4D	-5.66	109.54	118.98
23	4	301	CHL	C1A-CHA-C4D	-5.66	109.54	118.98
23	4	308	CHL	C1B-CHB-C4A	5.66	124.96	121.32
26	8	319	0UR	C19-C18-C17	-5.65	115.78	124.58
23	3	305	CHL	C1A-CHA-C4D	-5.65	109.55	118.98
23	9	305	CHL	C1A-CHA-C4D	-5.65	109.56	118.98
23	1	306	CHL	C4D-ND-C1D	5.63	109.49	105.22
23	4	315	CHL	C1A-CHA-C4D	-5.63	109.59	118.98
25	8	317	8CT	C30-C31-C32	-5.62	114.55	121.47
23	7	302	CHL	C1A-CHA-C4D	-5.62	109.61	118.98
25	7	319	8CT	C01-C02-C03	-5.62	118.36	124.48
23	5	304	CHL	C1A-CHA-C4D	-5.60	109.63	118.98
23	8	309	CHL	C1A-CHA-C4D	-5.60	109.63	118.98
23	1	312	CHL	C1A-CHA-C4D	-5.60	109.63	118.98
23	5	305	CHL	C1A-CHA-C4D	-5.60	109.64	118.98
23	8	301	CHL	C4D-ND-C1D	5.59	109.47	105.22
23	8	301	CHL	C1A-CHA-C4D	-5.59	109.65	118.98
25	B	846	8CT	C29-C28-C26	-5.58	114.32	126.32
23	6	315	CHL	C4D-ND-C1D	5.58	109.45	105.22
23	7	313	CHL	C4D-ND-C1D	5.58	109.45	105.22
23	0	306	CHL	C4D-ND-C1D	5.57	109.45	105.22
25	I	101	8CT	C14-C13-C12	-5.56	119.47	127.28
25	8	317	8CT	C18-C17-C16	-5.56	119.48	127.28
23	6	305	CHL	C1A-CHA-C4D	-5.56	109.71	118.98
25	7	319	8CT	C14-C13-C12	-5.56	119.49	127.28
23	6	323	CHL	C4D-ND-C1D	5.55	109.43	105.22
25	2	314	8CT	C14-C13-C12	-5.55	119.50	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4	307	CHL	C1A-CHA-C4D	-5.54	109.73	118.98
23	6	315	CHL	C1A-CHA-C4D	-5.54	109.73	118.98
24	B	804	CLA	C4A-NA-C1A	5.54	109.21	106.68
25	1	314	8CT	C01-C02-C03	-5.54	118.44	124.48
23	7	306	CHL	C4D-ND-C1D	5.54	109.42	105.22
24	B	826	CLA	CBD-CHA-C4D	-5.53	107.53	117.29
25	0	314	8CT	C04-C03-C02	-5.52	115.09	122.64
23	5	306	CHL	C1A-CHA-C4D	-5.52	109.78	118.98
25	B	850	8CT	C10-C11-C12	-5.51	118.08	126.23
25	A	847	8CT	C01-C02-C03	-5.51	118.47	124.48
25	L	204	8CT	C14-C13-C12	-5.51	119.55	127.28
25	M	102	8CT	C19-C20-C21	-5.51	119.55	127.28
25	B	845	8CT	C14-C13-C12	-5.51	119.56	127.28
23	3	302	CHL	C1A-CHA-C4D	-5.51	109.80	118.98
25	7	319	8CT	C10-C11-C12	-5.51	118.09	126.23
23	6	306	CHL	C1A-CHA-C4D	-5.50	109.80	118.98
23	8	307	CHL	C1A-CHA-C4D	-5.50	109.80	118.98
23	1	305	CHL	C1A-CHA-C4D	-5.50	109.80	118.98
26	3	318	0UR	C43-C3-C4	-5.50	118.53	125.03
23	4	305	CHL	C1A-CHA-C4D	-5.50	109.80	118.98
25	J	104	8CT	C11-C12-C13	5.47	127.61	119.01
23	1	306	CHL	OBD-CAD-CBD	5.47	133.85	125.82
23	0	301	CHL	C1A-CHA-C4D	-5.47	109.86	118.98
25	6	324	8CT	C10-C11-C12	-5.47	118.14	126.23
23	8	308	CHL	C1A-CHA-C4D	-5.47	109.86	118.98
25	A	849	8CT	C19-C20-C21	-5.46	119.62	127.28
23	2	305	CHL	C1A-CHA-C4D	-5.46	109.88	118.98
23	4	306	CHL	C1A-CHA-C4D	-5.45	109.89	118.98
23	6	301	CHL	C1A-CHA-C4D	-5.44	109.90	118.98
25	8	317	8CT	C30-C29-C28	-5.44	116.11	124.58
23	7	305	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
25	A	846	8CT	C14-C13-C12	-5.43	119.66	127.28
25	K	105	8CT	C07-C02-C03	-5.43	115.36	122.70
23	7	301	CHL	C1A-CHA-C4D	-5.43	109.92	118.98
25	7	319	8CT	C24-C25-C26	-5.43	119.67	127.28
23	5	304	CHL	C4D-ND-C1D	5.42	109.33	105.22
23	8	309	CHL	C4D-ND-C1D	5.42	109.33	105.22
23	4	307	CHL	OBD-CAD-C3D	-5.41	119.45	127.89
25	3	316	8CT	C01-C02-C03	-5.41	118.58	124.48
25	L	207	8CT	C01-C02-C03	-5.41	118.58	124.48
23	6	302	CHL	OBD-CAD-CBD	5.41	133.76	125.82
23	4	308	CHL	C1A-CHA-C4D	-5.40	109.97	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2	301	CHL	C1A-CHA-C4D	-5.40	109.97	118.98
25	8	317	8CT	C01-C02-C03	-5.40	118.59	124.48
23	7	306	CHL	C1A-CHA-C4D	-5.39	109.98	118.98
23	9	306	CHL	C4D-ND-C1D	5.39	109.31	105.22
25	3	323	8CT	C28-C26-C25	5.39	127.49	119.01
23	7	306	CHL	C1B-CHB-C4A	5.39	124.79	121.32
26	6	320	0UR	C10-C11-C12	-5.38	119.73	127.28
25	9	313	8CT	C01-C02-C03	-5.38	118.61	124.48
25	7	318	8CT	C18-C17-C16	-5.38	119.73	127.28
25	B	843	8CT	C24-C25-C26	-5.38	119.73	127.28
23	4	302	CHL	C1A-CHA-C4D	-5.38	110.01	118.98
23	1	301	CHL	C1A-CHA-C4D	-5.37	110.03	118.98
23	6	308	CHL	C4D-ND-C1D	5.37	109.29	105.22
26	O	207	0UR	C9-C8-C7	-5.35	119.77	127.28
23	8	303	CHL	C1A-CHA-C4D	-5.35	110.05	118.98
25	O	202	8CT	C07-C02-C03	-5.35	115.47	122.70
23	9	301	CHL	C1A-CHA-C4D	-5.35	110.05	118.98
25	4	316	8CT	C07-C02-C03	-5.35	115.47	122.70
25	0	314	8CT	C30-C31-C32	-5.35	114.89	121.47
26	7	320	0UR	C43-C3-C4	-5.34	118.73	125.03
23	3	301	CHL	C1A-CHA-C4D	-5.34	110.08	118.98
23	7	301	CHL	C4D-ND-C1D	5.33	109.27	105.22
23	1	312	CHL	C4D-ND-C1D	5.32	109.26	105.22
25	7	318	8CT	C19-C20-C21	-5.32	119.82	127.28
23	2	307	CHL	C1A-CHA-C4D	-5.31	110.12	118.98
23	0	302	CHL	C1A-CHA-C4D	-5.31	110.12	118.98
25	J	104	8CT	C13-C14-C15	-5.30	107.84	123.20
23	4	313	CHL	C1A-CHA-C4D	-5.30	110.15	118.98
25	G	104	8CT	C30-C31-C32	-5.27	114.99	121.47
23	6	302	CHL	C1A-CHA-C4D	-5.27	110.19	118.98
23	5	304	CHL	C1B-CHB-C4A	5.27	124.71	121.32
25	A	849	8CT	C30-C31-C32	-5.25	115.01	121.47
23	5	301	CHL	C1A-CHA-C4D	-5.25	110.22	118.98
25	K	105	8CT	C30-C31-C32	-5.25	115.01	121.47
25	0	314	8CT	C01-C02-C03	-5.25	118.76	124.48
25	4	316	8CT	C01-C02-C03	-5.25	118.76	124.48
23	9	306	CHL	C1A-CHA-C4D	-5.24	110.24	118.98
23	7	307	CHL	OBD-CAD-CBD	5.23	133.50	125.82
26	5	315	0UR	C9-C8-C7	-5.22	119.95	127.28
25	I	101	8CT	C10-C11-C12	-5.22	118.51	126.23
25	9	313	8CT	C18-C17-C16	-5.22	119.96	127.28
25	3	317	8CT	C14-C13-C12	-5.22	119.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	306	CHL	OBD-CAD-CBD	5.22	133.48	125.82
25	B	845	8CT	C18-C19-C20	5.21	134.18	123.52
23	1	312	CHL	C1B-CHB-C4A	5.21	124.67	121.32
25	3	317	8CT	C04-C03-C02	-5.21	115.52	122.64
23	7	307	CHL	C4D-ND-C1D	5.20	109.16	105.22
23	2	312	CHL	C4D-ND-C1D	5.19	109.16	105.22
25	B	848	8CT	C29-C28-C26	-5.19	115.16	126.32
25	K	105	8CT	C01-C02-C03	-5.19	118.83	124.48
23	0	305	CHL	C4D-ND-C1D	5.18	109.15	105.22
26	2	316	0UR	C19-C18-C17	-5.18	116.51	124.58
23	8	308	CHL	OBD-CAD-CBD	5.18	133.43	125.82
23	4	301	CHL	OBD-CAD-CBD	5.18	133.43	125.82
23	9	306	CHL	OBD-CAD-CBD	5.18	133.42	125.82
23	5	312	CHL	C1A-CHA-C4D	-5.16	110.37	118.98
26	4	318	0UR	C19-C18-C17	-5.16	116.55	124.58
23	9	301	CHL	C4D-ND-C1D	5.16	109.14	105.22
26	2	315	0UR	C43-C3-C4	-5.16	118.94	125.03
26	5	314	0UR	C10-C11-C12	-5.15	120.06	127.28
25	3	316	8CT	C19-C20-C21	-5.15	120.06	127.28
25	0	314	8CT	C24-C25-C26	-5.15	120.06	127.28
25	4	316	8CT	C04-C03-C02	-5.12	115.64	122.64
23	2	304	CHL	OBD-CAD-CBD	5.12	133.33	125.82
23	6	323	CHL	OBD-CAD-CBD	5.11	133.33	125.82
25	A	847	8CT	C13-C14-C15	-5.11	108.39	123.20
25	F	301	8CT	C01-C02-C03	-5.11	118.91	124.48
23	6	313	CHL	C4D-ND-C1D	5.11	109.10	105.22
25	6	324	8CT	C28-C26-C25	5.10	127.04	119.01
23	2	305	CHL	C4D-ND-C1D	5.09	109.08	105.22
25	L	205	8CT	C24-C25-C26	-5.08	120.15	127.28
26	0	316	0UR	C9-C8-C7	-5.07	120.17	127.28
25	A	845	8CT	C04-C03-C02	-5.05	115.74	122.64
25	G	104	8CT	C35-C30-C29	-5.04	107.03	112.83
23	7	301	CHL	OBD-CAD-CBD	5.03	133.21	125.82
23	3	301	CHL	C4D-ND-C1D	5.03	109.04	105.22
26	9	315	0UR	C19-C18-C17	-5.03	116.75	124.58
25	3	317	8CT	C19-C20-C21	-5.02	120.23	127.28
23	3	305	CHL	OBD-CAD-CBD	5.02	133.19	125.82
23	8	306	CHL	C4D-ND-C1D	5.02	109.03	105.22
25	2	314	8CT	C04-C03-C02	-5.01	115.79	122.64
23	8	307	CHL	C4D-ND-C1D	5.01	109.02	105.22
23	1	312	CHL	OBD-CAD-CBD	4.99	133.15	125.82
25	M	102	8CT	C24-C25-C26	-4.99	120.28	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	312	CHL	C4D-ND-C1D	4.98	109.00	105.22
26	6	320	0UR	C14-C15-C16	-4.98	120.29	127.28
23	2	312	CHL	OBD-CAD-CBD	4.98	133.13	125.82
25	L	205	8CT	C01-C02-C03	-4.97	119.06	124.48
23	0	301	CHL	C4D-ND-C1D	4.97	108.99	105.22
34	B	849	DGD	O2G-C1B-C2B	4.96	122.22	111.48
25	A	844	8CT	C30-C31-C32	-4.96	115.36	121.47
25	A	847	8CT	C15-C16-C17	-4.96	111.21	119.01
23	4	315	CHL	OBD-CAD-CBD	4.96	133.10	125.82
23	4	305	CHL	OBD-CAD-CBD	4.95	133.09	125.82
23	3	305	CHL	C4D-ND-C1D	4.95	108.98	105.22
25	3	323	8CT	C01-C02-C03	-4.95	119.09	124.48
25	L	207	8CT	C30-C29-C28	-4.94	116.89	124.58
25	7	318	8CT	C01-C02-C03	-4.94	119.09	124.48
26	O	207	0UR	C5-C4-C3	-4.93	121.02	126.92
25	B	846	8CT	C07-C02-C03	-4.93	116.05	122.70
23	2	307	CHL	C4D-ND-C1D	4.92	108.95	105.22
25	B	844	8CT	C30-C31-C32	-4.90	115.43	121.47
23	8	301	CHL	OBD-CAD-CBD	4.90	133.02	125.82
25	6	319	8CT	C14-C15-C16	-4.90	112.92	126.36
25	9	313	8CT	C04-C03-C02	-4.90	115.94	122.64
23	4	302	CHL	OBD-CAD-CBD	4.90	133.01	125.82
23	0	306	CHL	OBD-CAD-CBD	4.89	133.01	125.82
23	3	301	CHL	OBD-CAD-CBD	4.89	133.00	125.82
23	7	302	CHL	OBD-CAD-CBD	4.89	133.00	125.82
25	J	104	8CT	C30-C31-C32	-4.88	115.46	121.47
25	B	848	8CT	C19-C18-C17	-4.88	113.54	123.52
23	9	306	CHL	OBD-CAD-C3D	-4.86	120.31	127.89
25	6	324	8CT	C14-C13-C12	-4.86	120.46	127.28
26	9	315	0UR	C9-C8-C7	-4.86	120.47	127.28
23	6	307	CHL	C4D-ND-C1D	4.85	108.90	105.22
26	4	317	0UR	C19-C18-C17	-4.85	117.03	124.58
25	L	204	8CT	C19-C20-C21	-4.85	120.47	127.28
25	J	104	8CT	C01-C02-C03	-4.85	119.20	124.48
23	0	301	CHL	OBD-CAD-CBD	4.84	132.93	125.82
25	B	850	8CT	C19-C20-C21	-4.84	120.50	127.28
25	B	847	8CT	C07-C02-C03	-4.83	116.17	122.70
25	7	319	8CT	C18-C17-C16	-4.83	120.50	127.28
25	O	202	8CT	C10-C11-C12	-4.83	119.09	126.23
23	9	312	CHL	OBD-CAD-CBD	4.83	132.91	125.82
23	6	305	CHL	C4D-ND-C1D	4.81	108.87	105.22
23	5	306	CHL	OBD-CAD-C3D	-4.81	120.39	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	843	8CT	C10-C11-C12	-4.81	119.12	126.23
25	A	849	8CT	C18-C17-C16	-4.81	120.53	127.28
25	8	317	8CT	C19-C20-C21	-4.81	120.53	127.28
25	J	101	8CT	C07-C02-C03	-4.81	116.21	122.70
23	0	302	CHL	OBD-CAD-CBD	4.80	132.87	125.82
25	O	202	8CT	C19-C20-C21	-4.80	120.55	127.28
26	5	314	0UR	C19-C18-C17	-4.80	117.11	124.58
25	L	204	8CT	C29-C28-C26	-4.80	116.00	126.32
25	3	323	8CT	C14-C15-C16	-4.80	113.20	126.36
23	6	323	CHL	OBD-CAD-C3D	-4.79	120.41	127.89
23	7	305	CHL	C4D-ND-C1D	4.78	108.84	105.22
23	4	306	CHL	OBD-CAD-CBD	4.78	132.84	125.82
23	6	302	CHL	OBD-CAD-C3D	-4.78	120.44	127.89
23	2	304	CHL	C4D-ND-C1D	4.78	108.84	105.22
23	6	315	CHL	OBD-CAD-CBD	4.78	132.83	125.82
23	3	307	CHL	C4D-ND-C1D	4.77	108.84	105.22
25	J	104	8CT	C24-C25-C26	-4.77	120.58	127.28
23	6	306	CHL	C4D-ND-C1D	4.77	108.84	105.22
25	6	324	8CT	C01-C02-C03	-4.75	119.30	124.48
25	4	316	8CT	C14-C13-C12	-4.75	120.62	127.28
25	L	204	8CT	C10-C11-C12	-4.75	119.21	126.23
25	B	845	8CT	C30-C31-C32	-4.75	115.63	121.47
23	4	306	CHL	C4D-ND-C1D	4.74	108.82	105.22
25	4	316	8CT	C24-C25-C26	-4.73	120.64	127.28
25	B	846	8CT	C39-C16-C17	-4.73	115.15	122.82
23	8	314	CHL	C4D-ND-C1D	4.73	108.81	105.22
23	4	301	CHL	C4D-ND-C1D	4.73	108.81	105.22
25	I	101	8CT	C19-C20-C21	-4.73	120.64	127.28
25	B	847	8CT	C01-C02-C03	-4.72	119.33	124.48
23	1	306	CHL	OBD-CAD-C3D	-4.72	120.53	127.89
23	9	305	CHL	C4D-ND-C1D	4.72	108.80	105.22
25	F	304	8CT	C01-C02-C03	-4.72	119.33	124.48
23	2	305	CHL	OBD-CAD-CBD	4.72	132.75	125.82
25	A	849	8CT	C01-C02-C03	-4.72	119.34	124.48
23	7	301	CHL	OBD-CAD-C3D	-4.71	120.55	127.89
26	0	315	0UR	C19-C18-C17	-4.71	117.25	124.58
25	7	319	8CT	C19-C20-C21	-4.69	120.69	127.28
25	K	105	8CT	C10-C11-C12	-4.69	119.29	126.23
25	B	845	8CT	C39-C16-C17	-4.69	115.22	122.82
25	B	847	8CT	C29-C28-C26	-4.68	116.26	126.32
23	4	305	CHL	C4D-ND-C1D	4.68	108.77	105.22
23	1	304	CHL	C4D-ND-C1D	4.68	108.77	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	316	0UR	C9-C8-C7	-4.67	120.72	127.28
23	6	305	CHL	OBD-CAD-CBD	4.67	132.67	125.82
23	1	304	CHL	OBD-CAD-CBD	4.67	132.67	125.82
23	5	301	CHL	OBD-CAD-CBD	4.66	132.66	125.82
25	O	202	8CT	C18-C17-C16	-4.66	120.74	127.28
23	3	302	CHL	OBD-CAD-CBD	4.65	132.65	125.82
23	8	306	CHL	OBD-CAD-CBD	4.65	132.65	125.82
23	8	308	CHL	C4D-ND-C1D	4.65	108.75	105.22
23	0	305	CHL	OBD-CAD-CBD	4.65	132.65	125.82
23	4	301	CHL	OBD-CAD-C3D	-4.65	120.64	127.89
23	6	302	CHL	C4D-ND-C1D	4.64	108.74	105.22
25	I	101	8CT	C35-C30-C29	-4.64	107.49	112.83
26	0	315	0UR	C4-C3-C2	-4.63	116.13	120.16
25	3	317	8CT	C07-C02-C03	-4.63	116.45	122.70
23	6	301	CHL	C4D-ND-C1D	4.63	108.73	105.22
26	1	316	0UR	C5-C4-C3	-4.63	121.38	126.92
23	0	302	CHL	C4D-ND-C1D	4.61	108.72	105.22
23	8	316	CHL	OBD-CAD-CBD	4.61	132.59	125.82
25	K	105	8CT	C35-C30-C29	-4.60	107.54	112.83
25	B	846	8CT	C19-C18-C17	-4.60	114.11	123.52
23	6	313	CHL	OBD-CAD-CBD	4.59	132.57	125.82
25	J	104	8CT	C40-C12-C13	-4.59	115.38	122.82
25	B	844	8CT	C10-C11-C12	-4.59	119.45	126.23
26	6	321	0UR	C5-C4-C3	-4.58	121.44	126.92
23	4	315	CHL	OBD-CAD-C3D	-4.58	120.75	127.89
23	7	307	CHL	OBD-CAD-C3D	-4.58	120.75	127.89
25	O	208	8CT	C30-C29-C28	-4.57	117.47	124.58
23	7	305	CHL	OBD-CAD-CBD	4.57	132.53	125.82
23	1	301	CHL	OBD-CAD-CBD	4.56	132.52	125.82
25	B	845	8CT	C23-C21-C20	-4.56	111.83	119.01
25	4	316	8CT	C35-C30-C29	-4.55	107.59	112.83
23	8	303	CHL	OBD-CAD-CBD	4.55	132.50	125.82
23	9	301	CHL	OBD-CAD-CBD	4.54	132.49	125.82
25	3	323	8CT	C35-C30-C29	-4.54	107.60	112.83
23	4	302	CHL	C4D-ND-C1D	4.54	108.67	105.22
25	I	101	8CT	C18-C17-C16	-4.54	120.91	127.28
26	8	318	0UR	C19-C18-C17	-4.53	117.53	124.58
23	4	313	CHL	C4D-ND-C1D	4.53	108.66	105.22
25	3	316	8CT	C07-C02-C03	-4.52	116.59	122.70
23	7	302	CHL	OBD-CAD-C3D	-4.52	120.84	127.89
23	6	301	CHL	OBD-CAD-CBD	4.52	132.45	125.82
23	8	301	CHL	OBD-CAD-C3D	-4.51	120.85	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4	315	CHL	C4D-ND-C1D	4.51	108.64	105.22
25	1	314	8CT	C10-C11-C12	-4.50	119.58	126.23
23	4	307	CHL	C4D-ND-C1D	4.49	108.63	105.22
23	2	301	CHL	C4D-ND-C1D	4.49	108.63	105.22
23	7	302	CHL	C4D-ND-C1D	4.48	108.62	105.22
25	B	845	8CT	C19-C20-C21	4.48	133.56	127.28
25	J	101	8CT	C29-C28-C26	-4.47	116.70	126.32
26	6	320	0UR	C4-C3-C2	-4.47	116.27	120.16
23	2	312	CHL	OBD-CAD-C3D	-4.47	120.92	127.89
25	3	317	8CT	C01-C02-C03	-4.46	119.61	124.48
23	4	302	CHL	OBD-CAD-C3D	-4.46	120.93	127.89
23	0	306	CHL	C1A-CHA-CBD	4.46	143.78	132.36
25	A	845	8CT	C10-C11-C12	-4.46	119.64	126.23
25	B	850	8CT	C14-C13-C12	-4.45	121.04	127.28
23	1	312	CHL	OBD-CAD-C3D	-4.44	120.96	127.89
25	K	105	8CT	C04-C03-C02	-4.44	116.57	122.64
25	J	104	8CT	C15-C16-C17	4.44	125.99	119.01
23	8	308	CHL	OBD-CAD-C3D	-4.44	120.97	127.89
25	B	850	8CT	C24-C25-C26	-4.44	121.05	127.28
26	2	315	0UR	C19-C18-C17	-4.43	117.68	124.58
25	B	848	8CT	C01-C02-C03	-4.43	119.65	124.48
25	G	104	8CT	C24-C25-C26	-4.43	121.06	127.28
23	8	303	CHL	C4D-ND-C1D	4.43	108.58	105.22
25	A	844	8CT	C04-C03-C02	-4.43	116.58	122.64
25	I	101	8CT	C18-C19-C20	-4.43	114.46	123.52
23	3	301	CHL	OBD-CAD-C3D	-4.43	120.98	127.89
23	5	301	CHL	C4D-ND-C1D	4.43	108.58	105.22
23	6	308	CHL	OBD-CAD-CBD	4.42	132.31	125.82
23	1	301	CHL	C4D-ND-C1D	4.42	108.57	105.22
26	4	317	0UR	C43-C3-C2	4.41	126.83	116.56
23	8	307	CHL	OBD-CAD-CBD	4.41	132.29	125.82
25	L	205	8CT	C07-C02-C03	-4.41	116.75	122.70
25	B	845	8CT	C10-C11-C12	-4.40	119.72	126.23
23	8	309	CHL	OBD-CAD-CBD	4.40	132.28	125.82
25	3	317	8CT	C10-C11-C12	-4.40	119.73	126.23
26	3	318	0UR	C43-C3-C2	4.39	126.78	116.56
23	1	306	CHL	C1A-CHA-CBD	4.39	143.61	132.36
25	I	101	8CT	C24-C25-C26	-4.38	121.13	127.28
25	J	101	8CT	C01-C02-C03	-4.38	119.70	124.48
23	7	313	CHL	OBD-CAD-CBD	4.38	132.25	125.82
27	A	850	LHG	O7-C7-C8	4.38	120.96	111.48
23	6	306	CHL	OBD-CAD-CBD	4.38	132.25	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	102	8CT	C07-C02-C03	-4.37	116.80	122.70
27	B	852	LHG	O7-C7-C8	4.37	120.93	111.48
23	3	302	CHL	OBD-CAD-C3D	-4.37	121.08	127.89
23	5	304	CHL	OBD-CAD-CBD	4.37	132.23	125.82
23	2	304	CHL	OBD-CAD-C3D	-4.36	121.09	127.89
23	7	307	CHL	C1A-CHA-CBD	4.36	143.53	132.36
23	9	312	CHL	OBD-CAD-C3D	-4.36	121.09	127.89
23	6	315	CHL	OBD-CAD-C3D	-4.36	121.10	127.89
25	J	104	8CT	C29-C28-C26	-4.35	116.96	126.32
23	8	316	CHL	OBD-CAD-C3D	-4.35	121.11	127.89
25	B	845	8CT	C01-C02-C03	-4.35	119.74	124.48
25	A	845	8CT	C07-C02-C03	-4.34	116.84	122.70
26	2	315	0UR	C43-C3-C2	4.34	126.65	116.56
26	4	318	0UR	C10-C11-C12	-4.34	121.19	127.28
25	2	314	8CT	C24-C25-C26	-4.34	121.20	127.28
25	B	844	8CT	C01-C02-C03	-4.34	119.75	124.48
26	1	316	0UR	C14-C15-C16	-4.33	121.20	127.28
26	9	314	0UR	C19-C18-C17	-4.33	117.84	124.58
25	7	318	8CT	C04-C03-C02	-4.33	116.72	122.64
25	G	104	8CT	C01-C02-C03	-4.33	119.76	124.48
26	6	321	0UR	C9-C8-C7	-4.32	121.21	127.28
25	B	850	8CT	C01-C02-C03	-4.32	119.77	124.48
23	8	303	CHL	OBD-CAD-C3D	-4.32	121.16	127.89
25	L	204	8CT	C07-C02-C03	-4.31	116.88	122.70
25	L	204	8CT	C01-C02-C03	-4.31	119.78	124.48
23	6	323	CHL	C1A-CHA-CBD	4.30	143.38	132.36
23	4	305	CHL	OBD-CAD-C3D	-4.30	121.18	127.89
25	A	846	8CT	C24-C25-C26	-4.30	121.24	127.28
25	3	316	8CT	C24-C25-C26	-4.30	121.25	127.28
25	7	318	8CT	C07-C02-C03	-4.30	116.90	122.70
23	2	312	CHL	C1A-CHA-CBD	4.30	143.37	132.36
25	B	845	8CT	C07-C02-C03	-4.29	116.91	122.70
23	2	305	CHL	OBD-CAD-C3D	-4.29	121.20	127.89
23	0	301	CHL	OBD-CAD-C3D	-4.29	121.20	127.89
25	2	314	8CT	C35-C30-C29	-4.29	107.90	112.83
23	4	306	CHL	OBD-CAD-C3D	-4.29	121.21	127.89
26	7	320	0UR	C43-C3-C2	4.28	126.52	116.56
25	J	101	8CT	C18-C19-C20	-4.28	114.76	123.52
25	J	101	8CT	C04-C03-C02	-4.28	116.78	122.64
23	3	305	CHL	OBD-CAD-C3D	-4.28	121.21	127.89
23	3	302	CHL	C4D-ND-C1D	4.27	108.46	105.22
23	6	302	CHL	C1-C2-C3	-4.26	119.21	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	317	8CT	C14-C13-C12	-4.26	121.30	127.28
26	1	315	0UR	C10-C11-C12	-4.26	121.31	127.28
26	2	316	0UR	C9-C8-C7	-4.25	121.31	127.28
25	7	319	8CT	C30-C29-C28	-4.24	117.98	124.58
25	B	845	8CT	C35-C30-C29	-4.24	107.95	112.83
23	1	301	CHL	OBD-CAD-C3D	-4.24	121.28	127.89
25	I	101	8CT	C01-C02-C03	-4.24	119.86	124.48
23	8	309	CHL	OBD-CAD-C3D	-4.23	121.29	127.89
23	0	306	CHL	OBD-CAD-C3D	-4.23	121.29	127.89
25	A	846	8CT	C19-C20-C21	-4.23	121.35	127.28
25	F	304	8CT	C29-C28-C26	-4.23	117.23	126.32
26	5	314	0UR	C9-C8-C7	-4.22	121.36	127.28
23	7	313	CHL	C1A-CHA-CBD	4.22	143.17	132.36
25	B	847	8CT	C10-C11-C12	-4.22	120.00	126.23
25	B	844	8CT	C19-C20-C21	-4.21	121.37	127.28
25	3	317	8CT	C18-C17-C16	-4.21	121.38	127.28
25	M	102	8CT	C01-C02-C03	-4.20	119.90	124.48
23	4	308	CHL	OBD-CAD-CBD	4.20	131.98	125.82
23	6	307	CHL	C1A-CHA-CBD	4.19	143.10	132.36
23	0	302	CHL	OBD-CAD-C3D	-4.19	121.35	127.89
25	M	102	8CT	C18-C17-C16	-4.19	121.40	127.28
23	2	301	CHL	OBD-CAD-CBD	4.19	131.97	125.82
23	6	315	CHL	C1B-CHB-C4A	4.19	124.02	121.32
25	I	101	8CT	C04-C03-C02	-4.19	116.92	122.64
25	F	304	8CT	C10-C11-C12	-4.18	120.04	126.23
23	8	314	CHL	OBD-CAD-CBD	4.18	131.97	125.82
25	9	313	8CT	C07-C02-C03	-4.18	117.05	122.70
25	6	319	8CT	C30-C29-C28	-4.18	118.07	124.58
25	F	301	8CT	C35-C30-C29	-4.18	108.02	112.83
23	4	307	CHL	C1-C2-C3	-4.17	120.01	126.76
23	8	316	CHL	C1A-CHA-CBD	4.17	143.04	132.36
23	1	305	CHL	OBD-CAD-CBD	4.17	131.94	125.82
25	A	846	8CT	C01-C02-C03	-4.17	119.94	124.48
26	8	318	0UR	C4-C3-C2	-4.16	116.53	120.16
25	6	324	8CT	C18-C17-C16	-4.16	121.44	127.28
25	B	850	8CT	C07-C02-C03	-4.16	117.08	122.70
25	A	845	8CT	C01-C02-C03	-4.16	119.94	124.48
25	B	843	8CT	C07-C02-C03	-4.16	117.08	122.70
25	K	105	8CT	C24-C25-C26	-4.16	121.45	127.28
27	5	316	LHG	O7-C7-C8	4.16	120.47	111.48
25	L	205	8CT	C35-C30-C29	-4.16	108.05	112.83
26	2	316	0UR	C10-C11-C12	-4.15	121.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	313	CHL	C1A-CHA-CBD	4.15	143.00	132.36
27	1	317	LHG	O7-C7-C8	4.14	120.45	111.48
26	O	207	0UR	C43-C3-C4	-4.14	120.14	125.03
23	5	301	CHL	OBD-CAD-C3D	-4.14	121.44	127.89
27	3	324	LHG	O7-C7-C8	4.13	120.42	111.48
26	8	318	0UR	C10-C11-C12	-4.13	121.48	127.28
23	0	305	CHL	OBD-CAD-C3D	-4.13	121.45	127.89
23	3	305	CHL	C1A-CHA-CBD	4.13	142.94	132.36
25	O	208	8CT	C18-C17-C16	-4.12	121.50	127.28
25	L	207	8CT	C18-C17-C16	-4.12	121.50	127.28
25	3	316	8CT	C39-C16-C15	4.12	124.38	118.09
27	7	323	LHG	O7-C7-C8	4.11	120.38	111.48
27	9	316	LHG	O7-C7-C8	4.11	120.37	111.48
23	6	305	CHL	OBD-CAD-C3D	-4.11	121.48	127.89
26	7	320	0UR	C19-C18-C17	-4.11	118.18	124.58
27	3	322	LHG	O7-C7-C8	4.11	120.37	111.48
25	B	850	8CT	C18-C17-C16	-4.11	121.52	127.28
25	I	101	8CT	C30-C31-C32	-4.11	116.41	121.47
27	A	843	LHG	O7-C7-C8	4.11	120.36	111.48
25	O	202	8CT	C01-C02-C03	-4.10	120.01	124.48
23	6	308	CHL	C1A-CHA-CBD	4.10	142.85	132.36
27	L	208	LHG	O7-C7-C8	4.10	120.34	111.48
27	A	842	LHG	O7-C7-C8	4.10	120.34	111.48
23	1	304	CHL	OBD-CAD-C3D	-4.09	121.51	127.89
27	3	320	LHG	O7-C7-C8	4.08	120.30	111.48
25	A	844	8CT	C07-C02-C03	-4.08	117.19	122.70
23	8	314	CHL	C1A-CHA-CBD	4.08	142.80	132.36
23	7	301	CHL	C1B-CHB-C4A	4.08	123.94	121.32
25	3	323	8CT	C04-C03-C02	-4.07	117.07	122.64
25	J	101	8CT	C24-C25-C26	-4.07	121.57	127.28
26	6	320	0UR	C34-C27-C1	-4.07	119.37	124.45
25	3	317	8CT	C29-C28-C26	-4.06	117.59	126.32
25	O	208	8CT	C19-C20-C21	-4.06	121.58	127.28
23	2	306	CHL	C1A-CHA-CBD	4.06	142.76	132.36
27	6	322	LHG	O7-C7-C8	4.05	120.25	111.48
23	6	313	CHL	OBD-CAD-C3D	-4.05	121.57	127.89
23	1	301	CHL	C1-C2-C3	-4.05	119.56	126.20
25	A	847	8CT	C18-C19-C20	4.05	131.80	123.52
23	6	308	CHL	OBD-CAD-C3D	-4.05	121.58	127.89
26	1	315	0UR	C19-C18-C17	-4.05	118.28	124.58
25	B	844	8CT	C39-C16-C17	-4.05	116.26	122.82
25	O	208	8CT	C07-C02-C03	-4.05	117.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	314	0UR	C10-C11-C12	-4.05	121.60	127.28
23	1	305	CHL	C1A-CHA-CBD	4.05	142.72	132.36
23	0	301	CHL	C1A-CHA-CBD	4.04	142.71	132.36
25	0	314	8CT	C18-C17-C16	-4.03	121.62	127.28
23	0	305	CHL	C1A-CHA-CBD	4.03	142.69	132.36
23	8	308	CHL	C1A-CHA-CBD	4.03	142.69	132.36
25	L	207	8CT	C07-C02-C03	-4.03	117.26	122.70
23	2	304	CHL	C1A-CHA-CBD	4.03	142.67	132.36
23	2	306	CHL	C1-C2-C3	-4.02	120.25	126.76
23	7	305	CHL	OBD-CAD-C3D	-4.02	121.62	127.89
25	3	323	8CT	C11-C12-C13	4.02	125.33	119.01
23	4	308	CHL	OBD-CAD-C3D	-4.02	121.62	127.89
25	B	843	8CT	C01-C02-C03	-4.02	120.10	124.48
23	2	306	CHL	C4D-ND-C1D	4.02	108.27	105.22
25	4	316	8CT	C10-C11-C12	-4.01	120.31	126.23
23	1	312	CHL	C1A-CHA-CBD	4.00	142.62	132.36
27	2	317	LHG	O7-C7-C8	4.00	120.14	111.48
23	5	305	CHL	C1A-CHA-CBD	4.00	142.60	132.36
23	1	306	CHL	C1B-CHB-C4A	4.00	123.89	121.32
23	8	301	CHL	C1A-CHA-CBD	3.99	142.59	132.36
23	4	307	CHL	C1A-CHA-CBD	3.99	142.58	132.36
23	6	301	CHL	OBD-CAD-C3D	-3.99	121.67	127.89
23	8	306	CHL	OBD-CAD-C3D	-3.99	121.67	127.89
25	9	313	8CT	C14-C13-C12	-3.99	121.69	127.28
25	3	316	8CT	C10-C11-C12	-3.98	120.34	126.23
26	5	315	0UR	C5-C4-C3	-3.98	122.15	126.92
25	B	846	8CT	C30-C31-C32	-3.98	116.57	121.47
23	8	303	CHL	C1-C2-C3	-3.98	119.67	126.20
23	5	304	CHL	C1A-CHA-CBD	3.98	142.55	132.36
23	9	301	CHL	C1A-CHA-CBD	3.98	142.55	132.36
23	5	306	CHL	C1A-CHA-CBD	3.97	142.54	132.36
23	4	305	CHL	C1A-CHA-CBD	3.97	142.53	132.36
26	8	319	0UR	O44-C45-C46	3.97	121.34	111.55
26	2	315	0UR	C10-C11-C12	-3.97	121.72	127.28
23	9	305	CHL	C1A-CHA-CBD	3.97	142.51	132.36
23	1	304	CHL	C1A-CHA-CBD	3.96	142.51	132.36
23	4	301	CHL	C1A-CHA-CBD	3.96	142.51	132.36
26	8	318	0UR	C34-C27-C1	-3.96	119.51	124.45
27	1	318	LHG	O7-C7-C8	3.96	120.04	111.48
23	9	312	CHL	C1A-CHA-CBD	3.95	142.49	132.36
25	B	848	8CT	C14-C13-C12	-3.95	121.73	127.28
25	6	324	8CT	C19-C20-C21	-3.95	121.74	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	8	306	CHL	C1A-CHA-CBD	3.95	142.47	132.36
23	6	306	CHL	C1A-CHA-CBD	3.95	142.46	132.36
23	8	309	CHL	C1A-CHA-CBD	3.94	142.46	132.36
27	0	317	LHG	O7-C7-C8	3.94	120.01	111.48
23	5	312	CHL	OBD-CAD-CBD	3.94	131.61	125.82
25	I	101	8CT	C07-C02-C03	-3.94	117.38	122.70
23	5	304	CHL	OBD-CAD-C3D	-3.94	121.75	127.89
23	6	315	CHL	C1A-CHA-CBD	3.93	142.44	132.36
26	7	320	0UR	C10-C11-C12	-3.93	121.76	127.28
23	3	307	CHL	C1A-CHA-CBD	3.93	142.43	132.36
23	3	301	CHL	C1-C2-C3	-3.92	119.77	126.20
25	0	314	8CT	C10-C11-C12	-3.92	120.43	126.23
25	O	202	8CT	C14-C13-C12	-3.92	121.78	127.28
23	6	305	CHL	C1A-CHA-CBD	3.92	142.39	132.36
27	7	322	LHG	O7-C7-C8	3.91	119.95	111.48
23	2	307	CHL	C1A-CHA-CBD	3.91	142.38	132.36
23	7	313	CHL	OBD-CAD-C3D	-3.91	121.79	127.89
25	L	207	8CT	C14-C15-C16	-3.91	115.64	126.36
23	4	313	CHL	OBD-CAD-CBD	3.91	131.56	125.82
23	8	307	CHL	C1A-CHA-CBD	3.91	142.37	132.36
25	8	317	8CT	C10-C11-C12	-3.90	120.47	126.23
25	J	101	8CT	C13-C14-C15	-3.90	111.91	123.20
23	7	305	CHL	C1A-CHA-CBD	3.90	142.34	132.36
25	L	205	8CT	C29-C28-C26	-3.89	117.95	126.32
26	5	315	0UR	C34-C27-C1	-3.89	119.60	124.45
32	A	852	CL0	C1B-CHB-C4A	3.89	123.82	121.32
23	8	308	CHL	C1-C2-C3	-3.89	120.47	126.76
23	9	301	CHL	OBD-CAD-C3D	-3.88	121.83	127.89
23	8	307	CHL	OBD-CAD-C3D	-3.88	121.85	127.89
23	4	308	CHL	C1A-CHA-CBD	3.87	142.28	132.36
23	4	315	CHL	C1A-CHA-CBD	3.87	142.27	132.36
25	7	318	8CT	C24-C25-C26	-3.87	121.85	127.28
27	B	851	LHG	O7-C7-C8	3.87	119.85	111.48
25	L	205	8CT	C19-C20-C21	-3.86	121.86	127.28
25	9	313	8CT	C30-C31-C32	-3.86	116.72	121.47
23	7	301	CHL	C1A-CHA-CBD	3.85	142.23	132.36
23	6	306	CHL	OBD-CAD-C3D	-3.85	121.88	127.89
23	1	305	CHL	OBD-CAD-C3D	-3.85	121.89	127.89
23	5	312	CHL	C1A-CHA-CBD	3.85	142.22	132.36
23	5	305	CHL	OBD-CAD-CBD	3.85	131.47	125.82
25	6	324	8CT	C27-C26-C25	-3.85	116.58	122.82
26	1	315	0UR	C34-C27-C1	-3.84	119.66	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	323	CHL	C1-C2-C3	-3.84	119.91	126.20
26	8	319	0UR	C34-C27-C1	-3.84	119.67	124.45
23	4	306	CHL	C1A-CHA-CBD	3.83	142.18	132.36
27	8	320	LHG	O7-C7-C8	3.83	119.78	111.48
25	6	319	8CT	C19-C20-C21	-3.83	121.91	127.28
25	A	845	8CT	C19-C20-C21	-3.83	121.91	127.28
23	2	305	CHL	C1A-CHA-CBD	3.82	142.15	132.36
26	3	318	0UR	O44-C45-C46	3.82	120.98	111.55
25	I	101	8CT	C29-C28-C26	-3.82	118.11	126.32
26	2	316	0UR	C34-C27-C1	-3.82	119.69	124.45
23	6	301	CHL	C1A-CHA-CBD	3.80	142.10	132.36
23	0	302	CHL	C1A-CHA-CBD	3.80	142.09	132.36
26	8	319	0UR	C5-C4-C3	-3.80	122.38	126.92
25	B	845	8CT	C25-C24-C23	-3.79	112.21	123.20
25	B	845	8CT	C30-C29-C28	-3.79	118.67	124.58
23	2	301	CHL	OBD-CAD-C3D	-3.79	121.98	127.89
25	L	204	8CT	C04-C03-C02	-3.79	117.46	122.64
23	3	301	CHL	C1A-CHA-CBD	3.79	142.06	132.36
25	A	847	8CT	C39-C16-C15	3.78	123.87	118.09
25	6	319	8CT	C11-C12-C13	3.78	124.96	119.01
27	7	324	LHG	O7-C7-C8	3.78	119.66	111.48
27	8	302	LHG	O7-C7-C8	3.78	119.66	111.48
23	7	302	CHL	C1A-CHA-CBD	3.78	142.04	132.36
25	A	844	8CT	C01-C02-C03	-3.78	120.36	124.48
26	1	316	0UR	C34-C27-C1	-3.77	119.74	124.45
26	1	316	0UR	C43-C3-C4	-3.77	120.58	125.03
27	2	319	LHG	O7-C7-C8	3.77	119.64	111.48
25	1	314	8CT	C29-C28-C26	-3.76	118.23	126.32
25	B	848	8CT	C05-C04-C03	3.76	115.90	110.44
25	A	844	8CT	C19-C20-C21	-3.76	122.00	127.28
26	7	320	0UR	C9-C8-C7	-3.76	122.01	127.28
25	O	208	8CT	C30-C31-C32	-3.76	116.85	121.47
23	5	301	CHL	C1A-CHA-CBD	3.76	141.98	132.36
25	B	846	8CT	C11-C12-C13	3.75	124.91	119.01
23	2	301	CHL	C1A-CHA-CBD	3.75	141.96	132.36
25	B	847	8CT	C18-C19-C20	-3.74	115.86	123.52
26	6	321	0UR	C34-C27-C1	-3.74	119.79	124.45
26	8	319	0UR	C10-C11-C12	-3.74	122.03	127.28
23	6	302	CHL	C1A-CHA-CBD	3.74	141.93	132.36
25	A	847	8CT	C18-C17-C16	3.73	132.52	127.28
27	I	102	LHG	O7-C7-C8	3.73	119.55	111.48
23	5	312	CHL	OBD-CAD-C3D	-3.73	122.08	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	207	0UR	C28-C19-C18	-3.73	108.54	112.83
25	G	104	8CT	C19-C20-C21	-3.72	122.06	127.28
23	0	301	CHL	C1-C2-C3	-3.72	120.10	126.20
26	1	316	0UR	O44-C45-C46	3.72	120.72	111.55
23	2	307	CHL	OBD-CAD-CBD	3.72	131.28	125.82
25	9	313	8CT	C35-C30-C29	-3.71	108.56	112.83
25	B	844	8CT	C14-C13-C12	-3.71	122.07	127.28
26	3	318	0UR	C9-C8-C7	-3.71	122.08	127.28
23	5	301	CHL	C1-C2-C3	-3.71	120.12	126.20
23	7	306	CHL	OBD-CAD-C3D	-3.71	122.11	127.89
25	B	844	8CT	C07-C02-C03	-3.70	117.70	122.70
26	8	319	0UR	C9-C8-C7	-3.69	122.10	127.28
23	4	302	CHL	C1A-CHA-CBD	3.69	141.82	132.36
23	4	313	CHL	C1A-CHA-CBD	3.69	141.82	132.36
25	B	843	8CT	C04-C03-C02	-3.69	117.59	122.64
26	2	315	0UR	C9-C8-C7	-3.68	122.11	127.28
23	7	306	CHL	C1A-CHA-CBD	3.68	141.79	132.36
23	1	301	CHL	C1A-CHA-CBD	3.68	141.77	132.36
23	8	314	CHL	OBD-CAD-C3D	-3.67	122.16	127.89
25	B	844	8CT	C29-C28-C26	-3.67	118.42	126.32
23	0	306	CHL	O1D-CGD-CBD	-3.67	119.15	124.72
26	4	318	0UR	C34-C27-C1	-3.67	119.87	124.45
23	9	306	CHL	C1A-CHA-CBD	3.67	141.76	132.36
26	0	316	0UR	O44-C45-C46	3.67	120.60	111.55
23	6	308	CHL	CBC-CAC-C3C	-3.67	107.62	112.87
25	A	847	8CT	C11-C10-C03	-3.67	117.20	127.00
25	A	846	8CT	C18-C19-C20	-3.66	116.02	123.52
25	J	104	8CT	C14-C13-C12	3.66	132.41	127.28
25	2	314	8CT	C10-C11-C12	-3.65	120.83	126.23
23	2	301	CHL	C1-C2-C3	-3.65	120.21	126.20
23	0	306	CHL	C1B-CHB-C4A	3.65	123.67	121.32
26	5	315	0UR	O44-C45-C46	3.64	120.54	111.55
26	O	207	0UR	C14-C15-C16	-3.64	122.17	127.28
26	8	319	0UR	C43-C3-C4	-3.64	120.73	125.03
25	6	324	8CT	C25-C24-C23	-3.64	112.66	123.20
26	0	315	0UR	C9-C8-C7	-3.63	122.18	127.28
25	7	319	8CT	C07-C02-C03	-3.63	117.80	122.70
26	7	320	0UR	O44-C45-C46	3.63	120.50	111.55
26	7	320	0UR	C28-C19-C18	-3.63	108.66	112.83
23	8	314	CHL	CBC-CAC-C3C	-3.62	107.69	112.87
25	G	104	8CT	C14-C13-C12	-3.62	122.20	127.28
23	3	305	CHL	C1-C2-C3	-3.62	120.91	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	302	CHL	C1A-CHA-CBD	3.62	141.62	132.36
23	8	303	CHL	C1A-CHA-CBD	3.62	141.62	132.36
25	6	319	8CT	C18-C19-C20	-3.61	116.13	123.52
23	0	302	CHL	C1-C2-C3	-3.61	120.29	126.20
23	2	304	CHL	CMD-C2D-C3D	-3.60	117.48	124.68
25	A	846	8CT	C04-C03-C02	-3.60	117.71	122.64
23	7	306	CHL	C1-C2-C3	-3.58	120.33	126.20
25	3	323	8CT	C30-C31-C32	-3.58	117.07	121.47
25	8	317	8CT	C04-C03-C02	-3.58	117.75	122.64
23	7	306	CHL	OBD-CAD-CBD	3.58	131.07	125.82
26	9	315	0UR	O44-C45-C46	3.57	120.37	111.55
23	4	302	CHL	C1-C2-C3	-3.57	120.34	126.20
25	M	102	8CT	C30-C31-C32	-3.57	117.07	121.47
26	4	317	0UR	C9-C8-C7	-3.57	122.27	127.28
25	A	845	8CT	C24-C25-C26	-3.57	122.27	127.28
26	9	315	0UR	C24-C23-C1	-3.57	105.88	110.61
25	A	844	8CT	C10-C11-C12	-3.57	120.96	126.23
25	B	848	8CT	C25-C24-C23	-3.57	112.87	123.20
26	4	317	0UR	O44-C45-C46	3.56	120.35	111.55
23	3	302	CHL	C1-C2-C3	-3.56	120.36	126.20
23	2	312	CHL	C1-C2-C3	-3.56	121.00	126.76
25	7	319	8CT	C35-C30-C29	-3.56	108.73	112.83
24	A	834	CLA	O2D-CGD-O1D	-3.56	116.93	123.85
23	6	302	CHL	CBC-CAC-C3C	-3.56	107.78	112.87
25	O	202	8CT	C35-C30-C29	-3.55	108.74	112.83
25	K	105	8CT	C29-C28-C26	-3.55	118.69	126.32
25	B	845	8CT	C39-C16-C15	3.55	123.51	118.09
25	B	845	8CT	C22-C21-C23	3.55	123.50	118.09
26	2	315	0UR	O44-C45-C46	3.54	120.30	111.55
23	6	306	CHL	C1-C2-C3	-3.54	121.03	126.76
23	8	301	CHL	C1-C2-C3	-3.54	120.40	126.20
23	4	313	CHL	OBD-CAD-C3D	-3.53	122.38	127.89
24	B	811	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
23	5	305	CHL	OBD-CAD-C3D	-3.53	122.39	127.89
25	J	104	8CT	C05-C04-C03	3.52	115.55	110.44
25	7	318	8CT	C11-C10-C03	-3.51	117.61	127.00
25	4	316	8CT	C19-C20-C21	-3.51	122.35	127.28
23	6	306	CHL	CBC-CAC-C3C	-3.51	107.85	112.87
24	B	804	CLA	C1-C2-C3	-3.51	120.45	126.20
26	2	316	0UR	C5-C4-C3	-3.51	122.72	126.92
25	B	846	8CT	C01-C02-C03	-3.51	120.66	124.48
23	6	308	CHL	C1-C2-C3	-3.51	120.45	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	321	0UR	C43-C3-C4	-3.50	120.90	125.03
26	4	317	0UR	C28-C19-C18	-3.50	108.80	112.83
25	0	314	8CT	C19-C18-C17	-3.50	116.36	123.52
26	0	315	0UR	C10-C11-C12	-3.49	122.39	127.28
26	9	314	0UR	O44-C45-C46	3.49	120.16	111.55
25	B	844	8CT	C22-C21-C23	3.49	123.41	118.09
26	5	315	0UR	C10-C11-C12	-3.48	122.39	127.28
23	1	306	CHL	CMD-C2D-C3D	-3.48	117.73	124.68
24	A	853	CLA	C3B-C4B-NB	-3.48	107.43	110.53
25	A	844	8CT	C35-C30-C29	-3.46	108.85	112.83
26	6	321	0UR	O44-C45-C46	3.46	120.08	111.55
25	B	846	8CT	C28-C26-C25	3.46	124.45	119.01
25	O	208	8CT	C04-C03-C02	-3.45	117.92	122.64
25	B	848	8CT	C28-C26-C25	3.45	124.44	119.01
25	M	102	8CT	C30-C29-C28	-3.45	119.21	124.58
31	B	842	PQN	C14-C13-C15	3.44	121.20	115.23
24	A	829	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
26	1	315	0UR	O44-C45-C46	3.44	120.04	111.55
23	6	313	CHL	C4-C3-C5	3.44	120.17	116.13
23	9	305	CHL	OBD-CAD-CBD	3.44	130.87	125.82
25	J	101	8CT	C24-C23-C21	-3.44	116.94	126.36
23	2	307	CHL	OBD-CAD-C3D	-3.43	122.54	127.89
26	O	207	0UR	C34-C27-C1	-3.43	120.17	124.45
26	9	315	0UR	C34-C27-C26	3.43	120.73	114.42
25	A	849	8CT	C10-C11-C12	-3.43	121.16	126.23
23	4	313	CHL	C1-C2-C3	-3.43	121.22	126.76
23	5	306	CHL	CMD-C2D-C3D	-3.42	117.84	124.68
25	K	105	8CT	C19-C20-C21	-3.42	122.48	127.28
25	M	102	8CT	C29-C28-C26	-3.42	118.97	126.32
30	3	319	0IE	C10-C9-C8	3.42	130.51	123.52
25	6	319	8CT	C07-C02-C03	-3.41	118.09	122.70
25	L	204	8CT	C11-C10-C03	-3.41	117.88	127.00
26	O	207	0UR	C19-C18-C17	-3.41	119.28	124.58
25	G	104	8CT	C05-C04-C03	3.41	115.39	110.44
25	B	845	8CT	C29-C28-C26	-3.41	119.00	126.32
28	0	318	SQD	C44-O6-C1	3.41	121.10	113.80
25	B	848	8CT	C30-C31-C32	-3.41	117.28	121.47
28	0	318	SQD	O47-C7-C8	3.40	118.84	111.48
23	1	312	CHL	C1-C2-C3	-3.40	120.62	126.20
25	B	843	8CT	C39-C16-C15	3.40	123.29	118.09
25	B	844	8CT	C22-C21-C20	-3.40	117.31	122.82
23	1	305	CHL	C1B-CHB-C4A	3.40	123.51	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	811	CLA	C3B-C4B-NB	-3.40	107.50	110.53
25	0	314	8CT	C14-C13-C12	-3.40	122.51	127.28
25	2	314	8CT	C14-C15-C16	-3.39	117.06	126.36
25	2	314	8CT	C19-C20-C21	-3.39	122.52	127.28
34	B	849	DGD	O1G-C1A-C2A	3.39	122.16	111.83
25	B	844	8CT	C24-C25-C26	-3.39	122.53	127.28
23	1	304	CHL	CMD-C2D-C3D	-3.38	117.92	124.68
26	9	314	0UR	C34-C27-C1	-3.38	120.23	124.45
24	B	806	CLA	C3B-C4B-NB	-3.38	107.51	110.53
23	4	315	CHL	O2A-CGA-CBA	3.38	122.14	111.83
25	L	205	8CT	C10-C11-C12	-3.38	121.23	126.23
23	6	313	CHL	CBC-CAC-C3C	-3.38	108.03	112.87
26	O	207	0UR	O44-C45-C46	3.38	119.88	111.55
26	5	314	0UR	C34-C27-C1	-3.37	120.25	124.45
25	O	202	8CT	C25-C24-C23	-3.37	113.44	123.20
25	B	844	8CT	C39-C16-C15	3.36	123.22	118.09
25	O	208	8CT	C01-C02-C03	-3.36	120.82	124.48
23	6	313	CHL	C1-C2-C3	-3.36	120.69	126.20
25	3	323	8CT	C07-C02-C03	-3.36	118.17	122.70
24	B	818	CLA	C3B-C4B-NB	-3.36	107.53	110.53
30	7	321	0IE	C10-C9-C8	3.36	130.39	123.52
23	6	323	CHL	C1B-CHB-C4A	3.35	123.48	121.32
26	1	315	0UR	C9-C8-C7	-3.35	122.58	127.28
25	7	318	8CT	C14-C13-C12	-3.35	122.58	127.28
24	B	829	CLA	C3B-C4B-NB	-3.35	107.54	110.53
23	8	306	CHL	CMD-C2D-C3D	-3.35	117.99	124.68
26	4	318	0UR	C9-C8-C7	-3.35	122.58	127.28
23	0	301	CHL	O2A-CGA-CBA	3.35	122.04	111.83
23	6	313	CHL	CMD-C2D-C3D	-3.34	118.00	124.68
24	A	804	CLA	C3B-C4B-NB	-3.34	107.55	110.53
26	0	316	0UR	C9-C10-C11	-3.34	116.68	123.52
26	7	320	0UR	C34-C27-C1	-3.34	120.28	124.45
23	6	323	CHL	O1D-CGD-CBD	-3.34	119.66	124.72
23	8	316	CHL	CBC-CAC-C3C	-3.34	108.10	112.87
26	0	315	0UR	C34-C27-C1	-3.33	120.29	124.45
26	2	315	0UR	C28-C19-C18	-3.33	108.99	112.83
26	3	318	0UR	C10-C11-C12	-3.33	122.61	127.28
25	L	204	8CT	C01-C02-C07	3.33	120.70	113.60
24	A	816	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
24	H	201	CLA	O2D-CGD-O1D	-3.33	117.38	123.85
25	A	849	8CT	C04-C03-C02	-3.32	118.09	122.64
24	A	802	CLA	O2D-CGD-O1D	-3.32	117.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	0	316	0UR	C28-C19-C18	-3.32	109.01	112.83
25	K	105	8CT	C14-C15-C16	-3.32	117.26	126.36
24	A	807	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
24	B	808	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
25	0	314	8CT	C07-C02-C03	-3.31	118.23	122.70
26	9	315	0UR	C4-C3-C2	-3.31	117.27	120.16
25	B	850	8CT	C04-C03-C02	-3.31	118.11	122.64
26	9	314	0UR	C9-C8-C7	-3.31	122.64	127.28
25	B	847	8CT	C11-C10-C03	-3.30	118.17	127.00
25	7	318	8CT	C29-C28-C26	-3.30	119.22	126.32
23	5	304	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
26	8	318	0UR	C9-C8-C7	-3.30	122.66	127.28
25	B	843	8CT	C35-C30-C29	-3.30	109.04	112.83
25	F	301	8CT	C14-C15-C16	-3.29	117.33	126.36
24	B	809	CLA	C3B-C4B-NB	-3.29	107.59	110.53
23	3	307	CHL	C1-C2-C3	-3.29	120.80	126.20
24	B	810	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	2	314	8CT	C22-C21-C20	-3.29	117.48	122.82
25	B	847	8CT	C14-C15-C16	-3.29	117.35	126.36
24	B	801	CLA	CAA-C2A-C3A	-3.29	104.12	113.00
24	A	803	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
25	J	101	8CT	C11-C10-C03	-3.28	118.22	127.00
24	A	809	CLA	C3B-C4B-NB	-3.28	107.60	110.53
24	L	202	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
23	9	312	CHL	CMD-C2D-C3D	-3.28	118.13	124.68
25	B	846	8CT	C39-C16-C15	3.28	123.09	118.09
25	B	848	8CT	C14-C15-C16	-3.27	117.39	126.36
24	0	313	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
25	A	849	8CT	C07-C02-C03	-3.27	118.28	122.70
26	5	315	0UR	C43-C3-C4	-3.27	121.17	125.03
24	A	848	CLA	C3B-C4B-NB	-3.27	107.61	110.53
23	2	306	CHL	CBC-CAC-C3C	-3.27	108.20	112.87
26	6	320	0UR	C43-C3-C4	-3.26	121.18	125.03
24	A	832	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
23	6	301	CHL	C1-C2-C3	-3.26	120.86	126.20
30	3	319	0IE	C20-C3-C4	-3.26	120.21	124.72
26	O	207	0UR	C9-C10-C11	-3.26	116.85	123.52
24	B	827	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
23	4	301	CHL	O2A-CGA-CBA	3.26	121.77	111.83
23	7	302	CHL	C1-C2-C3	-3.26	120.86	126.20
23	0	306	CHL	O2D-CGD-O1D	-3.25	117.52	123.85
25	A	847	8CT	C10-C11-C12	-3.25	121.42	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	852	CL0	C4D-CHA-CBD	-3.25	105.69	108.97
25	A	846	8CT	C07-C02-C03	-3.25	118.31	122.70
25	9	313	8CT	C24-C25-C26	-3.25	122.72	127.28
25	L	207	8CT	C35-C30-C29	-3.25	109.09	112.83
25	L	207	8CT	C25-C24-C23	-3.25	113.79	123.20
25	B	844	8CT	C04-C03-C02	-3.25	118.20	122.64
23	2	301	CHL	OMC-CMC-C2C	-3.24	119.49	125.12
26	0	316	0UR	C19-C18-C17	-3.24	119.53	124.58
26	3	318	0UR	C19-C18-C17	-3.24	119.53	124.58
25	B	846	8CT	C40-C12-C13	-3.24	117.56	122.82
23	2	307	CHL	CBC-CAC-C3C	-3.24	108.24	112.87
24	B	841	CLA	C3B-C4B-NB	-3.24	107.64	110.53
25	L	207	8CT	C14-C13-C12	-3.23	122.75	127.28
25	6	324	8CT	C05-C04-C03	3.23	115.13	110.44
25	A	844	8CT	C11-C10-C03	-3.23	118.37	127.00
24	6	314	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
24	3	315	CLA	CAC-C3C-C4C	3.23	128.99	124.79
23	3	307	CHL	O2A-CGA-CBA	3.23	121.68	111.83
24	B	838	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
24	A	838	CLA	C3B-C4B-NB	-3.23	107.65	110.53
24	A	824	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
25	F	301	8CT	C30-C29-C28	-3.23	119.56	124.58
25	0	314	8CT	C30-C29-C28	-3.23	119.56	124.58
25	1	314	8CT	C07-C02-C03	-3.23	118.34	122.70
24	B	833	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
25	3	316	8CT	C29-C28-C26	-3.22	119.39	126.32
25	9	313	8CT	C30-C29-C28	-3.22	119.56	124.58
26	1	316	0UR	C48-C47-C46	-3.22	119.21	125.92
23	4	302	CHL	OMC-CMC-C2C	-3.22	119.53	125.12
25	A	849	8CT	C11-C10-C03	-3.22	118.40	127.00
24	F	303	CLA	C3B-C4B-NB	-3.22	107.66	110.53
25	2	314	8CT	C23-C21-C20	3.22	124.07	119.01
24	B	804	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
25	L	205	8CT	C11-C10-C03	-3.22	118.41	127.00
24	B	824	CLA	C3B-C4B-NB	-3.21	107.66	110.53
25	B	846	8CT	C01-C02-C07	3.21	120.45	113.60
24	B	818	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
25	4	316	8CT	C23-C21-C20	3.21	124.06	119.01
24	B	841	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
24	B	819	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
24	O	204	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
23	6	302	CHL	O2D-CGD-O1D	-3.21	117.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	817	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
24	B	833	CLA	C3B-C4B-NB	-3.20	107.67	110.53
24	3	314	CLA	C3B-C4B-NB	-3.20	107.67	110.53
26	4	317	0UR	C10-C11-C12	-3.20	122.79	127.28
24	B	830	CLA	CMB-C2B-C1B	-3.20	120.55	125.42
24	A	818	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
24	A	825	CLA	C3B-C4B-NB	-3.20	107.68	110.53
23	6	323	CHL	O2A-CGA-CBA	3.20	121.58	111.83
25	9	313	8CT	C18-C19-C20	-3.19	116.98	123.52
25	O	202	8CT	C11-C10-C03	-3.19	118.46	127.00
26	4	317	0UR	C48-C47-C46	-3.19	119.27	125.92
24	B	826	CLA	C3D-C4D-ND	3.19	111.79	109.68
23	8	301	CHL	O2A-CGA-CBA	3.19	121.57	111.83
23	6	313	CHL	O2A-CGA-CBA	3.19	121.57	111.83
30	7	321	0IE	C23-C16-C15	-3.19	117.65	122.82
23	3	307	CHL	CBC-CAC-C3C	-3.19	108.31	112.87
25	L	207	8CT	C19-C18-C17	-3.19	116.99	123.52
23	6	323	CHL	O2D-CGD-O1D	-3.19	117.64	123.85
23	2	306	CHL	O2A-CGA-CBA	3.19	121.55	111.83
30	3	319	0IE	C23-C16-C15	-3.19	117.66	122.82
24	8	312	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	0	314	8CT	C01-C02-C07	3.18	120.39	113.60
26	0	315	0UR	O44-C45-C46	3.18	119.40	111.55
25	A	847	8CT	C40-C12-C11	3.18	122.95	118.09
24	A	805	CLA	C3B-C4B-NB	-3.18	107.69	110.53
24	B	801	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	A	826	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	A	837	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	A	826	CLA	C3B-C4B-NB	-3.18	107.69	110.53
24	3	313	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
25	I	101	8CT	C01-C02-C07	3.17	120.35	113.60
24	B	814	CLA	C3B-C4B-NB	-3.17	107.70	110.53
24	K	101	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
24	L	201	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
26	1	316	0UR	C36-C28-C19	3.16	114.33	109.55
25	A	845	8CT	C18-C19-C20	-3.16	117.06	123.52
23	6	301	CHL	O2A-CGA-CBA	3.16	121.46	111.83
30	3	319	0IE	C20-C3-C2	3.16	122.25	115.01
23	7	302	CHL	C4-C3-C5	3.16	120.70	115.23
23	9	306	CHL	O1D-CGD-CBD	-3.15	119.94	124.72
25	3	316	8CT	C04-C03-C02	-3.15	118.33	122.64
23	3	307	CHL	CMD-C2D-C3D	-3.15	118.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	314	0UR	O44-C45-C46	3.15	119.32	111.55
24	6	316	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
24	B	820	CLA	C3B-C4B-NB	-3.15	107.72	110.53
24	K	104	CLA	C3B-C4B-NB	-3.14	107.72	110.53
23	6	301	CHL	O1D-CGD-CBD	-3.14	119.96	124.72
24	3	309	CLA	C3B-C4B-NB	-3.14	107.72	110.53
24	B	813	CLA	C3B-C4B-NB	-3.14	107.73	110.53
24	A	839	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
25	A	846	8CT	C14-C15-C16	-3.14	117.76	126.36
23	0	305	CHL	C1-C2-C3	-3.14	121.69	126.76
24	B	837	CLA	O2D-CGD-O1D	-3.14	117.75	123.85
31	A	841	PQN	C14-C13-C15	3.13	120.67	115.23
25	3	323	8CT	C40-C12-C13	-3.13	117.74	122.82
23	9	305	CHL	OBD-CAD-C3D	-3.13	123.01	127.89
25	O	202	8CT	C01-C02-C07	3.13	120.27	113.60
23	1	304	CHL	CBC-CAC-C3C	-3.13	108.39	112.87
26	5	315	0UR	C48-C47-C46	-3.13	119.41	125.92
24	4	303	CLA	C3B-C4B-NB	-3.13	107.74	110.53
24	B	825	CLA	O2D-CGD-O1D	-3.13	117.77	123.85
23	3	301	CHL	O2A-CGA-CBA	3.12	121.36	111.83
27	B	852	LHG	O8-C23-C24	3.12	121.36	111.83
24	B	834	CLA	C3B-C4B-NB	-3.12	107.74	110.53
24	2	313	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
26	2	315	0UR	C48-C47-C46	-3.12	119.42	125.92
24	B	807	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
24	A	835	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
23	7	306	CHL	CMA-C3A-C4A	-3.11	107.90	114.61
24	3	315	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
24	2	309	CLA	C3B-C4B-NB	-3.11	107.75	110.53
24	A	839	CLA	C3B-C4B-NB	-3.11	107.75	110.53
24	B	831	CLA	C3B-C4B-NB	-3.11	107.75	110.53
24	O	205	CLA	C3B-C4B-NB	-3.11	107.75	110.53
23	0	305	CHL	CMD-C2D-C3D	-3.11	118.47	124.68
24	A	830	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
24	A	823	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
24	6	312	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
24	A	840	CLA	C3B-C4B-NB	-3.10	107.76	110.53
23	8	314	CHL	C4-C3-C5	3.10	120.61	115.23
24	A	811	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
26	5	314	0UR	C43-C3-C4	-3.10	121.37	125.03
25	J	104	8CT	C07-C02-C03	-3.10	118.52	122.70
26	1	316	0UR	C10-C11-C12	-3.10	122.93	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	312	CHL	O1D-CGD-CBD	-3.10	120.03	124.72
24	A	822	CLA	C3B-C4B-NB	-3.10	107.77	110.53
24	1	313	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
23	5	304	CHL	CMD-C2D-C3D	-3.09	118.52	124.68
25	7	318	8CT	C30-C29-C28	-3.09	119.78	124.58
24	3	313	CLA	C3B-C4B-NB	-3.09	107.78	110.53
24	9	302	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	A	814	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	B	830	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
24	A	829	CLA	CMB-C2B-C1B	-3.09	120.72	125.42
25	A	847	8CT	C10-C03-C02	-3.08	114.45	121.56
25	8	317	8CT	C07-C02-C03	-3.08	118.54	122.70
24	A	853	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
24	5	308	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
26	6	320	0UR	C36-C28-C19	3.08	114.22	109.55
25	3	316	8CT	C19-C18-C17	-3.08	117.21	123.52
24	B	821	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
23	8	314	CHL	CMD-C2D-C3D	-3.08	118.53	124.68
23	7	306	CHL	O1D-CGD-CBD	-3.08	120.06	124.72
24	A	828	CLA	C1-C2-C3	-3.08	121.16	126.20
24	G	103	CLA	C3B-C4B-NB	-3.07	107.78	110.53
24	A	836	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
24	4	303	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
23	2	305	CHL	O1D-CGD-CBD	-3.07	120.06	124.72
26	2	315	0UR	C34-C27-C1	-3.07	120.62	124.45
24	6	317	CLA	C3B-C4B-NB	-3.07	107.79	110.53
23	8	316	CHL	CMD-C2D-C3D	-3.07	118.55	124.68
24	9	309	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	A	813	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
23	5	305	CHL	CMD-C2D-C3D	-3.07	118.55	124.68
24	3	306	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	7	303	CLA	C3B-C4B-NB	-3.07	107.79	110.53
23	2	312	CHL	O2A-CGA-CBA	3.07	121.19	111.83
25	B	850	8CT	C29-C28-C26	-3.07	119.72	126.32
24	A	830	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	A	815	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
24	F	303	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
24	6	311	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	3	306	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
24	B	815	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
24	B	813	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
25	G	104	8CT	C29-C28-C26	-3.07	119.73	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	310	CLA	C3B-C4B-NB	-3.07	107.79	110.53
23	3	302	CHL	O2A-CGA-CBA	3.07	121.18	111.83
23	8	307	CHL	CMD-C2D-C3D	-3.06	118.56	124.68
24	6	317	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	8	314	CHL	C1-C2-C3	-3.06	121.18	126.20
23	8	301	CHL	C4-C3-C5	3.06	119.73	116.13
24	K	101	CLA	C3B-C4B-NB	-3.06	107.80	110.53
23	6	315	CHL	CBC-CAC-C3C	-3.06	108.49	112.87
25	1	314	8CT	C24-C23-C21	-3.06	117.97	126.36
24	A	827	CLA	C1-C2-C3	-3.06	121.19	126.20
24	0	311	CLA	C3B-C4B-NB	-3.06	107.80	110.53
25	B	850	8CT	C18-C19-C20	-3.06	117.26	123.52
24	A	819	CLA	C3B-C4B-NB	-3.06	107.80	110.53
24	7	312	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
23	1	301	CHL	CBC-CAC-C3C	-3.05	108.50	112.87
26	5	314	0UR	C5-C4-C3	-3.05	123.27	126.92
24	7	308	CLA	C3B-C4B-NB	-3.05	107.80	110.53
24	B	817	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
23	5	312	CHL	CMD-C2D-C3D	-3.05	118.58	124.68
24	3	312	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
26	9	315	0UR	C15-C14-C13	-3.05	114.36	123.20
24	1	308	CLA	C3B-C4B-NB	-3.05	107.81	110.53
23	4	301	CHL	CMD-C2D-C3D	-3.05	118.59	124.68
23	6	302	CHL	OMC-CMC-C2C	-3.05	119.83	125.12
25	J	104	8CT	C35-C30-C29	-3.05	109.32	112.83
26	0	316	0UR	C10-C11-C12	-3.05	123.01	127.28
24	9	310	CLA	C3B-C4B-NB	-3.05	107.81	110.53
26	9	315	0UR	C9-C10-C11	-3.05	117.29	123.52
25	B	844	8CT	C18-C17-C16	-3.04	123.01	127.28
25	7	318	8CT	C25-C24-C23	-3.04	114.38	123.20
24	7	312	CLA	C3B-C4B-NB	-3.04	107.81	110.53
24	A	822	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
23	1	312	CHL	O2A-CGA-CBA	3.04	121.11	111.83
24	3	310	CLA	C3B-C4B-NB	-3.04	107.82	110.53
24	B	832	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
24	A	808	CLA	C3B-C4B-NB	-3.04	107.82	110.53
23	2	305	CHL	CMD-C2D-C3D	-3.04	118.61	124.68
25	1	314	8CT	C04-C03-C02	-3.04	118.48	122.64
30	3	319	0IE	C4-C3-C2	-3.04	117.51	120.16
26	4	317	0UR	C34-C27-C1	-3.04	120.66	124.45
24	B	840	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
24	3	314	CLA	O2D-CGD-O1D	-3.04	117.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	316	0UR	O44-C45-C46	3.03	119.04	111.55
24	0	319	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
24	0	307	CLA	C3B-C4B-NB	-3.03	107.82	110.53
23	7	307	CHL	C1B-CHB-C4A	3.03	123.27	121.32
24	2	311	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
26	8	318	0UR	C28-C19-C18	-3.03	109.34	112.83
23	0	305	CHL	O1D-CGD-CBD	-3.03	120.13	124.72
23	4	313	CHL	O1D-CGD-CBD	-3.03	120.13	124.72
26	4	318	0UR	C14-C15-C16	-3.03	123.03	127.28
25	B	845	8CT	C01-C02-C07	3.03	120.05	113.60
24	A	802	CLA	C3B-C4B-NB	-3.03	107.83	110.53
24	A	848	CLA	C1-C2-C3	-3.03	121.24	126.20
23	5	301	CHL	OMC-CMC-C2C	-3.03	119.86	125.12
24	F	302	CLA	C3B-C4B-NB	-3.03	107.83	110.53
30	7	321	0IE	C9-C10-C11	3.03	129.71	123.52
24	2	308	CLA	C3B-C4B-NB	-3.02	107.83	110.53
24	8	313	CLA	C3B-C4B-NB	-3.02	107.83	110.53
24	A	834	CLA	C3B-C4B-NB	-3.02	107.83	110.53
24	0	308	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
24	B	816	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
23	6	307	CHL	CMD-C2D-C3D	-3.02	118.64	124.68
24	B	807	CLA	C3B-C4B-NB	-3.02	107.83	110.53
23	6	313	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
26	8	318	0UR	O44-C45-C46	3.02	119.00	111.55
25	3	317	8CT	C11-C10-C03	-3.02	118.93	127.00
24	L	203	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	H	205	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	H	203	CLA	C3B-C4B-NB	-3.02	107.84	110.53
23	6	315	CHL	CMD-C2D-C3D	-3.02	118.65	124.68
24	A	831	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	A	812	CLA	C3B-C4B-NB	-3.02	107.84	110.53
25	B	850	8CT	C11-C10-C03	-3.02	118.94	127.00
24	B	820	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
24	B	828	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
25	6	319	8CT	C40-C12-C13	-3.01	117.93	122.82
24	B	836	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
23	7	307	CHL	CBC-CAC-C3C	-3.01	108.56	112.87
23	1	305	CHL	O2A-CGA-CBA	3.01	121.02	111.83
24	6	310	CLA	C3B-C4B-NB	-3.01	107.84	110.53
25	L	205	8CT	C14-C15-C16	-3.01	118.11	126.36
24	7	317	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
24	3	312	CLA	C3B-C4B-NB	-3.01	107.84	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	313	8CT	C01-C02-C07	3.00	120.00	113.60
25	A	846	8CT	C35-C30-C29	-3.00	109.37	112.83
24	6	310	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
23	6	302	CHL	O2A-CGA-CBA	3.00	120.99	111.83
23	1	301	CHL	OMC-CMC-C2C	-3.00	119.91	125.12
24	3	304	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
24	3	310	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
24	G	102	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
24	L	206	CLA	C3B-C4B-NB	-3.00	107.85	110.53
25	B	846	8CT	C22-C21-C23	3.00	122.67	118.09
24	A	823	CLA	C3B-C4B-NB	-3.00	107.85	110.53
23	8	301	CHL	CMD-C2D-C3D	-3.00	118.69	124.68
30	7	321	0IE	C4-C3-C2	-3.00	117.55	120.16
24	2	302	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	6	323	CHL	CMD-C2D-C3D	-3.00	118.69	124.68
23	0	301	CHL	C4-C3-C5	3.00	119.65	116.13
26	4	318	0UR	C5-C4-C3	-3.00	123.34	126.92
23	6	308	CHL	O2A-CGA-CBA	2.99	120.97	111.83
27	3	320	LHG	O8-C23-C24	2.99	120.97	111.83
24	B	829	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
24	G	101	CLA	C3B-C4B-NB	-2.99	107.86	110.53
25	A	844	8CT	C25-C24-C23	-2.99	114.53	123.20
25	O	208	8CT	C35-C30-C29	-2.99	109.39	112.83
23	7	301	CHL	CMD-C2D-C3D	-2.99	118.71	124.68
24	A	801	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	B	802	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	5	314	0UR	C14-C15-C16	-2.99	123.08	127.28
25	B	850	8CT	C01-C02-C07	2.99	119.97	113.60
25	7	319	8CT	C29-C28-C26	-2.99	119.89	126.32
24	J	103	CLA	C3B-C4B-NB	-2.99	107.86	110.53
26	4	317	0UR	C5-C4-C3	-2.99	123.34	126.92
25	B	848	8CT	C04-C03-C02	-2.99	118.55	122.64
24	8	305	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
25	G	104	8CT	C39-C16-C17	-2.99	117.98	122.82
24	A	840	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
24	G	101	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
24	B	814	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
25	B	848	8CT	C27-C26-C25	-2.98	117.98	122.82
25	G	104	8CT	C14-C15-C16	-2.98	118.19	126.36
26	3	318	0UR	C34-C27-C1	-2.98	120.73	124.45
26	6	320	0UR	C18-C17-C16	-2.98	119.91	126.32
25	F	304	8CT	C05-C04-C03	2.98	114.77	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	313	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	G	104	8CT	C01-C02-C07	2.98	119.94	113.60
25	F	301	8CT	C19-C20-C21	-2.98	123.10	127.28
25	J	101	8CT	C01-C02-C07	2.98	119.94	113.60
24	A	828	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	O	208	8CT	C24-C25-C26	-2.98	123.10	127.28
24	A	814	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	B	817	CLA	CHB-C4A-NA	2.98	128.69	124.40
24	A	853	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
24	A	804	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	A	819	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
24	O	201	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
23	9	301	CHL	O1D-CGD-CBD	-2.97	120.21	124.72
23	4	313	CHL	CBC-CAC-C3C	-2.97	108.61	112.87
23	9	305	CHL	O2A-CGA-CBA	2.97	120.90	111.83
25	B	843	8CT	C22-C21-C20	-2.97	118.00	122.82
24	9	311	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
26	6	321	0UR	C10-C11-C12	-2.97	123.11	127.28
24	5	303	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
24	6	312	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	7	310	CLA	C3B-C4B-NB	-2.97	107.88	110.53
25	6	319	8CT	C15-C16-C17	2.97	123.68	119.01
24	4	311	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
25	J	104	8CT	C39-C16-C17	-2.97	118.01	122.82
23	3	301	CHL	CMD-C2D-C3D	-2.97	118.76	124.68
24	B	823	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
25	A	847	8CT	C11-C12-C13	-2.96	114.35	119.01
26	3	318	0UR	O44-C43-C3	2.96	116.80	109.09
25	A	847	8CT	C25-C24-C23	-2.96	114.62	123.20
24	8	310	CLA	C3B-C4B-NB	-2.96	107.89	110.53
28	0	318	SQD	O6-C1-C2	2.96	112.77	108.27
24	O	205	CLA	C3A-C2A-C1A	-2.96	103.27	106.30
31	A	841	PQN	C11-C12-C13	-2.96	121.73	126.83
24	B	811	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	9	303	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	A	809	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	A	825	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
25	J	104	8CT	C22-C21-C23	2.96	122.60	118.09
24	O	204	CLA	C3B-C4B-NB	-2.96	107.89	110.53
24	9	304	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
24	A	809	CLA	C1-C2-C3	-2.95	121.36	126.20
25	A	846	8CT	C29-C28-C26	-2.95	119.97	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	313	CLA	C3B-C4B-NB	-2.95	107.89	110.53
24	8	311	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	2	309	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	4	312	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
23	7	302	CHL	CMD-C2D-C3D	-2.95	118.79	124.68
24	1	302	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	7	313	CHL	CMD-C2D-C3D	-2.95	118.79	124.68
24	0	309	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	7	305	CHL	CMD-C2D-C3D	-2.95	118.79	124.68
23	8	307	CHL	C1-C2-C3	-2.95	121.99	126.76
26	1	316	0UR	C9-C10-C11	-2.95	117.49	123.52
24	A	803	CLA	CHB-C4A-NA	2.95	128.65	124.40
26	4	318	0UR	O44-C45-C46	2.95	118.82	111.55
23	9	312	CHL	CBC-CAC-C3C	-2.94	108.66	112.87
24	A	818	CLA	C3B-C4B-NB	-2.94	107.90	110.53
26	3	318	0UR	C28-C19-C18	-2.94	109.44	112.83
23	4	315	CHL	O2D-CGD-O1D	-2.94	118.12	123.85
23	4	308	CHL	CMD-C2D-C3D	-2.94	118.81	124.68
26	7	320	0UR	C48-C47-C46	-2.94	119.80	125.92
27	8	302	LHG	O8-C23-C24	2.94	120.80	111.83
24	B	822	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
25	L	207	8CT	C04-C03-C02	-2.94	118.62	122.64
26	9	315	0UR	C10-C11-C12	-2.94	123.16	127.28
32	A	852	CL0	CHA-C1A-C2A	-2.94	126.41	133.31
24	A	820	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
23	0	306	CHL	CMD-C2D-C3D	-2.94	118.81	124.68
26	6	320	0UR	C9-C8-C7	-2.94	123.16	127.28
24	0	309	CLA	C3B-C4B-NB	-2.93	107.91	110.53
23	8	309	CHL	CBC-CAC-C3C	-2.93	108.67	112.87
24	5	308	CLA	C3B-C4B-NB	-2.93	107.91	110.53
24	7	309	CLA	C3B-C4B-NB	-2.93	107.91	110.53
24	B	839	CLA	C3B-C4B-NB	-2.93	107.91	110.53
23	9	306	CHL	CBC-CAC-C3C	-2.93	108.67	112.87
24	B	802	CLA	C3B-C4B-NB	-2.93	107.91	110.53
25	L	205	8CT	C18-C19-C20	-2.93	117.52	123.52
23	1	312	CHL	CMD-C2D-C3D	-2.93	118.83	124.68
24	B	831	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
23	4	307	CHL	O2A-CGA-CBA	2.93	120.76	111.83
23	8	309	CHL	CMD-C2D-C3D	-2.93	118.83	124.68
25	3	323	8CT	C27-C26-C25	-2.93	118.08	122.82
23	6	306	CHL	O2A-CGA-CBA	2.92	120.75	111.83
23	7	301	CHL	O2A-CGA-CBA	2.92	120.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	301	CHL	CMD-C2D-C3D	-2.92	118.84	124.68
23	6	302	CHL	CMB-C2B-C3B	2.92	130.53	124.68
23	1	305	CHL	CMD-C2D-C3D	-2.92	118.84	124.68
26	9	314	0UR	C48-C47-C46	-2.92	119.83	125.92
27	A	843	LHG	O8-C23-C24	2.92	120.02	111.15
24	A	831	CLA	C3B-C4B-NB	-2.92	107.92	110.53
26	0	315	0UR	C14-C15-C16	-2.92	123.18	127.28
24	9	311	CLA	C3B-C4B-NB	-2.92	107.92	110.53
23	7	307	CHL	CMD-C2D-C3D	-2.92	118.85	124.68
24	7	308	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	A	806	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	1	311	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
24	6	304	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
23	2	301	CHL	O2A-CGA-CBA	2.92	120.73	111.83
24	0	304	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
26	1	315	0UR	C48-C47-C46	-2.92	119.85	125.92
26	6	321	0UR	C14-C15-C16	-2.91	123.19	127.28
25	B	847	8CT	C01-C02-C07	2.91	119.81	113.60
23	7	306	CHL	O2A-CGA-CBA	2.91	120.72	111.83
23	8	308	CHL	CMD-C2D-C3D	-2.91	118.86	124.68
31	A	841	PQN	C11-C3-C2	-2.91	119.90	124.89
23	5	301	CHL	O2A-CGA-CBA	2.91	120.72	111.83
23	7	302	CHL	O2A-CGA-CBA	2.91	120.72	111.83
25	4	316	8CT	C14-C15-C16	-2.91	118.38	126.36
23	6	307	CHL	CBC-CAC-C3C	-2.91	108.70	112.87
23	7	305	CHL	CBC-CAC-C3C	-2.91	108.71	112.87
23	6	306	CHL	CMD-C2D-C3D	-2.91	118.87	124.68
23	4	305	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
24	7	315	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
30	7	321	0IE	C20-C3-C2	2.91	121.69	115.01
23	4	306	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
24	B	839	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
24	A	835	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	L	202	CLA	C3B-C4B-NB	-2.90	107.94	110.53
24	5	309	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
23	8	308	CHL	O2A-CGA-CBA	2.90	120.69	111.83
23	6	305	CHL	CMD-C2D-C3D	-2.90	118.88	124.68
23	8	303	CHL	CBC-CAC-C3C	-2.90	108.72	112.87
24	5	309	CLA	C3B-C4B-NB	-2.90	107.94	110.53
29	J	102	LMG	O6-C1-O1	-2.90	103.19	110.04
23	7	306	CHL	CMD-C2D-C3D	-2.90	118.89	124.68
25	A	844	8CT	C14-C15-C16	-2.90	118.41	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	8	303	CHL	OMC-CMC-C2C	-2.90	120.08	125.12
25	6	319	8CT	C29-C28-C26	-2.90	120.09	126.32
23	4	305	CHL	CMD-C2D-C3D	-2.90	118.89	124.68
24	2	313	CLA	C3B-C4B-NB	-2.90	107.94	110.53
25	B	848	8CT	C07-C02-C03	-2.90	118.79	122.70
25	A	846	8CT	C01-C02-C07	2.90	119.77	113.60
24	O	204	CLA	CAA-C2A-C3A	-2.90	109.59	116.23
25	F	304	8CT	C01-C02-C07	2.90	119.77	113.60
23	4	313	CHL	O2A-CGA-CBA	2.90	120.66	111.83
24	2	308	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
24	0	319	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	A	816	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	0	311	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	O	202	8CT	C19-C18-C17	-2.89	117.60	123.52
23	5	301	CHL	CBC-CAC-C3C	-2.89	108.73	112.87
30	3	319	0IE	C9-C10-C11	2.89	129.44	123.52
26	2	316	0UR	C43-C3-C4	-2.89	121.62	125.03
23	7	302	CHL	CBC-CAC-C3C	-2.89	108.73	112.87
24	F	302	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	B	844	8CT	C35-C30-C29	-2.89	109.50	112.83
26	1	315	0UR	C28-C19-C18	-2.89	109.50	112.83
32	A	852	CL0	CBC-CAC-C3C	-2.89	108.74	112.87
23	4	306	CHL	CMD-C2D-C3D	-2.89	118.91	124.68
23	9	312	CHL	O1D-CGD-CBD	-2.89	120.34	124.72
24	1	309	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	A	828	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	G	104	8CT	C15-C16-C17	2.89	123.55	119.01
24	7	314	CLA	C3B-C4B-NB	-2.88	107.95	110.53
23	8	314	CHL	O1D-CGD-CBD	-2.88	120.35	124.72
24	A	833	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
25	F	301	8CT	C04-C03-C02	-2.88	118.70	122.64
24	1	303	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
24	7	303	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
26	0	315	0UR	C4-C5-C6	-2.88	114.85	123.20
25	A	845	8CT	C11-C10-C03	-2.88	119.30	127.00
23	4	301	CHL	C4-C3-C5	2.88	120.23	115.23
23	0	301	CHL	CMD-C2D-C3D	-2.88	118.93	124.68
24	9	308	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
24	7	315	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	O	206	CLA	CAA-C2A-C3A	-2.88	109.63	116.23
24	B	835	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
24	8	311	CLA	C3B-C4B-NB	-2.88	107.96	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	309	CLA	C3B-C4B-NB	-2.88	107.96	110.53
24	K	102	CLA	C3B-C4B-NB	-2.88	107.96	110.53
25	6	324	8CT	C01-C02-C07	2.88	119.73	113.60
26	9	314	0UR	C4-C3-C2	-2.87	117.66	120.16
24	B	809	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
25	I	101	8CT	C11-C10-C03	-2.87	119.32	127.00
25	B	843	8CT	C22-C21-C23	2.87	122.48	118.09
26	4	318	0UR	C43-C3-C4	-2.87	121.64	125.03
25	F	301	8CT	C07-C02-C03	-2.87	118.82	122.70
26	5	315	0UR	C29-C30-C31	-2.87	106.92	111.18
24	B	805	CLA	C3B-C4B-NB	-2.87	107.97	110.53
23	6	302	CHL	O1D-CGD-CBD	-2.87	120.37	124.72
24	L	201	CLA	C3B-C4B-NB	-2.87	107.97	110.53
24	7	311	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
24	O	209	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
23	3	305	CHL	CMD-C2D-C3D	-2.87	118.95	124.68
24	B	805	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
26	8	319	0UR	C9-C10-C11	-2.87	117.65	123.52
24	A	836	CLA	C3B-C4B-NB	-2.87	107.97	110.53
25	B	846	8CT	C30-C29-C28	2.87	129.04	124.58
23	4	301	CHL	O1D-CGD-CBD	-2.87	120.38	124.72
25	L	205	8CT	C05-C04-C03	2.87	114.60	110.44
23	5	304	CHL	O1D-CGD-CBD	-2.87	120.38	124.72
24	2	303	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	B	812	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	0	303	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
24	3	308	CLA	C1-C2-C3	-2.86	121.51	126.20
24	J	103	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
24	3	308	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	3	323	8CT	C01-C02-C07	2.86	119.69	113.60
30	7	321	0IE	C20-C3-C4	-2.86	120.77	124.72
24	B	817	CLA	C3B-C4B-NB	-2.86	107.98	110.53
23	1	305	CHL	CBC-CAC-C3C	-2.86	108.78	112.87
24	A	810	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
23	8	301	CHL	O1D-CGD-CBD	-2.86	120.39	124.72
24	2	302	CLA	C3B-C4B-NB	-2.86	107.98	110.53
24	A	820	CLA	C3B-C4B-NB	-2.86	107.98	110.53
24	B	808	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	3	323	8CT	C15-C16-C17	2.86	123.50	119.01
24	6	311	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
24	8	312	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
27	2	319	LHG	O8-C23-C24	2.85	120.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	304	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	K	104	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	2	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	A	827	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	9	306	CHL	O2A-CGA-CBA	2.85	120.53	111.83
26	2	315	0UR	O44-C43-C3	2.85	116.50	109.09
25	B	848	8CT	C18-C19-C20	2.85	129.35	123.52
25	F	304	8CT	C11-C10-C03	-2.84	119.40	127.00
24	H	202	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	L	206	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	A	838	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	A	821	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	7	311	CLA	C3B-C4B-NB	-2.84	107.99	110.53
26	1	315	0UR	C43-C3-C4	-2.84	121.68	125.03
24	3	309	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	A	805	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	B	815	CLA	C3B-C4B-NB	-2.84	108.00	110.53
25	7	318	8CT	C01-C02-C07	2.84	119.65	113.60
23	7	313	CHL	O1D-CGD-CBD	-2.84	120.42	124.72
24	H	203	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
23	7	307	CHL	C1-C2-C3	-2.84	122.17	126.76
26	7	320	0UR	O44-C43-C3	2.84	116.47	109.09
25	B	846	8CT	C27-C26-C25	-2.84	118.22	122.82
24	8	315	CLA	C3B-C4B-NB	-2.84	108.00	110.53
24	4	312	CLA	C3B-C4B-NB	-2.84	108.00	110.53
23	3	305	CHL	O2A-CGA-CBA	2.83	120.48	111.83
25	J	101	8CT	C10-C11-C12	-2.83	122.04	126.23
23	1	306	CHL	C4-C3-C5	2.83	120.15	115.23
23	9	305	CHL	CMD-C2D-C3D	-2.83	119.02	124.68
24	1	302	CLA	C3B-C4B-NB	-2.83	108.00	110.53
24	A	808	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
26	9	314	0UR	C15-C14-C13	-2.83	115.00	123.20
25	L	207	8CT	C01-C02-C07	2.83	119.63	113.60
23	1	306	CHL	O2A-CGA-CBA	2.83	120.46	111.83
27	3	324	LHG	O8-C23-C24	2.83	120.46	111.83
24	L	201	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
25	2	314	8CT	C11-C10-C03	-2.83	119.44	127.00
24	4	310	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
23	5	301	CHL	CMD-C2D-C3D	-2.83	119.03	124.68
23	0	302	CHL	O1D-CGD-CBD	-2.83	120.44	124.72
24	5	311	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
24	1	307	CLA	C3B-C4B-NB	-2.83	108.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2	312	CHL	CMD-C2D-C3D	-2.82	119.04	124.68
24	B	822	CLA	C3B-C4B-NB	-2.82	108.01	110.53
26	9	314	0UR	C10-C9-C8	-2.82	117.74	123.52
23	6	301	CHL	CMD-C2D-C3D	-2.82	119.04	124.68
24	6	304	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	B	827	CLA	C1-C2-C3	-2.82	121.57	126.20
24	A	812	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	4	302	CHL	CMD-C2D-C3D	-2.82	119.05	124.68
25	O	208	8CT	C01-C02-C07	2.82	119.61	113.60
23	2	305	CHL	O2A-CGA-CBA	2.82	120.43	111.83
24	1	313	CLA	C3B-C4B-NB	-2.82	108.01	110.53
24	4	304	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
23	4	315	CHL	CMD-C2D-C3D	-2.82	119.05	124.68
25	A	845	8CT	C01-C02-C07	2.82	119.60	113.60
27	I	102	LHG	O8-C23-C24	2.82	120.42	111.83
23	7	301	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
24	6	309	CLA	C3B-C4B-NB	-2.82	108.02	110.53
23	1	304	CHL	O2A-CGA-CBA	2.81	120.42	111.83
24	5	313	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
23	4	305	CHL	CBC-CAC-C3C	-2.81	108.84	112.87
23	0	305	CHL	O2A-CGA-CBA	2.81	120.42	111.83
23	1	306	CHL	C1-C2-C3	-2.81	121.59	126.20
24	H	204	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
23	4	315	CHL	C4-C3-C5	2.81	120.11	115.23
25	3	323	8CT	C05-C04-C03	2.81	114.53	110.44
24	K	102	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	9	302	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	0	302	CHL	CBC-CAC-C3C	-2.81	108.85	112.87
24	3	303	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
24	A	824	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	9	306	CHL	CMD-C2D-C3D	-2.81	119.07	124.68
24	0	310	CLA	C3B-C4B-NB	-2.81	108.02	110.53
23	0	302	CHL	C4-C3-C5	2.81	120.10	115.23
24	3	308	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
24	1	307	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
24	B	824	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
23	9	301	CHL	CBC-CAC-C3C	-2.80	108.86	112.87
23	4	307	CHL	CMD-C2D-C3D	-2.80	119.08	124.68
25	L	205	8CT	C01-C02-C07	2.80	119.57	113.60
26	6	320	0UR	C48-C47-C46	-2.80	120.08	125.92
25	1	314	8CT	C35-C30-C29	-2.80	109.60	112.83
24	9	310	CLA	O2D-CGD-O1D	-2.80	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	815	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	7	305	CHL	O2A-CGA-CBA	2.80	120.37	111.83
30	7	321	0IE	C23-C16-C17	2.80	122.36	118.09
24	8	304	CLA	C3B-C4B-NB	-2.80	108.03	110.53
24	A	837	CLA	C3B-C4B-NB	-2.80	108.03	110.53
23	4	308	CHL	O1D-CGD-CBD	-2.80	120.48	124.72
24	0	312	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
25	F	301	8CT	C25-C24-C23	-2.80	115.10	123.20
25	I	101	8CT	C30-C29-C28	-2.79	120.23	124.58
23	8	303	CHL	C4-C3-C5	2.79	120.08	115.23
24	5	302	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
23	7	313	CHL	CBC-CAC-C3C	-2.79	108.87	112.87
25	4	316	8CT	C22-C21-C20	-2.79	118.29	122.82
24	1	310	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
27	A	850	LHG	O8-C23-C24	2.79	120.35	111.83
24	6	316	CLA	C3B-C4B-NB	-2.79	108.04	110.53
23	9	306	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
29	A	854	LMG	O6-C1-O1	-2.79	103.45	110.04
26	0	316	0UR	C34-C27-C1	-2.79	120.97	124.45
23	6	308	CHL	CMD-C2D-C3D	-2.79	119.11	124.68
26	0	316	0UR	C15-C14-C13	-2.79	115.12	123.20
25	B	843	8CT	C30-C29-C28	-2.79	120.24	124.58
24	0	307	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
26	8	318	0UR	C4-C5-C6	-2.79	115.13	123.20
24	1	310	CLA	C3B-C4B-NB	-2.78	108.04	110.53
23	4	301	CHL	O2D-CGD-O1D	-2.78	118.43	123.85
24	6	303	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
23	1	301	CHL	C4-C3-C5	2.78	120.06	115.23
24	8	305	CLA	C3B-C4B-NB	-2.78	108.05	110.53
32	A	852	CL0	C1C-CHC-C4B	2.78	126.02	116.07
24	K	103	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	4	311	CLA	C3B-C4B-NB	-2.78	108.05	110.53
25	B	843	8CT	C29-C28-C26	-2.78	120.35	126.32
25	O	208	8CT	C25-C24-C23	-2.78	115.15	123.20
23	0	302	CHL	CMD-C2D-C3D	-2.78	119.14	124.68
24	B	811	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
24	9	308	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	3	311	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
23	3	301	CHL	O1D-CGD-CBD	-2.78	120.51	124.72
25	O	202	8CT	C27-C26-C28	2.77	122.33	118.09
25	J	104	8CT	C23-C21-C20	-2.77	114.65	119.01
24	H	205	CLA	C3B-C4B-NB	-2.77	108.05	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	323	8CT	C25-C24-C23	-2.77	115.16	123.20
25	L	205	8CT	C40-C12-C13	-2.77	118.32	122.82
24	B	836	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	2	304	CHL	O1D-CGD-CBD	-2.77	120.52	124.72
25	A	849	8CT	C01-C02-C07	2.77	119.50	113.60
24	B	832	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	8	307	CHL	CBC-CAC-C3C	-2.77	108.91	112.87
25	8	317	8CT	C05-C04-C03	2.77	114.46	110.44
24	8	310	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	O	209	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	0	302	CHL	O2A-CGA-CBA	2.77	120.27	111.83
24	9	309	CLA	CAA-C2A-C3A	-2.77	109.88	116.23
24	9	307	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
24	A	806	CLA	CMB-C2B-C1B	-2.76	121.21	125.42
24	8	315	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	G	103	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	A	803	CLA	C3B-C4B-NB	-2.76	108.06	110.53
24	B	827	CLA	C3B-C4B-NB	-2.76	108.06	110.53
25	8	317	8CT	C24-C25-C26	-2.76	123.41	127.28
23	8	303	CHL	O2A-CGA-CBA	2.76	120.25	111.83
23	2	301	CHL	CMD-C2D-C3D	-2.76	119.17	124.68
23	1	312	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
23	3	302	CHL	CMD-C2D-C3D	-2.76	119.17	124.68
24	L	203	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	A	849	8CT	C14-C15-C16	-2.76	118.81	126.36
24	7	314	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
26	O	207	0UR	C10-C11-C12	-2.76	123.41	127.28
26	3	318	0UR	C5-C4-C3	-2.75	123.62	126.92
23	5	306	CHL	C1B-CHB-C4A	2.75	123.09	121.32
26	O	207	0UR	C18-C17-C16	-2.75	120.40	126.32
29	J	105	LMG	O6-C1-O1	-2.75	103.54	110.04
26	O	207	0UR	C15-C14-C13	-2.75	115.23	123.20
23	1	312	CHL	CBC-CAC-C3C	-2.75	108.94	112.87
25	3	323	8CT	C39-C16-C17	-2.75	118.36	122.82
24	B	825	CLA	C3B-C4B-NB	-2.75	108.08	110.53
24	4	309	CLA	C3B-C4B-NB	-2.75	108.08	110.53
23	3	305	CHL	O1D-CGD-CBD	-2.75	120.56	124.72
27	2	317	LHG	O8-C23-C24	2.75	120.21	111.83
27	5	316	LHG	O8-C23-C24	2.75	120.21	111.83
23	2	306	CHL	CMD-C2D-C3D	-2.75	119.19	124.68
25	1	314	8CT	C05-C04-C03	2.75	114.43	110.44
27	7	324	LHG	O8-C23-C24	2.75	120.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	O	202	8CT	C13-C14-C15	-2.75	115.25	123.20
24	B	834	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
23	1	301	CHL	O2A-CGA-CBA	2.74	120.20	111.83
24	G	102	CLA	C3B-C4B-NB	-2.74	108.08	110.53
24	6	318	CLA	C3B-C4B-NB	-2.74	108.08	110.53
25	M	102	8CT	C04-C03-C02	-2.74	118.89	122.64
25	6	319	8CT	C05-C04-C03	2.74	114.42	110.44
24	7	304	CLA	C3B-C4B-NB	-2.74	108.08	110.53
23	6	323	CHL	C4-C3-C5	2.74	119.98	115.23
23	6	307	CHL	C1-C2-C3	-2.74	122.33	126.76
27	7	323	LHG	O8-C23-C24	2.74	120.19	111.83
26	3	318	0UR	C15-C14-C13	-2.74	115.27	123.20
24	B	826	CLA	C3B-C4B-NB	-2.74	108.09	110.53
23	7	306	CHL	CBC-CAC-C3C	-2.74	108.95	112.87
23	7	301	CHL	O2D-CGD-O1D	-2.74	118.52	123.85
25	7	318	8CT	C30-C31-C32	-2.73	118.10	121.47
23	8	303	CHL	CMD-C2D-C3D	-2.73	119.22	124.68
25	L	207	8CT	C19-C20-C21	-2.73	123.45	127.28
24	4	314	CLA	C3B-C4B-NB	-2.73	108.09	110.53
23	8	306	CHL	O1D-CGD-CBD	-2.73	120.58	124.72
29	O	203	LMG	O6-C1-O1	-2.73	103.59	110.04
23	9	305	CHL	CBC-CAC-C3C	-2.73	108.96	112.87
24	3	311	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	B	819	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	7	309	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
24	B	840	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	7	319	8CT	C01-C02-C07	2.73	119.41	113.60
24	0	310	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
24	B	806	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	4	313	CHL	CMD-C2D-C3D	-2.73	119.24	124.68
25	G	104	8CT	C18-C19-C20	-2.73	117.94	123.52
24	8	304	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	2	307	CHL	CMD-C2D-C3D	-2.73	119.24	124.68
25	K	105	8CT	C01-C02-C07	2.72	119.41	113.60
27	L	208	LHG	O8-C23-C24	2.72	120.14	111.83
26	0	316	0UR	C14-C15-C16	-2.72	123.46	127.28
24	1	308	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	A	840	CLA	C1-C2-C3	-2.72	121.74	126.20
23	4	302	CHL	O2A-CGA-CBA	2.72	120.13	111.83
27	6	322	LHG	O8-C23-C24	2.72	120.13	111.83
23	2	304	CHL	CBC-CAC-C3C	-2.72	108.98	112.87
23	7	305	CHL	O1D-CGD-CBD	-2.72	120.60	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	307	CLA	C3B-C4B-NB	-2.72	108.10	110.53
23	4	302	CHL	C4-C3-C5	2.72	119.95	115.23
23	6	307	CHL	O2A-CGA-CBA	2.72	120.12	111.83
24	6	318	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
24	7	317	CLA	C3B-C4B-NB	-2.72	108.10	110.53
24	A	832	CLA	C3B-C4B-NB	-2.72	108.11	110.53
23	4	308	CHL	CBC-CAC-C3C	-2.72	108.98	112.87
25	O	208	8CT	C14-C15-C16	-2.72	118.92	126.36
24	A	807	CLA	C3B-C4B-NB	-2.72	108.11	110.53
25	3	317	8CT	C01-C02-C07	2.71	119.38	113.60
24	2	303	CLA	C3B-C4B-NB	-2.71	108.11	110.53
23	1	304	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
25	A	847	8CT	C27-C26-C28	2.71	122.23	118.09
26	5	314	0UR	C48-C47-C46	-2.71	120.27	125.92
25	7	318	8CT	C13-C14-C15	-2.71	115.34	123.20
25	7	319	8CT	C04-C03-C02	-2.71	118.93	122.64
23	8	309	CHL	CMA-C3A-C4A	-2.71	108.77	114.61
26	2	316	0UR	C17-C16-C15	2.71	123.27	119.01
31	A	841	PQN	C2M-C2-C3	-2.71	120.00	124.45
23	3	305	CHL	CBC-CAC-C3C	-2.71	108.99	112.87
25	4	316	8CT	C24-C23-C21	-2.71	118.93	126.36
24	K	103	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
24	5	307	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
24	7	316	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
23	4	301	CHL	C1-C2-C3	-2.71	121.76	126.20
25	G	104	8CT	C04-C03-C02	-2.71	118.94	122.64
23	8	306	CHL	CBC-CAC-C3C	-2.71	109.00	112.87
24	5	310	CLA	C3B-C4B-NB	-2.71	108.11	110.53
25	A	847	8CT	C28-C26-C25	-2.71	114.75	119.01
26	6	320	0UR	O44-C45-C46	2.71	118.23	111.55
23	4	306	CHL	CBC-CAC-C3C	-2.71	109.00	112.87
24	A	833	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	9	309	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
24	6	316	CLA	CAA-CBA-CGA	-2.70	105.53	113.21
31	A	841	PQN	C12-C11-C3	-2.70	105.42	112.08
23	8	314	CHL	O2A-CGA-CBA	2.70	120.08	111.83
30	3	319	0IE	C23-C16-C17	2.70	122.22	118.09
29	3	321	LMG	O6-C1-O1	-2.70	103.66	110.04
23	4	313	CHL	O2D-CGD-O1D	-2.70	118.59	123.85
24	4	309	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
25	F	304	8CT	C30-C31-C32	-2.70	118.14	121.47
26	1	316	0UR	C18-C17-C16	-2.70	120.52	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	316	CLA	CMB-C2B-C1B	-2.70	121.31	125.42
26	8	319	0UR	C48-C47-C46	-2.70	120.30	125.92
25	A	845	8CT	C25-C24-C23	-2.70	115.39	123.20
24	7	316	CLA	CHB-C4A-NA	2.70	128.29	124.40
24	3	304	CLA	CHB-C4A-NA	2.70	128.29	124.40
32	A	852	CL0	C4D-ND-C1D	2.70	107.27	105.22
26	4	317	0UR	C15-C14-C13	-2.69	115.39	123.20
25	7	318	8CT	C18-C19-C20	-2.69	118.01	123.52
26	8	318	0UR	C48-C47-C46	-2.69	120.31	125.92
24	B	816	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	6	305	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
25	6	319	8CT	C39-C16-C17	-2.69	118.45	122.82
25	B	847	8CT	C05-C04-C03	2.69	114.35	110.44
24	A	821	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	8	316	CHL	O1D-CGD-CBD	-2.69	120.64	124.72
27	A	842	LHG	O8-C23-C24	2.69	120.03	111.83
23	8	309	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
25	F	301	8CT	C05-C04-C03	2.69	114.34	110.44
23	0	301	CHL	OMC-CMC-C2C	-2.69	120.45	125.12
26	6	321	0UR	C48-C47-C46	-2.69	120.33	125.92
23	1	301	CHL	CMA-C3A-C4A	-2.69	108.82	114.61
23	6	315	CHL	O1D-CGD-CBD	-2.69	120.65	124.72
23	5	305	CHL	O2A-CGA-CBA	2.68	120.02	111.83
31	B	842	PQN	C11-C12-C13	-2.68	122.21	126.83
23	1	304	CHL	CMB-C2B-C3B	2.68	130.04	124.68
24	A	835	CLA	C1-C2-C3	-2.68	121.80	126.20
24	A	838	CLA	C1-C2-C3	-2.68	121.81	126.20
25	4	316	8CT	C11-C10-C03	-2.68	119.84	127.00
25	F	301	8CT	C24-C25-C26	-2.68	123.52	127.28
24	0	310	CLA	CHB-C4A-NA	2.68	128.26	124.40
30	7	321	0IE	C21-C7-C8	-2.68	118.48	122.82
25	A	846	8CT	C25-C24-C23	-2.67	115.45	123.20
24	A	848	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
24	B	807	CLA	CHB-C4A-NA	2.67	128.26	124.40
26	6	320	0UR	C10-C9-C8	-2.67	118.05	123.52
24	0	308	CLA	C3B-C4B-NB	-2.67	108.15	110.53
23	7	302	CHL	O2D-CGD-O1D	-2.67	118.65	123.85
30	3	319	0IE	C21-C7-C8	-2.67	118.49	122.82
25	B	845	8CT	C24-C25-C26	-2.67	123.53	127.28
24	5	302	CLA	C3B-C4B-NB	-2.67	108.15	110.53
24	4	314	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
25	9	313	8CT	C29-C28-C26	-2.67	120.59	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	0	317	LHG	O8-C23-C24	2.67	119.97	111.83
27	3	322	LHG	O8-C23-C24	2.67	119.96	111.83
27	7	322	LHG	O8-C23-C24	2.66	119.96	111.83
24	3	311	CLA	CHB-C4A-NA	2.66	128.24	124.40
27	1	318	LHG	O8-C23-C24	2.66	119.95	111.83
24	A	805	CLA	CHB-C4A-NA	2.66	128.24	124.40
23	8	307	CHL	O2D-CGD-O1D	-2.66	118.67	123.85
29	9	317	LMG	O1-C1-C2	-2.66	104.24	108.27
23	4	315	CHL	C1-C2-C3	-2.66	121.84	126.20
23	7	301	CHL	C1-C2-C3	-2.66	121.85	126.20
25	B	843	8CT	C01-C02-C07	2.65	119.25	113.60
24	5	310	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
23	3	301	CHL	CMB-C2B-C3B	2.65	129.98	124.68
24	H	201	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	6	309	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
25	A	845	8CT	C27-C26-C28	2.65	122.14	118.09
27	1	317	LHG	O8-C23-C24	2.65	119.91	111.83
26	0	316	0UR	C48-C47-C46	-2.64	120.41	125.92
24	B	812	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	A	805	CLA	C1-C2-C3	-2.64	121.86	126.20
24	B	825	CLA	CHB-C4A-NA	2.64	128.22	124.40
27	2	319	LHG	C26-C25-C24	2.64	122.84	113.13
23	9	305	CHL	CMB-C2B-C3B	2.64	129.96	124.68
24	B	830	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	1	307	CLA	CHB-C4A-NA	2.64	128.21	124.40
23	2	301	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
23	8	307	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
25	0	314	8CT	C11-C10-C03	-2.64	119.94	127.00
25	M	102	8CT	C01-C02-C07	2.64	119.22	113.60
24	A	806	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	9	305	CHL	CMA-C3A-C4A	-2.64	108.92	114.61
25	K	105	8CT	C11-C10-C03	-2.64	119.95	127.00
24	H	202	CLA	C3B-C4B-NB	-2.64	108.17	110.53
25	G	104	8CT	C07-C02-C03	-2.64	119.14	122.70
23	2	301	CHL	O2D-CGD-O1D	-2.64	118.72	123.85
27	9	316	LHG	O8-C23-C24	2.63	119.86	111.83
23	1	301	CHL	C6-C5-C3	-2.63	107.06	113.47
23	5	301	CHL	C4-C3-C5	2.63	119.80	115.23
25	6	319	8CT	C35-C30-C29	-2.63	109.80	112.83
29	O	210	LMG	O6-C1-O1	-2.63	103.83	110.04
25	J	101	8CT	C39-C16-C15	2.63	122.11	118.09
25	4	316	8CT	C04-C03-C10	2.63	122.78	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4	307	CHL	OMC-CMC-C2C	-2.63	120.56	125.12
24	0	303	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	O	201	CLA	C3B-C4B-NB	-2.63	108.18	110.53
23	5	305	CHL	O1D-CGD-CBD	-2.63	120.74	124.72
23	9	312	CHL	O2D-CGD-O1D	-2.63	118.74	123.85
24	0	313	CLA	C3B-C4B-NB	-2.63	108.19	110.53
24	9	307	CLA	C3B-C4B-NB	-2.63	108.19	110.53
23	2	304	CHL	CMA-C3A-C4A	-2.63	108.95	114.61
25	M	102	8CT	C14-C15-C16	-2.62	119.17	126.36
24	5	310	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	B	837	CLA	C3B-C4B-NB	-2.61	108.20	110.53
25	L	205	8CT	C11-C12-C13	2.61	123.12	119.01
29	9	317	LMG	O6-C1-O1	-2.61	103.87	110.04
25	A	849	8CT	C27-C26-C25	-2.61	118.58	122.82
24	7	310	CLA	CAA-C2A-C3A	-2.61	110.24	116.23
26	0	316	0UR	C43-C3-C2	2.61	122.64	116.56
27	8	320	LHG	O8-C23-C24	2.61	119.80	111.83
23	5	301	CHL	O1D-CGD-CBD	-2.61	120.76	124.72
25	F	301	8CT	C18-C19-C20	-2.61	118.17	123.52
23	6	308	CHL	CMA-C3A-C4A	-2.61	108.98	114.61
24	A	807	CLA	CHB-C4A-NA	2.61	128.17	124.40
26	3	318	0UR	C48-C47-C46	-2.61	120.48	125.92
25	A	849	8CT	C30-C29-C28	-2.61	120.52	124.58
23	7	306	CHL	C4-C3-C5	2.61	119.76	115.23
26	7	320	0UR	C10-C9-C8	-2.61	118.18	123.52
25	A	844	8CT	C01-C02-C07	2.61	119.16	113.60
25	7	318	8CT	C10-C11-C12	-2.61	122.38	126.23
23	6	306	CHL	O1D-CGD-CBD	-2.61	120.77	124.72
23	0	306	CHL	O2A-CGA-CBA	2.61	119.78	111.83
25	A	844	8CT	C24-C25-C26	-2.61	123.62	127.28
24	3	304	CLA	C3B-C4B-NB	-2.61	108.20	110.53
24	3	309	CLA	CHB-C4A-NA	2.61	128.16	124.40
23	6	301	CHL	O2D-CGD-O1D	-2.61	118.78	123.85
25	A	849	8CT	C24-C23-C21	-2.61	119.22	126.36
25	9	313	8CT	C25-C24-C23	-2.60	115.66	123.20
26	0	316	0UR	C34-C27-C26	2.60	119.21	114.42
23	4	306	CHL	O2A-CGA-CBA	2.60	119.77	111.83
23	2	301	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
25	1	314	8CT	C14-C15-C16	-2.60	119.23	126.36
24	A	839	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
23	7	301	CHL	CBC-CAC-C3C	-2.60	109.15	112.87
25	8	317	8CT	C11-C10-C03	-2.60	120.05	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	801	CLA	CHB-C4A-NA	2.60	128.15	124.40
26	2	315	0UR	C15-C14-C13	-2.60	115.66	123.20
23	8	303	CHL	CMB-C2B-C3B	2.60	129.88	124.68
23	3	307	CHL	O1D-CGD-CBD	-2.60	120.78	124.72
24	8	310	CLA	C1-C2-C3	-2.60	121.94	126.20
24	5	308	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
24	A	830	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	B	816	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	A	818	CLA	CMB-C2B-C1B	-2.60	121.47	125.42
23	3	302	CHL	O1D-CGD-CBD	-2.60	120.79	124.72
24	1	310	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	3	303	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	4	318	0UR	C15-C14-C13	-2.59	115.69	123.20
26	3	318	0UR	C18-C17-C16	-2.59	120.75	126.32
24	B	808	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	B	801	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	3	316	8CT	C15-C16-C17	-2.59	114.93	119.01
24	O	205	CLA	O2D-CGD-O1D	-2.59	118.20	124.08
25	K	105	8CT	C11-C12-C13	2.59	123.08	119.01
25	B	846	8CT	C25-C24-C23	2.59	130.71	123.20
24	B	823	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	O	202	8CT	C10-C03-C02	-2.59	115.59	121.56
23	7	302	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
23	8	307	CHL	O2A-CGA-CBA	2.59	119.73	111.83
23	4	308	CHL	O2D-CGD-O1D	-2.59	118.81	123.85
24	9	307	CLA	CHB-C4A-NA	2.59	128.13	124.40
23	6	305	CHL	CBC-CAC-C3C	-2.59	109.17	112.87
23	3	307	CHL	C4-C3-C5	2.59	119.72	115.23
24	2	310	CLA	CHB-C4A-NA	2.59	128.13	124.40
23	3	301	CHL	O2D-CGD-O1D	-2.58	118.82	123.85
24	A	819	CLA	CHB-C4A-NA	2.58	128.13	124.40
25	8	317	8CT	C25-C24-C23	-2.58	115.71	123.20
24	6	310	CLA	C1-C2-C3	-2.58	121.97	126.20
26	6	320	0UR	C43-C3-C2	2.58	122.55	116.56
26	5	315	0UR	C9-C10-C11	-2.58	118.25	123.52
24	B	808	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
25	B	844	8CT	C30-C29-C28	-2.57	120.57	124.58
26	4	317	0UR	C14-C15-C16	-2.57	123.67	127.28
24	0	311	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	B	835	CLA	C3B-C4B-NB	-2.57	108.23	110.53
24	6	303	CLA	C3B-C4B-NB	-2.57	108.23	110.53
23	4	315	CHL	CMB-C2B-C3B	2.57	129.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	305	CHL	O2D-CGD-O1D	-2.57	118.85	123.85
24	9	303	CLA	C3B-C4B-NB	-2.57	108.24	110.53
24	4	304	CLA	C3B-C4B-NB	-2.57	108.24	110.53
24	3	314	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	6	314	CLA	C3B-C4B-NB	-2.57	108.24	110.53
25	7	319	8CT	C11-C10-C03	-2.57	120.14	127.00
24	B	821	CLA	CHB-C4A-NA	2.57	128.10	124.40
23	3	302	CHL	C4-C3-C5	2.57	119.68	115.23
23	5	312	CHL	CMB-C2B-C3B	2.57	129.81	124.68
24	B	806	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	B	832	CLA	CAA-CBA-CGA	-2.56	105.93	113.21
26	4	317	0UR	C4-C5-C6	-2.56	115.78	123.20
24	5	302	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	A	826	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	2	311	CLA	C3B-C4B-NB	-2.56	108.25	110.53
30	7	321	0IE	C6-C7-C8	2.56	123.03	119.01
23	4	308	CHL	CMB-C2B-C3B	2.56	129.79	124.68
24	1	303	CLA	C3B-C4B-NB	-2.56	108.25	110.53
24	9	303	CLA	CHB-C4A-NA	2.56	128.09	124.40
26	4	317	0UR	O44-C43-C3	2.55	115.74	109.09
24	7	316	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	B	813	CLA	CHB-C4A-NA	2.55	128.08	124.40
23	9	305	CHL	O1D-CGD-CBD	-2.55	120.85	124.72
29	2	318	LMG	O6-C1-O1	-2.55	104.01	110.04
25	0	314	8CT	C29-C28-C26	-2.55	120.84	126.32
23	6	323	CHL	CBC-CAC-C3C	-2.55	109.22	112.87
24	0	313	CLA	CHB-C4A-NA	2.55	128.08	124.40
24	0	308	CLA	CHB-C4A-NA	2.55	128.08	124.40
25	B	845	8CT	C11-C10-C03	-2.55	120.19	127.00
25	L	207	8CT	C22-C21-C23	2.55	121.98	118.09
26	6	321	0UR	C28-C19-C18	2.55	115.75	112.83
26	7	320	0UR	C15-C14-C13	-2.55	115.82	123.20
24	A	830	CLA	C1-C2-C3	-2.55	122.64	126.76
24	3	309	CLA	CMB-C2B-C1B	-2.54	121.54	125.42
25	M	102	8CT	C18-C19-C20	-2.54	118.31	123.52
23	1	312	CHL	CMB-C2B-C3B	2.54	129.77	124.68
24	9	308	CLA	C1-C2-C3	-2.54	122.03	126.20
24	A	814	CLA	CHB-C4A-NA	2.54	128.07	124.40
24	A	817	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	1	302	CLA	CHB-C4A-NA	2.54	128.07	124.40
23	8	306	CHL	CMA-C3A-C4A	-2.54	109.14	114.61
24	7	309	CLA	CHB-C4A-NA	2.54	128.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	306	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
29	A	851	LMG	O6-C5-C4	2.54	114.28	109.70
23	1	305	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
23	9	301	CHL	OMC-CMC-C2C	-2.54	120.71	125.12
23	4	308	CHL	CMA-C3A-C4A	-2.54	109.14	114.61
24	A	810	CLA	C3B-C4B-NB	-2.54	108.26	110.53
25	B	846	8CT	C22-C21-C20	-2.54	118.70	122.82
25	4	316	8CT	C01-C02-C07	2.54	119.01	113.60
24	B	818	CLA	CHB-C4A-NA	2.54	128.06	124.40
24	9	304	CLA	C3B-C4B-NB	-2.54	108.27	110.53
24	B	815	CLA	CHB-C4A-NA	2.54	128.06	124.40
25	M	102	8CT	C11-C10-C03	-2.53	120.23	127.00
23	5	312	CHL	O2D-CGD-O1D	-2.53	118.92	123.85
23	6	301	CHL	C4-C3-C5	2.53	119.62	115.23
23	4	302	CHL	O1D-CGD-CBD	-2.53	120.88	124.72
26	8	318	0UR	C43-C3-C4	-2.53	122.04	125.03
25	L	204	8CT	C05-C04-C03	2.53	114.12	110.44
23	4	305	CHL	O2D-CGD-O1D	-2.53	118.92	123.85
24	B	837	CLA	CHB-C4A-NA	2.53	128.05	124.40
24	H	204	CLA	CHB-C4A-NA	2.53	128.05	124.40
25	1	314	8CT	C11-C10-C03	-2.53	120.24	127.00
32	A	852	CL0	C4C-CHD-C1D	2.53	125.12	116.07
24	1	311	CLA	C3B-C4B-NB	-2.53	108.27	110.53
23	6	308	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
23	5	304	CHL	CMB-C2B-C3B	2.53	129.74	124.68
25	2	314	8CT	C24-C23-C21	-2.53	119.43	126.36
25	K	105	8CT	C40-C12-C13	-2.53	118.72	122.82
24	B	806	CLA	CAC-C3C-C4C	2.53	128.08	124.79
24	A	824	CLA	C1-C2-C3	-2.53	122.06	126.20
23	2	312	CHL	CMB-C2B-C3B	2.53	129.73	124.68
24	B	830	CLA	CHB-C1B-NB	2.53	127.84	124.05
24	A	816	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	9	308	CLA	CHB-C4A-NA	2.52	128.04	124.40
24	B	828	CLA	C3B-C4B-NB	-2.52	108.28	110.53
23	4	301	CHL	CMB-C2B-C3B	2.52	129.72	124.68
24	7	314	CLA	CHB-C4A-NA	2.52	128.04	124.40
23	1	306	CHL	O1D-CGD-CBD	-2.52	120.90	124.72
24	A	808	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
23	2	312	CHL	CBC-CAC-C3C	-2.52	109.27	112.87
26	9	314	0UR	C28-C19-C18	-2.52	109.93	112.83
24	5	311	CLA	C3B-C4B-NB	-2.52	108.28	110.53
24	0	309	CLA	CAA-C2A-C3A	-2.51	110.47	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	835	CLA	CHB-C4A-NA	2.51	128.03	124.40
25	1	314	8CT	C01-C02-C07	2.51	118.95	113.60
25	O	208	8CT	C18-C19-C20	-2.51	118.38	123.52
23	6	315	CHL	CMB-C2B-C3B	2.51	129.70	124.68
25	3	316	8CT	C04-C03-C10	2.51	122.46	115.65
24	8	315	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	0	310	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
23	6	302	CHL	C4-C3-C5	2.51	119.58	115.23
24	B	827	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	4	311	CLA	CHB-C4A-NA	2.51	128.02	124.40
24	O	206	CLA	CMB-C2B-C3B	2.51	130.19	123.53
23	8	316	CHL	O2D-CGD-O1D	-2.51	118.97	123.85
24	L	201	CLA	CHB-C4A-NA	2.51	128.02	124.40
26	9	314	0UR	C4-C5-C6	-2.51	115.94	123.20
23	2	305	CHL	O2D-CGD-O1D	-2.51	118.97	123.85
23	4	313	CHL	CMB-C2B-C3B	2.51	129.69	124.68
24	6	311	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	2	301	CHL	C4-C3-C5	2.50	119.58	115.23
24	4	310	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	7	307	CHL	O2A-CGA-CBA	2.50	119.47	111.83
23	9	306	CHL	CMB-C2B-C3B	2.50	129.69	124.68
23	5	312	CHL	CBC-CAC-C3C	-2.50	109.29	112.87
24	H	202	CLA	C1-C2-C3	-2.50	122.10	126.20
24	K	102	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	6	307	CHL	O1D-CGD-CBD	-2.50	120.93	124.72
25	L	205	8CT	C30-C31-C32	-2.50	118.39	121.47
24	A	817	CLA	CHB-C4A-NA	2.50	128.01	124.40
25	J	104	8CT	C04-C03-C02	-2.50	119.22	122.64
23	7	313	CHL	CMB-C2B-C3B	2.50	129.68	124.68
24	J	103	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	B	847	8CT	C04-C03-C02	-2.50	119.22	122.64
29	J	105	LMG	C40-C39-C38	-2.50	101.75	114.37
24	1	308	CLA	CHB-C4A-NA	2.50	128.00	124.40
23	5	304	CHL	O2D-CGD-O1D	-2.50	118.99	123.85
24	A	808	CLA	CHB-C4A-NA	2.50	128.00	124.40
24	B	840	CLA	CHB-C4A-NA	2.50	128.00	124.40
23	7	306	CHL	O2D-CGD-O1D	-2.49	118.99	123.85
28	0	318	SQD	O48-C23-C24	2.49	119.44	111.83
24	5	303	CLA	C3B-C4B-NB	-2.49	108.30	110.53
26	2	315	0UR	C10-C9-C8	-2.49	118.42	123.52
25	8	317	8CT	C01-C02-C07	2.49	118.91	113.60
24	H	204	CLA	C3B-C4B-NB	-2.49	108.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	9	301	CHL	CMB-C2B-C3B	2.49	129.66	124.68
23	2	307	CHL	CMA-C3A-C4A	-2.49	109.24	114.61
29	9	317	LMG	O1-C7-C8	-2.49	104.76	110.82
24	A	838	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	8	303	CHL	CMA-C3A-C4A	-2.49	109.25	114.61
24	B	831	CLA	C1-C2-C3	-2.49	122.74	126.76
24	A	836	CLA	CHB-C4A-NA	2.49	127.99	124.40
23	7	313	CHL	O2D-CGD-O1D	-2.49	119.01	123.85
23	9	306	CHL	CMA-C3A-C4A	-2.49	109.25	114.61
23	4	302	CHL	CMB-C2B-C3B	2.49	129.65	124.68
24	5	311	CLA	CHB-C4A-NA	2.48	127.99	124.40
24	K	103	CLA	CHB-C4A-NA	2.48	127.99	124.40
24	B	836	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
24	B	820	CLA	CHB-C4A-NA	2.48	127.98	124.40
23	1	301	CHL	CMD-C2D-C3D	-2.48	119.72	124.68
24	2	311	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
24	B	815	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
23	6	307	CHL	CMB-C2B-C3B	2.48	129.64	124.68
23	4	306	CHL	OMC-CMC-C2C	-2.48	120.81	125.12
25	F	301	8CT	C27-C26-C28	2.48	121.88	118.09
24	L	202	CLA	CHB-C4A-NA	2.48	127.97	124.40
23	2	307	CHL	CMB-C2B-C3B	2.48	129.63	124.68
24	A	839	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	A	827	CLA	C3B-C4B-NB	-2.47	108.32	110.53
23	0	305	CHL	O2D-CGD-O1D	-2.47	119.03	123.85
25	K	105	8CT	C39-C16-C17	-2.47	118.81	122.82
25	6	319	8CT	C04-C03-C02	-2.47	119.26	122.64
25	L	204	8CT	C14-C15-C16	-2.47	119.59	126.36
24	0	304	CLA	C3B-C4B-NB	-2.47	108.32	110.53
24	B	841	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	3	308	CLA	CHB-C4A-NA	2.47	127.97	124.40
24	7	304	CLA	CHB-C4A-NA	2.47	127.97	124.40
23	3	302	CHL	OMC-CMC-C2C	-2.47	120.83	125.12
25	6	324	8CT	C04-C03-C02	-2.47	119.26	122.64
23	2	301	CHL	CMB-C2B-C3B	2.47	129.62	124.68
24	3	313	CLA	CHB-C4A-NA	2.47	127.96	124.40
25	M	102	8CT	C05-C04-C03	2.47	114.02	110.44
24	6	309	CLA	C1-C2-C3	-2.47	122.15	126.20
24	F	303	CLA	CHB-C4A-NA	2.47	127.96	124.40
26	0	316	0UR	C4-C5-C6	-2.47	116.05	123.20
23	6	307	CHL	OMC-CMC-C2C	-2.46	120.84	125.12
24	7	315	CLA	CHB-C4A-NA	2.46	127.96	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	301	CHL	CBC-CAC-C3C	-2.46	109.34	112.87
23	8	307	CHL	CMB-C2B-C3B	2.46	129.61	124.68
23	1	312	CHL	O2D-CGD-O1D	-2.46	119.05	123.85
24	7	308	CLA	CHB-C4A-NA	2.46	127.96	124.40
26	1	315	0UR	C10-C9-C8	-2.46	118.48	123.52
24	O	206	CLA	O2D-CGD-O1D	-2.46	118.49	124.08
26	1	315	0UR	C4-C3-C2	-2.46	118.02	120.16
25	J	104	8CT	C25-C24-C23	-2.46	116.07	123.20
24	A	836	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
24	B	817	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
23	5	304	CHL	OMC-CMC-C2C	-2.46	120.85	125.12
24	G	101	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	6	306	CHL	CMB-C2B-C3B	2.46	129.60	124.68
23	5	312	CHL	C1B-CHB-C4A	-2.46	119.74	121.32
24	B	821	CLA	C3B-C4B-NB	-2.46	108.33	110.53
24	7	311	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	8	313	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	6	310	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	6	302	CHL	CMD-C2D-C3D	-2.46	119.77	124.68
23	5	306	CHL	CMB-C2B-C3B	2.46	129.59	124.68
23	1	305	CHL	O2D-CGD-O1D	-2.46	119.07	123.85
26	1	315	0UR	C5-C4-C3	-2.46	123.98	126.92
24	A	804	CLA	CHB-C4A-NA	2.46	127.94	124.40
24	O	206	CLA	CAB-C3B-C2B	2.45	130.06	123.53
24	8	312	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	9	310	CLA	CHB-C4A-NA	2.45	127.94	124.40
24	G	102	CLA	CHB-C4A-NA	2.45	127.94	124.40
23	7	306	CHL	OMC-CMC-C2C	-2.45	120.86	125.12
24	B	826	CLA	CAA-C2A-C1A	-2.45	103.94	111.97
24	0	307	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	3	317	8CT	C30-C31-C32	-2.45	118.45	121.47
26	3	318	0UR	C29-C30-C31	-2.45	107.55	111.18
24	A	802	CLA	CHB-C4A-NA	2.45	127.94	124.40
25	B	848	8CT	C01-C02-C07	2.45	118.82	113.60
24	6	317	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	6	316	CLA	CHB-C4A-NA	2.45	127.93	124.40
26	8	318	0UR	C15-C14-C13	-2.45	116.11	123.20
24	3	315	CLA	CHB-C4A-NA	2.45	127.93	124.40
24	B	836	CLA	CHB-C4A-NA	2.45	127.93	124.40
23	1	306	CHL	CMB-C2B-C3B	2.45	129.57	124.68
23	1	301	CHL	O2D-CGD-O1D	-2.45	119.09	123.85
24	A	812	CLA	CHB-C4A-NA	2.44	127.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2	306	CHL	CMA-C3A-C4A	-2.44	109.35	114.61
24	A	826	CLA	C1-C2-C3	-2.44	122.19	126.20
24	B	811	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	A	813	CLA	C3B-C4B-NB	-2.44	108.35	110.53
24	B	814	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	B	839	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	O	204	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	A	833	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	3	306	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	H	202	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	B	810	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	8	308	CHL	CBC-CAC-C3C	-2.44	109.38	112.87
24	9	302	CLA	CHB-C4A-NA	2.44	127.92	124.40
23	0	301	CHL	CMB-C2B-C3B	2.44	129.55	124.68
26	9	315	0UR	C4-C5-C6	-2.44	116.14	123.20
30	3	319	0IE	C6-C7-C8	2.44	122.84	119.01
24	A	836	CLA	C1-C2-C3	-2.44	122.21	126.20
25	3	316	8CT	C11-C10-C03	-2.44	120.49	127.00
26	9	314	0UR	C43-C3-C4	-2.44	122.16	125.03
23	5	301	CHL	O2D-CGD-O1D	-2.44	119.11	123.85
24	6	309	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	A	824	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	B	810	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	5	305	CHL	CMB-C2B-C3B	2.43	129.55	124.68
26	9	315	0UR	C22-C16-C17	2.43	121.81	118.09
24	0	319	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	F	302	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	A	802	CLA	C1-C2-C3	-2.43	122.21	126.20
23	3	302	CHL	O2D-CGD-O1D	-2.43	119.11	123.85
24	2	308	CLA	CHB-C4A-NA	2.43	127.91	124.40
24	4	314	CLA	CHB-C4A-NA	2.43	127.91	124.40
23	2	306	CHL	O1D-CGD-CBD	-2.43	121.04	124.72
24	3	303	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	9	314	0UR	C5-C4-C3	-2.43	124.01	126.92
25	0	314	8CT	C35-C30-C29	-2.43	110.03	112.83
24	9	304	CLA	CHB-C4A-NA	2.43	127.91	124.40
26	8	318	0UR	C14-C15-C16	-2.43	123.87	127.28
23	6	301	CHL	CMA-C3A-C4A	-2.43	109.38	114.61
24	1	309	CLA	CHB-C4A-NA	2.43	127.90	124.40
24	B	809	CLA	CHB-C4A-NA	2.43	127.90	124.40
23	8	301	CHL	CMB-C2B-C3B	2.43	129.53	124.68
25	3	316	8CT	C01-C02-C07	2.43	118.77	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	9	317	LMG	O2-C2-C1	-2.43	104.30	110.08
23	6	307	CHL	CMA-C3A-C4A	-2.42	109.39	114.61
25	0	314	8CT	C10-C03-C02	-2.42	115.97	121.56
24	A	848	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
23	6	308	CHL	CMB-C2B-C3B	2.42	129.52	124.68
24	3	310	CLA	CHB-C4A-NA	2.42	127.90	124.40
30	7	321	0IE	C22-C12-C11	-2.42	118.89	122.82
24	G	101	CLA	C1-C2-C3	-2.42	122.84	126.76
23	8	308	CHL	O1D-CGD-CBD	-2.42	121.05	124.72
23	0	305	CHL	CBC-CAC-C3C	-2.42	109.41	112.87
24	B	833	CLA	C1-C2-C3	-2.42	122.23	126.20
24	2	309	CLA	CHB-C4A-NA	2.42	127.89	124.40
23	7	302	CHL	CMB-C2B-C3B	2.42	129.51	124.68
23	4	313	CHL	OMC-CMC-C2C	-2.42	120.93	125.12
23	9	301	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
24	A	806	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	4	307	CHL	CMB-C2B-C3B	2.41	129.51	124.68
24	2	303	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	B	822	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	3	304	CLA	C1-C2-C3	-2.41	122.24	126.20
23	6	315	CHL	CMA-C3A-C4A	-2.41	109.41	114.61
29	A	851	LMG	O3-C3-C2	-2.41	104.69	110.38
23	3	301	CHL	CMA-C3A-C4A	-2.41	109.41	114.61
24	6	309	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
24	K	104	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	8	308	CHL	CMB-C2B-C3B	2.41	129.50	124.68
24	A	816	CLA	O2D-CGD-CBD	2.41	115.44	111.23
24	0	312	CLA	C3B-C4B-NB	-2.41	108.38	110.53
24	H	203	CLA	CHB-C4A-NA	2.41	127.88	124.40
34	B	849	DGD	O1G-C1A-O1A	-2.41	117.61	123.63
23	8	308	CHL	C5-C3-C4	2.41	120.13	114.59
25	F	301	8CT	C01-C02-C07	2.41	118.73	113.60
24	A	815	CLA	CHB-C4A-NA	2.41	127.87	124.40
24	A	832	CLA	CHB-C4A-NA	2.41	127.87	124.40
24	A	829	CLA	O2D-CGD-CBD	2.41	115.44	111.23
25	L	205	8CT	C04-C03-C02	-2.41	119.35	122.64
23	1	312	CHL	OMC-CMC-C2C	-2.41	120.94	125.12
24	6	303	CLA	CHB-C4A-NA	2.40	127.87	124.40
23	7	301	CHL	CMB-C2B-C3B	2.40	129.48	124.68
24	A	853	CLA	CHB-C4A-NA	2.40	127.87	124.40
24	B	836	CLA	C1-C2-C3	-2.40	122.26	126.20
23	7	305	CHL	CMA-C3A-C4A	-2.40	109.44	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	832	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
24	9	309	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	G	103	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	A	829	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	H	205	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	M	102	8CT	C35-C30-C29	-2.40	110.07	112.83
23	6	306	CHL	CMA-C3A-C4A	-2.40	109.44	114.61
24	2	302	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	B	812	CLA	C1-C2-C3	-2.40	122.27	126.20
30	3	319	0IE	C22-C12-C11	-2.40	118.93	122.82
26	6	320	0UR	C4-C5-C6	-2.40	116.25	123.20
23	7	301	CHL	C6-C5-C3	-2.40	107.63	113.47
24	7	312	CLA	CHB-C4A-NA	2.40	127.86	124.40
24	2	310	CLA	C3B-C4B-NB	-2.40	108.39	110.53
24	A	820	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	9	313	8CT	C11-C10-C03	-2.40	120.60	127.00
25	K	105	8CT	C18-C19-C20	-2.40	118.62	123.52
24	B	834	CLA	CHB-C4A-NA	2.39	127.86	124.40
23	9	312	CHL	CMA-C3A-C4A	-2.39	109.45	114.61
25	8	317	8CT	C27-C26-C28	2.39	121.75	118.09
25	3	323	8CT	C27-C26-C28	-2.39	114.43	118.09
24	B	811	CLA	C1-C2-C3	-2.39	122.27	126.20
24	2	311	CLA	CHB-C4A-NA	2.39	127.86	124.40
24	A	818	CLA	CHB-C4A-NA	2.39	127.86	124.40
24	B	838	CLA	CHB-C4A-NA	2.39	127.86	124.40
25	A	846	8CT	C10-C03-C02	-2.39	116.04	121.56
26	5	314	0UR	C10-C9-C8	-2.39	118.62	123.52
23	4	306	CHL	CMA-C3A-C4A	-2.39	109.46	114.61
25	G	104	8CT	C10-C03-C02	-2.39	116.05	121.56
23	2	304	CHL	CMB-C2B-C3B	2.39	129.46	124.68
23	0	302	CHL	CMB-C2B-C3B	2.39	129.46	124.68
26	9	315	0UR	C21-C12-C13	2.39	121.74	118.09
23	7	301	CHL	C4-C3-C5	2.39	119.38	115.23
23	6	305	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
24	B	831	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	2	305	CHL	CMB-C2B-C3B	2.39	129.46	124.68
25	L	204	8CT	C18-C19-C20	-2.39	118.64	123.52
29	9	317	LMG	C40-C39-C38	-2.39	102.31	114.37
24	1	311	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	M	101	LMG	O1-C7-C8	-2.38	105.02	110.82
24	H	205	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
29	9	317	LMG	C38-C37-C36	-2.38	102.33	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	312	CLA	CHB-C4A-NA	2.38	127.84	124.40
24	A	813	CLA	CHB-C4A-NA	2.38	127.84	124.40
24	A	853	CLA	CMB-C2B-C3B	2.38	132.15	126.55
24	A	834	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	O	202	8CT	C24-C25-C26	-2.38	123.94	127.28
24	A	831	CLA	CHB-C4A-NA	2.38	127.83	124.40
25	J	104	8CT	C19-C18-C17	-2.38	118.66	123.52
23	3	302	CHL	CBC-CAC-C3C	-2.38	109.47	112.87
23	4	306	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
25	B	850	8CT	C30-C29-C28	-2.38	120.88	124.58
24	A	824	CLA	CMB-C2B-C1B	-2.37	121.80	125.42
24	K	101	CLA	CHB-C4A-NA	2.37	127.83	124.40
26	0	316	0UR	C18-C17-C16	-2.37	121.22	126.32
23	6	315	CHL	O2D-CGD-O1D	-2.37	119.23	123.85
25	A	845	8CT	C13-C14-C15	-2.37	116.33	123.20
24	2	313	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	B	805	CLA	C1-C2-C3	-2.37	122.31	126.20
23	5	306	CHL	CBC-CAC-C3C	-2.37	109.48	112.87
24	8	310	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
24	A	834	CLA	O2D-CGD-CBD	2.37	115.37	111.23
26	1	315	0UR	C15-C14-C13	-2.37	116.33	123.20
24	5	303	CLA	CHB-C4A-NA	2.37	127.82	124.40
25	A	849	8CT	C28-C26-C25	2.37	122.73	119.01
24	4	312	CLA	CHB-C4A-NA	2.37	127.82	124.40
24	3	303	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
24	O	201	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
23	8	309	CHL	O2D-CGD-O1D	-2.37	119.24	123.85
25	B	847	8CT	C19-C20-C21	-2.37	123.96	127.28
29	J	105	LMG	C38-C37-C36	-2.37	102.41	114.37
24	8	311	CLA	CHB-C4A-NA	2.37	127.81	124.40
25	B	844	8CT	C01-C02-C07	2.37	118.64	113.60
23	3	301	CHL	C6-C5-C3	-2.37	107.71	113.47
24	8	310	CLA	CHB-C4A-NA	2.37	127.81	124.40
24	4	303	CLA	CHB-C4A-NA	2.37	127.81	124.40
23	3	302	CHL	CMB-C2B-C3B	2.36	129.41	124.68
24	A	823	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	A	837	CLA	CHB-C4A-NA	2.36	127.81	124.40
25	B	850	8CT	C13-C14-C15	-2.36	116.35	123.20
24	A	807	CLA	O2D-CGD-CBD	2.36	115.36	111.23
25	6	324	8CT	C10-C03-C02	-2.36	116.11	121.56
23	4	306	CHL	CMB-C2B-C3B	2.36	129.40	124.68
24	L	206	CLA	CHB-C4A-NA	2.36	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	810	CLA	CHB-C4A-NA	2.36	127.81	124.40
24	B	833	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	7	307	CHL	CMB-C2B-C3B	2.36	129.40	124.68
26	2	315	0UR	C22-C16-C17	2.36	121.69	118.09
23	8	303	CHL	O1D-CGD-CBD	-2.36	121.14	124.72
24	A	814	CLA	C1-C2-C3	-2.36	122.33	126.20
24	A	853	CLA	C1-C2-C3	-2.36	122.33	126.20
24	8	304	CLA	CHB-C4A-NA	2.36	127.80	124.40
23	0	302	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
24	7	317	CLA	CHB-C4A-NA	2.36	127.80	124.40
23	6	305	CHL	CMB-C2B-C3B	2.36	129.39	124.68
25	L	207	8CT	C04-C03-C10	2.36	122.04	115.65
24	6	304	CLA	CHB-C4A-NA	2.36	127.80	124.40
24	5	307	CLA	CHB-C4A-NA	2.36	127.80	124.40
26	0	315	0UR	C15-C14-C13	-2.35	116.38	123.20
24	A	840	CLA	CHB-C4A-NA	2.35	127.80	124.40
24	B	802	CLA	CHB-C4A-NA	2.35	127.80	124.40
24	A	808	CLA	C1-C2-C3	-2.35	122.34	126.20
23	7	305	CHL	CMB-C2B-C3B	2.35	129.39	124.68
23	1	301	CHL	CMB-C2B-C3B	2.35	129.39	124.68
24	A	835	CLA	CHB-C4A-NA	2.35	127.80	124.40
23	7	313	CHL	OMC-CMC-C2C	-2.35	121.03	125.12
24	7	310	CLA	CHB-C4A-NA	2.35	127.80	124.40
29	3	321	LMG	O3-C3-C2	-2.35	104.83	110.38
24	0	303	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	B	809	CLA	C1-C2-C3	-2.35	122.34	126.20
26	8	318	0UR	C10-C9-C8	-2.35	118.71	123.52
24	A	825	CLA	CHB-C4A-NA	2.35	127.79	124.40
23	2	312	CHL	C5-C3-C4	2.35	120.00	114.59
23	2	312	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
24	0	309	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	K	104	CLA	C1-C2-C3	-2.35	122.97	126.76
23	8	309	CHL	CMB-C2B-C3B	2.34	129.37	124.68
24	A	821	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	6	321	0UR	C18-C17-C16	-2.34	121.28	126.32
24	A	825	CLA	CAA-C2A-C1A	-2.34	104.30	111.97
29	O	203	LMG	O1-C1-C2	-2.34	104.72	108.27
24	5	308	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	5	309	CLA	CHB-C4A-NA	2.34	127.78	124.40
26	2	315	0UR	C5-C4-C3	-2.34	124.12	126.92
24	5	308	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
26	0	315	0UR	C10-C9-C8	-2.34	118.73	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	845	8CT	C04-C03-C10	2.34	122.00	115.65
24	O	201	CLA	CHB-C4A-NA	2.34	127.78	124.40
27	B	852	LHG	C26-C25-C24	2.34	121.72	113.13
25	A	847	8CT	C01-C02-C07	2.34	118.58	113.60
24	A	809	CLA	CHB-C4A-NA	2.34	127.77	124.40
25	A	849	8CT	C29-C28-C26	-2.34	121.30	126.32
24	B	816	CLA	C1-C2-C3	-2.34	122.37	126.20
24	B	807	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
23	4	307	CHL	O1D-CGD-CBD	-2.34	121.18	124.72
23	2	304	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
29	J	102	LMG	O3-C3-C2	-2.34	104.87	110.38
24	9	311	CLA	CHB-C4A-NA	2.33	127.77	124.40
23	6	323	CHL	CMB-C2B-C3B	2.33	129.35	124.68
26	4	317	0UR	C22-C16-C17	2.33	121.65	118.09
24	A	820	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
25	J	101	8CT	C15-C16-C17	-2.33	115.34	119.01
29	J	105	LMG	O3-C3-C2	-2.33	104.88	110.38
24	3	315	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	6	312	CLA	CHB-C4A-NA	2.33	127.76	124.40
23	0	306	CHL	CMA-C3A-C4A	-2.33	109.59	114.61
24	4	304	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	A	804	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
24	0	304	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	B	819	CLA	CHB-C4A-NA	2.33	127.76	124.40
24	B	824	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	O	202	8CT	C18-C19-C20	-2.33	118.76	123.52
24	7	309	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
25	J	101	8CT	C40-C12-C11	2.33	121.64	118.09
24	A	838	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
24	5	313	CLA	CHB-C4A-NA	2.33	127.76	124.40
23	6	308	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
23	8	316	CHL	CMB-C2B-C3B	2.33	129.33	124.68
23	7	305	CHL	O2D-CGD-O1D	-2.33	119.32	123.85
24	2	308	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
25	F	301	8CT	C29-C28-C26	-2.32	121.32	126.32
24	6	314	CLA	CHB-C4A-NA	2.32	127.75	124.40
23	1	305	CHL	CMB-C2B-C3B	2.32	129.33	124.68
24	O	206	CLA	C3B-C4B-NB	-2.32	107.92	110.33
24	1	313	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	O	206	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	A	812	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
24	L	201	CLA	CMB-C2B-C3B	2.32	132.01	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	848	CLA	CHB-C4A-NA	2.32	127.75	124.40
25	K	105	8CT	C10-C03-C02	-2.32	116.21	121.56
24	4	309	CLA	C1-C2-C3	-2.32	122.40	126.20
25	A	844	8CT	C27-C26-C28	2.32	121.63	118.09
24	6	318	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	4	309	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	B	826	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
24	7	303	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	3	309	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
24	3	303	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
24	9	308	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
26	2	316	0UR	C22-C16-C15	-2.32	119.06	122.82
23	8	314	CHL	O2D-CGD-O1D	-2.31	119.34	123.85
24	A	828	CLA	CHB-C4A-NA	2.31	127.74	124.40
23	6	313	CHL	CMB-C2B-C3B	2.31	129.30	124.68
24	6	316	CLA	CMB-C2B-C3B	2.31	131.99	126.55
23	1	304	CHL	O2D-CGD-O1D	-2.31	119.35	123.85
25	K	105	8CT	C05-C04-C03	2.31	113.80	110.44
29	9	317	LMG	O3-C3-C2	-2.31	104.93	110.38
23	4	302	CHL	CBC-CAC-C3C	-2.31	109.56	112.87
25	A	847	8CT	C24-C23-C21	-2.31	120.03	126.36
23	2	306	CHL	CMB-C2B-C3B	2.31	129.30	124.68
24	B	826	CLA	CHB-C4A-NA	2.31	127.73	124.40
24	1	311	CLA	C1-C2-C3	-2.31	122.42	126.20
23	2	305	CHL	CMA-C3A-C4A	-2.31	109.64	114.61
25	3	323	8CT	C10-C03-C02	-2.30	116.25	121.56
25	F	301	8CT	C30-C31-C32	-2.30	118.63	121.47
25	I	101	8CT	C24-C23-C21	-2.30	120.05	126.36
23	6	305	CHL	CMA-C3A-C4A	-2.30	109.65	114.61
25	K	105	8CT	C25-C24-C23	-2.30	116.53	123.20
23	4	302	CHL	O2D-CGD-O1D	-2.30	119.37	123.85
24	B	823	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	3	321	LMG	O1-C7-C8	-2.30	105.22	110.82
25	F	301	8CT	C11-C10-C03	-2.30	120.85	127.00
24	B	812	CLA	CHB-C4A-NA	2.30	127.72	124.40
34	B	849	DGD	O2G-C1B-O1B	-2.30	118.33	123.70
24	7	309	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
23	8	307	CHL	OMC-CMC-C2C	-2.30	121.13	125.12
23	2	301	CHL	C6-C5-C3	-2.30	107.87	113.47
24	B	832	CLA	CHB-C4A-NA	2.30	127.72	124.40
23	8	303	CHL	O2D-CGD-O1D	-2.30	119.38	123.85
23	9	312	CHL	CMB-C2B-C3B	2.30	129.27	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	316	0UR	C5-C6-C7	-2.29	120.07	126.36
26	9	315	0UR	C28-C19-C18	-2.29	110.19	112.83
23	8	314	CHL	CMB-C2B-C3B	2.29	129.27	124.68
25	8	317	8CT	C39-C16-C15	2.29	121.59	118.09
24	7	317	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
23	9	312	CHL	O2A-CGA-CBA	2.29	120.80	112.14
24	A	806	CLA	C1-C2-C3	-2.29	122.44	126.20
26	5	315	0UR	C22-C16-C15	-2.29	119.10	122.82
24	0	308	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
24	B	810	CLA	O2D-CGD-CBD	2.29	115.23	111.23
24	A	813	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
29	9	317	LMG	O7-C10-O9	-2.29	118.35	123.70
24	B	806	CLA	C1-C2-C3	-2.29	122.45	126.20
24	B	821	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
24	B	833	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
25	6	324	8CT	C07-C02-C03	-2.29	119.61	122.70
23	5	306	CHL	OMC-CMC-C2C	-2.29	121.15	125.12
23	3	307	CHL	O2D-CGD-O1D	-2.29	119.40	123.85
24	A	817	CLA	C1-C2-C3	-2.29	122.45	126.20
23	3	305	CHL	CMB-C2B-C3B	2.29	129.25	124.68
26	6	321	0UR	C15-C14-C13	-2.29	116.58	123.20
24	G	101	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
25	F	304	8CT	C07-C02-C03	-2.28	119.62	122.70
25	O	202	8CT	C40-C12-C11	2.28	121.58	118.09
24	B	825	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	5	312	CHL	O2A-CGA-CBA	2.28	120.76	112.14
23	2	312	CHL	OMC-CMC-C2C	-2.28	121.16	125.12
23	1	301	CHL	O1D-CGD-CBD	-2.28	121.26	124.72
25	3	317	8CT	C19-C18-C17	-2.28	118.85	123.52
24	A	822	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	8	301	CHL	O2D-CGD-O1D	-2.28	119.41	123.85
23	7	307	CHL	O1D-CGD-CBD	-2.28	121.27	124.72
25	B	844	8CT	C11-C10-C03	-2.28	120.91	127.00
24	2	308	CLA	C1-C2-C3	-2.28	122.46	126.20
24	B	838	CLA	C3B-C4B-NB	-2.28	108.50	110.53
23	1	306	CHL	OMC-CMC-C2C	-2.28	121.16	125.12
24	7	310	CLA	CMA-C3A-C2A	-2.28	111.01	116.23
25	7	319	8CT	C14-C15-C16	-2.28	120.12	126.36
23	2	306	CHL	OMC-CMC-C2C	-2.28	121.17	125.12
25	6	319	8CT	C01-C02-C07	2.28	118.45	113.60
25	A	846	8CT	C11-C10-C03	-2.28	120.92	127.00
23	9	306	CHL	OMC-CMC-C2C	-2.28	121.17	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	831	CLA	C1-C2-C3	-2.27	122.47	126.20
24	K	101	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	A	818	CLA	C1-C2-C3	-2.27	122.47	126.20
23	8	307	CHL	C5-C3-C4	2.27	119.82	114.59
26	9	315	0UR	O44-C45-O57	-2.27	118.18	122.96
24	O	209	CLA	CHB-C4A-NA	2.27	127.68	124.40
28	0	318	SQD	C1-O5-C5	2.27	118.16	113.72
29	O	203	LMG	O1-C7-C8	-2.27	105.29	110.82
25	6	324	8CT	C18-C19-C20	-2.27	118.87	123.52
34	B	849	DGD	C1E-O6E-C5E	-2.27	109.29	113.72
24	B	830	CLA	CHB-C4A-NA	2.27	127.67	124.40
24	A	806	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
24	B	830	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
23	1	312	CHL	C4-C3-C5	2.27	119.17	115.23
24	B	819	CLA	C1-C2-C3	-2.26	122.49	126.20
24	B	817	CLA	CBA-CAA-C2A	2.26	120.53	113.79
24	0	312	CLA	CHB-C4A-NA	2.26	127.67	124.40
23	2	312	CHL	O2D-CGD-O1D	-2.26	119.44	123.85
29	O	210	LMG	O2-C2-C1	-2.26	104.68	110.08
24	9	308	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
29	2	318	LMG	O1-C1-C2	-2.26	104.84	108.27
24	1	311	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
26	8	319	0UR	C22-C16-C15	-2.26	119.15	122.82
25	B	847	8CT	C38-C31-C32	-2.26	114.77	122.37
25	F	304	8CT	C10-C03-C02	-2.26	116.35	121.56
23	2	305	CHL	CBC-CAC-C3C	-2.26	109.64	112.87
24	B	813	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
29	3	321	LMG	O2-C2-C1	-2.26	104.69	110.08
24	L	203	CLA	CHB-C4A-NA	2.26	127.66	124.40
26	5	314	0UR	C28-C19-C18	-2.26	110.23	112.83
29	M	101	LMG	O6-C1-O1	-2.26	104.72	110.04
24	H	201	CLA	CHB-C4A-NA	2.25	127.65	124.40
23	4	315	CHL	O2A-CGA-O1A	-2.25	118.00	123.63
29	M	101	LMG	O3-C3-C2	-2.25	105.07	110.38
24	B	821	CLA	C1-C2-C3	-2.25	123.12	126.76
24	H	202	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
23	4	307	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
23	1	305	CHL	CMA-C3A-C4A	-2.25	109.76	114.61
24	8	305	CLA	C1-C2-C3	-2.25	122.51	126.20
24	8	305	CLA	CHB-C4A-NA	2.25	127.64	124.40
23	0	302	CHL	OMC-CMC-C2C	-2.25	121.22	125.12
25	B	843	8CT	C39-C16-C17	-2.25	119.18	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1	301	CHL	CAC-C3C-C4C	2.25	129.81	124.03
23	2	307	CHL	O1D-CGD-CBD	-2.25	121.32	124.72
27	3	324	LHG	C26-C25-C24	2.25	121.38	113.13
24	B	804	CLA	C3B-C4B-NB	-2.25	108.53	110.53
24	9	310	CLA	C1-C2-C3	-2.25	122.52	126.20
24	A	825	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
24	7	316	CLA	C2A-C1A-CHA	2.24	127.76	123.87
26	7	320	0UR	C22-C16-C17	2.24	121.51	118.09
32	A	852	CL0	CMA-C3A-C4A	-2.24	109.78	114.61
26	7	320	0UR	C5-C4-C3	-2.24	124.24	126.92
25	M	102	8CT	C24-C23-C21	-2.24	120.22	126.36
23	0	305	CHL	C5-C3-C4	2.24	119.74	114.59
25	A	844	8CT	C19-C18-C17	-2.24	118.94	123.52
24	1	303	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	7	319	8CT	C30-C31-C32	-2.24	118.72	121.47
26	1	315	0UR	C4-C5-C6	-2.24	116.72	123.20
29	A	851	LMG	O2-C2-C1	-2.24	104.75	110.08
24	B	828	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
25	7	319	8CT	C18-C19-C20	-2.23	118.95	123.52
24	A	824	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
23	1	305	CHL	OMC-CMC-C2C	-2.23	121.24	125.12
24	A	806	CLA	CMB-C2B-C3B	2.23	131.80	126.55
29	A	854	LMG	O2-C2-C1	-2.23	104.75	110.08
26	6	321	0UR	C9-C10-C11	-2.23	118.96	123.52
23	1	304	CHL	CMA-C3A-C4A	-2.23	109.81	114.61
23	4	313	CHL	C5-C3-C4	2.23	119.72	114.59
24	B	832	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
24	A	811	CLA	CHB-C4A-NA	2.23	127.62	124.40
23	8	303	CHL	CAC-C3C-C4C	2.23	129.76	124.03
29	J	102	LMG	C6-C5-C4	-2.23	107.55	113.02
29	O	203	LMG	O3-C3-C2	-2.23	105.12	110.38
29	A	854	LMG	O3-C3-C2	-2.23	105.12	110.38
24	2	310	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
24	B	808	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
26	1	315	0UR	C14-C15-C16	-2.23	124.16	127.28
23	0	306	CHL	CMB-C2B-C3B	2.23	129.13	124.68
23	3	305	CHL	CMA-C3A-C4A	-2.23	109.82	114.61
23	2	301	CHL	CAC-C3C-C4C	2.23	129.75	124.03
23	6	313	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
24	K	102	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
25	2	314	8CT	C18-C19-C20	-2.22	118.97	123.52
23	6	307	CHL	C5-C3-C4	2.22	119.71	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	318	0UR	C4-C5-C6	-2.22	116.76	123.20
32	A	852	CL0	O2A-CGA-O1A	-2.22	118.07	123.63
23	8	316	CHL	CMA-C3A-C4A	-2.22	109.82	114.61
25	7	319	8CT	C19-C18-C17	-2.22	118.97	123.52
24	B	828	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	L	206	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	B	833	CLA	O2D-CGD-CBD	2.22	115.11	111.23
24	A	826	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
24	B	804	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	B	838	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
29	O	203	LMG	O2-C2-C1	-2.22	104.79	110.08
23	8	314	CHL	OMC-CMC-C2C	-2.22	121.27	125.12
24	B	811	CLA	O2D-CGD-CBD	2.22	115.10	111.23
29	2	318	LMG	O3-C3-C2	-2.22	105.15	110.38
25	6	324	8CT	C22-C21-C23	2.22	121.47	118.09
24	6	303	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
23	9	305	CHL	O2D-CGD-O1D	-2.21	119.54	123.85
24	A	817	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
24	L	202	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
26	0	315	0UR	C48-C47-C46	-2.21	121.31	125.92
24	A	807	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
25	8	317	8CT	C39-C16-C17	-2.21	119.23	122.82
24	B	808	CLA	CMB-C2B-C3B	2.21	131.75	126.55
23	4	305	CHL	CMA-C3A-C4A	-2.21	109.85	114.61
25	3	316	8CT	C18-C17-C16	-2.21	124.18	127.28
26	3	318	0UR	C14-C15-C16	-2.21	124.18	127.28
26	2	315	0UR	C29-C30-C31	-2.21	107.91	111.18
25	0	314	8CT	C24-C23-C21	-2.21	120.31	126.36
25	F	304	8CT	C04-C03-C02	-2.21	119.62	122.64
26	9	314	0UR	C22-C16-C17	2.21	121.46	118.09
24	3	308	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
23	7	302	CHL	OMC-CMC-C2C	-2.21	121.29	125.12
25	A	849	8CT	C05-C04-C03	2.21	113.64	110.44
24	B	841	CLA	C1-C2-C3	-2.21	122.58	126.20
25	F	304	8CT	C14-C15-C16	-2.20	120.32	126.36
24	A	829	CLA	C3B-C4B-NB	-2.20	108.56	110.53
26	0	316	0UR	C43-C3-C4	-2.20	122.43	125.03
23	1	306	CHL	CBC-CAC-C3C	-2.20	109.72	112.87
25	F	304	8CT	C24-C23-C21	-2.20	120.32	126.36
25	A	846	8CT	C22-C21-C23	2.20	121.45	118.09
24	A	816	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	B	810	CLA	O2A-CGA-O1A	-2.20	118.12	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	846	8CT	C30-C29-C28	-2.20	121.15	124.58
25	O	208	8CT	C05-C04-C03	2.20	113.64	110.44
25	6	319	8CT	C22-C21-C23	2.20	121.45	118.09
26	O	207	0UR	C5-C6-C7	-2.20	120.33	126.36
24	A	803	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
23	4	301	CHL	CMA-C3A-C4A	-2.20	109.87	114.61
23	4	305	CHL	CMB-C2B-C3B	2.20	129.08	124.68
26	8	319	0UR	O44-C45-O57	-2.20	118.34	122.96
24	A	812	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
23	6	306	CHL	OMC-CMC-C2C	-2.20	121.31	125.12
24	1	302	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
26	1	315	0UR	C22-C16-C17	2.20	121.44	118.09
24	2	310	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
23	8	306	CHL	O2D-CGD-O1D	-2.20	119.57	123.85
24	B	829	CLA	CHB-C4A-NA	2.19	127.57	124.40
23	4	301	CHL	O2A-CGA-O1A	-2.19	118.14	123.63
24	A	829	CLA	CHB-C1B-NB	2.19	127.34	124.05
24	7	317	CLA	C1-C2-C3	-2.19	122.60	126.20
24	A	829	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
23	2	305	CHL	OMC-CMC-C2C	-2.19	121.31	125.12
23	8	307	CHL	CMA-C3A-C4A	-2.19	109.89	114.61
23	5	301	CHL	CMB-C2B-C3B	2.19	129.06	124.68
29	2	318	LMG	O1-C7-C8	-2.19	105.49	110.82
23	6	301	CHL	CMB-C2B-C3B	2.19	129.06	124.68
23	0	301	CHL	O1D-CGD-CBD	-2.19	121.40	124.72
26	4	318	0UR	C25-C26-C27	-2.19	106.72	112.18
24	O	201	CLA	O1D-CGD-CBD	2.19	128.84	124.52
24	B	817	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
24	4	309	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	6	309	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	B	840	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
26	4	318	0UR	C9-C10-C11	-2.19	119.04	123.52
23	5	304	CHL	CMA-C3A-C4A	-2.19	109.90	114.61
24	B	802	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
24	7	304	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
27	A	842	LHG	C5-O7-C7	-2.18	112.57	117.80
24	B	836	CLA	CMB-C2B-C3B	2.18	131.69	126.55
24	A	835	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
29	O	210	LMG	O3-C3-C2	-2.18	105.23	110.38
26	3	318	0UR	C9-C10-C11	-2.18	119.05	123.52
24	B	825	CLA	C1-C2-C3	-2.18	122.62	126.20
24	4	310	CLA	O2A-CGA-O1A	-2.18	118.17	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	308	CHL	C4-C3-C5	2.18	119.01	115.23
24	3	312	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
23	7	307	CHL	C5-C3-C4	2.18	119.60	114.59
23	7	305	CHL	OMC-CMC-C2C	-2.18	121.34	125.12
26	4	317	0UR	C41-C2-C3	2.18	125.06	119.12
26	4	317	0UR	C10-C9-C8	-2.18	119.07	123.52
25	B	843	8CT	C11-C10-C03	-2.18	121.19	127.00
24	B	826	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
25	8	317	8CT	C13-C14-C15	-2.18	116.90	123.20
24	7	308	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
24	5	308	CLA	CMB-C2B-C3B	2.17	131.66	126.55
23	6	301	CHL	O2A-CGA-O1A	-2.17	118.19	123.63
23	2	306	CHL	C5-C3-C4	2.17	119.59	114.59
24	A	826	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
25	7	319	8CT	C05-C04-C03	2.17	113.59	110.44
24	B	827	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
25	1	314	8CT	C39-C16-C17	-2.17	119.30	122.82
29	J	105	LMG	C42-C41-C40	-2.17	103.40	114.37
24	O	205	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	A	817	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
23	6	307	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
29	A	851	LMG	O6-C1-C2	2.17	114.82	110.37
24	B	816	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
23	5	306	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
25	B	848	8CT	C22-C21-C23	2.17	121.40	118.09
26	0	316	0UR	C21-C12-C13	2.17	121.40	118.09
25	1	314	8CT	C27-C26-C25	-2.16	119.31	122.82
29	J	102	LMG	O7-C10-O9	-2.16	118.65	123.70
24	B	808	CLA	O2D-CGD-CBD	2.16	115.01	111.23
23	0	305	CHL	O2A-CGA-O1A	-2.16	118.22	123.63
24	1	308	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	4	302	CHL	CAC-C3C-C4C	2.16	129.59	124.03
24	B	806	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
23	5	306	CHL	O2A-CGA-CBA	2.16	120.30	112.14
26	5	314	0UR	C15-C14-C13	-2.16	116.94	123.20
24	B	812	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
24	B	809	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
25	A	849	8CT	C18-C19-C20	-2.16	119.10	123.52
25	3	317	8CT	C35-C30-C29	-2.16	110.34	112.83
29	2	318	LMG	O2-C2-C1	-2.16	104.94	110.08
23	0	301	CHL	CMA-C3A-C4A	-2.16	109.96	114.61
23	4	308	CHL	OMC-CMC-C2C	-2.16	121.38	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	814	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
24	K	102	CLA	C1-C2-C3	-2.16	122.67	126.20
24	9	304	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
24	A	813	CLA	C1-C2-C3	-2.15	122.67	126.20
27	B	852	LHG	C5-O7-C7	-2.15	112.64	117.80
23	8	301	CHL	CMA-C3A-C4A	-2.15	109.97	114.61
29	M	101	LMG	C1-C2-C3	-2.15	105.48	110.01
25	L	207	8CT	C30-C31-C32	-2.15	118.82	121.47
24	3	309	CLA	CMB-C2B-C3B	2.15	131.61	126.55
24	3	306	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
24	A	827	CLA	CHB-C4A-NA	2.15	127.50	124.40
24	B	830	CLA	C2D-C1D-ND	-2.15	108.00	110.13
24	4	314	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
24	B	818	CLA	O2D-CGD-CBD	2.15	114.99	111.23
24	B	823	CLA	C1-C2-C3	-2.15	122.68	126.20
26	9	314	0UR	C20-C7-C6	2.15	121.37	118.09
26	6	320	0UR	C23-C24-C25	-2.15	108.89	113.59
24	A	830	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
29	M	101	LMG	O2-C2-C1	-2.15	104.96	110.08
30	7	321	0IE	C13-C12-C11	2.15	122.38	119.01
24	3	315	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
23	8	308	CHL	OMC-CMC-C2C	-2.14	121.40	125.12
24	B	841	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
25	9	313	8CT	C14-C15-C16	-2.14	120.49	126.36
24	B	837	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
24	B	819	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
23	8	307	CHL	CAC-C3C-C4C	2.14	129.53	124.03
24	A	853	CLA	CHB-C1B-NB	2.14	127.26	124.05
23	5	305	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
26	2	315	0UR	C4-C5-C6	-2.14	117.00	123.20
23	0	302	CHL	CAC-C3C-C4C	2.14	129.53	124.03
23	2	306	CHL	CAA-CBA-CGA	-2.14	107.14	113.21
24	B	817	CLA	CAC-C3C-C4C	2.14	127.57	124.79
26	4	317	0UR	C9-C10-C11	-2.14	119.14	123.52
23	6	306	CHL	C5-C3-C4	2.14	119.51	114.59
29	J	105	LMG	C1-O6-C5	-2.14	109.55	113.72
24	B	808	CLA	C1-C2-C3	-2.14	122.70	126.20
24	A	817	CLA	O2D-CGD-CBD	2.14	114.96	111.23
24	3	304	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
29	9	317	LMG	C42-C41-C40	-2.14	103.57	114.37
24	B	818	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
26	2	316	0UR	C36-C28-C38	-2.13	104.77	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	M	101	LMG	O7-C10-O9	-2.13	118.71	123.70
24	A	827	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
24	A	832	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	B	820	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
23	1	306	CHL	O2D-CGD-O1D	-2.13	119.70	123.85
24	B	805	CLA	CHB-C4A-NA	2.13	127.48	124.40
24	B	814	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	2	311	CLA	CMB-C2B-C3B	2.13	131.56	126.55
24	O	201	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
25	A	845	8CT	C39-C16-C17	-2.13	119.36	122.82
23	3	307	CHL	CMA-C3A-C4A	-2.13	110.02	114.61
24	B	819	CLA	O2D-CGD-CBD	2.13	114.95	111.23
25	B	847	8CT	C22-C21-C23	2.13	121.34	118.09
24	A	828	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
24	5	302	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	B	805	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
25	O	202	8CT	C39-C16-C15	2.13	121.33	118.09
26	7	320	0UR	C18-C17-C16	-2.13	121.75	126.32
24	B	815	CLA	CMB-C2B-C3B	2.12	131.55	126.55
26	9	315	0UR	C43-C3-C4	-2.12	122.53	125.03
31	B	842	PQN	C11-C3-C2	-2.12	121.25	124.89
25	B	848	8CT	C23-C21-C20	-2.12	115.67	119.01
24	B	822	CLA	C1-C2-C3	-2.12	122.72	126.20
24	H	204	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
23	4	308	CHL	O2A-CGA-CBA	2.12	120.15	112.14
24	A	801	CLA	C1-C2-C3	-2.12	122.73	126.20
25	A	847	8CT	C35-C30-C29	-2.12	110.39	112.83
26	O	207	0UR	C21-C12-C13	2.12	121.32	118.09
23	4	313	CHL	CMA-C3A-C4A	-2.12	110.05	114.61
24	B	810	CLA	C1-C2-C3	-2.12	122.73	126.20
24	B	824	CLA	C1-C2-C3	-2.12	122.73	126.20
23	4	302	CHL	CMA-C3A-C4A	-2.11	110.06	114.61
23	5	306	CHL	CMA-C3A-C4A	-2.11	110.06	114.61
23	3	307	CHL	CMB-C2B-C3B	2.11	128.90	124.68
23	8	309	CHL	OMC-CMC-C2C	-2.11	121.45	125.12
24	9	310	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
26	9	315	0UR	C48-C47-C46	-2.11	121.53	125.92
23	8	306	CHL	O2A-CGA-CBA	2.11	120.11	112.14
24	B	812	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
32	A	852	CL0	CMB-C2B-C3B	2.11	128.90	124.68
26	9	315	0UR	C34-C27-C1	-2.11	121.82	124.45
25	B	844	8CT	C19-C18-C17	-2.11	119.21	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	308	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
23	8	308	CHL	O2D-CGD-O1D	-2.11	119.75	123.85
23	7	301	CHL	OMC-CMC-C2C	-2.11	121.47	125.12
29	O	210	LMG	O1-C7-C8	-2.10	105.70	110.82
24	9	303	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
24	A	823	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
23	9	301	CHL	O2A-CGA-CBA	2.10	120.09	112.14
24	9	311	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
24	B	804	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
24	7	311	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
24	6	309	CLA	CMB-C2B-C3B	2.10	131.50	126.55
25	B	850	8CT	C35-C30-C29	-2.10	110.41	112.83
23	9	305	CHL	C5-C3-C4	2.10	119.43	114.59
30	3	319	0IE	C13-C12-C11	2.10	122.31	119.01
23	2	307	CHL	O2A-CGA-CBA	2.10	120.08	112.14
24	7	311	CLA	C1-C2-C3	-2.10	122.75	126.20
24	A	824	CLA	CMB-C2B-C3B	2.10	131.49	126.55
26	2	315	0UR	C41-C2-C3	2.10	124.84	119.12
24	9	302	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
23	9	305	CHL	CAC-C3C-C4C	2.10	129.43	124.03
24	B	801	CLA	O2D-CGD-CBD	2.10	114.90	111.23
23	6	302	CHL	CMA-C3A-C4A	-2.10	110.09	114.61
23	2	304	CHL	CAC-C3C-C4C	2.10	129.43	124.03
24	6	314	CLA	O2D-CGD-CBD	2.10	114.90	111.23
26	2	315	0UR	C14-C15-C16	-2.10	124.33	127.28
23	3	301	CHL	C4-C3-C5	2.10	118.87	115.23
23	1	306	CHL	CMA-C3A-C4A	-2.10	110.09	114.61
26	7	320	0UR	C4-C5-C6	-2.10	117.12	123.20
24	B	830	CLA	CMB-C2B-C3B	2.10	131.48	126.55
24	3	303	CLA	C1-C2-C3	-2.10	122.76	126.20
25	L	204	8CT	C24-C23-C21	-2.10	120.62	126.36
24	6	311	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	6	312	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	K	102	CLA	CAC-C3C-C4C	2.09	127.52	124.79
24	3	311	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
23	5	301	CHL	CAC-C3C-C4C	2.09	129.41	124.03
25	7	318	8CT	C40-C12-C11	2.09	121.28	118.09
26	0	316	0UR	C29-C30-C31	-2.09	108.08	111.18
25	2	314	8CT	C06-C07-C02	-2.09	110.33	114.06
24	A	820	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
23	0	305	CHL	CMB-C2B-C3B	2.09	128.86	124.68
26	8	318	0UR	C23-C24-C25	-2.09	109.01	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	318	0UR	C43-C3-C2	2.09	121.42	116.56
24	B	826	CLA	CMB-C2B-C3B	2.09	131.46	126.55
23	6	323	CHL	O2A-CGA-O1A	-2.09	118.40	123.63
27	I	102	LHG	C5-O7-C7	-2.09	112.80	117.80
24	A	837	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
25	A	846	8CT	C27-C26-C28	2.09	121.28	118.09
24	A	827	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
24	B	816	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
25	A	847	8CT	C30-C29-C28	-2.09	121.33	124.58
25	A	845	8CT	C40-C12-C13	-2.09	119.44	122.82
23	7	307	CHL	OMC-CMC-C2C	-2.09	121.50	125.12
24	3	310	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
24	B	824	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
24	0	307	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
23	8	301	CHL	O2A-CGA-O1A	-2.08	118.41	123.63
24	6	318	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
24	4	311	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
23	0	305	CHL	CMA-C3A-C4A	-2.08	110.12	114.61
24	A	840	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	6	313	CHL	O2D-CGD-O1D	-2.08	119.79	123.85
23	1	304	CHL	CAC-C3C-C4C	2.08	129.38	124.03
24	A	835	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
23	4	307	CHL	C5-C3-C4	2.08	119.38	114.59
24	B	807	CLA	CMB-C2B-C3B	2.08	131.45	126.55
23	5	305	CHL	O2D-CGD-O1D	-2.08	119.80	123.85
24	K	101	CLA	O2D-CGD-CBD	2.08	114.87	111.23
24	7	304	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	0	308	CLA	CMB-C2B-C3B	2.08	131.45	126.55
24	1	310	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
24	A	839	CLA	C1-C2-C3	2.08	129.61	126.20
24	2	308	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
25	B	844	8CT	C05-C04-C03	2.08	113.46	110.44
24	8	305	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	B	815	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
25	A	844	8CT	C39-C16-C17	-2.08	119.44	122.82
23	3	301	CHL	CBC-CAC-C3C	-2.08	109.89	112.87
23	3	305	CHL	CAC-C3C-C4C	2.08	129.38	124.03
25	L	207	8CT	C39-C16-C15	2.08	121.27	118.09
29	J	105	LMG	O2-C2-C1	-2.08	105.12	110.08
26	7	320	0UR	C41-C2-C3	2.08	124.79	119.12
24	B	839	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
23	7	313	CHL	O2A-CGA-CBA	2.08	119.99	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	802	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
23	6	323	CHL	C6-C5-C3	-2.08	108.41	113.47
25	O	202	8CT	C28-C26-C25	-2.08	115.74	119.01
24	A	826	CLA	CMB-C2B-C3B	2.08	131.44	126.55
24	A	818	CLA	CMB-C2B-C3B	2.08	131.43	126.55
25	4	316	8CT	C39-C16-C17	-2.08	119.45	122.82
23	0	305	CHL	OMC-CMC-C2C	-2.08	121.52	125.12
23	6	306	CHL	O2D-CGD-O1D	-2.08	119.81	123.85
24	A	819	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
29	A	854	LMG	O1-C7-C8	-2.07	105.77	110.82
25	A	845	8CT	C35-C30-C29	-2.07	110.44	112.83
24	A	805	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	4	304	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	8	310	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
24	B	807	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
24	B	837	CLA	O2D-CGD-CBD	2.07	114.85	111.23
24	2	308	CLA	O2D-CGD-CBD	2.07	114.85	111.23
23	4	307	CHL	CMA-C3A-C4A	-2.07	110.15	114.61
26	3	318	0UR	C4-C5-C6	-2.07	117.20	123.20
29	O	210	LMG	O7-C10-O9	-2.07	118.87	123.70
26	O	207	0UR	C43-C3-C2	2.07	121.37	116.56
24	2	303	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
24	3	315	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
24	A	818	CLA	O2D-CGD-CBD	2.07	114.84	111.23
23	9	312	CHL	OMC-CMC-C2C	-2.07	121.53	125.12
32	A	852	CL0	C3C-C4C-NC	-2.07	109.60	114.65
24	A	818	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
24	B	827	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
23	7	306	CHL	CMB-C2B-C3B	2.06	128.81	124.68
24	B	801	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
24	B	837	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
25	2	314	8CT	C39-C16-C17	-2.06	119.47	122.82
25	A	849	8CT	C40-C12-C13	-2.06	119.47	122.82
24	9	307	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	A	811	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	A	803	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
27	A	850	LHG	C26-C25-C24	2.06	120.71	113.13
26	0	315	0UR	C28-C19-C18	-2.06	110.45	112.83
23	8	306	CHL	CAC-C3C-C4C	2.06	129.33	124.03
26	8	318	0UR	C20-C7-C6	2.06	121.24	118.09
24	H	202	CLA	CMB-C2B-C3B	2.06	131.40	126.55
24	B	836	CLA	O2A-CGA-O1A	-2.06	118.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	315	0UR	C34-C27-C26	2.06	118.21	114.42
25	B	844	8CT	C27-C26-C25	-2.06	119.48	122.82
24	0	304	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	1	303	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
26	4	318	0UR	C34-C27-C26	2.06	118.21	114.42
25	J	104	8CT	C01-C02-C07	2.06	117.98	113.60
24	7	304	CLA	C1-C2-C3	-2.06	122.83	126.20
26	5	315	0UR	C17-C16-C15	2.06	122.25	119.01
23	4	315	CHL	O1D-CGD-CBD	-2.06	121.60	124.72
25	B	848	8CT	C39-C16-C15	2.06	121.23	118.09
24	O	209	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	B	832	CLA	CMB-C2B-C3B	2.06	131.39	126.55
29	3	321	LMG	O7-C10-O9	-2.06	118.90	123.70
25	K	105	8CT	C15-C16-C17	2.05	122.24	119.01
25	B	843	8CT	C05-C04-C03	2.05	113.42	110.44
25	B	846	8CT	C37-C35-C30	2.05	112.66	109.55
24	A	802	CLA	O2D-CGD-CBD	2.05	114.82	111.23
23	1	304	CHL	C5-C3-C4	2.05	119.31	114.59
26	6	320	0UR	C14-C13-C12	-2.05	120.73	126.36
26	3	318	0UR	C10-C9-C8	-2.05	119.32	123.52
23	7	305	CHL	CAC-C3C-C4C	2.05	129.30	124.03
23	1	305	CHL	CAC-C3C-C4C	2.05	129.30	124.03
23	6	313	CHL	O2A-CGA-O1A	-2.05	118.50	123.63
24	9	308	CLA	CMB-C2B-C3B	2.05	131.37	126.55
24	B	817	CLA	CMB-C2B-C3B	2.05	131.37	126.55
24	A	811	CLA	CHB-C1B-NB	2.05	127.12	124.05
23	2	307	CHL	O2D-CGD-O1D	-2.05	119.86	123.85
23	6	323	CHL	CMA-C3A-C4A	-2.05	110.20	114.61
24	A	817	CLA	CMB-C2B-C3B	2.05	131.37	126.55
25	1	314	8CT	C40-C12-C13	-2.05	119.50	122.82
23	7	313	CHL	C1B-CHB-C4A	2.05	122.64	121.32
25	L	204	8CT	C19-C18-C17	-2.05	119.33	123.52
24	2	309	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
25	O	202	8CT	C22-C21-C23	2.05	121.21	118.09
24	B	818	CLA	C1-C2-C3	-2.04	122.85	126.20
23	3	307	CHL	O2A-CGA-O1A	-2.04	118.52	123.63
24	B	815	CLA	C1-C2-C3	-2.04	122.85	126.20
24	7	309	CLA	CMB-C2B-C3B	2.04	131.35	126.55
24	H	202	CLA	O1D-CGD-CBD	2.04	128.55	124.52
23	4	315	CHL	CMA-C3A-C4A	-2.04	110.21	114.61
27	3	324	LHG	C5-O7-C7	-2.04	112.91	117.80
24	A	837	CLA	C1-C2-C3	-2.04	122.85	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	317	LHG	C26-C25-C24	2.04	120.63	113.13
24	7	315	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
29	A	851	LMG	O1-C1-C2	-2.04	105.17	108.27
24	A	812	CLA	CMB-C2B-C3B	2.04	131.35	126.55
24	K	104	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
24	0	304	CLA	C1-C2-C3	-2.04	122.86	126.20
27	5	316	LHG	C26-C25-C24	2.04	120.61	113.13
24	A	825	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
23	2	301	CHL	CMA-C3A-C4A	-2.04	110.22	114.61
24	B	833	CLA	CAA-CBA-CGA	-2.04	107.43	113.21
24	L	201	CLA	O2D-CGD-CBD	2.04	114.79	111.23
25	3	316	8CT	C14-C15-C16	2.04	131.94	126.36
25	3	317	8CT	C24-C23-C21	-2.03	120.78	126.36
23	2	306	CHL	O2D-CGD-O1D	-2.03	119.89	123.85
23	7	313	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
25	9	313	8CT	C10-C03-C02	-2.03	116.87	121.56
23	8	306	CHL	OMC-CMC-C2C	-2.03	121.59	125.12
24	0	311	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	B	802	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	A	853	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
25	7	319	8CT	C22-C21-C23	2.03	121.19	118.09
25	O	208	8CT	C40-C12-C13	-2.03	119.53	122.82
26	5	314	0UR	C4-C5-C6	-2.03	117.32	123.20
25	L	207	8CT	C27-C26-C28	2.03	121.19	118.09
26	3	318	0UR	C41-C2-C3	2.03	124.65	119.12
24	3	303	CLA	CMB-C2B-C3B	2.03	131.32	126.55
24	B	814	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
24	F	302	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	L	207	8CT	C05-C04-C03	2.03	113.38	110.44
24	B	821	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
26	1	315	0UR	C20-C7-C6	2.02	121.18	118.09
26	5	315	0UR	C5-C6-C7	-2.02	120.82	126.36
25	B	850	8CT	C25-C24-C23	-2.02	117.34	123.20
23	6	302	CHL	CAC-C3C-C4C	2.02	129.23	124.03
24	B	804	CLA	CMB-C2B-C3B	2.02	131.30	126.55
26	4	317	0UR	C18-C17-C16	-2.02	121.98	126.32
24	A	826	CLA	O2D-CGD-CBD	2.02	114.76	111.23
26	1	315	0UR	C29-C30-C31	-2.02	108.19	111.18
23	8	309	CHL	O2A-CGA-CBA	2.02	119.77	112.14
24	1	310	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
26	0	315	0UR	C23-C24-C25	-2.02	109.17	113.59
24	A	822	CLA	C1-C2-C3	-2.02	122.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	313	CHL	OMC-CMC-C2C	-2.02	121.62	125.12
29	M	101	LMG	O1-C1-C2	-2.02	105.21	108.27
23	3	302	CHL	CMA-C3A-C4A	-2.02	110.27	114.61
25	3	323	8CT	C22-C21-C20	-2.02	119.55	122.82
26	8	319	0UR	C34-C27-C26	2.02	118.13	114.42
24	2	302	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	1	303	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
24	1	308	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
24	A	829	CLA	CMB-C2B-C3B	2.02	131.29	126.55
25	J	101	8CT	C27-C26-C28	2.01	121.17	118.09
24	O	201	CLA	CMB-C2B-C3B	2.01	131.29	126.55
25	G	104	8CT	C38-C31-C32	-2.01	115.60	122.37
24	A	836	CLA	O2D-CGD-CBD	2.01	114.75	111.23
23	0	301	CHL	O2A-CGA-O1A	-2.01	118.59	123.63
24	H	205	CLA	C1-C2-C3	-2.01	122.90	126.20
23	3	302	CHL	CAC-C3C-C4C	2.01	129.21	124.03
24	B	838	CLA	O2D-CGD-CBD	2.01	114.75	111.23
24	A	801	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	8	318	0UR	C22-C16-C17	2.01	121.16	118.09
24	A	821	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
26	6	321	0UR	C36-C28-C19	2.01	112.59	109.55
26	2	316	0UR	C48-C47-C46	-2.01	123.56	125.84
23	6	306	CHL	CAC-C3C-C4C	2.01	129.20	124.03
24	B	821	CLA	CMB-C2B-C3B	2.01	131.28	126.55
25	B	847	8CT	C06-C07-C02	-2.01	110.47	114.06
26	9	314	0UR	C14-C15-C16	-2.01	124.46	127.28
24	A	820	CLA	CMB-C2B-C3B	2.01	131.27	126.55
25	O	208	8CT	C27-C26-C28	2.01	121.15	118.09
24	A	827	CLA	CMB-C2B-C3B	2.01	131.27	126.55
24	A	822	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
24	7	314	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
24	A	835	CLA	CMB-C2B-C3B	2.00	131.27	126.55
25	L	204	8CT	C10-C03-C02	-2.00	116.94	121.56
23	8	309	CHL	CAC-C3C-C4C	2.00	129.18	124.03
25	I	101	8CT	C39-C16-C15	2.00	121.15	118.09
28	0	318	SQD	O5-C1-C2	2.00	114.49	110.37
23	3	301	CHL	O2A-CGA-O1A	-2.00	118.62	123.63
26	4	317	0UR	C20-C7-C6	2.00	121.15	118.09
26	3	318	0UR	C21-C12-C13	2.00	121.15	118.09
25	3	317	8CT	C18-C19-C20	-2.00	119.42	123.52
26	2	316	0UR	C9-C10-C11	-2.00	119.42	123.52
26	O	207	0UR	C34-C27-C26	2.00	118.10	114.42

All (373) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	0	301	CHL	NC
23	0	301	CHL	ND
23	0	301	CHL	NA
23	0	302	CHL	NC
23	0	302	CHL	ND
23	0	302	CHL	NA
23	0	305	CHL	NC
23	0	305	CHL	ND
23	0	305	CHL	NA
23	0	306	CHL	NC
23	0	306	CHL	ND
23	0	306	CHL	NA
23	1	301	CHL	NC
23	1	301	CHL	ND
23	1	301	CHL	NA
23	1	304	CHL	NC
23	1	304	CHL	ND
23	1	304	CHL	NA
23	1	305	CHL	NC
23	1	305	CHL	ND
23	1	305	CHL	NA
23	1	306	CHL	NC
23	1	306	CHL	ND
23	1	306	CHL	NA
23	1	312	CHL	NC
23	1	312	CHL	ND
23	1	312	CHL	NA
23	2	301	CHL	NC
23	2	301	CHL	ND
23	2	301	CHL	NA
23	2	304	CHL	NC
23	2	304	CHL	ND
23	2	304	CHL	NA
23	2	305	CHL	NC
23	2	305	CHL	ND
23	2	305	CHL	NA
23	2	306	CHL	NC
23	2	306	CHL	ND
23	2	306	CHL	NA
23	2	307	CHL	NC
23	2	307	CHL	ND
23	2	307	CHL	NA

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Mol	Chain	Res	Type	Atom
23	2	312	CHL	NC
23	2	312	CHL	ND
23	2	312	CHL	NA
23	3	301	CHL	NC
23	3	301	CHL	ND
23	3	301	CHL	NA
23	3	302	CHL	NC
23	3	302	CHL	ND
23	3	302	CHL	NA
23	3	305	CHL	NC
23	3	305	CHL	ND
23	3	305	CHL	NA
23	3	307	CHL	NC
23	3	307	CHL	ND
23	3	307	CHL	NA
23	5	301	CHL	NC
23	5	301	CHL	ND
23	5	301	CHL	NA
23	5	304	CHL	NC
23	5	304	CHL	ND
23	5	304	CHL	NA
23	5	305	CHL	NC
23	5	305	CHL	ND
23	5	305	CHL	NA
23	5	306	CHL	NC
23	5	306	CHL	ND
23	5	306	CHL	NA
23	5	312	CHL	NC
23	5	312	CHL	ND
23	5	312	CHL	NA
23	6	301	CHL	NC
23	6	301	CHL	ND
23	6	301	CHL	NA
23	6	302	CHL	NC
23	6	302	CHL	ND
23	6	302	CHL	NA
23	6	305	CHL	NC
23	6	305	CHL	ND
23	6	305	CHL	NA
23	6	306	CHL	NC
23	6	306	CHL	ND
23	6	306	CHL	NA

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Mol	Chain	Res	Type	Atom
23	6	307	CHL	NC
23	6	307	CHL	ND
23	6	307	CHL	NA
23	6	308	CHL	NC
23	6	308	CHL	ND
23	6	308	CHL	NA
23	6	313	CHL	NC
23	6	313	CHL	ND
23	6	313	CHL	NA
23	6	315	CHL	NC
23	6	315	CHL	ND
23	6	315	CHL	NA
23	6	323	CHL	NC
23	6	323	CHL	ND
23	6	323	CHL	NA
23	7	301	CHL	NC
23	7	301	CHL	ND
23	7	301	CHL	NA
23	7	302	CHL	NC
23	7	302	CHL	ND
23	7	302	CHL	NA
23	7	305	CHL	NC
23	7	305	CHL	ND
23	7	305	CHL	NA
23	7	306	CHL	NC
23	7	306	CHL	ND
23	7	306	CHL	NA
23	7	307	CHL	NC
23	7	307	CHL	ND
23	7	307	CHL	NA
23	7	313	CHL	NC
23	7	313	CHL	ND
23	7	313	CHL	NA
23	8	301	CHL	NC
23	8	301	CHL	ND
23	8	301	CHL	NA
23	8	303	CHL	NC
23	8	303	CHL	ND
23	8	303	CHL	NA
23	8	306	CHL	NC
23	8	306	CHL	ND
23	8	306	CHL	NA

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Mol	Chain	Res	Type	Atom
23	8	307	CHL	NC
23	8	307	CHL	ND
23	8	307	CHL	NA
23	8	308	CHL	NC
23	8	308	CHL	ND
23	8	308	CHL	NA
23	8	309	CHL	NC
23	8	309	CHL	ND
23	8	309	CHL	NA
23	8	314	CHL	NC
23	8	314	CHL	ND
23	8	314	CHL	NA
23	8	316	CHL	NC
23	8	316	CHL	ND
23	8	316	CHL	NA
23	9	301	CHL	NC
23	9	301	CHL	ND
23	9	301	CHL	NA
23	9	305	CHL	NC
23	9	305	CHL	ND
23	9	305	CHL	NA
23	9	306	CHL	NC
23	9	306	CHL	ND
23	9	306	CHL	NA
23	9	312	CHL	NC
23	9	312	CHL	ND
23	9	312	CHL	NA
23	4	301	CHL	NC
23	4	301	CHL	ND
23	4	301	CHL	NA
23	4	302	CHL	NC
23	4	302	CHL	ND
23	4	302	CHL	NA
23	4	305	CHL	NC
23	4	305	CHL	ND
23	4	305	CHL	NA
23	4	306	CHL	NC
23	4	306	CHL	ND
23	4	306	CHL	NA
23	4	307	CHL	NC
23	4	307	CHL	ND
23	4	307	CHL	NA

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Mol	Chain	Res	Type	Atom
23	4	308	CHL	NC
23	4	308	CHL	ND
23	4	308	CHL	NA
23	4	313	CHL	NC
23	4	313	CHL	ND
23	4	313	CHL	NA
23	4	315	CHL	NC
23	4	315	CHL	ND
23	4	315	CHL	NA
24	0	303	CLA	ND
24	0	304	CLA	ND
24	0	307	CLA	ND
24	0	308	CLA	ND
24	0	309	CLA	ND
24	0	310	CLA	ND
24	0	311	CLA	ND
24	0	312	CLA	ND
24	0	313	CLA	ND
24	0	319	CLA	ND
24	1	302	CLA	ND
24	1	303	CLA	ND
24	1	307	CLA	ND
24	1	308	CLA	ND
24	1	309	CLA	ND
24	1	310	CLA	ND
24	1	311	CLA	ND
24	1	313	CLA	ND
24	2	302	CLA	ND
24	2	303	CLA	ND
24	2	308	CLA	ND
24	2	309	CLA	ND
24	2	310	CLA	ND
24	2	311	CLA	ND
24	2	313	CLA	ND
24	3	303	CLA	ND
24	3	304	CLA	ND
24	3	306	CLA	ND
24	3	308	CLA	ND
24	3	309	CLA	ND
24	3	310	CLA	ND
24	3	311	CLA	ND
24	3	312	CLA	ND

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Mol	Chain	Res	Type	Atom
24	3	313	CLA	ND
24	3	314	CLA	ND
24	3	315	CLA	ND
24	5	302	CLA	ND
24	5	303	CLA	ND
24	5	307	CLA	ND
24	5	308	CLA	ND
24	5	309	CLA	ND
24	5	310	CLA	ND
24	5	311	CLA	ND
24	5	313	CLA	ND
24	6	303	CLA	ND
24	6	304	CLA	ND
24	6	309	CLA	ND
24	6	310	CLA	ND
24	6	311	CLA	ND
24	6	312	CLA	ND
24	6	314	CLA	ND
24	6	316	CLA	ND
24	6	317	CLA	ND
24	6	318	CLA	ND
24	7	303	CLA	ND
24	7	304	CLA	ND
24	7	308	CLA	ND
24	7	309	CLA	ND
24	7	310	CLA	ND
24	7	311	CLA	ND
24	7	312	CLA	ND
24	7	314	CLA	ND
24	7	315	CLA	ND
24	7	316	CLA	ND
24	7	317	CLA	ND
24	8	304	CLA	ND
24	8	305	CLA	ND
24	8	310	CLA	ND
24	8	311	CLA	ND
24	8	312	CLA	ND
24	8	313	CLA	ND
24	8	315	CLA	ND
24	9	302	CLA	ND
24	9	303	CLA	ND
24	9	304	CLA	ND

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Mol	Chain	Res	Type	Atom
24	9	307	CLA	ND
24	9	308	CLA	ND
24	9	309	CLA	ND
24	9	310	CLA	ND
24	9	311	CLA	ND
24	A	801	CLA	ND
24	A	802	CLA	ND
24	A	803	CLA	ND
24	A	804	CLA	ND
24	A	805	CLA	ND
24	A	806	CLA	ND
24	A	807	CLA	ND
24	A	808	CLA	ND
24	A	809	CLA	ND
24	A	810	CLA	ND
24	A	811	CLA	ND
24	A	812	CLA	ND
24	A	813	CLA	ND
24	A	814	CLA	ND
24	A	815	CLA	ND
24	A	816	CLA	ND
24	A	817	CLA	ND
24	A	818	CLA	ND
24	A	819	CLA	ND
24	A	820	CLA	ND
24	A	821	CLA	ND
24	A	822	CLA	ND
24	A	823	CLA	ND
24	A	824	CLA	ND
24	A	825	CLA	ND
24	A	826	CLA	ND
24	A	827	CLA	ND
24	A	828	CLA	ND
24	A	829	CLA	ND
24	A	830	CLA	ND
24	A	831	CLA	ND
24	A	832	CLA	ND
24	A	833	CLA	ND
24	A	834	CLA	ND
24	A	835	CLA	ND
24	A	836	CLA	ND
24	A	837	CLA	ND

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Mol	Chain	Res	Type	Atom
24	A	838	CLA	ND
24	A	839	CLA	ND
24	A	840	CLA	ND
24	A	848	CLA	ND
24	A	853	CLA	ND
24	B	801	CLA	ND
24	B	802	CLA	ND
24	B	804	CLA	ND
24	B	805	CLA	ND
24	B	806	CLA	ND
24	B	807	CLA	ND
24	B	808	CLA	ND
24	B	809	CLA	ND
24	B	810	CLA	ND
24	B	811	CLA	ND
24	B	812	CLA	ND
24	B	813	CLA	ND
24	B	814	CLA	ND
24	B	815	CLA	ND
24	B	816	CLA	ND
24	B	817	CLA	ND
24	B	818	CLA	ND
24	B	819	CLA	ND
24	B	820	CLA	ND
24	B	821	CLA	ND
24	B	822	CLA	ND
24	B	823	CLA	ND
24	B	824	CLA	ND
24	B	825	CLA	ND
24	B	826	CLA	ND
24	B	827	CLA	ND
24	B	828	CLA	ND
24	B	829	CLA	ND
24	B	830	CLA	ND
24	B	831	CLA	ND
24	B	832	CLA	ND
24	B	833	CLA	ND
24	B	834	CLA	ND
24	B	835	CLA	ND
24	B	836	CLA	ND
24	B	837	CLA	ND
24	B	838	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	839	CLA	ND
24	B	840	CLA	ND
24	B	841	CLA	ND
24	F	302	CLA	ND
24	F	303	CLA	ND
24	G	101	CLA	ND
24	G	102	CLA	ND
24	G	103	CLA	ND
24	J	103	CLA	ND
24	L	201	CLA	ND
24	L	202	CLA	ND
24	L	203	CLA	ND
24	L	206	CLA	ND
24	K	101	CLA	ND
24	K	102	CLA	ND
24	K	103	CLA	ND
24	K	104	CLA	ND
24	O	201	CLA	ND
24	O	204	CLA	ND
24	O	205	CLA	ND
24	O	206	CLA	ND
24	O	209	CLA	ND
24	H	201	CLA	ND
24	H	202	CLA	ND
24	H	203	CLA	ND
24	H	204	CLA	ND
24	H	205	CLA	ND
24	4	303	CLA	ND
24	4	304	CLA	ND
24	4	309	CLA	ND
24	4	310	CLA	ND
24	4	311	CLA	ND
24	4	312	CLA	ND
24	4	314	CLA	ND
32	A	852	CL0	NC
32	A	852	CL0	ND
32	A	852	CL0	NA

All (3316) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	0	301	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	0	301	CHL	C1C-C2C-CMC-OMC
23	0	301	CHL	C3C-C2C-CMC-OMC
23	0	301	CHL	C2-C3-C5-C6
23	0	301	CHL	C4-C3-C5-C6
23	0	302	CHL	C12-C13-C15-C16
23	0	305	CHL	C1A-C2A-CAA-CBA
23	0	305	CHL	C3A-C2A-CAA-CBA
23	0	305	CHL	C1C-C2C-CMC-OMC
23	0	305	CHL	C3C-C2C-CMC-OMC
23	0	306	CHL	C4C-C3C-CAC-CBC
23	1	301	CHL	C1C-C2C-CMC-OMC
23	1	301	CHL	C3C-C2C-CMC-OMC
23	1	306	CHL	C1C-C2C-CMC-OMC
23	1	306	CHL	C3C-C2C-CMC-OMC
23	1	306	CHL	C11-C10-C8-C9
23	1	312	CHL	C1C-C2C-CMC-OMC
23	1	312	CHL	C3C-C2C-CMC-OMC
23	2	301	CHL	C1C-C2C-CMC-OMC
23	2	301	CHL	C3C-C2C-CMC-OMC
23	2	301	CHL	C6-C7-C8-C9
23	2	301	CHL	C12-C13-C15-C16
23	2	305	CHL	C1C-C2C-CMC-OMC
23	2	305	CHL	C3C-C2C-CMC-OMC
23	2	306	CHL	CBD-CGD-O2D-CED
23	3	302	CHL	C1C-C2C-CMC-OMC
23	3	302	CHL	C3C-C2C-CMC-OMC
23	5	301	CHL	C1C-C2C-CMC-OMC
23	5	301	CHL	C3C-C2C-CMC-OMC
23	5	304	CHL	C1C-C2C-CMC-OMC
23	5	304	CHL	C3C-C2C-CMC-OMC
23	5	304	CHL	CHA-CBD-CGD-O1D
23	5	305	CHL	C4C-C3C-CAC-CBC
23	5	306	CHL	C1C-C2C-CMC-OMC
23	5	306	CHL	C3C-C2C-CMC-OMC
23	5	312	CHL	CHA-CBD-CGD-O1D
23	5	312	CHL	CHA-CBD-CGD-O2D
23	6	302	CHL	C1C-C2C-CMC-OMC
23	6	302	CHL	C3C-C2C-CMC-OMC
23	6	302	CHL	C11-C10-C8-C9
23	6	306	CHL	C1C-C2C-CMC-OMC
23	6	306	CHL	C3C-C2C-CMC-OMC
23	6	307	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
23	6	307	CHL	C3C-C2C-CMC-OMC
23	6	313	CHL	C2-C3-C5-C6
23	6	313	CHL	C4-C3-C5-C6
23	7	302	CHL	C14-C13-C15-C16
23	7	307	CHL	C3A-C2A-CAA-CBA
23	7	307	CHL	CBD-CGD-O2D-CED
23	8	301	CHL	C2-C3-C5-C6
23	8	301	CHL	C4-C3-C5-C6
23	8	303	CHL	C1C-C2C-CMC-OMC
23	8	303	CHL	C3C-C2C-CMC-OMC
23	8	307	CHL	C1A-C2A-CAA-CBA
23	8	307	CHL	C1C-C2C-CMC-OMC
23	8	307	CHL	C3C-C2C-CMC-OMC
23	8	307	CHL	CAD-CBD-CGD-O1D
23	8	307	CHL	CAD-CBD-CGD-O2D
23	8	308	CHL	C3A-C2A-CAA-CBA
23	8	314	CHL	C1C-C2C-CMC-OMC
23	8	314	CHL	C3C-C2C-CMC-OMC
23	9	301	CHL	C1C-C2C-CMC-OMC
23	9	301	CHL	C3C-C2C-CMC-OMC
23	9	306	CHL	C1C-C2C-CMC-OMC
23	9	312	CHL	C3A-C2A-CAA-CBA
23	4	301	CHL	CAD-CBD-CGD-O1D
23	4	301	CHL	CAD-CBD-CGD-O2D
23	4	302	CHL	C1C-C2C-CMC-OMC
23	4	302	CHL	C3C-C2C-CMC-OMC
23	4	306	CHL	C1C-C2C-CMC-OMC
23	4	306	CHL	C3C-C2C-CMC-OMC
23	4	307	CHL	C1C-C2C-CMC-OMC
23	4	307	CHL	C3C-C2C-CMC-OMC
23	4	307	CHL	CBD-CGD-O2D-CED
23	4	313	CHL	C1C-C2C-CMC-OMC
23	4	313	CHL	C3C-C2C-CMC-OMC
23	4	315	CHL	CAD-CBD-CGD-O1D
23	4	315	CHL	CAD-CBD-CGD-O2D
24	0	304	CLA	C1A-C2A-CAA-CBA
24	0	304	CLA	C3A-C2A-CAA-CBA
24	0	307	CLA	C1A-C2A-CAA-CBA
24	0	307	CLA	C3A-C2A-CAA-CBA
24	0	308	CLA	C2-C3-C5-C6
24	0	308	CLA	C4-C3-C5-C6
24	0	310	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	0	311	CLA	C6-C7-C8-C9
24	0	312	CLA	CBA-CGA-O2A-C1
24	0	312	CLA	CAD-CBD-CGD-O2D
24	0	312	CLA	CBD-CGD-O2D-CED
24	0	313	CLA	C1A-C2A-CAA-CBA
24	0	313	CLA	C3A-C2A-CAA-CBA
24	0	313	CLA	CAD-CBD-CGD-O1D
24	0	313	CLA	CAD-CBD-CGD-O2D
24	1	310	CLA	C1A-C2A-CAA-CBA
24	1	310	CLA	C3A-C2A-CAA-CBA
24	3	303	CLA	C1A-C2A-CAA-CBA
24	3	306	CLA	C1A-C2A-CAA-CBA
24	3	306	CLA	C3A-C2A-CAA-CBA
24	3	308	CLA	C1A-C2A-CAA-CBA
24	3	308	CLA	C3A-C2A-CAA-CBA
24	3	309	CLA	C1A-C2A-CAA-CBA
24	3	309	CLA	C3A-C2A-CAA-CBA
24	5	303	CLA	CAD-CBD-CGD-O1D
24	5	303	CLA	CAD-CBD-CGD-O2D
24	5	303	CLA	CBD-CGD-O2D-CED
24	5	307	CLA	C1A-C2A-CAA-CBA
24	5	307	CLA	C3A-C2A-CAA-CBA
24	5	310	CLA	CBD-CGD-O2D-CED
24	5	311	CLA	C1A-C2A-CAA-CBA
24	5	311	CLA	C3A-C2A-CAA-CBA
24	5	311	CLA	CBD-CGD-O2D-CED
24	6	303	CLA	C4-C3-C5-C6
24	6	312	CLA	C4B-C3B-CAB-CBB
24	6	316	CLA	CAD-CBD-CGD-O1D
24	6	316	CLA	CAD-CBD-CGD-O2D
24	6	317	CLA	C1A-C2A-CAA-CBA
24	6	317	CLA	C3A-C2A-CAA-CBA
24	7	303	CLA	CBD-CGD-O2D-CED
24	7	304	CLA	CHA-CBD-CGD-O1D
24	7	304	CLA	CHA-CBD-CGD-O2D
24	7	308	CLA	C1A-C2A-CAA-CBA
24	7	308	CLA	C3A-C2A-CAA-CBA
24	7	309	CLA	C1A-C2A-CAA-CBA
24	7	309	CLA	C3A-C2A-CAA-CBA
24	7	314	CLA	CBD-CGD-O2D-CED
24	7	316	CLA	CHA-CBD-CGD-O1D
24	7	316	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	7	317	CLA	C3A-C2A-CAA-CBA
24	8	304	CLA	CBA-CGA-O2A-C1
24	8	305	CLA	C1A-C2A-CAA-CBA
24	8	305	CLA	C3A-C2A-CAA-CBA
24	8	315	CLA	C3A-C2A-CAA-CBA
24	9	302	CLA	CHA-CBD-CGD-O1D
24	9	302	CLA	CHA-CBD-CGD-O2D
24	9	310	CLA	CBD-CGD-O2D-CED
24	A	803	CLA	C1A-C2A-CAA-CBA
24	A	803	CLA	C3A-C2A-CAA-CBA
24	A	803	CLA	CHA-CBD-CGD-O1D
24	A	803	CLA	CHA-CBD-CGD-O2D
24	A	804	CLA	CAD-CBD-CGD-O1D
24	A	804	CLA	CAD-CBD-CGD-O2D
24	A	805	CLA	C3A-C2A-CAA-CBA
24	A	805	CLA	C4B-C3B-CAB-CBB
24	A	807	CLA	C3A-C2A-CAA-CBA
24	A	807	CLA	CHA-CBD-CGD-O1D
24	A	807	CLA	CHA-CBD-CGD-O2D
24	A	810	CLA	C1A-C2A-CAA-CBA
24	A	815	CLA	CHA-CBD-CGD-O1D
24	A	815	CLA	CHA-CBD-CGD-O2D
24	A	816	CLA	CHA-CBD-CGD-O1D
24	A	816	CLA	CHA-CBD-CGD-O2D
24	A	817	CLA	C3A-C2A-CAA-CBA
24	A	818	CLA	C1A-C2A-CAA-CBA
24	A	818	CLA	C3A-C2A-CAA-CBA
24	A	819	CLA	C1A-C2A-CAA-CBA
24	A	819	CLA	C3A-C2A-CAA-CBA
24	A	819	CLA	C2B-C3B-CAB-CBB
24	A	819	CLA	C4B-C3B-CAB-CBB
24	A	821	CLA	C1A-C2A-CAA-CBA
24	A	821	CLA	C3A-C2A-CAA-CBA
24	A	827	CLA	CBD-CGD-O2D-CED
24	A	829	CLA	CHA-CBD-CGD-O1D
24	A	829	CLA	CHA-CBD-CGD-O2D
24	A	832	CLA	CHA-CBD-CGD-O1D
24	A	832	CLA	CHA-CBD-CGD-O2D
24	A	836	CLA	C4-C3-C5-C6
24	A	848	CLA	CBD-CGD-O2D-CED
24	A	848	CLA	O1D-CGD-O2D-CED
24	A	853	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	801	CLA	C1A-C2A-CAA-CBA
24	B	801	CLA	CHA-CBD-CGD-O1D
24	B	801	CLA	CHA-CBD-CGD-O2D
24	B	802	CLA	C12-C13-C15-C16
24	B	804	CLA	CAD-CBD-CGD-O1D
24	B	804	CLA	CAD-CBD-CGD-O2D
24	B	808	CLA	C1A-C2A-CAA-CBA
24	B	808	CLA	C3A-C2A-CAA-CBA
24	B	814	CLA	C1A-C2A-CAA-CBA
24	B	817	CLA	C1A-C2A-CAA-CBA
24	B	818	CLA	C1A-C2A-CAA-CBA
24	B	818	CLA	C3A-C2A-CAA-CBA
24	B	818	CLA	C2B-C3B-CAB-CBB
24	B	818	CLA	C4B-C3B-CAB-CBB
24	B	819	CLA	C1A-C2A-CAA-CBA
24	B	819	CLA	C3A-C2A-CAA-CBA
24	B	820	CLA	C1A-C2A-CAA-CBA
24	B	820	CLA	C2B-C3B-CAB-CBB
24	B	820	CLA	C4B-C3B-CAB-CBB
24	B	825	CLA	CHA-CBD-CGD-O2D
24	B	827	CLA	C1A-C2A-CAA-CBA
24	B	828	CLA	C3A-C2A-CAA-CBA
24	B	829	CLA	C1A-C2A-CAA-CBA
24	B	829	CLA	C3A-C2A-CAA-CBA
24	B	830	CLA	C4-C3-C5-C6
24	B	831	CLA	C1A-C2A-CAA-CBA
24	B	831	CLA	C3A-C2A-CAA-CBA
24	B	833	CLA	C1A-C2A-CAA-CBA
24	B	833	CLA	C3A-C2A-CAA-CBA
24	B	833	CLA	C4B-C3B-CAB-CBB
24	B	833	CLA	CHA-CBD-CGD-O1D
24	B	833	CLA	CHA-CBD-CGD-O2D
24	B	834	CLA	C1A-C2A-CAA-CBA
24	B	834	CLA	C3A-C2A-CAA-CBA
24	B	836	CLA	C1A-C2A-CAA-CBA
24	G	101	CLA	C1A-C2A-CAA-CBA
24	G	101	CLA	C3A-C2A-CAA-CBA
24	G	101	CLA	CHA-CBD-CGD-O1D
24	G	101	CLA	CHA-CBD-CGD-O2D
24	G	103	CLA	CBA-CGA-O2A-C1
24	L	202	CLA	C1A-C2A-CAA-CBA
24	L	202	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	L	202	CLA	CAD-CBD-CGD-O2D
24	L	203	CLA	C1A-C2A-CAA-CBA
24	L	203	CLA	C3A-C2A-CAA-CBA
24	L	203	CLA	CBA-CGA-O2A-C1
24	L	206	CLA	CHA-CBD-CGD-O1D
24	L	206	CLA	CHA-CBD-CGD-O2D
24	K	103	CLA	CBA-CGA-O2A-C1
24	K	103	CLA	O1A-CGA-O2A-C1
24	K	104	CLA	C1A-C2A-CAA-CBA
24	K	104	CLA	C3A-C2A-CAA-CBA
24	O	201	CLA	C3A-C2A-CAA-CBA
24	O	201	CLA	CBD-CGD-O2D-CED
24	O	204	CLA	CAD-CBD-CGD-O1D
24	O	204	CLA	CAD-CBD-CGD-O2D
24	O	204	CLA	CBD-CGD-O2D-CED
24	O	209	CLA	CAD-CBD-CGD-O1D
24	O	209	CLA	CAD-CBD-CGD-O2D
24	O	209	CLA	CBD-CGD-O2D-CED
24	O	209	CLA	C2-C3-C5-C6
24	O	209	CLA	C4-C3-C5-C6
24	H	201	CLA	C1A-C2A-CAA-CBA
24	H	202	CLA	C1A-C2A-CAA-CBA
24	H	202	CLA	CAD-CBD-CGD-O1D
24	H	202	CLA	CAD-CBD-CGD-O2D
24	H	205	CLA	C2-C3-C5-C6
24	H	205	CLA	C4-C3-C5-C6
25	0	314	8CT	C02-C03-C10-C11
25	1	314	8CT	C22-C21-C23-C24
25	1	314	8CT	C28-C29-C30-C31
25	1	314	8CT	C28-C29-C30-C35
25	2	314	8CT	C20-C21-C23-C24
25	2	314	8CT	C22-C21-C23-C24
25	3	316	8CT	C02-C03-C10-C11
25	3	316	8CT	C28-C29-C30-C31
25	3	316	8CT	C28-C29-C30-C35
25	3	317	8CT	C10-C11-C12-C13
25	3	317	8CT	C28-C29-C30-C31
25	3	323	8CT	C10-C11-C12-C13
25	6	319	8CT	C10-C11-C12-C13
25	6	319	8CT	C16-C17-C18-C19
25	6	324	8CT	C02-C03-C10-C11
25	6	324	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	7	318	8CT	C10-C11-C12-C40
25	7	318	8CT	C14-C15-C16-C39
25	7	318	8CT	C20-C21-C23-C24
25	7	318	8CT	C22-C21-C23-C24
25	7	318	8CT	C25-C26-C28-C29
25	7	318	8CT	C27-C26-C28-C29
25	7	318	8CT	C28-C29-C30-C31
25	7	319	8CT	C02-C03-C10-C11
25	8	317	8CT	C14-C15-C16-C17
25	8	317	8CT	C18-C19-C20-C21
25	8	317	8CT	C28-C29-C30-C31
25	8	317	8CT	C28-C29-C30-C35
25	9	313	8CT	C20-C21-C23-C24
25	9	313	8CT	C22-C21-C23-C24
25	9	313	8CT	C28-C29-C30-C31
25	A	845	8CT	C14-C15-C16-C17
25	A	846	8CT	C16-C17-C18-C19
25	A	846	8CT	C28-C29-C30-C31
25	A	847	8CT	C04-C03-C10-C11
25	A	847	8CT	C14-C15-C16-C17
25	A	847	8CT	C18-C19-C20-C21
25	A	849	8CT	C20-C21-C23-C24
25	A	849	8CT	C22-C21-C23-C24
25	B	843	8CT	C10-C11-C12-C13
25	B	843	8CT	C20-C21-C23-C24
25	B	843	8CT	C28-C29-C30-C31
25	B	843	8CT	C28-C29-C30-C35
25	B	844	8CT	C10-C11-C12-C13
25	B	844	8CT	C10-C11-C12-C40
25	B	845	8CT	C10-C11-C12-C13
25	B	845	8CT	C10-C11-C12-C40
25	B	845	8CT	C18-C19-C20-C21
25	B	846	8CT	C14-C15-C16-C17
25	B	846	8CT	C14-C15-C16-C39
25	B	846	8CT	C28-C29-C30-C31
25	B	846	8CT	C28-C29-C30-C35
25	B	847	8CT	C28-C29-C30-C31
25	B	848	8CT	C14-C15-C16-C17
25	B	848	8CT	C14-C15-C16-C39
25	B	850	8CT	C14-C15-C16-C17
25	B	850	8CT	C16-C17-C18-C19
25	B	850	8CT	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
25	B	850	8CT	C28-C29-C30-C35
25	F	301	8CT	C10-C11-C12-C13
25	F	301	8CT	C10-C11-C12-C40
25	F	301	8CT	C20-C21-C23-C24
25	F	301	8CT	C28-C29-C30-C31
25	F	301	8CT	C28-C29-C30-C35
25	F	304	8CT	C02-C03-C10-C11
25	F	304	8CT	C14-C15-C16-C17
25	F	304	8CT	C14-C15-C16-C39
25	F	304	8CT	C28-C29-C30-C31
25	F	304	8CT	C28-C29-C30-C35
25	G	104	8CT	C10-C11-C12-C13
25	G	104	8CT	C12-C13-C14-C15
25	G	104	8CT	C14-C15-C16-C17
25	G	104	8CT	C14-C15-C16-C39
25	G	104	8CT	C20-C21-C23-C24
25	G	104	8CT	C22-C21-C23-C24
25	G	104	8CT	C25-C26-C28-C29
25	G	104	8CT	C27-C26-C28-C29
25	G	104	8CT	C28-C29-C30-C31
25	I	101	8CT	C25-C26-C28-C29
25	I	101	8CT	C27-C26-C28-C29
25	I	101	8CT	C28-C29-C30-C31
25	J	101	8CT	C18-C19-C20-C21
25	J	101	8CT	C20-C21-C23-C24
25	J	101	8CT	C28-C29-C30-C31
25	J	101	8CT	C28-C29-C30-C35
25	J	104	8CT	C18-C19-C20-C21
25	J	104	8CT	C28-C29-C30-C31
25	J	104	8CT	C28-C29-C30-C35
25	L	204	8CT	C25-C26-C28-C29
25	L	204	8CT	C27-C26-C28-C29
25	L	204	8CT	C28-C29-C30-C31
25	L	205	8CT	C28-C29-C30-C31
25	L	207	8CT	C02-C03-C10-C11
25	L	207	8CT	C10-C11-C12-C13
25	K	105	8CT	C10-C11-C12-C13
25	K	105	8CT	C10-C11-C12-C40
25	K	105	8CT	C28-C29-C30-C31
25	M	102	8CT	C25-C26-C28-C29
25	O	202	8CT	C10-C11-C12-C13
25	O	202	8CT	C10-C11-C12-C40

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Mol	Chain	Res	Type	Atoms
25	O	202	8CT	C14-C15-C16-C17
25	O	208	8CT	C10-C11-C12-C13
25	O	208	8CT	C10-C11-C12-C40
25	O	208	8CT	C14-C15-C16-C17
25	4	316	8CT	C20-C21-C23-C24
25	4	316	8CT	C22-C21-C23-C24
26	0	316	0UR	C2-C3-C43-O44
26	0	316	0UR	C4-C3-C43-O44
26	0	316	0UR	C46-C45-O44-C43
26	1	316	0UR	C17-C18-C19-C28
26	1	316	0UR	C17-C18-C19-C32
26	1	316	0UR	C46-C45-O44-C43
26	1	316	0UR	O57-C45-O44-C43
26	2	315	0UR	C2-C3-C43-O44
26	2	315	0UR	C4-C3-C43-O44
26	2	315	0UR	C46-C45-O44-C43
26	2	315	0UR	O57-C45-O44-C43
26	2	316	0UR	C2-C3-C43-O44
26	2	316	0UR	C4-C3-C43-O44
26	2	316	0UR	C41-C2-C3-C4
26	3	318	0UR	C2-C3-C43-O44
26	3	318	0UR	C4-C3-C43-O44
26	3	318	0UR	C46-C45-O44-C43
26	3	318	0UR	O57-C45-O44-C43
26	5	314	0UR	O42-C2-C3-C43
26	5	314	0UR	C5-C6-C7-C8
26	5	315	0UR	C2-C3-C43-O44
26	5	315	0UR	C4-C3-C43-O44
26	5	315	0UR	C17-C18-C19-C28
26	5	315	0UR	C17-C18-C19-C32
26	6	320	0UR	C17-C18-C19-C28
26	6	320	0UR	C17-C18-C19-C32
26	6	320	0UR	C46-C45-O44-C43
26	6	321	0UR	C4-C3-C43-O44
26	6	321	0UR	C17-C18-C19-C28
26	6	321	0UR	C17-C18-C19-C32
26	7	320	0UR	C2-C3-C43-O44
26	7	320	0UR	C4-C3-C43-O44
26	7	320	0UR	C46-C45-O44-C43
26	7	320	0UR	O57-C45-O44-C43
26	8	319	0UR	C46-C45-O44-C43
26	9	315	0UR	C2-C3-C43-O44

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Mol	Chain	Res	Type	Atoms
26	9	315	0UR	C4-C3-C43-O44
26	9	315	0UR	O42-C2-C3-C43
26	9	315	0UR	C46-C45-O44-C43
26	O	207	0UR	C46-C45-O44-C43
26	4	317	0UR	C2-C3-C43-O44
26	4	317	0UR	C4-C3-C43-O44
26	4	317	0UR	C46-C45-O44-C43
26	4	317	0UR	O57-C45-O44-C43
26	4	318	0UR	C2-C3-C43-O44
26	4	318	0UR	C4-C3-C43-O44
26	4	318	0UR	C11-C12-C13-C14
26	4	318	0UR	C21-C12-C13-C14
27	0	317	LHG	C3-O3-P-O6
27	0	317	LHG	C4-O6-P-O3
27	0	317	LHG	C4-O6-P-O4
27	1	317	LHG	O2-C2-C3-O3
27	1	317	LHG	C3-O3-P-O4
27	1	317	LHG	C3-O3-P-O6
27	1	318	LHG	C4-O6-P-O5
27	2	317	LHG	O1-C1-C2-C3
27	2	317	LHG	O2-C2-C3-O3
27	2	317	LHG	C3-O3-P-O6
27	2	319	LHG	C3-O3-P-O4
27	2	319	LHG	C3-O3-P-O6
27	3	320	LHG	O1-C1-C2-C3
27	3	320	LHG	C3-O3-P-O4
27	3	320	LHG	C3-O3-P-O5
27	3	320	LHG	C3-O3-P-O6
27	3	320	LHG	O7-C5-C6-O8
27	3	322	LHG	O1-C1-C2-C3
27	3	322	LHG	O2-C2-C3-O3
27	3	322	LHG	C4-O6-P-O3
27	3	322	LHG	C4-O6-P-O4
27	3	322	LHG	C4-O6-P-O5
27	3	324	LHG	C5-C4-O6-P
27	5	316	LHG	C3-O3-P-O4
27	5	316	LHG	C3-O3-P-O6
27	6	322	LHG	C3-O3-P-O4
27	6	322	LHG	C3-O3-P-O6
27	7	322	LHG	C1-C2-C3-O3
27	7	323	LHG	C3-O3-P-O5
27	7	323	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
27	7	323	LHG	C4-O6-P-O3
27	7	323	LHG	C4-O6-P-O5
27	7	323	LHG	C8-C7-O7-C5
27	7	324	LHG	C4-O6-P-O3
27	7	324	LHG	C4-O6-P-O4
27	7	324	LHG	C4-O6-P-O5
27	8	302	LHG	C4-O6-P-O3
27	8	302	LHG	C4-O6-P-O5
27	8	302	LHG	C5-C4-O6-P
27	8	320	LHG	C3-O3-P-O5
27	8	320	LHG	C3-O3-P-O6
27	8	320	LHG	C4-O6-P-O3
27	8	320	LHG	C4-O6-P-O5
27	9	316	LHG	C3-O3-P-O5
27	9	316	LHG	C4-O6-P-O3
27	9	316	LHG	C4-O6-P-O5
27	9	316	LHG	C18-C19-C20-C21
27	A	843	LHG	O2-C2-C3-O3
27	A	843	LHG	C3-O3-P-O4
27	A	843	LHG	C4-O6-P-O3
27	A	843	LHG	C4-O6-P-O4
27	A	843	LHG	C4-O6-P-O5
27	A	843	LHG	O6-C4-C5-O7
27	A	843	LHG	C8-C7-O7-C5
27	A	850	LHG	C3-O3-P-O5
27	A	850	LHG	C3-O3-P-O6
27	A	850	LHG	O9-C7-O7-C5
27	A	850	LHG	C24-C23-O8-C6
27	B	851	LHG	C1-C2-C3-O3
27	B	851	LHG	C3-O3-P-O4
27	B	851	LHG	C3-O3-P-O5
27	B	851	LHG	C3-O3-P-O6
27	B	851	LHG	C4-O6-P-O4
27	B	851	LHG	C8-C7-O7-C5
27	B	852	LHG	C1-C2-C3-O3
27	B	852	LHG	O2-C2-C3-O3
27	B	852	LHG	C3-O3-P-O5
27	B	852	LHG	C3-O3-P-O6
27	B	852	LHG	C4-O6-P-O3
27	B	852	LHG	C4-O6-P-O4
27	I	102	LHG	O1-C1-C2-C3
27	I	102	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	I	102	LHG	C8-C7-O7-C5
27	L	208	LHG	O1-C1-C2-C3
28	0	318	SQD	O5-C1-O6-C44
29	2	318	LMG	O6-C1-O1-C7
29	3	321	LMG	C2-C1-O1-C7
29	3	321	LMG	O6-C1-O1-C7
29	3	321	LMG	O7-C8-C9-O8
29	3	321	LMG	O9-C10-O7-C8
29	A	851	LMG	C11-C10-O7-C8
29	A	854	LMG	O7-C8-C9-O8
29	J	102	LMG	O6-C1-O1-C7
29	M	101	LMG	O6-C1-O1-C7
34	B	849	DGD	O1B-C1B-O2G-C2G
24	0	312	CLA	O1D-CGD-O2D-CED
24	0	313	CLA	O1D-CGD-O2D-CED
24	7	315	CLA	O1D-CGD-O2D-CED
24	B	806	CLA	O1D-CGD-O2D-CED
24	7	303	CLA	O1D-CGD-O2D-CED
24	9	308	CLA	O1D-CGD-O2D-CED
24	B	805	CLA	O1D-CGD-O2D-CED
24	O	201	CLA	O1D-CGD-O2D-CED
24	4	314	CLA	O1D-CGD-O2D-CED
23	1	306	CHL	CBD-CGD-O2D-CED
23	5	306	CHL	CBD-CGD-O2D-CED
23	6	307	CHL	CBD-CGD-O2D-CED
23	8	308	CHL	CBD-CGD-O2D-CED
24	0	304	CLA	CBD-CGD-O2D-CED
24	0	313	CLA	CBD-CGD-O2D-CED
24	1	310	CLA	CBD-CGD-O2D-CED
24	1	313	CLA	CBD-CGD-O2D-CED
24	2	310	CLA	CBD-CGD-O2D-CED
24	3	303	CLA	CBD-CGD-O2D-CED
24	5	307	CLA	CBD-CGD-O2D-CED
24	6	310	CLA	CBD-CGD-O2D-CED
24	7	315	CLA	CBD-CGD-O2D-CED
24	8	304	CLA	CBD-CGD-O2D-CED
24	8	305	CLA	CBD-CGD-O2D-CED
24	8	312	CLA	CBD-CGD-O2D-CED
24	8	313	CLA	CBD-CGD-O2D-CED
24	9	308	CLA	CBD-CGD-O2D-CED
24	B	805	CLA	CBD-CGD-O2D-CED
24	B	806	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	807	CLA	CBD-CGD-O2D-CED
24	G	102	CLA	CBD-CGD-O2D-CED
24	K	102	CLA	CBD-CGD-O2D-CED
24	4	314	CLA	CBD-CGD-O2D-CED
24	3	309	CLA	O1A-CGA-O2A-C1
24	A	804	CLA	O1A-CGA-O2A-C1
24	B	802	CLA	O1A-CGA-O2A-C1
24	B	813	CLA	O1A-CGA-O2A-C1
24	B	823	CLA	O1A-CGA-O2A-C1
27	3	324	LHG	O10-C23-O8-C6
27	5	316	LHG	O10-C23-O8-C6
27	A	850	LHG	O10-C23-O8-C6
29	J	102	LMG	O10-C28-O8-C9
24	0	312	CLA	O1A-CGA-O2A-C1
24	G	103	CLA	O1A-CGA-O2A-C1
24	L	203	CLA	O1A-CGA-O2A-C1
24	6	304	CLA	CBA-CGA-O2A-C1
24	3	303	CLA	O1D-CGD-O2D-CED
24	B	813	CLA	CBA-CGA-O2A-C1
27	3	324	LHG	C24-C23-O8-C6
27	5	316	LHG	C24-C23-O8-C6
29	J	102	LMG	C29-C28-O8-C9
24	1	307	CLA	CBD-CGD-O2D-CED
24	9	302	CLA	CBD-CGD-O2D-CED
24	2	309	CLA	O1A-CGA-O2A-C1
24	7	309	CLA	O1A-CGA-O2A-C1
24	7	314	CLA	O1A-CGA-O2A-C1
24	F	302	CLA	O1A-CGA-O2A-C1
24	L	202	CLA	O1A-CGA-O2A-C1
24	H	203	CLA	O1A-CGA-O2A-C1
27	1	317	LHG	O10-C23-O8-C6
27	I	102	LHG	O10-C23-O8-C6
29	9	317	LMG	O10-C28-O8-C9
29	M	101	LMG	O10-C28-O8-C9
24	8	304	CLA	O1A-CGA-O2A-C1
24	7	314	CLA	O1D-CGD-O2D-CED
24	O	209	CLA	O1D-CGD-O2D-CED
23	2	306	CHL	O1D-CGD-O2D-CED
23	7	307	CHL	O1D-CGD-O2D-CED
24	5	310	CLA	O1D-CGD-O2D-CED
24	5	311	CLA	O1D-CGD-O2D-CED
24	9	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	827	CLA	O1D-CGD-O2D-CED
24	O	204	CLA	O1D-CGD-O2D-CED
23	6	306	CHL	CBD-CGD-O2D-CED
27	7	323	LHG	O9-C7-O7-C5
27	A	843	LHG	O9-C7-O7-C5
27	B	851	LHG	O9-C7-O7-C5
29	9	317	LMG	O9-C10-O7-C8
29	A	851	LMG	O9-C10-O7-C8
29	A	854	LMG	O9-C10-O7-C8
29	J	102	LMG	O9-C10-O7-C8
29	M	101	LMG	O9-C10-O7-C8
24	5	313	CLA	O1A-CGA-O2A-C1
26	0	316	0UR	O57-C45-O44-C43
26	6	320	0UR	O57-C45-O44-C43
26	9	315	0UR	O57-C45-O44-C43
23	2	301	CHL	C3-C5-C6-C7
24	0	303	CLA	C3-C5-C6-C7
24	2	302	CLA	C3-C5-C6-C7
24	3	303	CLA	C3-C5-C6-C7
24	5	308	CLA	C3-C5-C6-C7
24	7	308	CLA	C3-C5-C6-C7
24	A	805	CLA	C3-C5-C6-C7
24	A	807	CLA	C3-C5-C6-C7
24	A	820	CLA	C3-C5-C6-C7
24	A	831	CLA	C3-C5-C6-C7
24	B	801	CLA	C3-C5-C6-C7
24	B	811	CLA	C3-C5-C6-C7
24	B	822	CLA	C3-C5-C6-C7
24	B	836	CLA	C3-C5-C6-C7
24	L	201	CLA	C3-C5-C6-C7
31	B	842	PQN	C13-C15-C16-C17
26	5	314	0UR	C46-C45-O44-C43
26	8	318	0UR	C46-C45-O44-C43
24	8	312	CLA	O1D-CGD-O2D-CED
24	3	309	CLA	CBA-CGA-O2A-C1
24	3	310	CLA	CBA-CGA-O2A-C1
24	5	302	CLA	CBA-CGA-O2A-C1
24	A	804	CLA	CBA-CGA-O2A-C1
24	A	807	CLA	CBA-CGA-O2A-C1
24	B	802	CLA	CBA-CGA-O2A-C1
24	B	819	CLA	CBA-CGA-O2A-C1
24	B	824	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	1	317	LHG	C24-C23-O8-C6
29	9	317	LMG	C29-C28-O8-C9
29	M	101	LMG	C29-C28-O8-C9
23	0	301	CHL	CBD-CGD-O2D-CED
23	1	305	CHL	CBD-CGD-O2D-CED
23	3	302	CHL	CBD-CGD-O2D-CED
23	3	307	CHL	CBD-CGD-O2D-CED
23	5	301	CHL	CBD-CGD-O2D-CED
23	5	305	CHL	CBD-CGD-O2D-CED
23	7	305	CHL	CBD-CGD-O2D-CED
24	0	311	CLA	CBD-CGD-O2D-CED
24	2	309	CLA	CBD-CGD-O2D-CED
24	2	311	CLA	CBD-CGD-O2D-CED
24	5	308	CLA	CBD-CGD-O2D-CED
24	5	313	CLA	CBD-CGD-O2D-CED
24	6	316	CLA	CBD-CGD-O2D-CED
24	7	312	CLA	CBD-CGD-O2D-CED
24	A	832	CLA	CBD-CGD-O2D-CED
24	A	838	CLA	CBD-CGD-O2D-CED
24	B	815	CLA	CBD-CGD-O2D-CED
24	B	816	CLA	CBD-CGD-O2D-CED
24	B	820	CLA	CBD-CGD-O2D-CED
24	F	303	CLA	CBD-CGD-O2D-CED
24	G	101	CLA	CBD-CGD-O2D-CED
24	4	310	CLA	CBD-CGD-O2D-CED
24	4	312	CLA	CBD-CGD-O2D-CED
27	A	850	LHG	C8-C7-O7-C5
28	0	318	SQD	C8-C7-O47-C45
34	B	849	DGD	C2B-C1B-O2G-C2G
23	0	306	CHL	C2C-C3C-CAC-CBC
23	4	307	CHL	O1D-CGD-O2D-CED
24	5	303	CLA	O1D-CGD-O2D-CED
24	5	307	CLA	O1D-CGD-O2D-CED
24	8	304	CLA	O1D-CGD-O2D-CED
24	8	313	CLA	O1D-CGD-O2D-CED
24	A	853	CLA	O1D-CGD-O2D-CED
24	G	102	CLA	O1D-CGD-O2D-CED
24	6	304	CLA	O1A-CGA-O2A-C1
23	8	314	CHL	C4-C3-C5-C6
23	4	301	CHL	C4-C3-C5-C6
23	4	315	CHL	C4-C3-C5-C6
24	0	303	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	1	302	CLA	C4-C3-C5-C6
24	1	311	CLA	C4-C3-C5-C6
24	2	302	CLA	C4-C3-C5-C6
24	3	309	CLA	C4-C3-C5-C6
24	7	309	CLA	C4-C3-C5-C6
24	A	839	CLA	C4-C3-C5-C6
24	A	840	CLA	C4-C3-C5-C6
24	B	823	CLA	C4-C3-C5-C6
23	8	314	CHL	C2-C3-C5-C6
23	4	301	CHL	C2-C3-C5-C6
23	4	315	CHL	C2-C3-C5-C6
24	1	302	CLA	C2-C3-C5-C6
24	2	302	CLA	C2-C3-C5-C6
24	3	309	CLA	C2-C3-C5-C6
24	6	303	CLA	C2-C3-C5-C6
24	7	309	CLA	C2-C3-C5-C6
24	A	836	CLA	C2-C3-C5-C6
24	B	823	CLA	C2-C3-C5-C6
24	B	830	CLA	C2-C3-C5-C6
24	5	313	CLA	CBA-CGA-O2A-C1
24	6	317	CLA	CBA-CGA-O2A-C1
24	A	831	CLA	CBD-CGD-O2D-CED
24	H	205	CLA	CBD-CGD-O2D-CED
26	0	316	0UR	O44-C45-C46-C47
26	5	315	0UR	O44-C45-C46-C47
27	7	323	LHG	O10-C23-O8-C6
24	0	308	CLA	C3-C5-C6-C7
24	9	307	CLA	C3-C5-C6-C7
24	B	804	CLA	C3-C5-C6-C7
23	5	301	CHL	CBA-CGA-O2A-C1
24	1	310	CLA	CBA-CGA-O2A-C1
24	2	309	CLA	CBA-CGA-O2A-C1
24	7	309	CLA	CBA-CGA-O2A-C1
24	7	314	CLA	CBA-CGA-O2A-C1
24	9	310	CLA	CBA-CGA-O2A-C1
24	A	805	CLA	CBA-CGA-O2A-C1
24	B	822	CLA	CBA-CGA-O2A-C1
24	B	823	CLA	CBA-CGA-O2A-C1
24	F	302	CLA	CBA-CGA-O2A-C1
24	L	202	CLA	CBA-CGA-O2A-C1
24	H	203	CLA	CBA-CGA-O2A-C1
24	4	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	2	319	LHG	C24-C23-O8-C6
27	I	102	LHG	C24-C23-O8-C6
28	0	318	SQD	C24-C23-O48-C46
27	1	318	LHG	C24-C25-C26-C27
27	B	852	LHG	C24-C25-C26-C27
27	0	317	LHG	C24-C25-C26-C27
27	2	317	LHG	C24-C25-C26-C27
27	A	850	LHG	C24-C25-C26-C27
29	9	317	LMG	C4-C5-C6-O5
25	3	317	8CT	C18-C19-C20-C21
25	3	323	8CT	C16-C17-C18-C19
25	7	318	8CT	C16-C17-C18-C19
25	8	317	8CT	C12-C13-C14-C15
25	F	301	8CT	C12-C13-C14-C15
25	F	304	8CT	C12-C13-C14-C15
25	I	101	8CT	C16-C17-C18-C19
25	I	101	8CT	C18-C19-C20-C21
25	J	101	8CT	C23-C24-C25-C26
25	K	105	8CT	C12-C13-C14-C15
25	M	102	8CT	C18-C19-C20-C21
25	O	208	8CT	C18-C19-C20-C21
24	1	310	CLA	O1A-CGA-O2A-C1
24	5	302	CLA	O1A-CGA-O2A-C1
24	A	807	CLA	O1A-CGA-O2A-C1
24	A	818	CLA	O1A-CGA-O2A-C1
24	B	819	CLA	O1A-CGA-O2A-C1
24	B	822	CLA	O1A-CGA-O2A-C1
24	B	824	CLA	O1A-CGA-O2A-C1
24	B	833	CLA	O1A-CGA-O2A-C1
24	4	310	CLA	O1A-CGA-O2A-C1
27	1	318	LHG	O10-C23-O8-C6
27	B	852	LHG	O10-C23-O8-C6
32	A	852	CL0	O1A-CGA-O2A-C1
28	0	318	SQD	O49-C7-O47-C45
27	2	319	LHG	C24-C25-C26-C27
27	3	322	LHG	C24-C25-C26-C27
27	3	324	LHG	C24-C25-C26-C27
27	5	316	LHG	C24-C25-C26-C27
27	L	208	LHG	C24-C25-C26-C27
26	2	316	0UR	O57-C45-O44-C43
26	5	314	0UR	O57-C45-O44-C43
26	8	319	0UR	O57-C45-O44-C43

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Mol	Chain	Res	Type	Atoms
26	O	207	0UR	O57-C45-O44-C43
26	4	318	0UR	O57-C45-O44-C43
23	6	307	CHL	O1D-CGD-O2D-CED
24	8	305	CLA	O1D-CGD-O2D-CED
23	1	312	CHL	C3-C5-C6-C7
23	3	301	CHL	C3-C5-C6-C7
24	5	302	CLA	C3-C5-C6-C7
24	7	309	CLA	C3-C5-C6-C7
23	9	305	CHL	CBD-CGD-O2D-CED
24	0	309	CLA	CBD-CGD-O2D-CED
24	6	312	CLA	CBD-CGD-O2D-CED
24	7	311	CLA	CBD-CGD-O2D-CED
24	7	317	CLA	CBD-CGD-O2D-CED
24	B	804	CLA	CBD-CGD-O2D-CED
24	B	824	CLA	CBD-CGD-O2D-CED
24	B	836	CLA	CBD-CGD-O2D-CED
26	2	316	0UR	C46-C45-O44-C43
26	4	318	0UR	C46-C45-O44-C43
27	1	318	LHG	O2-C2-C3-O3
27	7	322	LHG	O2-C2-C3-O3
27	7	324	LHG	O2-C2-C3-O3
23	8	308	CHL	O1D-CGD-O2D-CED
24	1	310	CLA	O1D-CGD-O2D-CED
24	2	310	CLA	O1D-CGD-O2D-CED
24	6	310	CLA	O1D-CGD-O2D-CED
23	7	301	CHL	CBA-CGA-O2A-C1
24	A	818	CLA	CBA-CGA-O2A-C1
24	A	836	CLA	CBA-CGA-O2A-C1
24	B	833	CLA	CBA-CGA-O2A-C1
24	B	840	CLA	CBA-CGA-O2A-C1
24	K	102	CLA	CBA-CGA-O2A-C1
24	4	304	CLA	CBA-CGA-O2A-C1
27	1	318	LHG	C24-C23-O8-C6
32	A	852	CL0	CBA-CGA-O2A-C1
29	J	102	LMG	O6-C5-C6-O5
24	3	310	CLA	O1A-CGA-O2A-C1
24	A	836	CLA	O1A-CGA-O2A-C1
28	0	318	SQD	O10-C23-O48-C46
24	0	304	CLA	O1D-CGD-O2D-CED
26	6	320	0UR	O44-C45-C46-C47
26	7	320	0UR	O44-C45-C46-C47
26	9	315	0UR	O44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
26	O	207	0UR	O44-C45-C46-C47
29	M	101	LMG	O6-C5-C6-O5
24	B	822	CLA	CBD-CGD-O2D-CED
29	9	317	LMG	C11-C10-O7-C8
29	M	101	LMG	C11-C10-O7-C8
24	8	312	CLA	CBA-CGA-O2A-C1
24	B	840	CLA	O1A-CGA-O2A-C1
27	2	319	LHG	O10-C23-O8-C6
29	3	321	LMG	O6-C5-C6-O5
34	B	849	DGD	O6E-C5E-C6E-O5E
23	5	306	CHL	O1D-CGD-O2D-CED
23	6	308	CHL	C3-C5-C6-C7
24	A	837	CLA	C3-C5-C6-C7
24	B	820	CLA	C3-C5-C6-C7
31	A	841	PQN	C13-C15-C16-C17
24	1	302	CLA	CBD-CGD-O2D-CED
24	7	316	CLA	CBD-CGD-O2D-CED
24	H	202	CLA	CBD-CGD-O2D-CED
23	1	306	CHL	O1D-CGD-O2D-CED
24	B	807	CLA	O1D-CGD-O2D-CED
24	K	102	CLA	O1D-CGD-O2D-CED
27	7	323	LHG	C24-C23-O8-C6
27	B	852	LHG	C24-C23-O8-C6
24	1	308	CLA	C4-C3-C5-C6
24	7	304	CLA	C4-C3-C5-C6
24	A	827	CLA	C4-C3-C5-C6
24	B	819	CLA	C4-C3-C5-C6
31	A	841	PQN	C14-C13-C15-C16
24	0	303	CLA	C2-C3-C5-C6
24	A	827	CLA	C2-C3-C5-C6
24	A	839	CLA	C2-C3-C5-C6
24	B	819	CLA	C2-C3-C5-C6
23	5	301	CHL	O1A-CGA-O2A-C1
24	9	310	CLA	O1A-CGA-O2A-C1
24	A	805	CLA	O1A-CGA-O2A-C1
24	K	102	CLA	O1A-CGA-O2A-C1
24	4	304	CLA	O1A-CGA-O2A-C1
29	9	317	LMG	O6-C5-C6-O5
29	3	321	LMG	C4-C5-C6-O5
24	3	315	CLA	C2C-C3C-CAC-CBC
24	1	311	CLA	CBD-CGD-O2D-CED
24	4	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	6	317	CLA	O1A-CGA-O2A-C1
24	1	313	CLA	O1D-CGD-O2D-CED
27	I	102	LHG	C2-C3-O3-P
29	O	203	LMG	O6-C5-C6-O5
23	2	312	CHL	C2A-CAA-CBA-CGA
24	A	823	CLA	C2A-CAA-CBA-CGA
26	8	319	0UR	O44-C45-C46-C47
24	B	834	CLA	O1A-CGA-O2A-C1
29	3	321	LMG	O10-C28-O8-C9
34	B	849	DGD	O6D-C1D-O3G-C3G
29	M	101	LMG	C4-C5-C6-O5
24	9	302	CLA	O1D-CGD-O2D-CED
24	2	303	CLA	CBA-CGA-O2A-C1
24	3	304	CLA	CBA-CGA-O2A-C1
24	A	806	CLA	CBA-CGA-O2A-C1
24	A	840	CLA	CBA-CGA-O2A-C1
24	B	831	CLA	CBA-CGA-O2A-C1
24	B	834	CLA	CBA-CGA-O2A-C1
23	5	312	CHL	CBD-CGD-O2D-CED
23	8	303	CHL	CBD-CGD-O2D-CED
23	8	307	CHL	CBD-CGD-O2D-CED
24	2	313	CLA	CBD-CGD-O2D-CED
24	A	805	CLA	CBD-CGD-O2D-CED
24	A	818	CLA	CBD-CGD-O2D-CED
24	L	206	CLA	CBD-CGD-O2D-CED
29	O	210	LMG	O6-C5-C6-O5
23	7	301	CHL	O1A-CGA-O2A-C1
27	A	842	LHG	C12-C13-C14-C15
24	1	307	CLA	O1D-CGD-O2D-CED
23	6	315	CHL	CBD-CGD-O2D-CED
24	3	310	CLA	CBD-CGD-O2D-CED
24	3	313	CLA	CBD-CGD-O2D-CED
24	B	817	CLA	CBD-CGD-O2D-CED
29	J	102	LMG	C11-C10-O7-C8
25	0	314	8CT	C16-C17-C18-C19
25	0	314	8CT	C18-C19-C20-C21
25	7	318	8CT	C18-C19-C20-C21
25	G	104	8CT	C16-C17-C18-C19
25	G	104	8CT	C18-C19-C20-C21
25	J	101	8CT	C16-C17-C18-C19
25	L	207	8CT	C12-C13-C14-C15
25	L	207	8CT	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	8	307	CHL	O1A-CGA-O2A-C1
24	2	303	CLA	O1A-CGA-O2A-C1
24	A	840	CLA	O1A-CGA-O2A-C1
27	0	317	LHG	C1-C2-C3-O3
27	2	317	LHG	C1-C2-C3-O3
27	3	322	LHG	C1-C2-C3-O3
27	7	324	LHG	C1-C2-C3-O3
23	2	306	CHL	CBA-CGA-O2A-C1
23	3	301	CHL	CBA-CGA-O2A-C1
23	8	307	CHL	CBA-CGA-O2A-C1
23	8	308	CHL	CBA-CGA-O2A-C1
23	4	307	CHL	CBA-CGA-O2A-C1
24	A	803	CLA	CBA-CGA-O2A-C1
24	A	809	CLA	CBA-CGA-O2A-C1
24	A	816	CLA	CBA-CGA-O2A-C1
24	A	830	CLA	CBA-CGA-O2A-C1
24	A	832	CLA	CBA-CGA-O2A-C1
24	H	205	CLA	CBA-CGA-O2A-C1
29	3	321	LMG	C29-C28-O8-C9
29	J	105	LMG	C29-C28-O8-C9
24	8	311	CLA	CBA-CGA-O2A-C1
23	0	302	CHL	CBD-CGD-O2D-CED
23	5	304	CHL	CBD-CGD-O2D-CED
23	7	306	CHL	CBD-CGD-O2D-CED
24	L	203	CLA	CBD-CGD-O2D-CED
26	1	316	0UR	O44-C45-C46-C47
26	6	321	0UR	O44-C45-C46-C47
26	8	318	0UR	O44-C45-C46-C47
27	0	317	LHG	C12-C13-C14-C15
27	A	850	LHG	C12-C13-C14-C15
27	I	102	LHG	C12-C13-C14-C15
23	6	306	CHL	O1D-CGD-O2D-CED
26	8	318	0UR	O57-C45-O44-C43
23	8	308	CHL	O1A-CGA-O2A-C1
27	1	317	LHG	C31-C32-C33-C34
24	1	311	CLA	C2-C3-C5-C6
24	7	304	CLA	C2-C3-C5-C6
24	A	840	CLA	C2-C3-C5-C6
31	A	841	PQN	C12-C13-C15-C16
24	A	802	CLA	C3-C5-C6-C7
24	B	834	CLA	C3-C5-C6-C7
23	2	301	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	5	301	CHL	C14-C13-C15-C16
23	6	301	CHL	C11-C10-C8-C9
23	6	302	CHL	C6-C7-C8-C9
23	6	308	CHL	C11-C10-C8-C9
23	7	301	CHL	C14-C13-C15-C16
23	4	301	CHL	C6-C7-C8-C9
23	4	301	CHL	C11-C10-C8-C9
24	2	302	CLA	C6-C7-C8-C9
24	2	309	CLA	C11-C10-C8-C9
24	3	309	CLA	C14-C13-C15-C16
24	3	310	CLA	C6-C7-C8-C9
24	5	308	CLA	C6-C7-C8-C9
24	6	310	CLA	C6-C7-C8-C9
24	7	308	CLA	C11-C12-C13-C14
24	7	309	CLA	C11-C10-C8-C9
24	9	307	CLA	C11-C12-C13-C14
24	9	308	CLA	C6-C7-C8-C9
24	A	838	CLA	C11-C12-C13-C14
24	A	848	CLA	C6-C7-C8-C9
24	B	806	CLA	C11-C12-C13-C14
24	B	808	CLA	C6-C7-C8-C9
24	B	814	CLA	C11-C12-C13-C14
24	B	836	CLA	C11-C10-C8-C9
24	L	201	CLA	C6-C7-C8-C9
26	6	321	0UR	C46-C45-O44-C43
23	3	307	CHL	O1D-CGD-O2D-CED
24	5	313	CLA	O1D-CGD-O2D-CED
29	J	102	LMG	C2-C1-O1-C7
29	M	101	LMG	C2-C1-O1-C7
34	B	849	DGD	C2D-C1D-O3G-C3G
27	0	317	LHG	O2-C2-C3-O3
24	B	815	CLA	O1D-CGD-O2D-CED
24	4	310	CLA	O1D-CGD-O2D-CED
26	O	207	0UR	O57-C45-C46-C47
23	2	306	CHL	O1A-CGA-O2A-C1
23	3	301	CHL	O1A-CGA-O2A-C1
24	A	816	CLA	O1A-CGA-O2A-C1
34	B	849	DGD	C4E-C5E-C6E-O5E
25	2	314	8CT	C27-C26-C28-C29
25	3	323	8CT	C10-C11-C12-C40
25	6	319	8CT	C10-C11-C12-C40
25	6	319	8CT	C22-C21-C23-C24

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Mol	Chain	Res	Type	Atoms
25	7	319	8CT	C14-C15-C16-C39
25	8	317	8CT	C10-C11-C12-C40
25	8	317	8CT	C14-C15-C16-C39
25	A	844	8CT	C10-C11-C12-C40
25	A	845	8CT	C14-C15-C16-C39
25	A	845	8CT	C27-C26-C28-C29
25	A	846	8CT	C10-C11-C12-C40
25	A	847	8CT	C10-C11-C12-C40
25	A	847	8CT	C14-C15-C16-C39
25	A	849	8CT	C27-C26-C28-C29
25	B	843	8CT	C10-C11-C12-C40
25	B	843	8CT	C22-C21-C23-C24
25	B	847	8CT	C10-C11-C12-C40
25	B	850	8CT	C14-C15-C16-C39
25	F	301	8CT	C14-C15-C16-C39
25	F	301	8CT	C22-C21-C23-C24
25	F	301	8CT	C27-C26-C28-C29
25	G	104	8CT	C10-C11-C12-C40
25	I	101	8CT	C10-C11-C12-C40
25	J	101	8CT	C22-C21-C23-C24
25	J	101	8CT	C27-C26-C28-C29
25	L	205	8CT	C10-C11-C12-C40
25	L	207	8CT	C14-C15-C16-C39
25	K	105	8CT	C14-C15-C16-C39
25	K	105	8CT	C22-C21-C23-C24
25	M	102	8CT	C10-C11-C12-C40
25	M	102	8CT	C27-C26-C28-C29
25	O	202	8CT	C14-C15-C16-C39
25	O	208	8CT	C14-C15-C16-C39
26	1	316	0UR	C22-C16-C17-C18
26	5	314	0UR	C5-C6-C7-C20
29	J	105	LMG	O6-C5-C6-O5
25	1	314	8CT	C20-C21-C23-C24
25	2	314	8CT	C25-C26-C28-C29
25	6	319	8CT	C20-C21-C23-C24
25	6	324	8CT	C14-C15-C16-C17
25	7	318	8CT	C10-C11-C12-C13
25	7	318	8CT	C14-C15-C16-C17
25	8	317	8CT	C10-C11-C12-C13
25	A	844	8CT	C10-C11-C12-C13
25	A	846	8CT	C10-C11-C12-C13
25	A	847	8CT	C20-C21-C23-C24

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Mol	Chain	Res	Type	Atoms
25	A	849	8CT	C25-C26-C28-C29
25	B	847	8CT	C10-C11-C12-C13
25	F	301	8CT	C14-C15-C16-C17
25	F	301	8CT	C25-C26-C28-C29
25	I	101	8CT	C10-C11-C12-C13
25	J	101	8CT	C25-C26-C28-C29
25	L	207	8CT	C14-C15-C16-C17
25	K	105	8CT	C14-C15-C16-C17
25	4	316	8CT	C25-C26-C28-C29
26	1	316	0UR	C15-C16-C17-C18
27	A	850	LHG	C10-C11-C12-C13
23	6	307	CHL	C2A-CAA-CBA-CGA
23	4	302	CHL	C3-C5-C6-C7
24	0	319	CLA	C2A-CAA-CBA-CGA
24	B	813	CLA	C2A-CAA-CBA-CGA
24	B	823	CLA	C3-C5-C6-C7
24	O	209	CLA	C2A-CAA-CBA-CGA
24	A	838	CLA	O1D-CGD-O2D-CED
24	F	303	CLA	O1D-CGD-O2D-CED
24	4	312	CLA	O1D-CGD-O2D-CED
24	8	312	CLA	O1A-CGA-O2A-C1
29	A	854	LMG	C11-C10-O7-C8
27	1	317	LHG	O7-C5-C6-O8
27	7	324	LHG	O7-C5-C6-O8
28	0	318	SQD	O47-C45-C46-O48
29	2	318	LMG	O7-C8-C9-O8
23	7	302	CHL	C5-C6-C7-C8
24	A	804	CLA	C2-C1-O2A-CGA
32	A	852	CL0	C2-C1-O2A-CGA
23	0	301	CHL	O1D-CGD-O2D-CED
23	8	316	CHL	CBD-CGD-O2D-CED
27	A	850	LHG	C11-C10-C9-C8
23	1	306	CHL	C8-C10-C11-C12
24	2	309	CLA	C5-C6-C7-C8
24	9	307	CLA	C10-C11-C12-C13
24	A	805	CLA	C8-C10-C11-C12
24	A	808	CLA	C8-C10-C11-C12
24	A	840	CLA	C5-C6-C7-C8
24	B	827	CLA	C8-C10-C11-C12
23	7	301	CHL	C3-C5-C6-C7
24	A	832	CLA	C3-C5-C6-C7
29	J	102	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
27	7	324	LHG	C7-C8-C9-C10
24	5	308	CLA	O1D-CGD-O2D-CED
24	7	312	CLA	O1D-CGD-O2D-CED
24	A	832	CLA	O1D-CGD-O2D-CED
24	B	806	CLA	C8-C10-C11-C12
27	3	322	LHG	C28-C29-C30-C31
27	9	316	LHG	C12-C13-C14-C15
27	I	102	LHG	C28-C29-C30-C31
23	5	301	CHL	C6-C7-C8-C10
24	7	308	CLA	C12-C13-C15-C16
24	A	802	CLA	C11-C10-C8-C7
24	A	805	CLA	C6-C7-C8-C10
24	A	816	CLA	C11-C12-C13-C15
24	B	828	CLA	C6-C7-C8-C10
23	5	305	CHL	O1D-CGD-O2D-CED
24	B	820	CLA	O1D-CGD-O2D-CED
23	7	306	CHL	CBA-CGA-O2A-C1
26	5	315	0UR	O57-C45-C46-C47
26	6	320	0UR	O57-C45-C46-C47
26	6	321	0UR	O57-C45-C46-C47
26	7	320	0UR	O57-C45-C46-C47
26	8	318	0UR	O57-C45-C46-C47
26	9	315	0UR	O57-C45-C46-C47
24	B	808	CLA	C15-C16-C17-C18
34	B	849	DGD	C1B-C2B-C3B-C4B
25	6	319	8CT	C18-C19-C20-C21
25	6	324	8CT	C18-C19-C20-C21
25	A	849	8CT	C23-C24-C25-C26
25	B	845	8CT	C12-C13-C14-C15
25	J	104	8CT	C16-C17-C18-C19
26	4	318	0UR	C13-C14-C15-C16
27	0	317	LHG	C30-C31-C32-C33
27	2	317	LHG	C11-C10-C9-C8
27	I	102	LHG	C14-C15-C16-C17
24	2	309	CLA	O1D-CGD-O2D-CED
23	1	306	CHL	C15-C16-C17-C18
23	3	307	CHL	C13-C15-C16-C17
24	B	805	CLA	C8-C10-C11-C12
24	4	310	CLA	C5-C6-C7-C8
27	A	842	LHG	C28-C29-C30-C31
27	0	317	LHG	C23-C24-C25-C26
27	I	102	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	J	102	LMG	C28-C29-C30-C31
23	4	307	CHL	O1A-CGA-O2A-C1
24	A	803	CLA	O1A-CGA-O2A-C1
23	8	301	CHL	CBD-CGD-O2D-CED
24	A	813	CLA	CBD-CGD-O2D-CED
24	6	316	CLA	O1D-CGD-O2D-CED
23	1	312	CHL	C8-C10-C11-C12
23	6	302	CHL	C13-C15-C16-C17
23	8	303	CHL	C10-C11-C12-C13
24	A	802	CLA	C8-C10-C11-C12
24	A	829	CLA	C5-C6-C7-C8
24	A	839	CLA	C5-C6-C7-C8
24	B	802	CLA	C13-C15-C16-C17
24	B	809	CLA	C5-C6-C7-C8
24	B	814	CLA	C8-C10-C11-C12
24	B	814	CLA	C15-C16-C17-C18
24	B	819	CLA	C5-C6-C7-C8
24	B	839	CLA	C13-C15-C16-C17
23	1	304	CHL	C2A-CAA-CBA-CGA
23	1	306	CHL	C2A-CAA-CBA-CGA
23	5	305	CHL	C2A-CAA-CBA-CGA
23	5	312	CHL	C2A-CAA-CBA-CGA
23	7	307	CHL	C2A-CAA-CBA-CGA
23	9	305	CHL	C2A-CAA-CBA-CGA
24	8	305	CLA	C2A-CAA-CBA-CGA
24	8	315	CLA	C2A-CAA-CBA-CGA
24	A	821	CLA	C2A-CAA-CBA-CGA
24	A	828	CLA	C2A-CAA-CBA-CGA
24	B	834	CLA	C2A-CAA-CBA-CGA
24	0	311	CLA	O1D-CGD-O2D-CED
23	2	301	CHL	C8-C10-C11-C12
23	3	302	CHL	C8-C10-C11-C12
23	5	301	CHL	C13-C15-C16-C17
23	8	303	CHL	C13-C15-C16-C17
24	1	311	CLA	C13-C15-C16-C17
24	A	810	CLA	C13-C15-C16-C17
24	A	828	CLA	C15-C16-C17-C18
24	A	831	CLA	C5-C6-C7-C8
24	A	834	CLA	C5-C6-C7-C8
24	B	804	CLA	C13-C15-C16-C17
24	B	814	CLA	C5-C6-C7-C8
24	B	827	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	0	317	LHG	C7-C8-C9-C10
27	2	317	LHG	C23-C24-C25-C26
23	5	301	CHL	O1D-CGD-O2D-CED
23	7	305	CHL	O1D-CGD-O2D-CED
24	B	816	CLA	O1D-CGD-O2D-CED
24	H	201	CLA	CBA-CGA-O2A-C1
24	A	830	CLA	O1A-CGA-O2A-C1
24	H	205	CLA	O1A-CGA-O2A-C1
24	9	311	CLA	C3-C5-C6-C7
24	6	316	CLA	C10-C11-C12-C13
24	A	810	CLA	C8-C10-C11-C12
24	A	810	CLA	C15-C16-C17-C18
24	A	825	CLA	C5-C6-C7-C8
24	A	848	CLA	C5-C6-C7-C8
24	B	834	CLA	C8-C10-C11-C12
24	B	836	CLA	C5-C6-C7-C8
24	B	836	CLA	C8-C10-C11-C12
24	L	202	CLA	C13-C15-C16-C17
27	B	851	LHG	O2-C2-C3-O3
23	4	315	CHL	CBA-CGA-O2A-C1
24	0	308	CLA	CBA-CGA-O2A-C1
26	0	316	0UR	O57-C45-C46-C47
27	A	850	LHG	C14-C15-C16-C17
24	3	304	CLA	O1A-CGA-O2A-C1
24	A	806	CLA	O1A-CGA-O2A-C1
24	A	809	CLA	O1A-CGA-O2A-C1
24	A	832	CLA	O1A-CGA-O2A-C1
24	B	831	CLA	O1A-CGA-O2A-C1
23	7	301	CHL	C13-C15-C16-C17
27	3	324	LHG	C23-C24-C25-C26
29	9	317	LMG	C28-C29-C30-C31
23	4	301	CHL	C5-C6-C7-C8
23	4	301	CHL	C8-C10-C11-C12
24	A	812	CLA	C13-C15-C16-C17
24	B	828	CLA	C8-C10-C11-C12
24	A	831	CLA	O1D-CGD-O2D-CED
23	1	305	CHL	O1D-CGD-O2D-CED
23	3	302	CHL	O1D-CGD-O2D-CED
23	9	305	CHL	O1D-CGD-O2D-CED
24	B	836	CLA	O1D-CGD-O2D-CED
24	G	101	CLA	O1D-CGD-O2D-CED
24	H	205	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	817	CLA	C13-C15-C16-C17
24	A	825	CLA	C15-C16-C17-C18
24	B	830	CLA	C5-C6-C7-C8
23	7	313	CHL	CBD-CGD-O2D-CED
24	0	309	CLA	O1D-CGD-O2D-CED
24	2	311	CLA	O1D-CGD-O2D-CED
24	6	312	CLA	O1D-CGD-O2D-CED
24	7	311	CLA	O1D-CGD-O2D-CED
24	1	302	CLA	C5-C6-C7-C8
24	8	310	CLA	C5-C6-C7-C8
24	A	828	CLA	C8-C10-C11-C12
24	B	806	CLA	C10-C11-C12-C13
23	4	301	CHL	CBA-CGA-O2A-C1
24	2	311	CLA	CBA-CGA-O2A-C1
26	6	321	0UR	O57-C45-O44-C43
24	6	311	CLA	O2A-C1-C2-C3
24	B	806	CLA	C2C-C3C-CAC-CBC
24	B	817	CLA	C2C-C3C-CAC-CBC
24	8	315	CLA	CBD-CGD-O2D-CED
24	B	804	CLA	O1D-CGD-O2D-CED
27	A	850	LHG	C28-C29-C30-C31
24	2	311	CLA	C3-C5-C6-C7
23	9	301	CHL	CBD-CGD-O2D-CED
25	1	314	8CT	C18-C19-C20-C21
25	3	323	8CT	C18-C19-C20-C21
25	9	313	8CT	C18-C19-C20-C21
25	A	845	8CT	C12-C13-C14-C15
25	B	848	8CT	C12-C13-C14-C15
25	B	850	8CT	C18-C19-C20-C21
25	O	202	8CT	C16-C17-C18-C19
24	3	308	CLA	C10-C11-C12-C13
24	A	805	CLA	C15-C16-C17-C18
27	1	317	LHG	C1-C2-C3-O3
27	1	318	LHG	C1-C2-C3-O3
27	A	843	LHG	C1-C2-C3-O3
24	3	306	CLA	C2A-CAA-CBA-CGA
24	3	308	CLA	C2A-CAA-CBA-CGA
24	B	823	CLA	C2A-CAA-CBA-CGA
24	L	206	CLA	C2A-CAA-CBA-CGA
23	0	302	CHL	CBA-CGA-O2A-C1
23	8	303	CHL	CBA-CGA-O2A-C1
24	1	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	801	CLA	CBA-CGA-O2A-C1
23	1	301	CHL	C13-C15-C16-C17
24	2	303	CLA	C10-C11-C12-C13
24	3	303	CLA	C5-C6-C7-C8
24	7	308	CLA	C5-C6-C7-C8
24	A	807	CLA	C15-C16-C17-C18
24	B	802	CLA	C10-C11-C12-C13
24	B	814	CLA	C10-C11-C12-C13
24	B	827	CLA	C5-C6-C7-C8
31	A	841	PQN	C15-C16-C17-C18
31	B	842	PQN	C18-C20-C21-C22
24	B	824	CLA	O1D-CGD-O2D-CED
23	9	312	CHL	CBD-CGD-O2D-CED
26	2	316	0UR	O44-C45-C46-C47
24	B	809	CLA	C3-C5-C6-C7
24	7	317	CLA	O1D-CGD-O2D-CED
27	1	317	LHG	C7-C8-C9-C10
23	2	301	CHL	C5-C6-C7-C8
23	6	302	CHL	C8-C10-C11-C12
24	5	311	CLA	C5-C6-C7-C8
24	9	307	CLA	C5-C6-C7-C8
23	6	302	CHL	C5-C6-C7-C8
24	1	308	CLA	C5-C6-C7-C8
24	A	818	CLA	C15-C16-C17-C18
24	B	802	CLA	C5-C6-C7-C8
24	B	802	CLA	C8-C10-C11-C12
24	B	809	CLA	C15-C16-C17-C18
24	B	811	CLA	C5-C6-C7-C8
24	B	839	CLA	C15-C16-C17-C18
24	L	202	CLA	C5-C6-C7-C8
24	B	822	CLA	O1D-CGD-O2D-CED
23	7	302	CHL	CBA-CGA-O2A-C1
26	1	316	0UR	O57-C45-C46-C47
26	8	319	0UR	O57-C45-C46-C47
27	A	842	LHG	C23-C24-C25-C26
24	A	829	CLA	C4-C3-C5-C6
24	B	817	CLA	C4-C3-C5-C6
24	1	308	CLA	C2-C3-C5-C6
23	7	302	CHL	C13-C15-C16-C17
24	0	311	CLA	C5-C6-C7-C8
24	A	814	CLA	C13-C15-C16-C17
24	0	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	5	311	CLA	C3-C5-C6-C7
23	7	301	CHL	CBD-CGD-O2D-CED
34	B	849	DGD	C2E-C1E-O5D-C6D
24	A	839	CLA	C13-C15-C16-C17
24	B	828	CLA	C10-C11-C12-C13
24	L	201	CLA	C5-C6-C7-C8
26	5	314	0UR	O44-C45-C46-C47
23	2	307	CHL	CBA-CGA-O2A-C1
24	H	202	CLA	O1D-CGD-O2D-CED
24	1	302	CLA	CBA-CGA-O2A-C1
24	1	309	CLA	CBA-CGA-O2A-C1
27	2	317	LHG	C24-C23-O8-C6
23	7	306	CHL	O1A-CGA-O2A-C1
24	A	836	CLA	C5-C6-C7-C8
25	1	314	8CT	C10-C11-C12-C40
25	3	317	8CT	C10-C11-C12-C40
25	6	324	8CT	C14-C15-C16-C39
25	7	319	8CT	C27-C26-C28-C29
25	9	313	8CT	C10-C11-C12-C40
25	9	313	8CT	C27-C26-C28-C29
25	A	845	8CT	C10-C11-C12-C40
25	A	847	8CT	C22-C21-C23-C24
25	A	847	8CT	C27-C26-C28-C29
25	B	843	8CT	C14-C15-C16-C39
25	B	850	8CT	C10-C11-C12-C40
25	L	207	8CT	C10-C11-C12-C40
25	4	316	8CT	C27-C26-C28-C29
26	2	316	0UR	C22-C16-C17-C18
26	5	315	0UR	C22-C16-C17-C18
26	6	320	0UR	C22-C16-C17-C18
26	6	321	0UR	C22-C16-C17-C18
27	B	851	LHG	C5-C4-O6-P
25	1	314	8CT	C10-C11-C12-C13
25	9	313	8CT	C10-C11-C12-C13
25	9	313	8CT	C25-C26-C28-C29
25	A	845	8CT	C10-C11-C12-C13
25	A	847	8CT	C10-C11-C12-C13
25	A	847	8CT	C25-C26-C28-C29
25	F	304	8CT	C10-C11-C12-C13
25	L	205	8CT	C10-C11-C12-C13
25	M	102	8CT	C10-C11-C12-C13
26	2	316	0UR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	5	315	0UR	C15-C16-C17-C18
26	6	320	0UR	C15-C16-C17-C18
23	8	303	CHL	O1A-CGA-O2A-C1
23	4	315	CHL	O1A-CGA-O2A-C1
23	0	301	CHL	C2A-CAA-CBA-CGA
23	0	302	CHL	C2A-CAA-CBA-CGA
23	0	305	CHL	C2A-CAA-CBA-CGA
23	1	312	CHL	C2A-CAA-CBA-CGA
23	2	301	CHL	C2A-CAA-CBA-CGA
23	2	305	CHL	C2A-CAA-CBA-CGA
23	3	307	CHL	C2A-CAA-CBA-CGA
23	7	302	CHL	C2A-CAA-CBA-CGA
23	8	308	CHL	C2A-CAA-CBA-CGA
23	9	306	CHL	C2A-CAA-CBA-CGA
23	4	306	CHL	C2A-CAA-CBA-CGA
24	5	303	CLA	C2A-CAA-CBA-CGA
24	5	307	CLA	C2A-CAA-CBA-CGA
24	5	313	CLA	C2A-CAA-CBA-CGA
24	6	317	CLA	C2A-CAA-CBA-CGA
24	A	839	CLA	C2A-CAA-CBA-CGA
24	B	801	CLA	C2A-CAA-CBA-CGA
24	B	804	CLA	C2A-CAA-CBA-CGA
24	B	816	CLA	C2A-CAA-CBA-CGA
24	B	828	CLA	C2A-CAA-CBA-CGA
24	B	829	CLA	C2A-CAA-CBA-CGA
24	G	103	CLA	C2A-CAA-CBA-CGA
24	H	203	CLA	C2A-CAA-CBA-CGA
27	6	322	LHG	O1-C1-C2-C3
27	7	324	LHG	O1-C1-C2-C3
27	8	302	LHG	O1-C1-C2-C3
27	A	843	LHG	O1-C1-C2-C3
27	B	851	LHG	O1-C1-C2-C3
24	3	315	CLA	C4C-C3C-CAC-CBC
24	A	839	CLA	O2A-C1-C2-C3
28	0	318	SQD	C44-C45-O47-C7
29	9	317	LMG	C9-C8-O7-C10
25	9	313	8CT	C16-C17-C18-C19
24	7	316	CLA	O1D-CGD-O2D-CED
23	4	301	CHL	O1A-CGA-O2A-C1
24	0	308	CLA	O1A-CGA-O2A-C1
24	1	309	CLA	C3-C5-C6-C7
24	K	102	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	J	105	LMG	O6-C1-O1-C7
34	B	849	DGD	O6E-C1E-O5D-C6D
24	1	302	CLA	O1D-CGD-O2D-CED
24	1	311	CLA	O1D-CGD-O2D-CED
24	7	311	CLA	CBA-CGA-O2A-C1
24	7	312	CLA	C5-C6-C7-C8
24	A	806	CLA	CBD-CGD-O2D-CED
24	A	825	CLA	CBD-CGD-O2D-CED
23	1	306	CHL	C16-C17-C18-C20
24	2	311	CLA	O1A-CGA-O2A-C1
24	B	801	CLA	O1A-CGA-O2A-C1
29	9	317	LMG	C14-C15-C16-C17
26	3	318	0UR	O44-C45-C46-C47
23	6	308	CHL	C10-C11-C12-C13
27	1	318	LHG	C34-C35-C36-C37
27	8	320	LHG	C30-C31-C32-C33
27	A	842	LHG	C30-C31-C32-C33
29	M	101	LMG	C16-C17-C18-C19
34	B	849	DGD	C2A-C3A-C4A-C5A
24	A	837	CLA	C11-C10-C8-C9
27	8	320	LHG	C11-C12-C13-C14
28	0	318	SQD	C26-C27-C28-C29
34	B	849	DGD	C2A-C1A-O1G-C1G
27	0	317	LHG	C15-C16-C17-C18
27	8	320	LHG	C14-C15-C16-C17
27	A	842	LHG	C10-C11-C12-C13
29	9	317	LMG	C20-C21-C22-C23
34	B	849	DGD	C4B-C5B-C6B-C7B
27	2	317	LHG	O1-C1-C2-O2
27	3	320	LHG	O1-C1-C2-O2
27	3	322	LHG	O1-C1-C2-O2
27	I	102	LHG	O1-C1-C2-O2
27	L	208	LHG	O1-C1-C2-O2
27	3	324	LHG	C9-C10-C11-C12
24	2	313	CLA	O1D-CGD-O2D-CED
24	A	805	CLA	O1D-CGD-O2D-CED
24	4	304	CLA	O1D-CGD-O2D-CED
24	0	311	CLA	C4B-C3B-CAB-CBB
24	1	307	CLA	C4B-C3B-CAB-CBB
24	1	309	CLA	C4B-C3B-CAB-CBB
24	3	310	CLA	C4B-C3B-CAB-CBB
24	A	823	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	A	838	CLA	C4B-C3B-CAB-CBB
24	B	824	CLA	C4B-C3B-CAB-CBB
24	G	103	CLA	C4B-C3B-CAB-CBB
24	O	204	CLA	C4B-C3B-CAB-CBB
24	0	308	CLA	C11-C12-C13-C14
24	A	823	CLA	C6-C7-C8-C9
24	L	206	CLA	O1D-CGD-O2D-CED
23	1	301	CHL	C2A-CAA-CBA-CGA
24	6	303	CLA	C3-C5-C6-C7
24	A	807	CLA	C2A-CAA-CBA-CGA
24	B	807	CLA	C2A-CAA-CBA-CGA
27	2	319	LHG	C10-C11-C12-C13
23	6	301	CHL	C8-C10-C11-C12
24	2	303	CLA	CBD-CGD-O2D-CED
27	B	852	LHG	C8-C7-O7-C5
29	3	321	LMG	C11-C10-O7-C8
27	8	320	LHG	C25-C26-C27-C28
23	1	312	CHL	C11-C12-C13-C15
24	0	311	CLA	C12-C13-C15-C16
24	5	311	CLA	C6-C7-C8-C10
24	A	807	CLA	C11-C12-C13-C15
24	A	829	CLA	C12-C13-C15-C16
24	B	814	CLA	C11-C12-C13-C15
24	B	839	CLA	C11-C12-C13-C15
24	L	201	CLA	C6-C7-C8-C10
32	A	852	CL0	C12-C13-C15-C16
29	O	203	LMG	C10-C11-C12-C13
23	8	303	CHL	C8-C10-C11-C12
24	3	308	CLA	C8-C10-C11-C12
27	1	318	LHG	C25-C26-C27-C28
27	5	316	LHG	C28-C29-C30-C31
27	7	323	LHG	C15-C16-C17-C18
27	A	842	LHG	C15-C16-C17-C18
27	A	842	LHG	C26-C27-C28-C29
29	9	317	LMG	C30-C31-C32-C33
29	9	317	LMG	C34-C35-C36-C37
29	J	105	LMG	C32-C33-C34-C35
34	B	849	DGD	C7A-C8A-C9A-CAA
34	B	849	DGD	C3B-C4B-C5B-C6B
24	8	311	CLA	O1A-CGA-O2A-C1
24	1	311	CLA	O1A-CGA-O2A-C1
23	4	315	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	A	827	CLA	C3-C5-C6-C7
23	6	301	CHL	C3A-C2A-CAA-CBA
24	0	303	CLA	C3A-C2A-CAA-CBA
24	0	310	CLA	C3A-C2A-CAA-CBA
24	0	312	CLA	C3A-C2A-CAA-CBA
24	3	303	CLA	C3A-C2A-CAA-CBA
24	7	316	CLA	C3A-C2A-CAA-CBA
24	9	310	CLA	C3A-C2A-CAA-CBA
24	A	802	CLA	C3A-C2A-CAA-CBA
24	A	831	CLA	C3A-C2A-CAA-CBA
24	A	835	CLA	C3A-C2A-CAA-CBA
24	B	801	CLA	C4-C3-C5-C6
24	B	814	CLA	C3A-C2A-CAA-CBA
24	B	817	CLA	C3A-C2A-CAA-CBA
24	B	827	CLA	C3A-C2A-CAA-CBA
24	B	836	CLA	C3A-C2A-CAA-CBA
24	H	201	CLA	C3A-C2A-CAA-CBA
24	H	202	CLA	C3A-C2A-CAA-CBA
23	8	307	CHL	O1D-CGD-O2D-CED
23	7	313	CHL	CBA-CGA-O2A-C1
27	1	317	LHG	C15-C16-C17-C18
23	3	307	CHL	C8-C10-C11-C12
24	A	839	CLA	C10-C11-C12-C13
24	B	817	CLA	C8-C10-C11-C12
23	5	312	CHL	O1D-CGD-O2D-CED
23	8	303	CHL	O1D-CGD-O2D-CED
24	A	818	CLA	O1D-CGD-O2D-CED
25	B	843	8CT	C18-C19-C20-C21
25	B	846	8CT	C16-C17-C18-C19
25	M	102	8CT	C16-C17-C18-C19
23	3	307	CHL	C16-C17-C18-C20
23	6	301	CHL	C11-C12-C13-C15
24	A	823	CLA	C6-C7-C8-C10
23	0	302	CHL	O1A-CGA-O2A-C1
23	7	302	CHL	O1A-CGA-O2A-C1
29	9	317	LMG	C33-C34-C35-C36
27	A	842	LHG	C1-C2-C3-O3
23	3	307	CHL	CBA-CGA-O2A-C1
24	1	303	CLA	CBA-CGA-O2A-C1
24	4	311	CLA	CBA-CGA-O2A-C1
27	7	322	LHG	C4-C5-C6-O8
29	3	321	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	0	317	LHG	C28-C29-C30-C31
34	B	849	DGD	C9B-CAB-CBB-CCB
24	1	302	CLA	O1A-CGA-O2A-C1
29	J	105	LMG	O10-C28-O8-C9
29	O	203	LMG	C4-C5-C6-O5
27	3	322	LHG	C9-C10-C11-C12
27	1	317	LHG	C28-C29-C30-C31
27	3	322	LHG	C11-C10-C9-C8
24	1	309	CLA	O1A-CGA-O2A-C1
24	0	310	CLA	C2B-C3B-CAB-CBB
24	0	311	CLA	C2B-C3B-CAB-CBB
24	0	313	CLA	C2B-C3B-CAB-CBB
24	1	307	CLA	C2B-C3B-CAB-CBB
24	3	310	CLA	C2B-C3B-CAB-CBB
24	5	310	CLA	C2B-C3B-CAB-CBB
24	6	312	CLA	C2B-C3B-CAB-CBB
24	7	316	CLA	C2B-C3B-CAB-CBB
24	A	805	CLA	C2B-C3B-CAB-CBB
24	A	823	CLA	C2B-C3B-CAB-CBB
24	B	824	CLA	C2B-C3B-CAB-CBB
24	B	833	CLA	C2B-C3B-CAB-CBB
24	G	103	CLA	C2B-C3B-CAB-CBB
24	O	204	CLA	C2B-C3B-CAB-CBB
25	1	314	8CT	C02-C03-C10-C11
25	2	314	8CT	C02-C03-C10-C11
25	3	316	8CT	C04-C03-C10-C11
25	3	323	8CT	C02-C03-C10-C11
25	6	324	8CT	C04-C03-C10-C11
25	7	318	8CT	C04-C03-C10-C11
25	A	849	8CT	C02-C03-C10-C11
25	B	845	8CT	C02-C03-C10-C11
25	B	847	8CT	C02-C03-C10-C11
25	B	847	8CT	C04-C03-C10-C11
25	I	101	8CT	C02-C03-C10-C11
25	J	101	8CT	C04-C03-C10-C11
25	L	205	8CT	C02-C03-C10-C11
25	L	205	8CT	C04-C03-C10-C11
25	L	207	8CT	C04-C03-C10-C11
25	K	105	8CT	C04-C03-C10-C11
25	O	202	8CT	C04-C03-C10-C11
27	1	318	LHG	C28-C29-C30-C31
27	B	852	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	6	303	CLA	CBD-CGD-O2D-CED
24	5	311	CLA	CBA-CGA-O2A-C1
27	3	320	LHG	C5-C4-O6-P
24	B	819	CLA	C3-C5-C6-C7
23	2	306	CHL	C2A-CAA-CBA-CGA
23	8	306	CHL	C2A-CAA-CBA-CGA
24	H	201	CLA	C2A-CAA-CBA-CGA
27	3	320	LHG	C13-C14-C15-C16
27	3	324	LHG	C31-C32-C33-C34
29	9	317	LMG	C12-C13-C14-C15
29	M	101	LMG	C14-C15-C16-C17
24	7	311	CLA	O1A-CGA-O2A-C1
27	2	317	LHG	O10-C23-O8-C6
34	B	849	DGD	O1A-C1A-O1G-C1G
23	4	313	CHL	CBD-CGD-O2D-CED
27	8	320	LHG	C12-C13-C14-C15
29	J	105	LMG	C30-C31-C32-C33
23	5	301	CHL	C8-C10-C11-C12
24	9	302	CLA	C13-C15-C16-C17
24	A	829	CLA	C2-C3-C5-C6
24	B	817	CLA	C2-C3-C5-C6
27	5	316	LHG	C26-C27-C28-C29
27	A	842	LHG	C9-C10-C11-C12
23	2	301	CHL	CBA-CGA-O2A-C1
23	6	302	CHL	CBA-CGA-O2A-C1
23	4	302	CHL	CBA-CGA-O2A-C1
24	6	310	CLA	CBA-CGA-O2A-C1
24	A	839	CLA	CBA-CGA-O2A-C1
26	2	316	0UR	O57-C45-C46-C47
27	0	317	LHG	C24-C23-O8-C6
24	B	825	CLA	CBD-CGD-O2D-CED
24	7	317	CLA	C6-C7-C8-C9
24	A	827	CLA	C6-C7-C8-C9
24	A	839	CLA	C11-C10-C8-C9
27	3	324	LHG	C15-C16-C17-C18
28	0	318	SQD	C11-C10-C9-C8
24	B	820	CLA	C5-C6-C7-C8
29	A	854	LMG	C13-C14-C15-C16
27	3	320	LHG	C14-C15-C16-C17
24	3	313	CLA	O1D-CGD-O2D-CED
27	1	317	LHG	C14-C15-C16-C17
24	K	104	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	844	8CT	C18-C19-C20-C21
25	L	204	8CT	C16-C17-C18-C19
25	K	105	8CT	C16-C17-C18-C19
25	O	202	8CT	C18-C19-C20-C21
29	A	851	LMG	O6-C5-C6-O5
27	3	324	LHG	C8-C7-O7-C5
29	O	203	LMG	C11-C10-O7-C8
27	3	320	LHG	C15-C16-C17-C18
27	3	324	LHG	C14-C15-C16-C17
27	L	208	LHG	C26-C27-C28-C29
27	B	852	LHG	O9-C7-O7-C5
27	I	102	LHG	C25-C26-C27-C28
24	K	102	CLA	C2C-C3C-CAC-CBC
24	1	303	CLA	O1A-CGA-O2A-C1
24	A	827	CLA	C5-C6-C7-C8
24	B	837	CLA	C5-C6-C7-C8
25	F	304	8CT	C10-C11-C12-C40
25	J	104	8CT	C14-C15-C16-C39
25	L	204	8CT	C10-C11-C12-C40
27	1	317	LHG	C10-C11-C12-C13
23	4	301	CHL	C3-C5-C6-C7
25	J	104	8CT	C14-C15-C16-C17
25	L	204	8CT	C10-C11-C12-C13
29	3	321	LMG	C8-C7-O1-C1
24	3	304	CLA	C15-C16-C17-C18
23	7	305	CHL	C2A-CAA-CBA-CGA
23	8	303	CHL	C2A-CAA-CBA-CGA
23	8	307	CHL	C2A-CAA-CBA-CGA
23	3	302	CHL	C14-C13-C15-C16
23	8	314	CHL	C6-C7-C8-C9
24	0	308	CLA	C11-C12-C13-C15
24	A	827	CLA	C16-C17-C18-C19
24	B	827	CLA	C16-C17-C18-C19
24	A	816	CLA	CBD-CGD-O2D-CED
29	9	317	LMG	C13-C14-C15-C16
26	4	318	0UR	O44-C45-C46-C47
27	7	324	LHG	C12-C13-C14-C15
23	3	307	CHL	O1A-CGA-O2A-C1
24	4	311	CLA	O1A-CGA-O2A-C1
24	A	834	CLA	C3-C5-C6-C7
24	A	853	CLA	C10-C11-C12-C13
26	3	318	0UR	O57-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
27	5	316	LHG	C23-C24-C25-C26
27	B	852	LHG	C23-C24-C25-C26
29	J	105	LMG	C34-C35-C36-C37
23	0	302	CHL	C13-C15-C16-C17
23	7	302	CHL	C8-C10-C11-C12
23	7	306	CHL	C8-C10-C11-C12
24	B	817	CLA	C11-C12-C13-C14
29	M	101	LMG	C31-C32-C33-C34
24	B	817	CLA	O1D-CGD-O2D-CED
24	3	310	CLA	C3-C5-C6-C7
24	A	822	CLA	CBD-CGD-O2D-CED
27	7	322	LHG	O7-C5-C6-O8
27	1	317	LHG	C26-C27-C28-C29
27	2	319	LHG	C9-C10-C11-C12
23	1	301	CHL	CBA-CGA-O2A-C1
24	B	818	CLA	CBA-CGA-O2A-C1
24	1	311	CLA	C8-C10-C11-C12
24	9	308	CLA	C5-C6-C7-C8
24	B	811	CLA	C8-C10-C11-C12
29	M	101	LMG	C10-C11-C12-C13
24	B	823	CLA	CBD-CGD-O2D-CED
23	4	308	CHL	CBA-CGA-O2A-C1
27	9	316	LHG	C11-C10-C9-C8
24	H	201	CLA	O1A-CGA-O2A-C1
25	A	849	8CT	C18-C19-C20-C21
24	K	101	CLA	C11-C12-C13-C14
27	7	324	LHG	C5-C4-O6-P
29	9	317	LMG	C38-C39-C40-C41
27	A	842	LHG	C25-C26-C27-C28
23	7	306	CHL	C4-C3-C5-C6
23	3	305	CHL	C2A-CAA-CBA-CGA
23	5	301	CHL	C2A-CAA-CBA-CGA
23	5	304	CHL	C2A-CAA-CBA-CGA
23	4	302	CHL	C2A-CAA-CBA-CGA
24	0	307	CLA	C2A-CAA-CBA-CGA
24	7	308	CLA	C2A-CAA-CBA-CGA
24	A	819	CLA	C2A-CAA-CBA-CGA
24	A	840	CLA	C2A-CAA-CBA-CGA
24	B	831	CLA	C2A-CAA-CBA-CGA
24	K	103	CLA	C2A-CAA-CBA-CGA
23	8	306	CHL	CBD-CGD-O2D-CED
24	B	814	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	7	306	CHL	O1D-CGD-O2D-CED
24	0	310	CLA	CBA-CGA-O2A-C1
24	A	813	CLA	CBA-CGA-O2A-C1
26	4	318	0UR	O57-C45-C46-C47
27	7	324	LHG	C28-C29-C30-C31
23	5	304	CHL	O1D-CGD-O2D-CED
24	L	203	CLA	O1D-CGD-O2D-CED
23	1	306	CHL	C13-C15-C16-C17
23	7	301	CHL	C10-C11-C12-C13
24	3	309	CLA	C5-C6-C7-C8
27	2	319	LHG	C23-C24-C25-C26
24	3	310	CLA	O1D-CGD-O2D-CED
29	9	317	LMG	C17-C18-C19-C20
24	B	810	CLA	C2C-C3C-CAC-CBC
23	0	302	CHL	O1D-CGD-O2D-CED
23	6	315	CHL	O1D-CGD-O2D-CED
23	4	302	CHL	O1A-CGA-O2A-C1
24	5	311	CLA	O1A-CGA-O2A-C1
27	0	317	LHG	O10-C23-O8-C6
24	A	816	CLA	C3-C5-C6-C7
24	4	310	CLA	C3-C5-C6-C7
29	J	105	LMG	C14-C15-C16-C17
24	0	303	CLA	C1A-C2A-CAA-CBA
24	0	310	CLA	C1A-C2A-CAA-CBA
24	0	312	CLA	C1A-C2A-CAA-CBA
24	1	308	CLA	C1A-C2A-CAA-CBA
24	5	308	CLA	C1A-C2A-CAA-CBA
24	7	316	CLA	C1A-C2A-CAA-CBA
24	7	317	CLA	C1A-C2A-CAA-CBA
24	8	315	CLA	C1A-C2A-CAA-CBA
24	9	307	CLA	C1A-C2A-CAA-CBA
24	9	310	CLA	C1A-C2A-CAA-CBA
24	A	802	CLA	C1A-C2A-CAA-CBA
24	A	805	CLA	C1A-C2A-CAA-CBA
24	A	807	CLA	C1A-C2A-CAA-CBA
24	A	817	CLA	C1A-C2A-CAA-CBA
24	A	831	CLA	C1A-C2A-CAA-CBA
24	A	835	CLA	C1A-C2A-CAA-CBA
24	B	828	CLA	C1A-C2A-CAA-CBA
24	K	101	CLA	C1A-C2A-CAA-CBA
24	O	201	CLA	C1A-C2A-CAA-CBA
24	H	203	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	5	314	0UR	O57-C45-C46-C47
24	7	309	CLA	C5-C6-C7-C8
24	B	840	CLA	C15-C16-C17-C18
29	O	210	LMG	C33-C34-C35-C36
23	2	301	CHL	O1A-CGA-O2A-C1
23	6	302	CHL	O1A-CGA-O2A-C1
24	6	310	CLA	O1A-CGA-O2A-C1
24	A	839	CLA	O1A-CGA-O2A-C1
27	3	324	LHG	C27-C28-C29-C30
23	1	312	CHL	C10-C11-C12-C13
31	B	842	PQN	C20-C21-C22-C23
27	B	851	LHG	O6-C4-C5-C6
23	6	301	CHL	C3-C5-C6-C7
23	1	306	CHL	C6-C7-C8-C10
23	2	301	CHL	C6-C7-C8-C10
23	3	301	CHL	C6-C7-C8-C10
23	3	307	CHL	C6-C7-C8-C10
23	3	307	CHL	C12-C13-C15-C16
23	5	301	CHL	C11-C10-C8-C7
23	5	301	CHL	C11-C12-C13-C15
23	5	301	CHL	C12-C13-C15-C16
23	7	301	CHL	C12-C13-C15-C16
24	1	311	CLA	C6-C7-C8-C10
24	2	303	CLA	C11-C10-C8-C7
24	3	309	CLA	C11-C12-C13-C15
24	3	310	CLA	C6-C7-C8-C10
24	6	316	CLA	C11-C10-C8-C7
24	8	305	CLA	C11-C10-C8-C7
24	9	308	CLA	C11-C10-C8-C7
24	A	802	CLA	C12-C13-C15-C16
24	A	807	CLA	C11-C10-C8-C7
24	A	812	CLA	C6-C7-C8-C10
24	A	816	CLA	C11-C10-C8-C7
24	A	818	CLA	C6-C7-C8-C10
24	A	818	CLA	C11-C10-C8-C7
24	A	818	CLA	C11-C12-C13-C15
24	A	818	CLA	C12-C13-C15-C16
24	A	824	CLA	C11-C10-C8-C7
24	A	827	CLA	C11-C12-C13-C15
24	A	838	CLA	C11-C12-C13-C15
24	A	853	CLA	C11-C10-C8-C7
24	B	801	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	817	CLA	C11-C10-C8-C7
24	B	834	CLA	C6-C7-C8-C10
24	B	834	CLA	C11-C10-C8-C7
28	0	318	SQD	C9-C10-C11-C12
24	B	816	CLA	C10-C11-C12-C13
24	1	309	CLA	C10-C11-C12-C13
24	B	837	CLA	C15-C16-C17-C18
23	7	306	CHL	C2-C3-C5-C6
24	K	104	CLA	O1A-CGA-O2A-C1
23	3	302	CHL	C2A-CAA-CBA-CGA
23	6	302	CHL	C2A-CAA-CBA-CGA
24	1	303	CLA	C2A-CAA-CBA-CGA
24	1	311	CLA	C2A-CAA-CBA-CGA
24	7	316	CLA	C2A-CAA-CBA-CGA
23	1	306	CHL	C6-C7-C8-C9
23	1	306	CHL	C11-C12-C13-C14
23	1	312	CHL	C11-C10-C8-C9
23	3	301	CHL	C6-C7-C8-C9
23	3	307	CHL	C6-C7-C8-C9
23	3	307	CHL	C14-C13-C15-C16
24	3	308	CLA	C6-C7-C8-C9
24	3	309	CLA	C11-C12-C13-C14
24	3	310	CLA	C11-C12-C13-C14
24	8	305	CLA	C11-C10-C8-C9
24	9	308	CLA	C11-C10-C8-C9
24	A	807	CLA	C11-C10-C8-C9
24	A	818	CLA	C6-C7-C8-C9
24	A	818	CLA	C11-C10-C8-C9
24	A	818	CLA	C14-C13-C15-C16
24	A	827	CLA	C11-C12-C13-C14
24	A	828	CLA	C11-C12-C13-C14
24	A	831	CLA	C6-C7-C8-C9
24	A	832	CLA	C6-C7-C8-C9
24	B	801	CLA	C6-C7-C8-C9
24	B	809	CLA	C11-C12-C13-C14
24	B	817	CLA	C11-C10-C8-C9
24	B	819	CLA	C11-C10-C8-C9
24	B	839	CLA	C11-C12-C13-C14
24	B	839	CLA	C14-C13-C15-C16
24	4	310	CLA	C11-C10-C8-C9
34	B	849	DGD	CBB-CCB-CDB-CEB
24	3	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	A	814	CLA	CBA-CGA-O2A-C1
24	O	201	CLA	CBA-CGA-O2A-C1
27	1	318	LHG	C27-C28-C29-C30
27	7	323	LHG	C10-C11-C12-C13
27	1	317	LHG	C4-C5-C6-O8
27	2	317	LHG	C4-C5-C6-O8
27	7	324	LHG	C4-C5-C6-O8
27	B	852	LHG	C4-C5-C6-O8
28	0	318	SQD	O6-C44-C45-C46
28	0	318	SQD	C44-C45-C46-O48
29	A	851	LMG	C7-C8-C9-O8
23	8	301	CHL	O1D-CGD-O2D-CED
27	9	316	LHG	C31-C32-C33-C34
24	B	830	CLA	CBA-CGA-O2A-C1
23	1	306	CHL	C16-C17-C18-C19
24	A	829	CLA	C16-C17-C18-C19
24	A	829	CLA	C16-C17-C18-C20
24	K	101	CLA	C11-C12-C13-C15
27	L	208	LHG	C25-C26-C27-C28
29	A	851	LMG	C30-C31-C32-C33
29	M	101	LMG	C15-C16-C17-C18
29	M	101	LMG	C17-C18-C19-C20
23	0	306	CHL	CHA-CBD-CGD-O1D
23	0	306	CHL	CHA-CBD-CGD-O2D
23	1	301	CHL	CHA-CBD-CGD-O1D
23	1	301	CHL	CHA-CBD-CGD-O2D
23	1	305	CHL	CHA-CBD-CGD-O1D
23	1	305	CHL	CHA-CBD-CGD-O2D
23	1	312	CHL	CHA-CBD-CGD-O1D
23	1	312	CHL	CHA-CBD-CGD-O2D
23	2	301	CHL	CHA-CBD-CGD-O1D
23	2	301	CHL	CHA-CBD-CGD-O2D
23	3	302	CHL	CHA-CBD-CGD-O1D
23	3	302	CHL	CHA-CBD-CGD-O2D
23	3	307	CHL	CHA-CBD-CGD-O1D
23	3	307	CHL	CHA-CBD-CGD-O2D
23	5	304	CHL	CHA-CBD-CGD-O2D
23	5	305	CHL	CHA-CBD-CGD-O1D
23	5	305	CHL	CHA-CBD-CGD-O2D
23	6	306	CHL	CHA-CBD-CGD-O1D
23	6	306	CHL	CHA-CBD-CGD-O2D
23	6	315	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	6	315	CHL	CHA-CBD-CGD-O2D
23	7	302	CHL	CHA-CBD-CGD-O1D
23	7	302	CHL	CHA-CBD-CGD-O2D
23	8	303	CHL	CHA-CBD-CGD-O1D
23	8	303	CHL	CHA-CBD-CGD-O2D
23	8	316	CHL	CHA-CBD-CGD-O1D
23	8	316	CHL	CHA-CBD-CGD-O2D
23	9	301	CHL	CHA-CBD-CGD-O1D
23	9	301	CHL	CHA-CBD-CGD-O2D
23	9	306	CHL	CHA-CBD-CGD-O1D
23	4	307	CHL	CHA-CBD-CGD-O2D
29	A	854	LMG	O6-C5-C6-O5
23	1	301	CHL	O1A-CGA-O2A-C1
23	2	301	CHL	CBD-CGD-O2D-CED
23	3	307	CHL	C2-C3-C5-C6
24	B	801	CLA	C2-C3-C5-C6
24	2	302	CLA	CBA-CGA-O2A-C1
25	A	849	8CT	C10-C11-C12-C40
26	4	318	0UR	C22-C16-C17-C18
27	L	208	LHG	C2-C3-O3-P
27	7	324	LHG	C26-C27-C28-C29
25	0	314	8CT	C25-C26-C28-C29
25	6	324	8CT	C25-C26-C28-C29
25	7	319	8CT	C14-C15-C16-C17
25	B	848	8CT	C10-C11-C12-C13
26	4	318	0UR	C15-C16-C17-C18
24	3	304	CLA	C13-C15-C16-C17
24	7	308	CLA	C8-C10-C11-C12
24	A	803	CLA	C5-C6-C7-C8
24	A	853	CLA	C15-C16-C17-C18
24	4	304	CLA	C8-C10-C11-C12
29	J	105	LMG	C4-C5-C6-O5
24	A	808	CLA	C2A-CAA-CBA-CGA
23	5	312	CHL	CBA-CGA-O2A-C1
24	B	818	CLA	O1A-CGA-O2A-C1
27	I	102	LHG	C26-C27-C28-C29
29	2	318	LMG	C30-C31-C32-C33
23	8	316	CHL	O1D-CGD-O2D-CED
24	2	310	CLA	O2A-C1-C2-C3
24	A	804	CLA	O2A-C1-C2-C3
27	B	851	LHG	C6-C5-O7-C7
29	3	321	LMG	C7-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
27	8	320	LHG	C10-C11-C12-C13
27	B	852	LHG	C25-C26-C27-C28
29	2	318	LMG	C32-C33-C34-C35
27	I	102	LHG	C30-C31-C32-C33
23	1	305	CHL	C3C-C2C-CMC-OMC
23	2	312	CHL	C3C-C2C-CMC-OMC
23	7	305	CHL	C3C-C2C-CMC-OMC
23	7	306	CHL	C3C-C2C-CMC-OMC
23	7	313	CHL	C3C-C2C-CMC-OMC
23	8	308	CHL	C3C-C2C-CMC-OMC
23	8	309	CHL	C3C-C2C-CMC-OMC
23	9	306	CHL	C3C-C2C-CMC-OMC
23	9	312	CHL	C3C-C2C-CMC-OMC
25	8	317	8CT	C16-C17-C18-C19
29	A	851	LMG	C29-C30-C31-C32
27	A	850	LHG	C23-C24-C25-C26
24	5	307	CLA	CBA-CGA-O2A-C1
24	B	833	CLA	C3-C5-C6-C7
24	B	802	CLA	CBD-CGD-O2D-CED
24	B	819	CLA	C10-C11-C12-C13
27	I	102	LHG	C9-C10-C11-C12
23	3	302	CHL	CBA-CGA-O2A-C1
24	6	318	CLA	CBA-CGA-O2A-C1
24	K	101	CLA	CBA-CGA-O2A-C1
29	A	851	LMG	C29-C28-O8-C9
24	8	310	CLA	CBD-CGD-O2D-CED
24	3	308	CLA	O1A-CGA-O2A-C1
29	3	321	LMG	C32-C33-C34-C35
24	B	839	CLA	C5-C6-C7-C8
24	L	201	CLA	C4-C3-C5-C6
23	1	306	CHL	C2-C3-C5-C6
29	M	101	LMG	C18-C19-C20-C21
27	0	317	LHG	C14-C15-C16-C17
27	3	324	LHG	C32-C33-C34-C35
27	B	852	LHG	C9-C10-C11-C12
29	2	318	LMG	C12-C13-C14-C15
27	A	850	LHG	O7-C5-C6-O8
29	A	851	LMG	O1-C7-C8-O7
29	M	101	LMG	C32-C33-C34-C35
23	2	307	CHL	O1A-CGA-O2A-C1
23	5	301	CHL	C15-C16-C17-C18
27	L	208	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	O	201	CLA	O1A-CGA-O2A-C1
24	A	813	CLA	O1D-CGD-O2D-CED
23	4	301	CHL	CAA-CBA-CGA-O2A
24	6	317	CLA	CAA-CBA-CGA-O2A
23	4	307	CHL	C2A-CAA-CBA-CGA
24	7	303	CLA	C2A-CAA-CBA-CGA
23	8	314	CHL	C3-C5-C6-C7
23	8	314	CHL	C5-C6-C7-C8
24	2	309	CLA	C8-C10-C11-C12
24	9	302	CLA	C8-C10-C11-C12
24	9	302	CLA	C10-C11-C12-C13
24	B	805	CLA	C15-C16-C17-C18
27	3	324	LHG	O9-C7-O7-C5
24	A	838	CLA	C13-C15-C16-C17
24	K	101	CLA	C10-C11-C12-C13
23	7	313	CHL	O1D-CGD-O2D-CED
27	7	324	LHG	C10-C11-C12-C13
23	1	305	CHL	C1C-C2C-CMC-OMC
23	7	313	CHL	C1C-C2C-CMC-OMC
23	8	308	CHL	C1C-C2C-CMC-OMC
23	8	309	CHL	C1C-C2C-CMC-OMC
23	9	312	CHL	C1C-C2C-CMC-OMC
24	A	834	CLA	CBD-CGD-O2D-CED
24	J	103	CLA	CBD-CGD-O2D-CED
34	B	849	DGD	CAB-CBB-CCB-CDB
23	3	307	CHL	C15-C16-C17-C18
24	A	813	CLA	O1A-CGA-O2A-C1
24	A	814	CLA	O1A-CGA-O2A-C1
23	0	302	CHL	C15-C16-C17-C18
23	6	308	CHL	C8-C10-C11-C12
23	4	301	CHL	C11-C12-C13-C14
23	3	307	CHL	C4-C3-C5-C6
24	A	838	CLA	C4-C3-C5-C6
24	5	302	CLA	C10-C11-C12-C13
27	7	323	LHG	C11-C10-C9-C8
24	A	823	CLA	CBA-CGA-O2A-C1
24	A	829	CLA	CBA-CGA-O2A-C1
24	B	829	CLA	CBA-CGA-O2A-C1
24	B	836	CLA	CBA-CGA-O2A-C1
27	3	324	LHG	C30-C31-C32-C33
28	0	318	SQD	C10-C11-C12-C13
29	9	317	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	9	316	LHG	C27-C28-C29-C30
29	A	854	LMG	C17-C18-C19-C20
27	0	317	LHG	O1-C1-C2-O2
24	B	832	CLA	C3-C5-C6-C7
23	5	301	CHL	C6-C7-C8-C9
23	5	301	CHL	C11-C10-C8-C9
23	5	301	CHL	C11-C12-C13-C14
24	0	311	CLA	C14-C13-C15-C16
24	1	311	CLA	C6-C7-C8-C9
24	2	303	CLA	C11-C10-C8-C9
24	2	309	CLA	C6-C7-C8-C9
24	9	302	CLA	C14-C13-C15-C16
24	A	802	CLA	C14-C13-C15-C16
24	A	804	CLA	C6-C7-C8-C9
24	A	812	CLA	C6-C7-C8-C9
24	A	814	CLA	C14-C13-C15-C16
24	A	816	CLA	C11-C10-C8-C9
24	A	817	CLA	C11-C12-C13-C14
24	A	818	CLA	C11-C12-C13-C14
24	A	824	CLA	C11-C10-C8-C9
24	A	829	CLA	C14-C13-C15-C16
24	A	853	CLA	C11-C10-C8-C9
24	B	804	CLA	C14-C13-C15-C16
24	B	809	CLA	C14-C13-C15-C16
24	B	832	CLA	C14-C13-C15-C16
24	B	834	CLA	C11-C10-C8-C9
24	4	304	CLA	C11-C10-C8-C9
24	8	315	CLA	O1D-CGD-O2D-CED
24	3	308	CLA	C13-C15-C16-C17
24	6	309	CLA	C5-C6-C7-C8
24	A	828	CLA	C10-C11-C12-C13
27	B	852	LHG	C2-C3-O3-P
24	0	310	CLA	O1A-CGA-O2A-C1
24	0	313	CLA	C4B-C3B-CAB-CBB
24	2	313	CLA	C4B-C3B-CAB-CBB
24	3	306	CLA	C4B-C3B-CAB-CBB
24	3	313	CLA	C4B-C3B-CAB-CBB
24	5	309	CLA	C4B-C3B-CAB-CBB
24	5	310	CLA	C4B-C3B-CAB-CBB
24	6	304	CLA	C4B-C3B-CAB-CBB
24	6	318	CLA	C4B-C3B-CAB-CBB
24	7	316	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	8	313	CLA	C4B-C3B-CAB-CBB
24	A	808	CLA	C4B-C3B-CAB-CBB
24	A	831	CLA	C4B-C3B-CAB-CBB
24	A	834	CLA	C4B-C3B-CAB-CBB
24	B	805	CLA	C4B-C3B-CAB-CBB
24	K	104	CLA	C4B-C3B-CAB-CBB
24	H	203	CLA	C4B-C3B-CAB-CBB
24	H	205	CLA	C4B-C3B-CAB-CBB
27	0	317	LHG	C33-C34-C35-C36
23	9	312	CHL	O1D-CGD-O2D-CED
23	3	307	CHL	C5-C6-C7-C8
24	A	825	CLA	C13-C15-C16-C17
24	B	841	CLA	C13-C15-C16-C17
23	1	301	CHL	C15-C16-C17-C18
24	0	313	CLA	C2A-CAA-CBA-CGA
24	5	303	CLA	C3-C5-C6-C7
27	7	322	LHG	C25-C26-C27-C28
27	8	320	LHG	C28-C29-C30-C31
28	0	318	SQD	C2-C1-O6-C44
24	6	310	CLA	C5-C6-C7-C8
27	1	317	LHG	C27-C28-C29-C30
29	9	317	LMG	C37-C38-C39-C40
23	6	302	CHL	C3-C5-C6-C7
23	6	323	CHL	C3-C5-C6-C7
29	J	105	LMG	C42-C43-C44-C45
24	A	840	CLA	CBD-CGD-O2D-CED
29	A	851	LMG	C32-C33-C34-C35
23	5	305	CHL	CAA-CBA-CGA-O2A
23	1	306	CHL	C11-C10-C8-C7
23	1	306	CHL	C11-C12-C13-C15
23	1	312	CHL	C11-C10-C8-C7
23	6	302	CHL	C6-C7-C8-C10
23	6	302	CHL	C11-C10-C8-C7
23	7	301	CHL	C11-C12-C13-C15
23	7	302	CHL	C12-C13-C15-C16
23	8	303	CHL	C12-C13-C15-C16
24	0	307	CLA	C11-C10-C8-C7
24	0	311	CLA	C6-C7-C8-C10
24	3	310	CLA	C11-C12-C13-C15
24	6	310	CLA	C6-C7-C8-C10
24	7	308	CLA	C11-C12-C13-C15
24	8	310	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	9	302	CLA	C12-C13-C15-C16
24	A	804	CLA	C6-C7-C8-C10
24	A	810	CLA	C11-C10-C8-C7
24	A	810	CLA	C11-C12-C13-C15
24	A	814	CLA	C6-C7-C8-C10
24	A	817	CLA	C11-C12-C13-C15
24	A	828	CLA	C11-C12-C13-C15
24	A	832	CLA	C6-C7-C8-C10
24	A	839	CLA	C6-C7-C8-C10
24	B	804	CLA	C12-C13-C15-C16
24	B	809	CLA	C11-C12-C13-C15
24	B	809	CLA	C12-C13-C15-C16
24	B	819	CLA	C11-C10-C8-C7
24	B	820	CLA	C6-C7-C8-C10
24	B	832	CLA	C12-C13-C15-C16
24	B	839	CLA	C12-C13-C15-C16
24	4	304	CLA	C11-C10-C8-C7
24	A	827	CLA	C15-C16-C17-C18
24	B	830	CLA	O1A-CGA-O2A-C1
23	8	303	CHL	C15-C16-C17-C18
24	L	202	CLA	C15-C16-C17-C18
27	2	319	LHG	C12-C13-C14-C15
23	8	306	CHL	CBA-CGA-O2A-C1
23	6	302	CHL	C15-C16-C17-C18
29	9	317	LMG	C36-C37-C38-C39
26	4	317	0UR	O44-C45-C46-C47
24	B	819	CLA	C8-C10-C11-C12
23	9	301	CHL	O1D-CGD-O2D-CED
23	6	308	CHL	C11-C12-C13-C14
23	1	306	CHL	C4-C3-C5-C6
23	6	306	CHL	C3A-C2A-CAA-CBA
23	6	307	CHL	C3A-C2A-CAA-CBA
23	4	308	CHL	C3A-C2A-CAA-CBA
24	5	313	CLA	C3A-C2A-CAA-CBA
24	6	316	CLA	C3A-C2A-CAA-CBA
24	9	307	CLA	C3A-C2A-CAA-CBA
24	A	848	CLA	C4-C3-C5-C6
24	B	820	CLA	C3A-C2A-CAA-CBA
24	L	202	CLA	C3A-C2A-CAA-CBA
24	A	838	CLA	C2-C3-C5-C6
23	1	306	CHL	C5-C6-C7-C8
23	8	301	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	0	311	CLA	CBA-CGA-O2A-C1
24	7	304	CLA	CBA-CGA-O2A-C1
24	7	312	CLA	CBA-CGA-O2A-C1
25	3	317	8CT	C16-C17-C18-C19
25	7	318	8CT	C23-C24-C25-C26
25	7	319	8CT	C12-C13-C14-C15
25	A	844	8CT	C16-C17-C18-C19
25	A	846	8CT	C18-C19-C20-C21
25	B	848	8CT	C18-C19-C20-C21
25	L	205	8CT	C16-C17-C18-C19
25	K	105	8CT	C18-C19-C20-C21
25	O	208	8CT	C16-C17-C18-C19
26	5	315	0UR	C3-C4-C5-C6
24	A	839	CLA	C3-C5-C6-C7
25	0	314	8CT	C27-C26-C28-C29
25	2	314	8CT	C14-C15-C16-C39
25	6	324	8CT	C27-C26-C28-C29
25	B	848	8CT	C10-C11-C12-C40
23	3	302	CHL	O1A-CGA-O2A-C1
24	2	302	CLA	O1A-CGA-O2A-C1
24	B	802	CLA	C2A-CAA-CBA-CGA
29	O	203	LMG	C30-C31-C32-C33
23	6	323	CHL	C10-C11-C12-C13
24	9	307	CLA	C13-C15-C16-C17
27	2	319	LHG	C4-C5-C6-O8
27	8	320	LHG	C4-C5-C6-O8
29	2	318	LMG	C7-C8-C9-O8
29	A	854	LMG	O1-C7-C8-C9
24	9	309	CLA	CBD-CGD-O2D-CED
29	J	105	LMG	C13-C14-C15-C16
29	O	210	LMG	C32-C33-C34-C35
23	1	312	CHL	C4-C3-C5-C6
24	3	310	CLA	C4-C3-C5-C6
24	A	834	CLA	C4-C3-C5-C6
24	A	848	CLA	C2-C3-C5-C6
24	5	302	CLA	C11-C12-C13-C15
29	3	321	LMG	C30-C31-C32-C33
29	M	101	LMG	C11-C12-C13-C14
23	4	301	CHL	C11-C12-C13-C15
24	2	313	CLA	C2B-C3B-CAB-CBB
24	3	306	CLA	C2B-C3B-CAB-CBB
24	A	831	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	K	104	CLA	C2B-C3B-CAB-CBB
24	H	205	CLA	C2B-C3B-CAB-CBB
25	3	317	8CT	C04-C03-C10-C11
25	7	319	8CT	C04-C03-C10-C11
25	9	313	8CT	C02-C03-C10-C11
24	1	311	CLA	C3-C5-C6-C7
27	8	320	LHG	C26-C27-C28-C29
24	2	308	CLA	C10-C11-C12-C13
24	A	806	CLA	O1D-CGD-O2D-CED
27	L	208	LHG	O8-C23-C24-C25
24	0	308	CLA	C5-C6-C7-C8
27	0	317	LHG	O7-C5-C6-O8
27	1	318	LHG	O7-C5-C6-O8
27	2	317	LHG	O7-C5-C6-O8
27	2	319	LHG	O7-C5-C6-O8
27	5	316	LHG	O7-C5-C6-O8
27	B	852	LHG	O7-C5-C6-O8
28	0	318	SQD	O6-C44-C45-O47
29	A	854	LMG	O1-C7-C8-O7
34	B	849	DGD	O2G-C2G-C3G-O3G
29	J	105	LMG	C37-C38-C39-C40
23	7	301	CHL	O1D-CGD-O2D-CED
24	2	303	CLA	O1D-CGD-O2D-CED
24	A	837	CLA	C11-C10-C8-C7
24	4	310	CLA	C8-C10-C11-C12
23	1	312	CHL	C2-C3-C5-C6
24	A	834	CLA	C2-C3-C5-C6
29	A	854	LMG	C18-C19-C20-C21
27	1	318	LHG	C26-C27-C28-C29
24	6	318	CLA	O1A-CGA-O2A-C1
23	3	302	CHL	C11-C12-C13-C14
23	6	301	CHL	C6-C7-C8-C9
23	7	301	CHL	C11-C12-C13-C14
24	2	311	CLA	C11-C10-C8-C9
24	A	836	CLA	C6-C7-C8-C9
27	1	318	LHG	C31-C32-C33-C34
24	A	808	CLA	C5-C6-C7-C8
29	9	317	LMG	O6-C1-O1-C7
24	K	101	CLA	O1A-CGA-O2A-C1
27	2	319	LHG	C11-C12-C13-C14
24	7	309	CLA	C11-C12-C13-C14
23	3	307	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	8	314	CHL	C6-C7-C8-C10
24	B	817	CLA	C11-C12-C13-C15
24	B	827	CLA	C16-C17-C18-C20
24	A	825	CLA	O1D-CGD-O2D-CED
24	A	813	CLA	C3-C5-C6-C7
27	3	324	LHG	C10-C11-C12-C13
27	0	317	LHG	C18-C19-C20-C21
23	7	313	CHL	C2A-CAA-CBA-CGA
27	6	322	LHG	C11-C10-C9-C8
26	1	316	0UR	C46-C47-C48-C49
27	1	317	LHG	C23-C24-C25-C26
27	B	851	LHG	O1-C1-C2-O2
24	B	810	CLA	C3-C5-C6-C7
25	A	849	8CT	C16-C17-C18-C19
25	L	207	8CT	C16-C17-C18-C19
23	6	301	CHL	C11-C12-C13-C14
26	0	315	0UR	O42-C2-C3-C4
26	0	316	0UR	O42-C2-C3-C4
26	1	315	0UR	O42-C2-C3-C4
26	2	315	0UR	O42-C2-C3-C4
26	2	316	0UR	O42-C2-C3-C4
26	3	318	0UR	O42-C2-C3-C4
26	5	314	0UR	O42-C2-C3-C4
26	6	320	0UR	O42-C2-C3-C4
26	7	320	0UR	O42-C2-C3-C4
26	8	318	0UR	O42-C2-C3-C4
26	9	314	0UR	O42-C2-C3-C4
26	9	315	0UR	O42-C2-C3-C4
26	4	317	0UR	O42-C2-C3-C4
30	3	319	0IE	O1-C2-C3-C4
30	7	321	0IE	O1-C2-C3-C4
24	A	817	CLA	C15-C16-C17-C18
23	7	306	CHL	C12-C13-C15-C16
29	O	210	LMG	C31-C32-C33-C34
27	9	316	LHG	C10-C11-C12-C13
23	1	312	CHL	CBD-CGD-O2D-CED
24	4	312	CLA	C3-C5-C6-C7
23	1	304	CHL	CBA-CGA-O2A-C1
24	7	308	CLA	CBA-CGA-O2A-C1
23	3	301	CHL	C10-C11-C12-C13
27	0	317	LHG	O6-C4-C5-C6
27	6	322	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	8	302	LHG	O6-C4-C5-C6
27	L	208	LHG	O6-C4-C5-C6
24	A	827	CLA	C16-C17-C18-C20
24	7	304	CLA	O1A-CGA-O2A-C1
23	2	301	CHL	C13-C15-C16-C17
24	8	305	CLA	C13-C15-C16-C17
25	B	847	8CT	C27-C26-C28-C29
25	B	850	8CT	C27-C26-C28-C29
26	8	319	0UR	C22-C16-C17-C18
23	1	306	CHL	C12-C13-C15-C16
23	3	302	CHL	C11-C12-C13-C15
24	2	302	CLA	C6-C7-C8-C10
24	2	311	CLA	C11-C10-C8-C7
24	3	308	CLA	C11-C10-C8-C7
24	5	302	CLA	C6-C7-C8-C10
24	A	825	CLA	C6-C7-C8-C10
24	A	836	CLA	C6-C7-C8-C10
24	A	848	CLA	C12-C13-C15-C16
23	7	302	CHL	C15-C16-C17-C18
27	A	842	LHG	C27-C28-C29-C30
24	A	807	CLA	C8-C10-C11-C12
25	7	319	8CT	C25-C26-C28-C29
25	A	845	8CT	C25-C26-C28-C29
25	A	849	8CT	C10-C11-C12-C13
25	B	843	8CT	C14-C15-C16-C17
25	B	847	8CT	C25-C26-C28-C29
25	B	850	8CT	C10-C11-C12-C13
25	B	850	8CT	C25-C26-C28-C29
25	K	105	8CT	C20-C21-C23-C24
26	6	321	0UR	C15-C16-C17-C18
26	8	319	0UR	C15-C16-C17-C18
24	B	812	CLA	CBA-CGA-O2A-C1
24	B	817	CLA	CBA-CGA-O2A-C1
27	9	316	LHG	C34-C35-C36-C37
24	A	829	CLA	O1A-CGA-O2A-C1
24	B	836	CLA	O1A-CGA-O2A-C1
23	7	306	CHL	C11-C12-C13-C15
24	A	824	CLA	C15-C16-C17-C18
23	5	306	CHL	C2A-CAA-CBA-CGA
23	6	301	CHL	C2A-CAA-CBA-CGA
23	2	301	CHL	C15-C16-C17-C18
27	7	322	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	2	318	LMG	C11-C10-O7-C8
23	8	306	CHL	O1D-CGD-O2D-CED
24	A	816	CLA	O1D-CGD-O2D-CED
27	8	320	LHG	C13-C14-C15-C16
23	8	301	CHL	O1A-CGA-O2A-C1
24	B	829	CLA	O1A-CGA-O2A-C1
23	4	313	CHL	O1D-CGD-O2D-CED
34	B	849	DGD	C3G-C2G-O2G-C1B
24	7	312	CLA	O1A-CGA-O2A-C1
25	7	318	8CT	C12-C13-C14-C15
25	F	301	8CT	C16-C17-C18-C19
34	B	849	DGD	C5A-C6A-C7A-C8A
24	B	819	CLA	C11-C12-C13-C15
24	6	303	CLA	O1D-CGD-O2D-CED
24	0	311	CLA	O1A-CGA-O2A-C1
24	A	823	CLA	O1A-CGA-O2A-C1
23	3	307	CHL	C3-C5-C6-C7
27	9	316	LHG	C30-C31-C32-C33
29	2	318	LMG	C13-C14-C15-C16
24	3	304	CLA	C8-C10-C11-C12
24	A	818	CLA	C13-C15-C16-C17
27	0	317	LHG	O6-C4-C5-O7
27	6	322	LHG	O6-C4-C5-O7
27	7	324	LHG	O6-C4-C5-O7
27	8	302	LHG	O6-C4-C5-O7
27	8	320	LHG	O6-C4-C5-O7
27	B	851	LHG	O6-C4-C5-O7
27	B	852	LHG	O6-C4-C5-O7
27	L	208	LHG	O6-C4-C5-O7
24	A	822	CLA	O1D-CGD-O2D-CED
27	3	320	LHG	C4-C5-C6-O8
27	7	323	LHG	C4-C5-C6-O8
29	3	321	LMG	C7-C8-C9-O8
29	A	851	LMG	O1-C7-C8-C9
24	A	804	CLA	C4-C3-C5-C6
24	A	805	CLA	C4-C3-C5-C6
27	7	323	LHG	C14-C15-C16-C17
26	6	321	0UR	C2-C3-C43-O44
27	8	320	LHG	O7-C5-C6-O8
29	A	851	LMG	O7-C8-C9-O8
29	J	105	LMG	O7-C8-C9-O8
24	B	825	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	829	CLA	C8-C10-C11-C12
23	3	302	CHL	C6-C7-C8-C9
24	2	303	CLA	C6-C7-C8-C9
24	6	316	CLA	C11-C10-C8-C9
24	A	810	CLA	C11-C10-C8-C9
24	A	824	CLA	C11-C12-C13-C14
24	A	825	CLA	C14-C13-C15-C16
24	A	832	CLA	C11-C10-C8-C9
24	A	853	CLA	C11-C12-C13-C14
24	B	827	CLA	C11-C12-C13-C14
31	A	841	PQN	C24-C23-C25-C26
23	5	306	CHL	CBA-CGA-O2A-C1
29	9	317	LMG	C41-C42-C43-C44
23	1	304	CHL	O1A-CGA-O2A-C1
24	7	308	CLA	O1A-CGA-O2A-C1
24	A	816	CLA	C8-C10-C11-C12
24	A	848	CLA	C13-C15-C16-C17
24	B	817	CLA	C10-C11-C12-C13
25	2	314	8CT	C26-C28-C29-C30
25	4	316	8CT	C26-C28-C29-C30
24	B	825	CLA	O1D-CGD-O2D-CED
29	M	101	LMG	C34-C35-C36-C37
23	7	313	CHL	O1A-CGA-O2A-C1
24	A	805	CLA	C5-C6-C7-C8
27	A	850	LHG	C2-C3-O3-P
27	5	316	LHG	C12-C13-C14-C15
34	B	849	DGD	C2B-C3B-C4B-C5B
26	2	315	0UR	O42-C2-C3-C43
24	3	315	CLA	C4-C3-C5-C6
24	A	804	CLA	C2-C3-C5-C6
27	A	842	LHG	O2-C2-C3-O3
24	3	315	CLA	C2A-CAA-CBA-CGA
29	O	210	LMG	C4-C5-C6-O5
24	6	316	CLA	C16-C17-C18-C20
24	B	817	CLA	O1A-CGA-O2A-C1
24	A	840	CLA	C3-C5-C6-C7
24	B	813	CLA	C3-C5-C6-C7
23	2	307	CHL	C4C-C3C-CAC-CBC
23	8	303	CHL	C4C-C3C-CAC-CBC
23	4	302	CHL	C4C-C3C-CAC-CBC
24	8	313	CLA	C11-C10-C8-C9
24	9	302	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	B	837	CLA	C16-C17-C18-C19
27	B	852	LHG	C15-C16-C17-C18
26	0	316	0UR	C22-C16-C17-C18
24	0	308	CLA	C1A-C2A-CAA-CBA
24	2	302	CLA	C4B-C3B-CAB-CBB
24	2	309	CLA	C1A-C2A-CAA-CBA
24	2	309	CLA	C4B-C3B-CAB-CBB
24	3	312	CLA	C4B-C3B-CAB-CBB
24	5	313	CLA	C1A-C2A-CAA-CBA
24	5	313	CLA	C4B-C3B-CAB-CBB
24	6	309	CLA	C1A-C2A-CAA-CBA
24	6	310	CLA	C4B-C3B-CAB-CBB
24	6	316	CLA	C1A-C2A-CAA-CBA
24	6	317	CLA	C4B-C3B-CAB-CBB
24	7	310	CLA	C4B-C3B-CAB-CBB
24	7	311	CLA	C4B-C3B-CAB-CBB
24	7	312	CLA	C4B-C3B-CAB-CBB
24	7	314	CLA	C4B-C3B-CAB-CBB
24	8	310	CLA	C1A-C2A-CAA-CBA
24	8	311	CLA	C4B-C3B-CAB-CBB
24	8	312	CLA	C4B-C3B-CAB-CBB
24	9	309	CLA	C4B-C3B-CAB-CBB
24	A	822	CLA	C4B-C3B-CAB-CBB
24	A	823	CLA	C1A-C2A-CAA-CBA
24	A	839	CLA	C4B-C3B-CAB-CBB
24	B	809	CLA	C4B-C3B-CAB-CBB
24	B	811	CLA	C4B-C3B-CAB-CBB
24	B	822	CLA	C4B-C3B-CAB-CBB
24	B	834	CLA	C4B-C3B-CAB-CBB
24	F	302	CLA	C4B-C3B-CAB-CBB
24	F	303	CLA	C4B-C3B-CAB-CBB
24	L	206	CLA	C4B-C3B-CAB-CBB
24	K	101	CLA	C4B-C3B-CAB-CBB
24	O	209	CLA	C4B-C3B-CAB-CBB
24	4	303	CLA	C4B-C3B-CAB-CBB
24	4	309	CLA	C1A-C2A-CAA-CBA
24	4	310	CLA	C4B-C3B-CAB-CBB
24	B	823	CLA	O1D-CGD-O2D-CED
24	1	309	CLA	C4-C3-C5-C6
24	A	828	CLA	C4-C3-C5-C6
23	9	312	CHL	CAA-CBA-CGA-O2A
29	O	203	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	2	314	8CT	C14-C15-C16-C17
25	A	846	8CT	C14-C15-C16-C17
24	3	308	CLA	C16-C17-C18-C19
24	B	810	CLA	C5-C6-C7-C8
24	B	806	CLA	C4C-C3C-CAC-CBC
24	B	812	CLA	O1A-CGA-O2A-C1
24	B	810	CLA	C2A-CAA-CBA-CGA
27	9	316	LHG	C25-C26-C27-C28
24	A	810	CLA	C10-C11-C12-C13
24	B	824	CLA	C8-C10-C11-C12
27	7	324	LHG	O6-C4-C5-C6
27	8	320	LHG	O6-C4-C5-C6
27	A	843	LHG	O6-C4-C5-C6
27	B	852	LHG	O6-C4-C5-C6
29	2	318	LMG	C33-C34-C35-C36
24	0	303	CLA	CBD-CGD-O2D-CED
24	J	103	CLA	O1D-CGD-O2D-CED
24	6	318	CLA	C2-C3-C5-C6
24	A	835	CLA	C2-C3-C5-C6
24	B	826	CLA	C2-C3-C5-C6
24	B	811	CLA	C10-C11-C12-C13
27	9	316	LHG	C28-C29-C30-C31
24	L	202	CLA	C3-C5-C6-C7
23	1	301	CHL	C11-C12-C13-C15
23	3	307	CHL	C11-C12-C13-C15
24	1	302	CLA	C6-C7-C8-C10
24	5	308	CLA	C6-C7-C8-C10
24	9	307	CLA	C12-C13-C15-C16
24	9	308	CLA	C6-C7-C8-C10
24	B	808	CLA	C11-C10-C8-C7
24	B	810	CLA	C6-C7-C8-C10
24	B	817	CLA	C6-C7-C8-C10
24	B	841	CLA	C12-C13-C15-C16
23	6	323	CHL	C11-C12-C13-C15
27	A	842	LHG	C19-C20-C21-C22
23	0	306	CHL	CBA-CGA-O2A-C1
29	M	101	LMG	C35-C36-C37-C38
24	B	814	CLA	O1D-CGD-O2D-CED
24	9	311	CLA	C5-C6-C7-C8
27	0	317	LHG	C17-C18-C19-C20
27	8	320	LHG	C15-C16-C17-C18
24	B	816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	804	CLA	C16-C17-C18-C19
29	9	317	LMG	C11-C12-C13-C14
24	0	307	CLA	C8-C10-C11-C12
27	6	322	LHG	C11-C12-C13-C14
24	H	205	CLA	C2A-CAA-CBA-CGA
23	1	301	CHL	C14-C13-C15-C16
23	1	306	CHL	C14-C13-C15-C16
24	0	307	CLA	C11-C10-C8-C9
24	5	302	CLA	C6-C7-C8-C9
24	7	308	CLA	C14-C13-C15-C16
24	A	810	CLA	C11-C12-C13-C14
24	A	816	CLA	C11-C12-C13-C14
24	A	848	CLA	C14-C13-C15-C16
24	B	820	CLA	C6-C7-C8-C9
23	4	308	CHL	O1A-CGA-O2A-C1
27	1	318	LHG	C32-C33-C34-C35
29	9	317	LMG	C32-C33-C34-C35
25	6	324	8CT	C16-C17-C18-C19
25	7	319	8CT	C16-C17-C18-C19
25	A	845	8CT	C18-C19-C20-C21
25	L	205	8CT	C18-C19-C20-C21
24	B	805	CLA	C16-C17-C18-C19
23	2	301	CHL	O1D-CGD-O2D-CED
24	8	310	CLA	O1D-CGD-O2D-CED
24	9	309	CLA	O1D-CGD-O2D-CED
24	B	802	CLA	O1D-CGD-O2D-CED
24	B	818	CLA	C8-C10-C11-C12
27	6	322	LHG	C25-C26-C27-C28
27	A	850	LHG	C27-C28-C29-C30
24	A	821	CLA	C1-C2-C3-C4
25	9	313	8CT	C28-C29-C30-C35
26	0	316	0UR	C17-C18-C19-C28
26	O	207	0UR	C17-C18-C19-C28
27	0	317	LHG	C10-C11-C12-C13
27	3	324	LHG	O7-C5-C6-O8
27	7	323	LHG	O7-C5-C6-O8
29	2	318	LMG	O1-C7-C8-O7
29	9	317	LMG	O7-C8-C9-O8
29	M	101	LMG	O7-C8-C9-O8
24	A	807	CLA	C5-C6-C7-C8
27	3	324	LHG	C4-C5-C6-O8
29	2	318	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	9	317	LMG	C7-C8-C9-O8
29	A	854	LMG	C7-C8-C9-O8
29	J	105	LMG	C7-C8-C9-O8
29	M	101	LMG	C7-C8-C9-O8
29	O	203	LMG	O1-C7-C8-C9
29	O	203	LMG	C7-C8-C9-O8
29	O	210	LMG	C7-C8-C9-O8
24	A	813	CLA	C4-C3-C5-C6
24	A	805	CLA	C2-C3-C5-C6
23	3	301	CHL	CAD-CBD-CGD-O2D
23	6	301	CHL	CAD-CBD-CGD-O2D
24	A	834	CLA	CAD-CBD-CGD-O2D
24	B	822	CLA	C4C-C3C-CAC-CBC
23	6	313	CHL	CBA-CGA-O2A-C1
26	0	315	0UR	C46-C47-C48-C49
27	3	324	LHG	C26-C27-C28-C29
28	0	318	SQD	O5-C5-C6-S
27	7	322	LHG	C26-C27-C28-C29
23	6	313	CHL	O1A-CGA-O2A-C1
24	A	820	CLA	C13-C15-C16-C17
26	4	317	0UR	O57-C45-C46-C47
23	0	306	CHL	O1A-CGA-O2A-C1
23	0	301	CHL	CHA-CBD-CGD-O1D
23	0	301	CHL	CHA-CBD-CGD-O2D
23	0	302	CHL	CHA-CBD-CGD-O1D
23	0	302	CHL	CHA-CBD-CGD-O2D
23	2	306	CHL	CHA-CBD-CGD-O2D
23	3	301	CHL	CAD-CBD-CGD-O1D
23	6	301	CHL	CAD-CBD-CGD-O1D
23	6	323	CHL	CHA-CBD-CGD-O1D
23	6	323	CHL	CHA-CBD-CGD-O2D
23	7	301	CHL	CHA-CBD-CGD-O1D
23	7	301	CHL	CHA-CBD-CGD-O2D
23	7	305	CHL	CHA-CBD-CGD-O2D
23	7	313	CHL	CHA-CBD-CGD-O2D
23	9	306	CHL	CHA-CBD-CGD-O2D
23	4	302	CHL	CHA-CBD-CGD-O1D
23	4	302	CHL	CHA-CBD-CGD-O2D
23	4	307	CHL	CHA-CBD-CGD-O1D
24	0	312	CLA	CAD-CBD-CGD-O1D
24	1	302	CLA	CHA-CBD-CGD-O1D
24	1	302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	2	309	CLA	CHA-CBD-CGD-O1D
24	2	309	CLA	CHA-CBD-CGD-O2D
24	3	304	CLA	CHA-CBD-CGD-O1D
24	3	304	CLA	CHA-CBD-CGD-O2D
24	5	302	CLA	CHA-CBD-CGD-O1D
24	5	302	CLA	CHA-CBD-CGD-O2D
24	6	304	CLA	CHA-CBD-CGD-O1D
24	6	304	CLA	CHA-CBD-CGD-O2D
24	9	303	CLA	CHA-CBD-CGD-O1D
24	9	303	CLA	CHA-CBD-CGD-O2D
24	A	805	CLA	CHA-CBD-CGD-O1D
24	A	805	CLA	CHA-CBD-CGD-O2D
24	A	834	CLA	CAD-CBD-CGD-O1D
24	A	839	CLA	CHA-CBD-CGD-O1D
24	B	825	CLA	CHA-CBD-CGD-O1D
24	J	103	CLA	CHA-CBD-CGD-O1D
24	K	104	CLA	CAD-CBD-CGD-O1D
24	O	205	CLA	CHA-CBD-CGD-O2D
24	O	205	CLA	CAD-CBD-CGD-O2D
24	4	310	CLA	CHA-CBD-CGD-O1D
24	4	310	CLA	CHA-CBD-CGD-O2D
25	B	846	8CT	C18-C19-C20-C21
26	5	314	0UR	C41-C2-C3-C4
26	5	314	0UR	C3-C2-C41-C1
27	3	322	LHG	C3-O3-P-O4
27	3	322	LHG	C3-O3-P-O5
27	3	322	LHG	C3-O3-P-O6
27	3	324	LHG	C4-O6-P-O5
27	6	322	LHG	C4-O6-P-O3
27	6	322	LHG	C4-O6-P-O4
27	6	322	LHG	C4-O6-P-O5
27	7	323	LHG	C4-O6-P-O4
27	8	302	LHG	C4-O6-P-O4
27	8	320	LHG	C3-O3-P-O4
27	9	316	LHG	C4-O6-P-O4
27	A	842	LHG	C4-O6-P-O3
27	A	843	LHG	C3-O3-P-O5
27	A	843	LHG	C3-O3-P-O6
27	A	850	LHG	C3-O3-P-O4
27	A	850	LHG	C4-O6-P-O4
27	B	851	LHG	C4-O6-P-O3
27	B	851	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
27	B	852	LHG	C4-O6-P-O5
32	A	852	CL0	CHA-CBD-CGD-O1D
32	A	852	CL0	CHA-CBD-CGD-O2D
24	8	313	CLA	C3-C5-C6-C7
24	A	826	CLA	C3-C5-C6-C7
24	A	840	CLA	O1D-CGD-O2D-CED
27	I	102	LHG	C34-C35-C36-C37
27	3	324	LHG	C7-C8-C9-C10
24	A	829	CLA	C13-C15-C16-C17
24	B	827	CLA	C10-C11-C12-C13
24	1	309	CLA	C2B-C3B-CAB-CBB
24	3	312	CLA	C2B-C3B-CAB-CBB
24	3	313	CLA	C2B-C3B-CAB-CBB
24	5	313	CLA	C2B-C3B-CAB-CBB
24	6	304	CLA	C2B-C3B-CAB-CBB
24	7	310	CLA	C2B-C3B-CAB-CBB
24	8	312	CLA	C2B-C3B-CAB-CBB
24	8	313	CLA	C2B-C3B-CAB-CBB
24	9	309	CLA	C2B-C3B-CAB-CBB
24	A	834	CLA	C2B-C3B-CAB-CBB
24	A	838	CLA	C2B-C3B-CAB-CBB
24	F	302	CLA	C2B-C3B-CAB-CBB
24	H	203	CLA	C2B-C3B-CAB-CBB
24	4	303	CLA	C2B-C3B-CAB-CBB
24	4	310	CLA	C2B-C3B-CAB-CBB
25	F	301	8CT	C02-C03-C10-C11
24	B	817	CLA	C4C-C3C-CAC-CBC
24	B	840	CLA	C13-C15-C16-C17
25	3	317	8CT	C22-C21-C23-C24
25	A	846	8CT	C14-C15-C16-C39
27	1	318	LHG	C2-C3-O3-P
27	3	320	LHG	C2-C3-O3-P
27	3	322	LHG	C5-C4-O6-P
27	7	322	LHG	C2-C3-O3-P
27	8	320	LHG	C2-C3-O3-P
27	A	850	LHG	C5-C4-O6-P
27	B	851	LHG	C2-C3-O3-P
27	3	324	LHG	C12-C13-C14-C15
24	0	307	CLA	C10-C11-C12-C13
29	9	317	LMG	C21-C22-C23-C24
27	1	317	LHG	C12-C13-C14-C15
28	0	318	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
24	A	816	CLA	C12-C13-C15-C16
23	1	304	CHL	O2A-C1-C2-C3
29	M	101	LMG	C9-C8-O7-C10
27	1	317	LHG	C35-C36-C37-C38
25	3	316	8CT	C13-C14-C15-C16
25	6	319	8CT	C21-C23-C24-C25
25	B	843	8CT	C13-C14-C15-C16
25	B	843	8CT	C21-C23-C24-C25
25	B	844	8CT	C13-C14-C15-C16
25	B	844	8CT	C21-C23-C24-C25
25	B	845	8CT	C13-C14-C15-C16
25	B	846	8CT	C13-C14-C15-C16
25	B	846	8CT	C21-C23-C24-C25
24	B	801	CLA	CAA-CBA-CGA-O2A
24	3	312	CLA	C6-C7-C8-C10
24	6	316	CLA	C16-C17-C18-C19
24	4	304	CLA	C10-C11-C12-C13
23	5	312	CHL	O1A-CGA-O2A-C1
24	5	307	CLA	O1A-CGA-O2A-C1
23	8	303	CHL	C14-C13-C15-C16
24	8	310	CLA	C11-C10-C8-C9
24	A	805	CLA	C14-C13-C15-C16
24	A	810	CLA	C14-C13-C15-C16
24	A	814	CLA	C6-C7-C8-C9
24	A	820	CLA	C14-C13-C15-C16
24	A	827	CLA	C14-C13-C15-C16
23	6	302	CHL	C12-C13-C15-C16
24	A	827	CLA	C12-C13-C15-C16
24	B	806	CLA	C11-C12-C13-C15
24	L	202	CLA	C11-C10-C8-C7
24	0	310	CLA	CBD-CGD-O2D-CED
27	I	102	LHG	C13-C14-C15-C16
24	3	308	CLA	C16-C17-C18-C20
27	0	317	LHG	C31-C32-C33-C34
24	2	303	CLA	C8-C10-C11-C12
24	A	848	CLA	C15-C16-C17-C18
29	9	317	LMG	C15-C16-C17-C18
24	0	303	CLA	O1D-CGD-O2D-CED
23	9	306	CHL	CAA-CBA-CGA-O2A
23	4	315	CHL	CAA-CBA-CGA-O2A
27	6	322	LHG	C27-C28-C29-C30
24	7	312	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	1	304	CHL	O1D-CGD-O2D-CED
24	9	302	CLA	C16-C17-C18-C19
24	B	805	CLA	C16-C17-C18-C20
27	B	852	LHG	C12-C13-C14-C15
27	B	852	LHG	C7-C8-C9-C10
29	O	203	LMG	O7-C8-C9-O8
27	8	302	LHG	O8-C23-C24-C25
26	2	316	0UR	C46-C47-C48-C49
23	1	304	CHL	CBD-CGD-O2D-CED
27	8	302	LHG	C24-C23-O8-C6
25	A	845	8CT	C23-C24-C25-C26
25	F	301	8CT	C18-C19-C20-C21
27	A	850	LHG	C15-C16-C17-C18
24	A	817	CLA	CAA-CBA-CGA-O2A
24	A	801	CLA	C2A-CAA-CBA-CGA
24	A	816	CLA	C2A-CAA-CBA-CGA
24	K	104	CLA	C2A-CAA-CBA-CGA
24	B	822	CLA	C2C-C3C-CAC-CBC
23	1	312	CHL	O1D-CGD-O2D-CED
24	L	202	CLA	C2-C1-O2A-CGA
24	9	311	CLA	C4-C3-C5-C6
24	B	808	CLA	C4-C3-C5-C6
24	L	201	CLA	C2-C3-C5-C6
27	3	324	LHG	C29-C30-C31-C32
27	I	102	LHG	C15-C16-C17-C18
27	A	850	LHG	C4-C5-C6-O8
34	B	849	DGD	C1G-C2G-C3G-O3G
27	6	322	LHG	O8-C23-C24-C25
25	3	316	8CT	C10-C11-C12-C40
27	2	317	LHG	C10-C11-C12-C13
24	B	814	CLA	C16-C17-C18-C19
23	2	312	CHL	C1C-C2C-CMC-OMC
23	7	305	CHL	C1C-C2C-CMC-OMC
23	7	306	CHL	C1C-C2C-CMC-OMC
23	8	301	CHL	C2A-CAA-CBA-CGA
24	2	311	CLA	C2A-CAA-CBA-CGA
24	A	834	CLA	C2A-CAA-CBA-CGA
24	A	836	CLA	C2A-CAA-CBA-CGA
24	A	838	CLA	C2A-CAA-CBA-CGA
25	B	847	8CT	C23-C24-C25-C26
29	2	318	LMG	C10-C11-C12-C13
29	A	854	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	B	805	CLA	CAA-CBA-CGA-O2A
24	1	309	CLA	C2-C3-C5-C6
24	A	828	CLA	C2-C3-C5-C6
24	B	824	CLA	C5-C6-C7-C8
23	8	306	CHL	O1A-CGA-O2A-C1
23	4	301	CHL	CAA-CBA-CGA-O1A
27	A	843	LHG	O1-C1-C2-O2
24	A	802	CLA	C16-C17-C18-C20
24	A	828	CLA	C16-C17-C18-C20
23	1	312	CHL	C6-C7-C8-C9
24	6	316	CLA	C11-C12-C13-C14
24	B	804	CLA	C11-C12-C13-C14
24	B	808	CLA	C11-C10-C8-C9
24	B	817	CLA	C6-C7-C8-C9
31	B	842	PQN	C21-C22-C23-C24
32	A	852	CL0	C14-C13-C15-C16
27	8	302	LHG	C2-C3-O3-P
27	A	850	LHG	C11-C12-C13-C14
24	8	304	CLA	C4B-C3B-CAB-CBB
24	B	840	CLA	C4B-C3B-CAB-CBB
27	2	317	LHG	C7-C8-C9-C10
24	A	812	CLA	CBA-CGA-O2A-C1
27	8	320	LHG	C24-C23-O8-C6
23	6	308	CHL	C5-C6-C7-C8
23	9	301	CHL	C2A-CAA-CBA-CGA
24	3	312	CLA	C2A-CAA-CBA-CGA
23	2	301	CHL	C4-C3-C5-C6
23	4	302	CHL	C4-C3-C5-C6
24	A	818	CLA	C4-C3-C5-C6
26	6	320	0UR	C46-C47-C48-C49
26	8	319	0UR	C46-C47-C48-C49
27	8	302	LHG	O10-C23-O8-C6
27	3	320	LHG	C25-C26-C27-C28
24	A	828	CLA	C16-C17-C18-C19
27	2	317	LHG	C12-C13-C14-C15
23	5	312	CHL	CAA-CBA-CGA-O2A
23	2	301	CHL	C11-C10-C8-C7
23	7	306	CHL	C11-C10-C8-C7
24	0	307	CLA	C6-C7-C8-C10
24	9	302	CLA	C11-C10-C8-C7
24	9	307	CLA	C11-C10-C8-C7
24	A	805	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	A	817	CLA	C12-C13-C15-C16
24	A	826	CLA	C6-C7-C8-C10
24	A	812	CLA	O1A-CGA-O2A-C1
24	A	834	CLA	O1D-CGD-O2D-CED
24	5	308	CLA	CBA-CGA-O2A-C1
24	7	316	CLA	CAA-CBA-CGA-O2A
24	8	305	CLA	C16-C17-C18-C20
26	8	318	0UR	C46-C47-C48-C49
27	8	320	LHG	O10-C23-O8-C6
29	O	210	LMG	O7-C8-C9-O8
29	O	210	LMG	C12-C13-C14-C15
23	3	307	CHL	C3A-C2A-CAA-CBA
23	9	306	CHL	C3A-C2A-CAA-CBA
24	5	303	CLA	C3A-C2A-CAA-CBA
24	A	827	CLA	C3A-C2A-CAA-CBA
24	B	829	CLA	C4-C3-C5-C6
24	F	303	CLA	C3A-C2A-CAA-CBA
24	K	102	CLA	C4-C3-C5-C6
24	9	311	CLA	C2-C3-C5-C6
24	B	808	CLA	C2-C3-C5-C6
29	A	854	LMG	C30-C31-C32-C33
24	0	303	CLA	C10-C11-C12-C13
24	2	303	CLA	C5-C6-C7-C8
25	2	314	8CT	C19-C20-C21-C22
25	3	316	8CT	C40-C12-C13-C14
25	3	323	8CT	C24-C25-C26-C27
25	6	324	8CT	C24-C25-C26-C27
25	7	319	8CT	C24-C25-C26-C27
25	B	843	8CT	C39-C16-C17-C18
25	B	844	8CT	C39-C16-C17-C18
25	B	844	8CT	C19-C20-C21-C22
25	B	844	8CT	C24-C25-C26-C27
25	B	845	8CT	C39-C16-C17-C18
25	B	845	8CT	C24-C25-C26-C27
25	B	846	8CT	C40-C12-C13-C14
25	B	846	8CT	C39-C16-C17-C18
25	B	848	8CT	C24-C25-C26-C27
25	B	850	8CT	C40-C12-C13-C14
25	J	104	8CT	C40-C12-C13-C14
25	4	316	8CT	C19-C20-C21-C22
24	B	834	CLA	C10-C11-C12-C13
24	B	830	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	6	301	CHL	C5-C6-C7-C8
23	1	304	CHL	C2-C1-O2A-CGA
23	7	306	CHL	C2-C1-O2A-CGA
23	8	301	CHL	C2-C1-O2A-CGA
23	9	305	CHL	C2-C1-O2A-CGA
25	B	847	8CT	C12-C13-C14-C15
26	8	319	0UR	C3-C4-C5-C6
27	7	323	LHG	C13-C14-C15-C16
24	3	308	CLA	C5-C6-C7-C8
24	B	806	CLA	C15-C16-C17-C18
25	2	314	8CT	C10-C11-C12-C40
26	4	318	0UR	C5-C6-C7-C20
24	8	315	CLA	CAA-CBA-CGA-O1A
24	6	318	CLA	C4-C3-C5-C6
24	A	835	CLA	C4-C3-C5-C6
23	2	307	CHL	C2C-C3C-CAC-CBC
29	A	851	LMG	C33-C34-C35-C36
23	5	305	CHL	C2C-C3C-CAC-CBC
24	B	832	CLA	C15-C16-C17-C18
26	0	316	0UR	C15-C16-C17-C18
24	0	310	CLA	O1D-CGD-O2D-CED
24	6	318	CLA	O1D-CGD-O2D-CED
24	K	102	CLA	C5-C6-C7-C8
24	6	317	CLA	CAA-CBA-CGA-O1A
24	8	305	CLA	C16-C17-C18-C19
23	1	312	CHL	C5-C6-C7-C8
24	B	801	CLA	C5-C6-C7-C8
29	9	317	LMG	C31-C32-C33-C34
24	9	311	CLA	C2A-CAA-CBA-CGA
24	A	828	CLA	CBA-CGA-O2A-C1
27	0	317	LHG	C9-C10-C11-C12
24	7	316	CLA	CAA-CBA-CGA-O1A
23	7	306	CHL	C11-C10-C8-C9
24	0	307	CLA	C6-C7-C8-C9
24	1	309	CLA	C11-C12-C13-C14
24	7	308	CLA	C11-C10-C8-C9
24	9	302	CLA	C11-C10-C8-C9
24	A	808	CLA	C11-C10-C8-C9
24	B	806	CLA	C14-C13-C15-C16
24	B	816	CLA	C6-C7-C8-C9
24	B	827	CLA	C11-C10-C8-C9
24	B	813	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	A	819	CLA	C5-C6-C7-C8
24	6	318	CLA	CBD-CGD-O2D-CED
27	2	317	LHG	C9-C10-C11-C12
23	9	305	CHL	O2A-C1-C2-C3
29	J	102	LMG	C7-C8-O7-C10
24	A	828	CLA	C5-C6-C7-C8
23	2	301	CHL	C1A-C2A-CAA-CBA
23	5	305	CHL	C1A-C2A-CAA-CBA
23	5	312	CHL	C1A-C2A-CAA-CBA
23	6	301	CHL	C1A-C2A-CAA-CBA
23	7	302	CHL	C1A-C2A-CAA-CBA
23	9	312	CHL	C1A-C2A-CAA-CBA
23	4	307	CHL	C1A-C2A-CAA-CBA
27	6	322	LHG	C23-C24-C25-C26
24	B	840	CLA	C16-C17-C18-C20
26	6	321	0UR	C46-C47-C48-C49
24	5	309	CLA	CBD-CGD-O2D-CED
24	A	815	CLA	CBD-CGD-O2D-CED
27	8	302	LHG	O1-C1-C2-O2
24	A	828	CLA	O1A-CGA-O2A-C1
24	4	312	CLA	O1A-CGA-O2A-C1
24	5	310	CLA	C2A-CAA-CBA-CGA
24	6	312	CLA	C2A-CAA-CBA-CGA
24	7	312	CLA	C2A-CAA-CBA-CGA
24	A	817	CLA	C2A-CAA-CBA-CGA
24	A	815	CLA	O1D-CGD-O2D-CED
24	5	309	CLA	C1A-C2A-CAA-CBA
24	6	310	CLA	C1A-C2A-CAA-CBA
24	A	801	CLA	C1A-C2A-CAA-CBA
24	A	827	CLA	C1A-C2A-CAA-CBA
24	B	813	CLA	C1A-C2A-CAA-CBA
24	B	816	CLA	C1A-C2A-CAA-CBA
25	2	314	8CT	C19-C20-C21-C23
25	3	316	8CT	C11-C12-C13-C14
25	3	323	8CT	C24-C25-C26-C28
25	6	324	8CT	C24-C25-C26-C28
25	7	319	8CT	C24-C25-C26-C28
25	B	843	8CT	C15-C16-C17-C18
25	B	844	8CT	C15-C16-C17-C18
25	B	844	8CT	C19-C20-C21-C23
25	B	844	8CT	C24-C25-C26-C28
25	B	845	8CT	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	845	8CT	C24-C25-C26-C28
25	B	846	8CT	C11-C12-C13-C14
25	B	846	8CT	C15-C16-C17-C18
25	B	848	8CT	C24-C25-C26-C28
25	B	850	8CT	C11-C12-C13-C14
25	J	104	8CT	C11-C12-C13-C14
25	4	316	8CT	C19-C20-C21-C23
27	9	316	LHG	C29-C30-C31-C32
24	A	803	CLA	C6-C7-C8-C10
27	A	850	LHG	O6-C4-C5-O7
24	5	308	CLA	O1A-CGA-O2A-C1
24	2	302	CLA	C2B-C3B-CAB-CBB
24	2	309	CLA	C2B-C3B-CAB-CBB
24	6	310	CLA	C2B-C3B-CAB-CBB
24	6	317	CLA	C2B-C3B-CAB-CBB
24	7	311	CLA	C2B-C3B-CAB-CBB
24	7	312	CLA	C2B-C3B-CAB-CBB
24	7	314	CLA	C2B-C3B-CAB-CBB
24	8	304	CLA	C2B-C3B-CAB-CBB
24	8	311	CLA	C2B-C3B-CAB-CBB
24	8	315	CLA	C2B-C3B-CAB-CBB
24	A	814	CLA	C2B-C3B-CAB-CBB
24	A	822	CLA	C2B-C3B-CAB-CBB
24	A	836	CLA	C2B-C3B-CAB-CBB
24	A	839	CLA	C2B-C3B-CAB-CBB
24	B	805	CLA	C2B-C3B-CAB-CBB
24	B	809	CLA	C2B-C3B-CAB-CBB
24	B	811	CLA	C2B-C3B-CAB-CBB
24	B	822	CLA	C2B-C3B-CAB-CBB
24	B	831	CLA	C2B-C3B-CAB-CBB
24	B	834	CLA	C2B-C3B-CAB-CBB
24	B	840	CLA	C2B-C3B-CAB-CBB
24	F	303	CLA	C2B-C3B-CAB-CBB
24	L	206	CLA	C2B-C3B-CAB-CBB
24	K	101	CLA	C2B-C3B-CAB-CBB
24	O	209	CLA	C2B-C3B-CAB-CBB
25	6	319	8CT	C02-C03-C10-C11
25	8	317	8CT	C02-C03-C10-C11
25	A	845	8CT	C04-C03-C10-C11
25	B	843	8CT	C04-C03-C10-C11
25	B	844	8CT	C04-C03-C10-C11
25	B	848	8CT	C02-C03-C10-C11

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Mol	Chain	Res	Type	Atoms
25	B	850	8CT	C02-C03-C10-C11
25	F	304	8CT	C04-C03-C10-C11
25	G	104	8CT	C02-C03-C10-C11
25	4	316	8CT	C02-C03-C10-C11
24	8	315	CLA	CAA-CBA-CGA-O2A
24	4	303	CLA	CAA-CBA-CGA-O2A
27	L	208	LHG	C24-C23-O8-C6
27	0	317	LHG	C16-C17-C18-C19
27	8	320	LHG	C9-C10-C11-C12
23	1	312	CHL	C14-C13-C15-C16
23	6	302	CHL	C4-C3-C5-C6
24	B	813	CLA	C4-C3-C5-C6
24	B	822	CLA	C4-C3-C5-C6
27	6	322	LHG	C28-C29-C30-C31
23	4	302	CHL	C2-C3-C5-C6
24	5	302	CLA	C8-C10-C11-C12
24	A	839	CLA	C15-C16-C17-C18
23	1	312	CHL	C6-C7-C8-C10
23	2	301	CHL	C11-C12-C13-C15
24	3	309	CLA	C12-C13-C15-C16
24	6	316	CLA	C11-C12-C13-C15
24	9	307	CLA	C11-C12-C13-C15
24	9	311	CLA	C6-C7-C8-C10
24	A	853	CLA	C12-C13-C15-C16
31	B	842	PQN	C21-C22-C23-C25
27	7	324	LHG	C9-C10-C11-C12
23	9	312	CHL	C2A-CAA-CBA-CGA
24	1	302	CLA	C2A-CAA-CBA-CGA
27	6	322	LHG	C7-C8-C9-C10
26	3	318	0UR	C46-C47-C48-C49
24	A	836	CLA	CBD-CGD-O2D-CED
24	K	101	CLA	CBD-CGD-O2D-CED
24	2	308	CLA	C11-C12-C13-C15
27	2	317	LHG	C25-C26-C27-C28
23	1	312	CHL	C12-C13-C15-C16
23	3	302	CHL	C12-C13-C15-C16
24	8	313	CLA	C11-C10-C8-C7
24	B	830	CLA	C11-C10-C8-C7
27	6	322	LHG	C10-C11-C12-C13
23	7	302	CHL	C4-C3-C5-C6
24	A	816	CLA	C4-C3-C5-C6
24	L	202	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	3	301	CHL	C8-C10-C11-C12
23	2	301	CHL	C2-C3-C5-C6
24	3	310	CLA	C2-C3-C5-C6
24	A	818	CLA	C2-C3-C5-C6
24	L	202	CLA	C2-C3-C5-C6
23	5	306	CHL	O1A-CGA-O2A-C1
24	B	841	CLA	CBD-CGD-O2D-CED
24	A	824	CLA	C8-C10-C11-C12
24	A	827	CLA	C8-C10-C11-C12
24	4	309	CLA	C10-C11-C12-C13
24	4	303	CLA	CAA-CBA-CGA-O1A
24	B	832	CLA	C13-C15-C16-C17
23	4	306	CHL	O1D-CGD-O2D-CED
23	0	302	CHL	C14-C13-C15-C16
23	2	301	CHL	C14-C13-C15-C16
23	6	308	CHL	C6-C7-C8-C9
24	A	817	CLA	C11-C10-C8-C9
24	A	825	CLA	C11-C12-C13-C14
24	B	814	CLA	C14-C13-C15-C16
24	B	818	CLA	C11-C12-C13-C14
23	5	305	CHL	C2-C1-O2A-CGA
25	K	105	8CT	C23-C24-C25-C26
24	K	102	CLA	C4C-C3C-CAC-CBC
24	7	303	CLA	CAA-CBA-CGA-O2A
24	1	308	CLA	CBA-CGA-O2A-C1
24	A	807	CLA	C4-C3-C5-C6
24	A	808	CLA	C4-C3-C5-C6
24	A	809	CLA	C4-C3-C5-C6
24	B	811	CLA	C4-C3-C5-C6
24	3	315	CLA	C2-C3-C5-C6
32	A	852	CL0	C8-C10-C11-C12
24	B	813	CLA	C6-C7-C8-C9
24	A	835	CLA	C2C-C3C-CAC-CBC
23	5	305	CHL	CAA-CBA-CGA-O1A
27	A	843	LHG	C4-C5-C6-O8
24	1	308	CLA	O1A-CGA-O2A-C1
27	L	208	LHG	O10-C23-O8-C6
24	B	806	CLA	C2A-CAA-CBA-CGA
24	B	808	CLA	CAA-CBA-CGA-O2A
24	0	313	CLA	CAA-CBA-CGA-O2A
24	B	813	CLA	C5-C6-C7-C8
27	7	324	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
24	G	102	CLA	CAA-CBA-CGA-O2A
24	B	811	CLA	C2-C3-C5-C6
24	6	317	CLA	CBD-CGD-O2D-CED
27	A	850	LHG	C9-C10-C11-C12
23	1	305	CHL	C2-C1-O2A-CGA
24	5	302	CLA	C4B-C3B-CAB-CBB
24	8	315	CLA	C4B-C3B-CAB-CBB
24	A	814	CLA	C4B-C3B-CAB-CBB
24	A	836	CLA	C4B-C3B-CAB-CBB
24	B	831	CLA	C4B-C3B-CAB-CBB
24	L	202	CLA	C4B-C3B-CAB-CBB
26	4	318	0UR	O42-C2-C3-C4
23	0	301	CHL	O1A-CGA-O2A-C1
27	B	852	LHG	C10-C11-C12-C13
27	I	102	LHG	C10-C11-C12-C13
27	9	316	LHG	C26-C27-C28-C29
24	6	312	CLA	O1A-CGA-O2A-C1
24	A	802	CLA	C16-C17-C18-C19
24	A	807	CLA	C16-C17-C18-C19
24	A	836	CLA	O1D-CGD-O2D-CED
23	7	306	CHL	CHA-CBD-CGD-O2D
23	7	313	CHL	CHA-CBD-CGD-O1D
23	4	315	CHL	CHA-CBD-CGD-O1D
23	4	315	CHL	CHA-CBD-CGD-O2D
23	5	304	CHL	CAA-CBA-CGA-O2A
29	9	317	LMG	C35-C36-C37-C38
29	O	203	LMG	O1-C7-C8-O7
26	2	315	0UR	C46-C47-C48-C49
26	9	314	0UR	C46-C47-C48-C49
24	7	304	CLA	C3-C5-C6-C7
24	A	807	CLA	C13-C15-C16-C17
27	3	320	LHG	C12-C13-C14-C15
34	B	849	DGD	C6A-C7A-C8A-C9A
24	A	817	CLA	C11-C10-C8-C7
24	A	820	CLA	C6-C7-C8-C10
24	B	808	CLA	C6-C7-C8-C10
24	4	314	CLA	CAA-CBA-CGA-O2A
23	1	306	CHL	C3-C5-C6-C7
24	7	303	CLA	CAA-CBA-CGA-O1A
25	3	316	8CT	C10-C11-C12-C13
24	0	303	CLA	C11-C12-C13-C14
24	1	302	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	5	311	CLA	C6-C7-C8-C9
24	A	820	CLA	C6-C7-C8-C9
24	B	802	CLA	C14-C13-C15-C16
24	4	309	CLA	C6-C7-C8-C9
24	A	840	CLA	C8-C10-C11-C12
29	2	318	LMG	C8-C7-O1-C1
24	A	827	CLA	CAA-CBA-CGA-O2A
29	A	854	LMG	C29-C30-C31-C32
26	5	314	0UR	C46-C47-C48-C49
26	4	317	0UR	C46-C47-C48-C49
24	0	311	CLA	C2A-CAA-CBA-CGA
24	7	317	CLA	C2A-CAA-CBA-CGA
24	8	313	CLA	C2A-CAA-CBA-CGA
24	A	835	CLA	C2A-CAA-CBA-CGA
24	4	312	CLA	C2A-CAA-CBA-CGA
23	1	301	CHL	C2-C1-O2A-CGA
23	3	302	CHL	C2-C1-O2A-CGA
23	6	313	CHL	C2-C1-O2A-CGA
23	7	302	CHL	C2-C1-O2A-CGA
23	8	303	CHL	C2-C1-O2A-CGA
23	4	302	CHL	C2-C1-O2A-CGA
24	A	820	CLA	C2-C1-O2A-CGA
24	K	102	CLA	C2-C1-O2A-CGA
32	A	852	CL0	C13-C15-C16-C17
23	0	301	CHL	CBA-CGA-O2A-C1
23	3	305	CHL	CBA-CGA-O2A-C1
24	4	312	CLA	CBA-CGA-O2A-C1
24	3	313	CLA	C3A-C2A-CAA-CBA
24	A	801	CLA	C3A-C2A-CAA-CBA
24	A	820	CLA	C4-C3-C5-C6
24	B	840	CLA	C2C-C3C-CAC-CBC
23	3	305	CHL	O1A-CGA-O2A-C1
24	A	813	CLA	C2-C3-C5-C6
27	1	318	LHG	C35-C36-C37-C38
24	6	317	CLA	O1D-CGD-O2D-CED
27	7	323	LHG	C11-C12-C13-C14
27	L	208	LHG	O10-C23-C24-C25
24	B	807	CLA	CAA-CBA-CGA-O2A
27	B	852	LHG	C14-C15-C16-C17
24	6	312	CLA	CBA-CGA-O2A-C1
26	0	316	0UR	C46-C47-C48-C49
26	1	315	0UR	C46-C47-C48-C49

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Mol	Chain	Res	Type	Atoms
26	5	315	0UR	C46-C47-C48-C49
24	A	831	CLA	C13-C15-C16-C17
27	8	320	LHG	C31-C32-C33-C34
23	0	306	CHL	C3C-C2C-CMC-OMC
23	6	313	CHL	C3C-C2C-CMC-OMC
23	7	301	CHL	C3C-C2C-CMC-OMC
23	8	306	CHL	C3C-C2C-CMC-OMC
24	7	317	CLA	C11-C12-C13-C14
24	B	819	CLA	C11-C12-C13-C14
24	0	313	CLA	CAA-CBA-CGA-O1A
24	9	302	CLA	C15-C16-C17-C18
27	8	320	LHG	O2-C2-C3-O3
23	5	304	CHL	CAA-CBA-CGA-O1A
26	1	316	0UR	C4-C3-C43-O44
24	G	102	CLA	CAA-CBA-CGA-O1A
27	9	316	LHG	C5-C4-O6-P
23	7	305	CHL	C2-C1-O2A-CGA
24	A	821	CLA	O2A-C1-C2-C3
29	O	210	LMG	O6-C1-O1-C7
23	3	307	CHL	C10-C11-C12-C13
27	5	316	LHG	C27-C28-C29-C30
27	0	317	LHG	C4-C5-C6-O8
27	1	318	LHG	C4-C5-C6-O8
29	J	102	LMG	O1-C7-C8-C9
23	4	315	CHL	C5-C6-C7-C8
24	6	314	CLA	CAA-CBA-CGA-O2A
27	A	843	LHG	C10-C11-C12-C13
24	A	820	CLA	CBA-CGA-O2A-C1
24	A	812	CLA	C4-C3-C5-C6
24	B	815	CLA	C2A-CAA-CBA-CGA
24	A	835	CLA	CBD-CGD-O2D-CED
24	4	309	CLA	C11-C12-C13-C15
31	B	842	PQN	C15-C16-C17-C18
24	B	807	CLA	CAA-CBA-CGA-O1A
24	A	816	CLA	C14-C13-C15-C16
24	K	104	CLA	CAA-CBA-CGA-O2A
23	1	301	CHL	C11-C12-C13-C14
23	3	302	CHL	C11-C10-C8-C9
23	3	307	CHL	C11-C12-C13-C14
24	3	308	CLA	C11-C10-C8-C9
24	A	848	CLA	C11-C12-C13-C14
24	B	832	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	841	CLA	C14-C13-C15-C16
31	A	841	PQN	C21-C22-C23-C24
24	0	312	CLA	CAA-CBA-CGA-O2A
27	7	323	LHG	O7-C7-C8-C9
29	2	318	LMG	O8-C28-C29-C30
24	4	314	CLA	CAA-CBA-CGA-O1A
27	8	320	LHG	C11-C10-C9-C8
23	9	305	CHL	CAA-CBA-CGA-O2A
23	6	302	CHL	C2-C3-C5-C6
23	0	306	CHL	C2A-CAA-CBA-CGA
23	8	314	CHL	C2A-CAA-CBA-CGA
23	3	302	CHL	C11-C10-C8-C7
23	6	308	CHL	C6-C7-C8-C10
23	7	302	CHL	C6-C7-C8-C10
23	4	301	CHL	C6-C7-C8-C10
24	7	309	CLA	C11-C10-C8-C7
24	9	307	CLA	C6-C7-C8-C10
24	A	825	CLA	C11-C12-C13-C15
24	B	804	CLA	C6-C7-C8-C10
24	B	814	CLA	C12-C13-C15-C16
24	B	816	CLA	C6-C7-C8-C10
24	A	804	CLA	C3-C5-C6-C7
27	3	324	LHG	C35-C36-C37-C38
24	1	313	CLA	C2B-C3B-CAB-CBB
24	5	309	CLA	C2B-C3B-CAB-CBB
24	6	318	CLA	C2B-C3B-CAB-CBB
24	A	808	CLA	C2B-C3B-CAB-CBB
24	B	841	CLA	C2B-C3B-CAB-CBB
25	7	318	8CT	C02-C03-C10-C11
25	J	101	8CT	C02-C03-C10-C11
25	M	102	8CT	C02-C03-C10-C11
27	A	843	LHG	O8-C23-C24-C25
27	8	320	LHG	C27-C28-C29-C30
24	5	302	CLA	CAA-CBA-CGA-O2A
24	A	819	CLA	CAA-CBA-CGA-O2A
26	7	320	0UR	C46-C47-C48-C49
23	1	312	CHL	C2-C1-O2A-CGA
23	8	308	CHL	C2-C1-O2A-CGA
24	7	308	CLA	C2-C1-O2A-CGA
24	A	838	CLA	C2-C1-O2A-CGA
24	A	848	CLA	C2-C1-O2A-CGA
24	B	812	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	0	305	CHL	CAA-CBA-CGA-O2A
24	L	202	CLA	CAA-CBA-CGA-O2A
23	4	306	CHL	CBD-CGD-O2D-CED
29	3	321	LMG	C33-C34-C35-C36
27	1	317	LHG	C16-C17-C18-C19
26	0	315	0UR	O42-C2-C3-C43
26	0	316	0UR	O42-C2-C3-C43
26	1	315	0UR	O42-C2-C3-C43
26	3	318	0UR	O42-C2-C3-C43
26	6	320	0UR	O42-C2-C3-C43
26	7	320	0UR	O42-C2-C3-C43
26	8	318	0UR	O42-C2-C3-C43
26	9	314	0UR	O42-C2-C3-C43
26	4	317	0UR	O42-C2-C3-C43
30	3	319	0IE	O1-C2-C3-C20
30	7	321	0IE	O1-C2-C3-C20
34	B	849	DGD	C3A-C4A-C5A-C6A
24	B	839	CLA	C8-C10-C11-C12
23	0	302	CHL	CAA-CBA-CGA-O2A
23	8	301	CHL	CAA-CBA-CGA-O2A
27	A	842	LHG	O7-C7-C8-C9
27	A	842	LHG	O8-C23-C24-C25
24	A	820	CLA	C2-C3-C5-C6
24	B	840	CLA	C4C-C3C-CAC-CBC
24	A	801	CLA	C13-C15-C16-C17
24	7	316	CLA	C2C-C3C-CAC-CBC
24	A	853	CLA	C2A-CAA-CBA-CGA
24	4	309	CLA	C2A-CAA-CBA-CGA
23	7	306	CHL	CAA-CBA-CGA-O2A
24	1	302	CLA	CAA-CBA-CGA-O2A
24	B	840	CLA	C16-C17-C18-C19
24	K	101	CLA	O1D-CGD-O2D-CED
24	B	837	CLA	C13-C15-C16-C17
24	2	310	CLA	CAA-CBA-CGA-O2A
27	3	322	LHG	O8-C23-C24-C25
23	3	307	CHL	CAA-CBA-CGA-O2A
24	A	804	CLA	CAA-CBA-CGA-O2A
24	A	824	CLA	CAA-CBA-CGA-O2A
24	H	204	CLA	CAA-CBA-CGA-O2A
27	7	324	LHG	O7-C7-C8-C9
24	B	829	CLA	C2-C3-C5-C6
24	K	102	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	A	820	CLA	O1A-CGA-O2A-C1
23	4	313	CHL	C2A-CAA-CBA-CGA
24	1	309	CLA	C2A-CAA-CBA-CGA
24	5	310	CLA	CAA-CBA-CGA-O1A
24	6	314	CLA	CAA-CBA-CGA-O1A
23	8	307	CHL	CAA-CBA-CGA-O2A
24	B	809	CLA	CAA-CBA-CGA-O2A
27	8	320	LHG	O8-C23-C24-C25
24	A	817	CLA	C10-C11-C12-C13
24	A	838	CLA	C15-C16-C17-C18
34	B	849	DGD	O6D-C5D-C6D-O5D
24	0	303	CLA	C6-C7-C8-C9
24	A	834	CLA	C11-C10-C8-C9
24	L	202	CLA	C11-C10-C8-C9
24	L	202	CLA	C14-C13-C15-C16
27	B	852	LHG	C28-C29-C30-C31
23	2	301	CHL	CAA-CBA-CGA-O2A
27	7	322	LHG	O8-C23-C24-C25
27	5	316	LHG	C4-C5-C6-O8
29	J	105	LMG	O1-C7-C8-C9
24	0	307	CLA	C4B-C3B-CAB-CBB
24	1	313	CLA	C4B-C3B-CAB-CBB
24	3	313	CLA	C1A-C2A-CAA-CBA
24	5	303	CLA	C1A-C2A-CAA-CBA
24	5	310	CLA	C1A-C2A-CAA-CBA
24	7	303	CLA	C4B-C3B-CAB-CBB
24	9	303	CLA	C4B-C3B-CAB-CBB
24	A	815	CLA	C4B-C3B-CAB-CBB
24	A	825	CLA	C1A-C2A-CAA-CBA
24	B	841	CLA	C4B-C3B-CAB-CBB
24	F	303	CLA	C1A-C2A-CAA-CBA
24	4	310	CLA	C1A-C2A-CAA-CBA
24	3	308	CLA	CAA-CBA-CGA-O2A
24	7	314	CLA	CAA-CBA-CGA-O2A
24	A	832	CLA	CAA-CBA-CGA-O2A
24	B	838	CLA	CAA-CBA-CGA-O2A
27	0	317	LHG	O8-C23-C24-C25
25	3	317	8CT	C20-C21-C23-C24
24	6	316	CLA	C8-C10-C11-C12
24	7	317	CLA	O1A-CGA-O2A-C1
24	1	307	CLA	CAA-CBA-CGA-O2A
24	5	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	5	309	CLA	O1D-CGD-O2D-CED
23	1	301	CHL	CAA-CBA-CGA-O2A
24	2	311	CLA	CAA-CBA-CGA-O2A
24	A	807	CLA	CAA-CBA-CGA-O2A
24	B	823	CLA	CAA-CBA-CGA-O2A
27	A	850	LHG	O7-C7-C8-C9
24	B	841	CLA	O1D-CGD-O2D-CED
29	O	210	LMG	C28-C29-C30-C31
32	A	852	CL0	C16-C17-C18-C19
24	A	813	CLA	CAA-CBA-CGA-O2A
24	K	103	CLA	CAA-CBA-CGA-O2A
27	3	320	LHG	O8-C23-C24-C25
23	2	305	CHL	O1D-CGD-O2D-CED
23	3	305	CHL	O1D-CGD-O2D-CED
27	8	320	LHG	C1-C2-C3-O3
24	B	829	CLA	C10-C11-C12-C13
24	2	303	CLA	C4-C3-C5-C6
23	0	302	CHL	C2-C1-O2A-CGA
24	0	307	CLA	C2-C1-O2A-CGA
24	6	318	CLA	C2-C1-O2A-CGA
24	7	311	CLA	C2-C1-O2A-CGA
24	A	813	CLA	C2-C1-O2A-CGA
24	A	830	CLA	C2-C1-O2A-CGA
24	8	312	CLA	CAA-CBA-CGA-O2A
23	6	301	CHL	C11-C10-C8-C7
24	B	802	CLA	C6-C7-C8-C10
24	B	825	CLA	C6-C7-C8-C10
24	B	832	CLA	C6-C7-C8-C10
24	B	836	CLA	C11-C10-C8-C7
24	A	808	CLA	C13-C15-C16-C17
24	A	839	CLA	C16-C17-C18-C19
24	4	310	CLA	C11-C12-C13-C14
29	J	102	LMG	C9-C8-O7-C10
27	0	317	LHG	O7-C7-C8-C9
29	9	317	LMG	C19-C20-C21-C22
34	B	849	DGD	C7B-C8B-C9B-CAB
24	K	104	CLA	CAA-CBA-CGA-O1A
24	6	318	CLA	C2A-CAA-CBA-CGA
24	H	204	CLA	C2A-CAA-CBA-CGA
29	O	203	LMG	O9-C10-O7-C8
24	B	811	CLA	C13-C15-C16-C17
24	A	810	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	A	841	PQN	C26-C27-C28-C30
24	L	201	CLA	C8-C10-C11-C12
23	0	305	CHL	CAA-CBA-CGA-O1A
24	6	303	CLA	O1A-CGA-O2A-C1
24	3	309	CLA	C15-C16-C17-C18
23	9	301	CHL	CBA-CGA-O2A-C1
23	8	301	CHL	C3A-C2A-CAA-CBA
23	8	307	CHL	C3A-C2A-CAA-CBA
24	3	312	CLA	C4-C3-C5-C6
24	A	810	CLA	C3A-C2A-CAA-CBA
24	9	303	CLA	O1A-CGA-O2A-C1
24	B	832	CLA	C16-C17-C18-C20
24	B	813	CLA	C2-C3-C5-C6
29	O	203	LMG	C28-C29-C30-C31
24	7	316	CLA	C4C-C3C-CAC-CBC
24	2	309	CLA	C3-C5-C6-C7
24	0	312	CLA	CAA-CBA-CGA-O1A
24	A	824	CLA	CAA-CBA-CGA-O1A
24	B	823	CLA	CAA-CBA-CGA-O1A
24	7	317	CLA	CBA-CGA-O2A-C1
27	5	316	LHG	O6-C4-C5-O7
27	A	842	LHG	C17-C18-C19-C20
23	9	305	CHL	CAA-CBA-CGA-O1A
23	2	305	CHL	C2-C1-O2A-CGA
24	6	316	CLA	C2A-CAA-CBA-CGA
24	A	811	CLA	C2A-CAA-CBA-CGA
24	B	814	CLA	C2A-CAA-CBA-CGA
23	6	302	CHL	C14-C13-C15-C16
24	9	307	CLA	C14-C13-C15-C16
24	A	807	CLA	C11-C12-C13-C14
24	A	853	CLA	C14-C13-C15-C16
24	B	825	CLA	C6-C7-C8-C9
23	9	312	CHL	CAA-CBA-CGA-O1A
24	2	310	CLA	CAA-CBA-CGA-O1A
24	3	308	CLA	CAA-CBA-CGA-O1A
27	7	322	LHG	O10-C23-C24-C25
24	1	302	CLA	CAA-CBA-CGA-O1A
24	A	807	CLA	CAA-CBA-CGA-O1A
24	3	303	CLA	CAA-CBA-CGA-O2A
24	B	822	CLA	C2-C3-C5-C6
24	O	206	CLA	CAD-CBD-CGD-O1D
25	3	317	8CT	C28-C29-C30-C35

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Mol	Chain	Res	Type	Atoms
25	L	204	8CT	C28-C29-C30-C35
25	L	205	8CT	C28-C29-C30-C35
25	M	102	8CT	C28-C29-C30-C35
24	5	302	CLA	CAA-CBA-CGA-O1A
24	A	813	CLA	CAA-CBA-CGA-O1A
27	A	850	LHG	O9-C7-C8-C9
24	B	834	CLA	CAA-CBA-CGA-O2A
24	1	307	CLA	CAA-CBA-CGA-O1A
25	2	314	8CT	C10-C11-C12-C13
24	9	303	CLA	CBA-CGA-O2A-C1
27	7	323	LHG	O9-C7-C8-C9
27	7	324	LHG	O9-C7-C8-C9
27	A	842	LHG	O10-C23-C24-C25
29	A	854	LMG	O9-C10-C11-C12
29	M	101	LMG	C8-C7-O1-C1
29	O	203	LMG	C8-C7-O1-C1
29	A	851	LMG	C11-C12-C13-C14
24	4	311	CLA	O2A-C1-C2-C3
24	B	838	CLA	CAA-CBA-CGA-O1A
24	A	824	CLA	C13-C15-C16-C17
24	2	308	CLA	C2A-CAA-CBA-CGA
24	9	302	CLA	C2A-CAA-CBA-CGA
23	2	301	CHL	CAA-CBA-CGA-O1A
24	2	311	CLA	CAA-CBA-CGA-O1A
24	A	819	CLA	CAA-CBA-CGA-O1A
24	B	809	CLA	CAA-CBA-CGA-O1A
24	H	204	CLA	CAA-CBA-CGA-O1A
27	8	320	LHG	O10-C23-C24-C25
23	6	301	CHL	C10-C11-C12-C13
23	7	302	CHL	CAA-CBA-CGA-O2A
25	B	846	8CT	C23-C24-C25-C26
23	3	307	CHL	CAA-CBA-CGA-O1A
23	7	306	CHL	CAA-CBA-CGA-O1A
24	L	202	CLA	CAA-CBA-CGA-O1A
27	A	842	LHG	O9-C7-C8-C9
24	A	835	CLA	O1D-CGD-O2D-CED
27	3	322	LHG	C26-C27-C28-C29
24	B	804	CLA	C16-C17-C18-C20
23	6	302	CHL	CAD-CBD-CGD-O2D
24	6	310	CLA	CAD-CBD-CGD-O2D
24	6	311	CLA	CAD-CBD-CGD-O2D
24	7	311	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	A	812	CLA	CAD-CBD-CGD-O2D
24	B	802	CLA	CAD-CBD-CGD-O2D
24	B	814	CLA	CAD-CBD-CGD-O2D
24	K	104	CLA	CAD-CBD-CGD-O2D
24	4	311	CLA	CAD-CBD-CGD-O2D
23	4	306	CHL	C2-C1-O2A-CGA
23	1	301	CHL	CAA-CBA-CGA-O1A
24	8	312	CLA	CAA-CBA-CGA-O1A
24	A	804	CLA	CAA-CBA-CGA-O1A
27	0	317	LHG	O10-C23-C24-C25
27	7	323	LHG	O6-C4-C5-C6
24	B	810	CLA	C4C-C3C-CAC-CBC
29	A	854	LMG	O6-C1-O1-C7
24	G	101	CLA	C2-C1-O2A-CGA
24	2	313	CLA	CAA-CBA-CGA-O2A
23	8	307	CHL	CAA-CBA-CGA-O1A
24	7	314	CLA	CAA-CBA-CGA-O1A
23	6	307	CHL	CAA-CBA-CGA-O2A
24	6	311	CLA	CAA-CBA-CGA-O2A
23	1	301	CHL	C1A-C2A-CAA-CBA
24	A	807	CLA	C16-C17-C18-C20
24	A	832	CLA	CAA-CBA-CGA-O1A
27	3	322	LHG	O10-C23-C24-C25
24	H	202	CLA	C5-C6-C7-C8
24	3	311	CLA	CAA-CBA-CGA-O2A
24	7	308	CLA	CAA-CBA-CGA-O2A
24	7	312	CLA	CAA-CBA-CGA-O2A
27	9	316	LHG	O8-C23-C24-C25
23	0	302	CHL	CAA-CBA-CGA-O1A
24	1	309	CLA	CBD-CGD-O2D-CED
23	4	302	CHL	CAA-CBA-CGA-O2A
24	A	808	CLA	CAA-CBA-CGA-O2A
24	B	812	CLA	CAA-CBA-CGA-O2A
24	B	841	CLA	CAA-CBA-CGA-O2A
27	1	317	LHG	O8-C23-C24-C25
27	I	102	LHG	O8-C23-C24-C25
24	3	313	CLA	CAA-CBA-CGA-O2A
24	B	834	CLA	CAA-CBA-CGA-O1A
24	K	103	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

268 monomers are involved in 685 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	1	306	CHL	4	0
34	B	849	DGD	3	0
24	9	302	CLA	4	0
23	7	302	CHL	3	0
24	7	309	CLA	3	0
24	A	837	CLA	3	0
24	3	312	CLA	2	0
24	5	310	CLA	2	0
24	8	310	CLA	1	0
23	7	306	CHL	4	0
23	7	305	CHL	4	0
24	B	809	CLA	10	0
24	1	311	CLA	8	0
24	B	818	CLA	11	0
24	A	853	CLA	8	0
23	7	301	CHL	3	0
31	A	841	PQN	4	0
24	A	818	CLA	4	0
24	A	826	CLA	3	0
24	B	827	CLA	4	0
31	B	842	PQN	1	0
24	A	825	CLA	2	0
23	2	312	CHL	6	0
23	3	301	CHL	1	0
23	6	308	CHL	3	0
24	B	814	CLA	7	0
24	H	204	CLA	1	0
24	B	813	CLA	4	0
27	A	850	LHG	3	0
24	A	802	CLA	3	0
24	3	306	CLA	2	0
26	4	317	0UR	3	0
24	B	817	CLA	8	0
24	3	315	CLA	1	0
23	5	306	CHL	2	0
24	A	820	CLA	6	0
24	A	828	CLA	4	0
23	8	309	CHL	2	0
26	1	315	0UR	1	0
24	B	806	CLA	6	0
24	1	302	CLA	2	0
27	3	324	LHG	3	0
24	A	806	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	316	8CT	1	0
27	3	322	LHG	3	0
23	5	305	CHL	1	0
23	6	302	CHL	2	0
24	5	303	CLA	2	0
24	A	812	CLA	7	0
24	A	824	CLA	5	0
24	L	202	CLA	5	0
24	B	810	CLA	4	0
24	O	209	CLA	1	0
27	0	317	LHG	2	0
25	J	104	8CT	1	0
24	4	304	CLA	1	0
24	H	202	CLA	3	0
24	B	829	CLA	3	0
23	3	302	CHL	3	0
23	5	304	CHL	4	0
24	4	311	CLA	4	0
23	4	307	CHL	3	0
24	B	840	CLA	1	0
23	8	307	CHL	1	0
24	5	307	CLA	2	0
24	0	310	CLA	2	0
24	B	819	CLA	4	0
24	3	304	CLA	1	0
26	2	315	0UR	3	0
24	3	314	CLA	3	0
24	4	314	CLA	1	0
23	3	307	CHL	5	0
24	F	302	CLA	1	0
27	B	852	LHG	1	0
24	5	311	CLA	3	0
24	6	309	CLA	1	0
24	5	308	CLA	3	0
23	6	306	CHL	2	0
24	6	312	CLA	3	0
24	A	835	CLA	1	0
23	6	315	CHL	1	0
23	2	307	CHL	1	0
24	A	805	CLA	5	0
27	I	102	LHG	4	0
24	0	309	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	826	CLA	3	0
24	B	811	CLA	8	0
24	A	816	CLA	2	0
24	3	309	CLA	4	0
24	6	303	CLA	1	0
24	A	829	CLA	5	0
24	0	312	CLA	2	0
24	B	835	CLA	1	0
23	8	301	CHL	6	0
24	9	310	CLA	2	0
26	5	314	0UR	4	0
25	A	847	8CT	1	0
23	1	301	CHL	4	0
23	6	301	CHL	9	0
24	A	808	CLA	7	0
24	6	311	CLA	1	0
29	9	317	LMG	4	0
24	B	837	CLA	3	0
24	6	316	CLA	4	0
25	L	204	8CT	1	0
26	6	321	0UR	1	0
23	3	305	CHL	1	0
24	A	838	CLA	6	0
23	0	301	CHL	6	0
24	0	307	CLA	1	0
24	A	827	CLA	7	0
23	0	306	CHL	5	0
24	K	102	CLA	3	0
27	1	318	LHG	2	0
23	5	312	CHL	1	0
23	8	308	CHL	4	0
23	0	305	CHL	5	0
24	B	838	CLA	4	0
27	5	316	LHG	1	0
24	A	814	CLA	2	0
27	3	320	LHG	1	0
32	A	852	CL0	8	0
24	1	303	CLA	1	0
23	4	306	CHL	2	0
24	G	102	CLA	1	0
23	4	315	CHL	7	0
24	B	841	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	0	311	CLA	6	0
27	6	322	LHG	5	0
24	B	804	CLA	9	0
24	6	310	CLA	3	0
24	B	839	CLA	5	0
24	F	303	CLA	3	0
23	6	323	CHL	4	0
25	3	323	8CT	1	0
26	O	207	0UR	2	0
24	O	204	CLA	1	0
24	4	310	CLA	2	0
24	1	308	CLA	2	0
24	7	304	CLA	5	0
24	B	822	CLA	4	0
27	A	842	LHG	5	0
23	1	312	CHL	3	0
25	3	316	8CT	1	0
23	7	307	CHL	6	0
23	2	306	CHL	3	0
23	8	314	CHL	3	0
24	9	308	CLA	4	0
24	7	308	CLA	8	0
23	2	305	CHL	2	0
24	6	304	CLA	2	0
24	0	308	CLA	2	0
23	4	313	CHL	3	0
23	6	307	CHL	3	0
24	A	848	CLA	4	0
24	A	836	CLA	3	0
23	0	302	CHL	3	0
26	3	318	0UR	1	0
23	5	301	CHL	5	0
24	2	313	CLA	1	0
24	J	103	CLA	2	0
33	B	803	SF4	1	0
29	A	854	LMG	3	0
24	B	830	CLA	6	0
24	O	201	CLA	4	0
23	8	303	CHL	1	0
24	B	802	CLA	5	0
24	B	816	CLA	2	0
24	2	309	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	840	CLA	4	0
24	A	830	CLA	3	0
24	B	825	CLA	4	0
26	9	314	0UR	2	0
24	1	307	CLA	2	0
24	B	812	CLA	1	0
24	3	308	CLA	1	0
25	B	847	8CT	1	0
24	B	808	CLA	6	0
27	7	323	LHG	3	0
23	9	312	CHL	1	0
24	A	815	CLA	1	0
29	M	101	LMG	1	0
24	8	305	CLA	3	0
25	F	301	8CT	1	0
24	A	821	CLA	2	0
23	6	313	CHL	2	0
29	3	321	LMG	2	0
24	B	831	CLA	3	0
24	L	203	CLA	2	0
24	A	831	CLA	4	0
24	A	807	CLA	7	0
24	0	303	CLA	4	0
24	7	316	CLA	6	0
24	1	310	CLA	2	0
24	3	303	CLA	3	0
24	A	810	CLA	6	0
24	B	801	CLA	1	0
24	4	312	CLA	2	0
23	1	304	CHL	3	0
27	B	851	LHG	1	0
24	A	823	CLA	1	0
24	8	315	CLA	2	0
24	B	805	CLA	4	0
24	B	834	CLA	7	0
29	A	851	LMG	4	0
27	7	322	LHG	2	0
29	J	105	LMG	2	0
24	8	312	CLA	2	0
24	5	313	CLA	1	0
24	G	103	CLA	1	0
24	A	813	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	317	LHG	5	0
23	9	301	CHL	1	0
24	K	104	CLA	2	0
24	A	803	CLA	1	0
24	K	103	CLA	1	0
24	A	839	CLA	5	0
24	7	312	CLA	5	0
24	2	308	CLA	2	0
27	2	317	LHG	2	0
26	8	318	0UR	2	0
24	A	804	CLA	2	0
27	A	843	LHG	3	0
24	9	303	CLA	1	0
24	B	820	CLA	4	0
23	4	302	CHL	2	0
24	7	317	CLA	1	0
24	B	824	CLA	5	0
27	9	316	LHG	5	0
26	0	315	0UR	1	0
24	B	836	CLA	3	0
24	A	801	CLA	2	0
24	A	811	CLA	2	0
29	O	210	LMG	1	0
26	7	320	0UR	2	0
24	B	833	CLA	6	0
24	L	201	CLA	3	0
24	8	313	CLA	3	0
24	9	311	CLA	2	0
24	9	307	CLA	6	0
24	H	201	CLA	2	0
24	A	817	CLA	8	0
24	5	302	CLA	3	0
23	9	305	CHL	1	0
23	6	305	CHL	2	0
24	0	313	CLA	4	0
28	0	318	SQD	2	0
23	8	316	CHL	3	0
24	7	314	CLA	1	0
24	3	313	CLA	1	0
23	1	305	CHL	2	0
23	2	301	CHL	3	0
24	4	309	CLA	5	0

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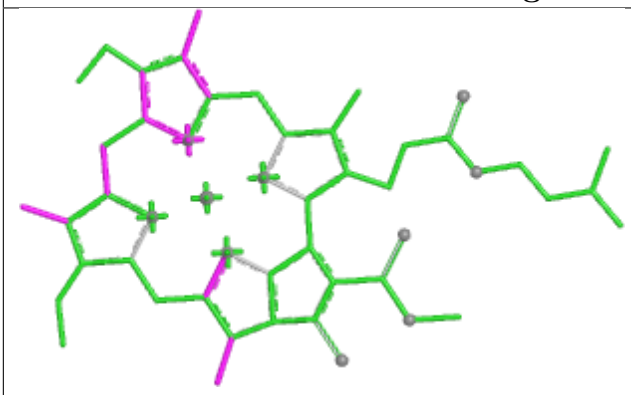
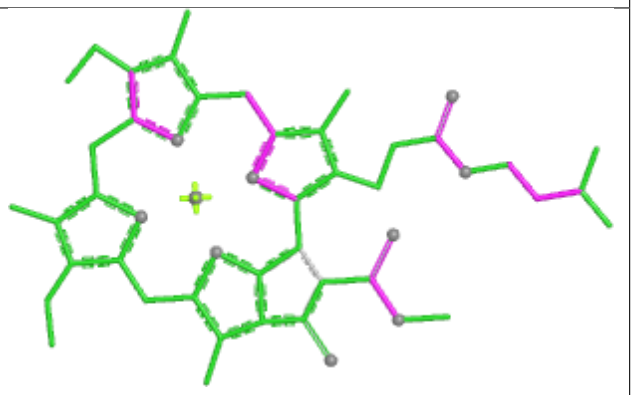
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	832	CLA	3	0
24	B	823	CLA	4	0
29	J	102	LMG	1	0
24	B	828	CLA	3	0
23	4	301	CHL	7	0
23	4	308	CHL	2	0
24	B	807	CLA	1	0
24	O	206	CLA	4	0
25	8	317	8CT	1	0
24	2	311	CLA	2	0
26	9	315	0UR	1	0
23	9	306	CHL	2	0
23	8	306	CHL	3	0
23	4	305	CHL	3	0
24	A	809	CLA	4	0

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.

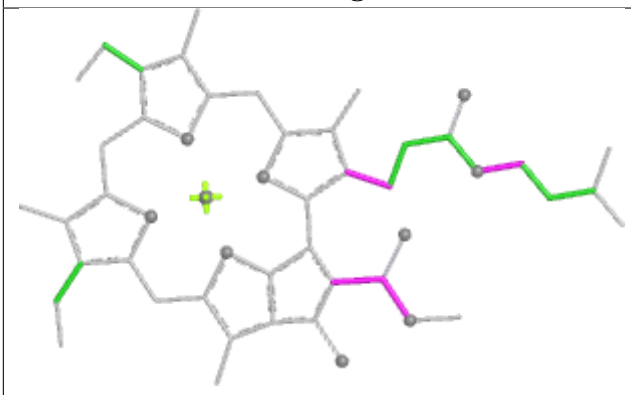
Ligand CLA G 101



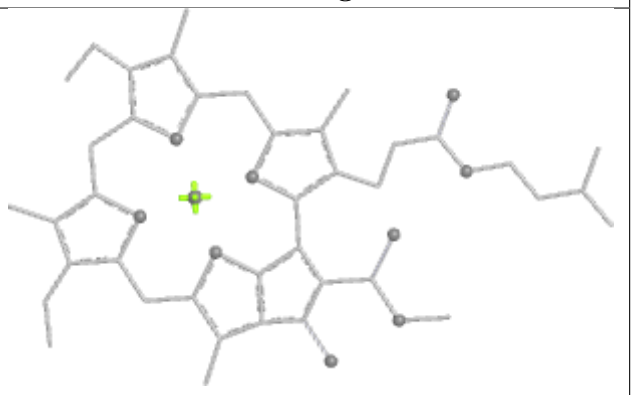
Bond lengths



Bond angles

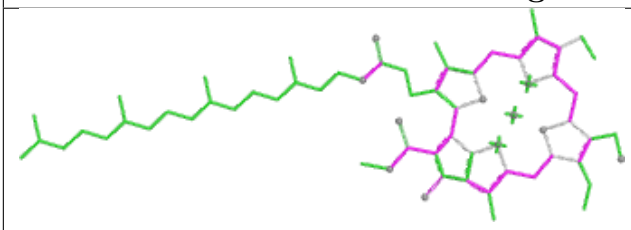


Torsions

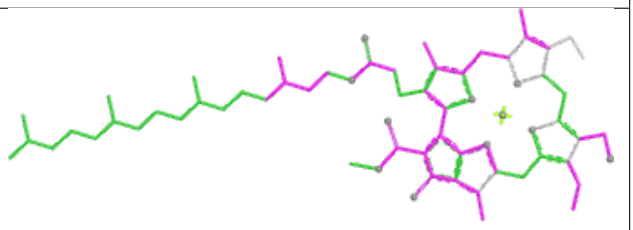


Rings

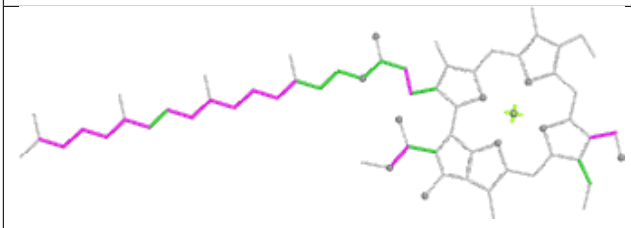
Ligand CHL 1 306



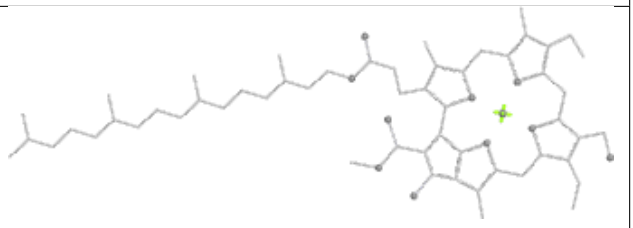
Bond lengths



Bond angles

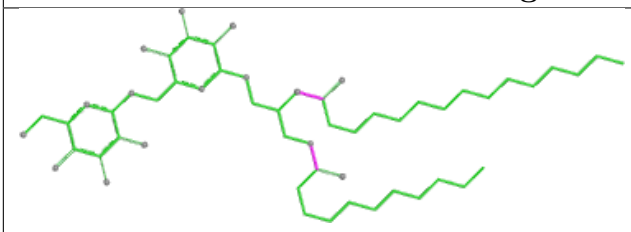


Torsions

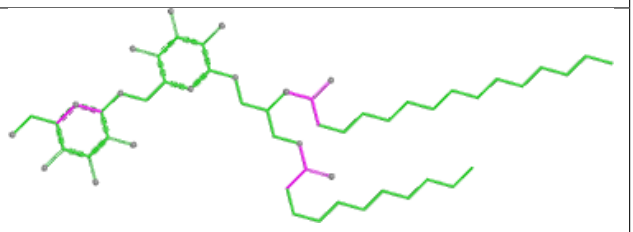


Rings

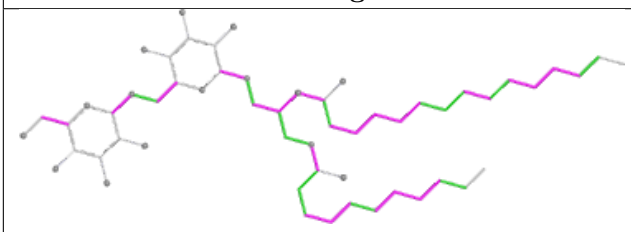
Ligand DGD B 849



Bond lengths



Bond angles



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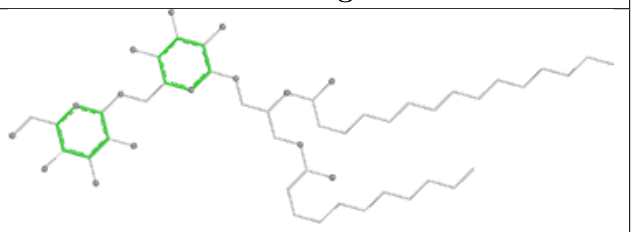
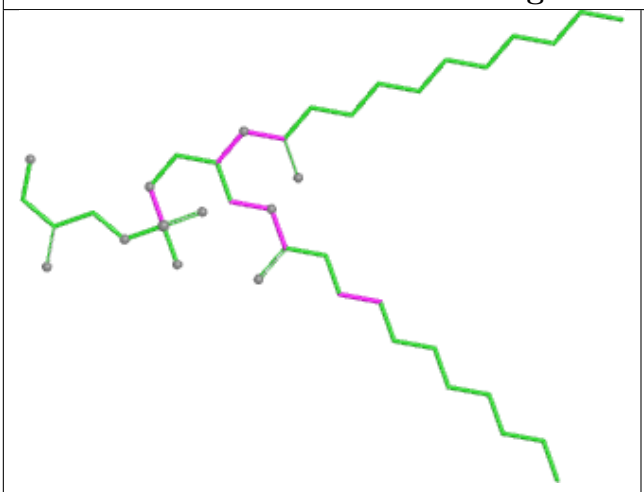
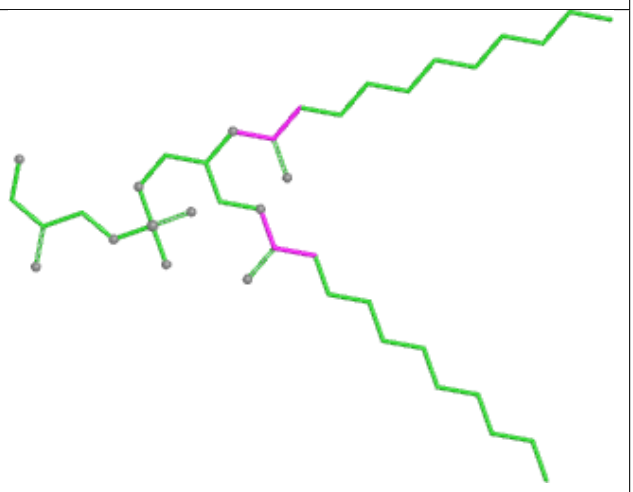


Rings

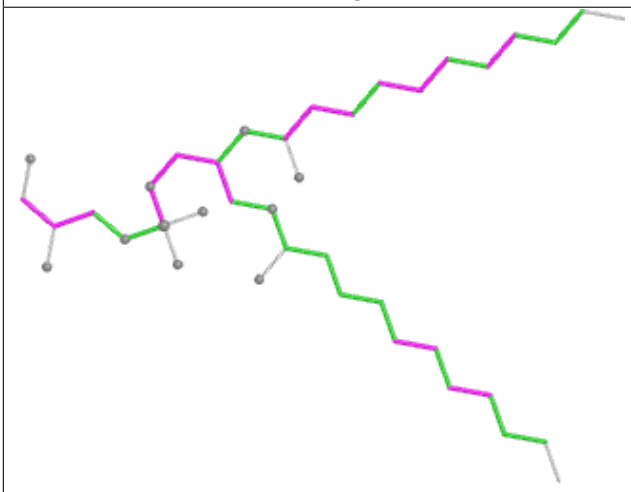
Ligand LHG 7 324



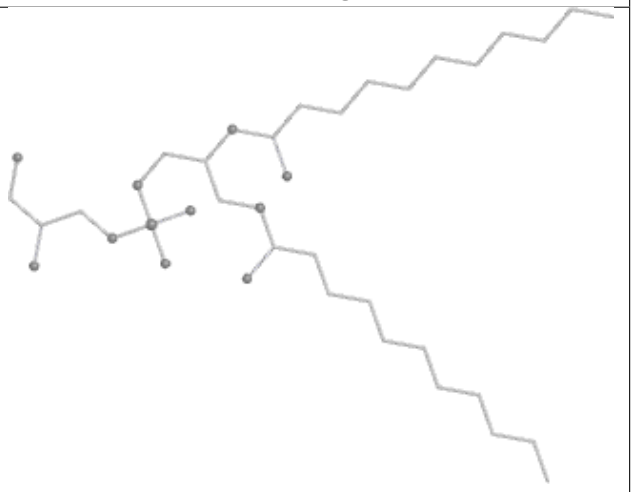
Bond lengths



Bond angles

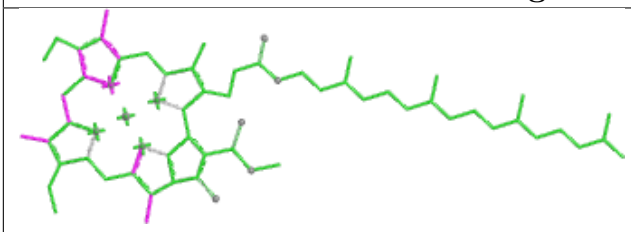


Torsions

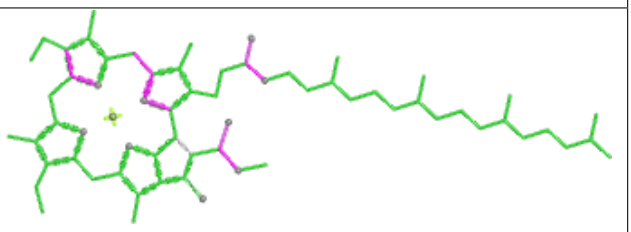


Rings

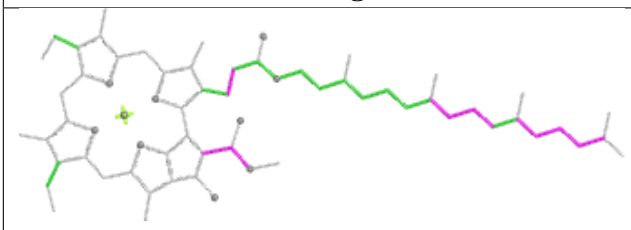
Ligand CLA 9 302



Bond lengths



Bond angles



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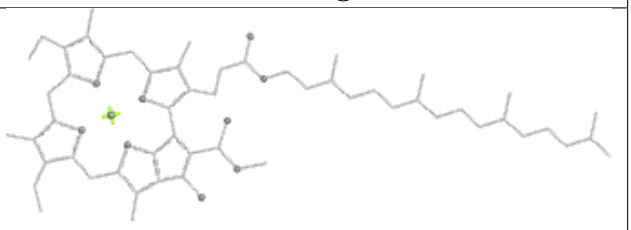
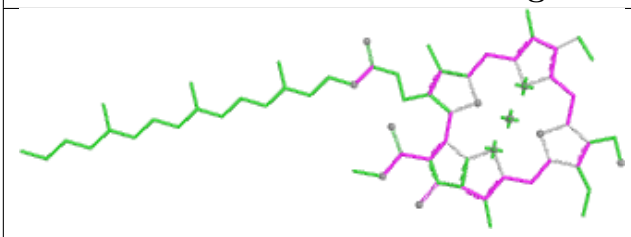
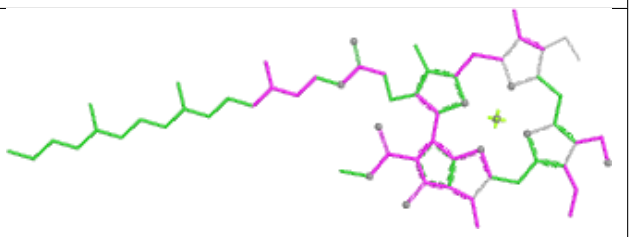


Rings

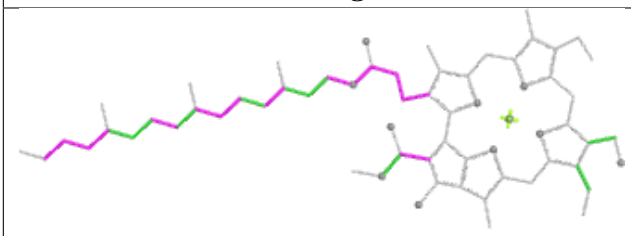
Ligand CHL 7 302



Bond lengths



Bond angles



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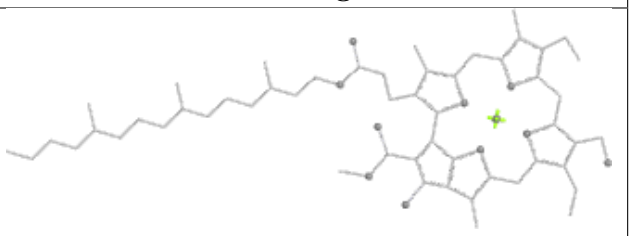

Rings

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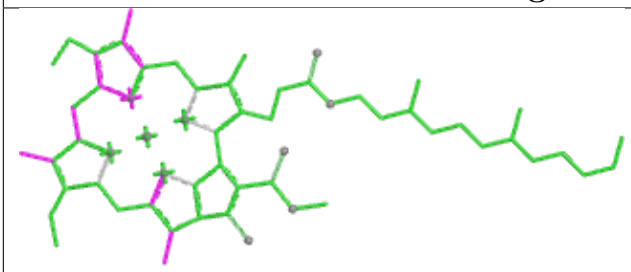
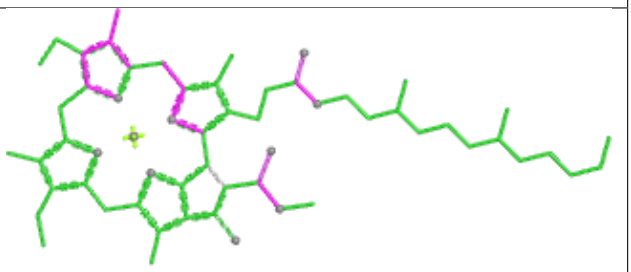
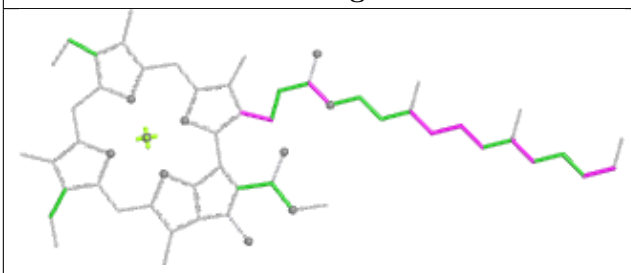
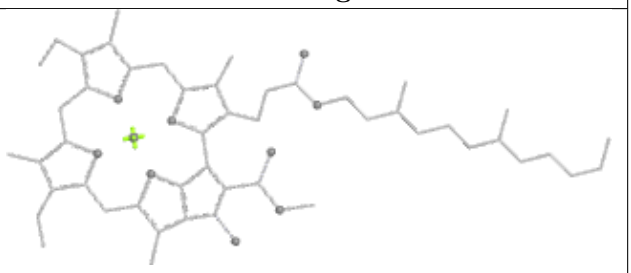
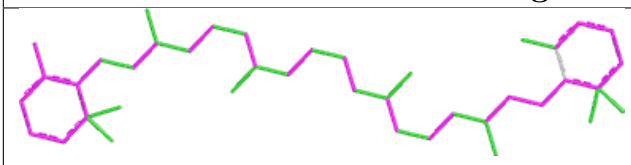
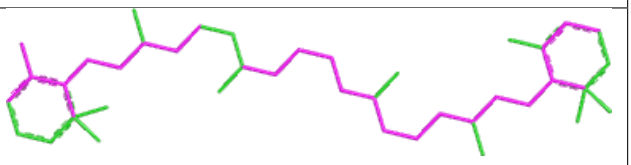
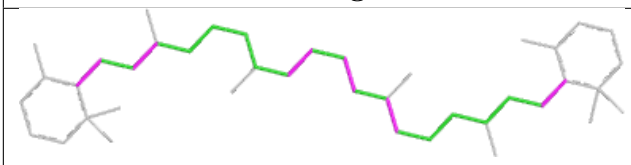
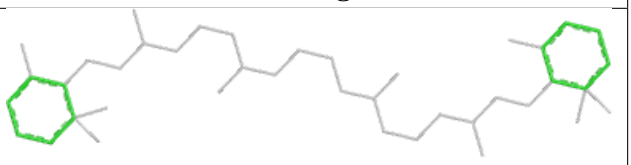
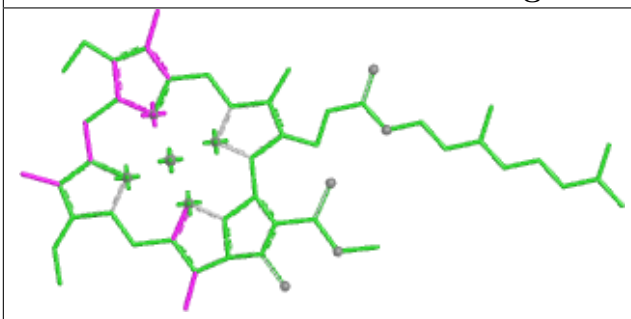
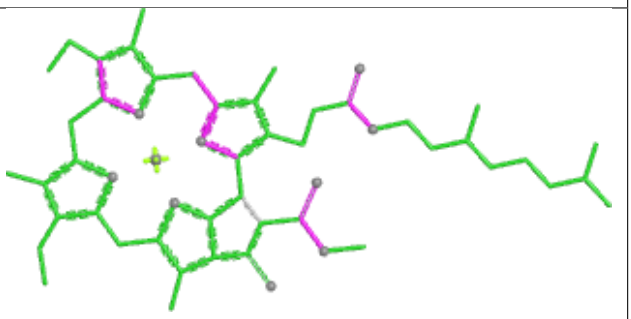
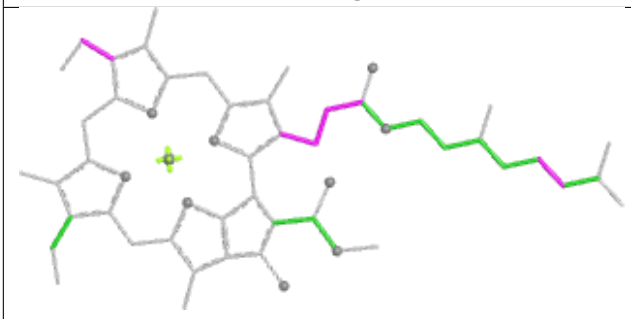
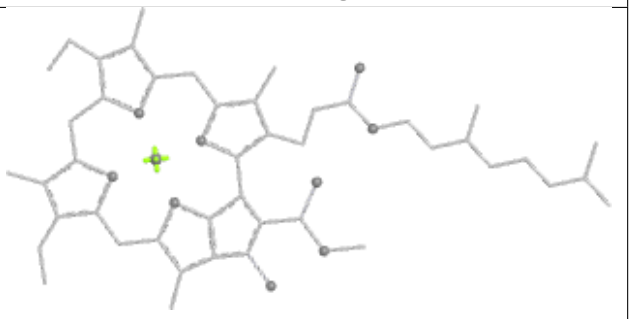
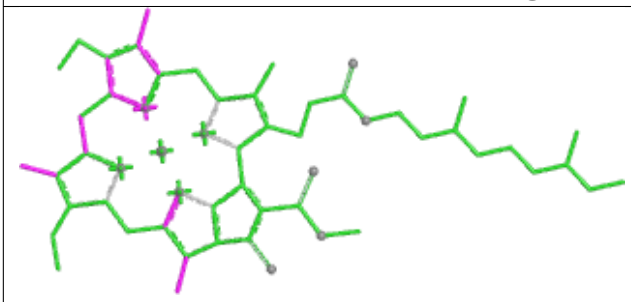
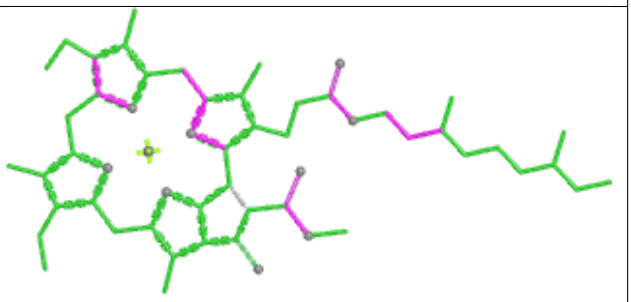
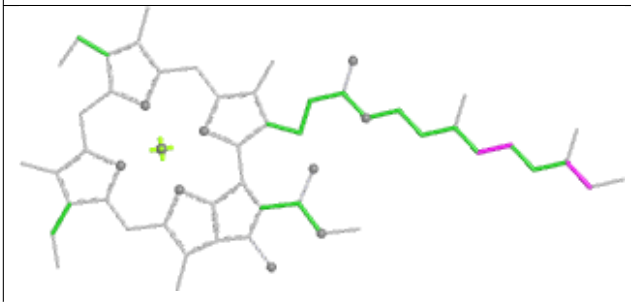
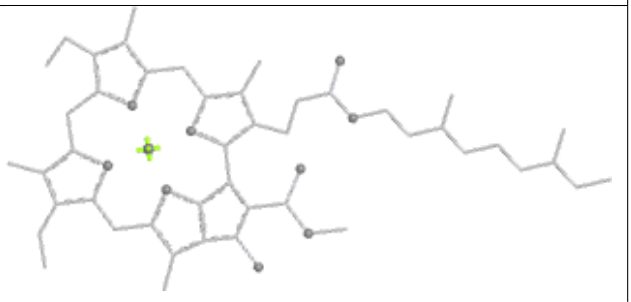
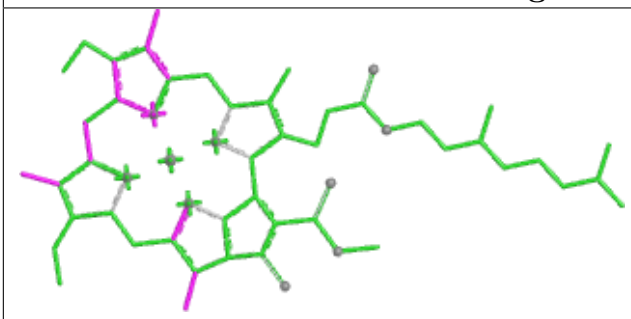
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT 3 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 312



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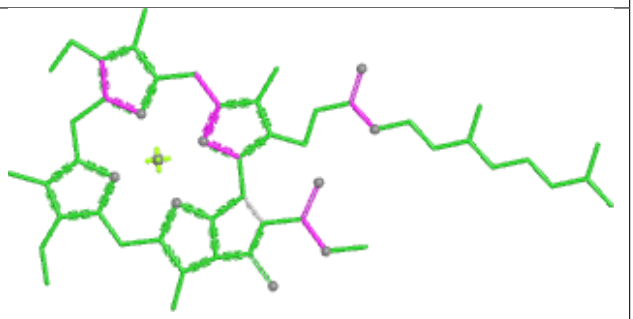

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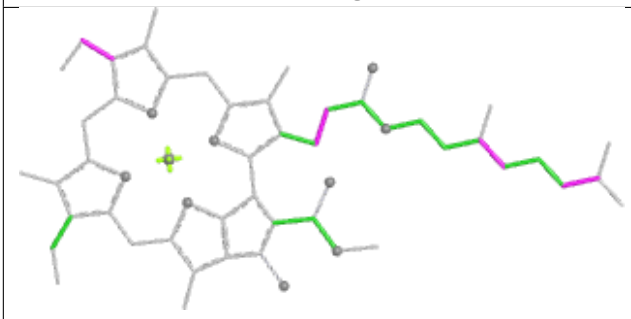
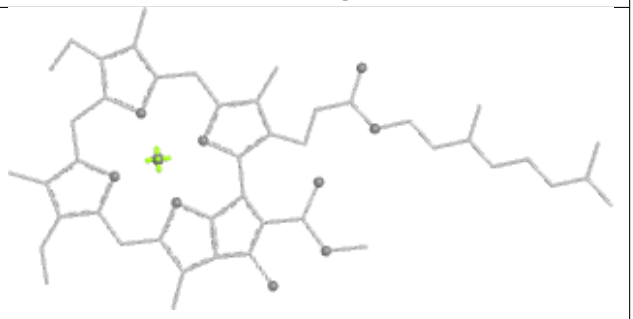
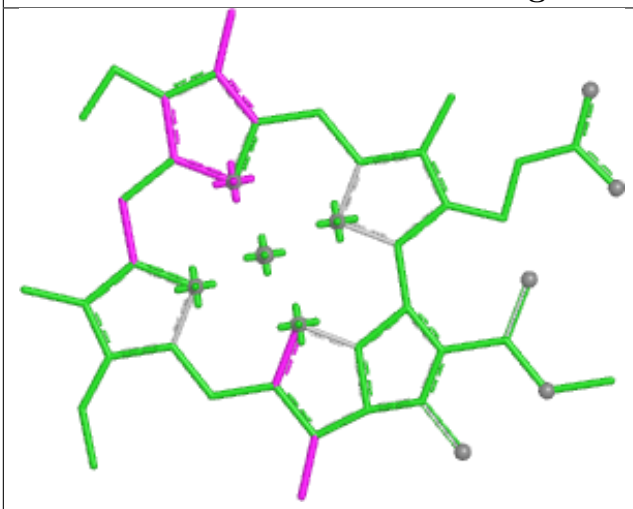


Torsions



Rings

Ligand CLA 5 310



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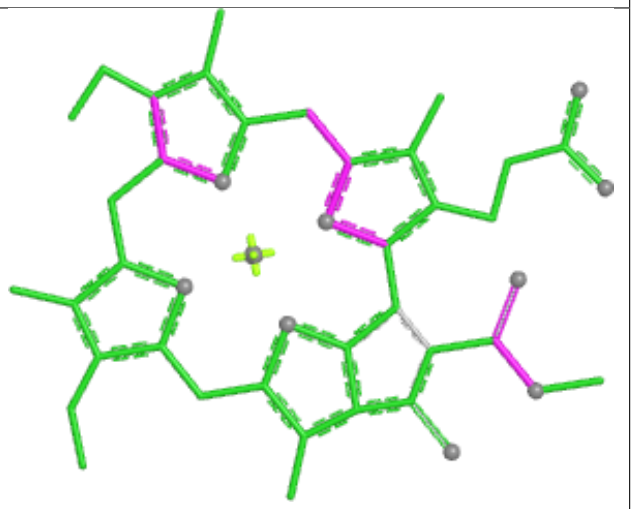

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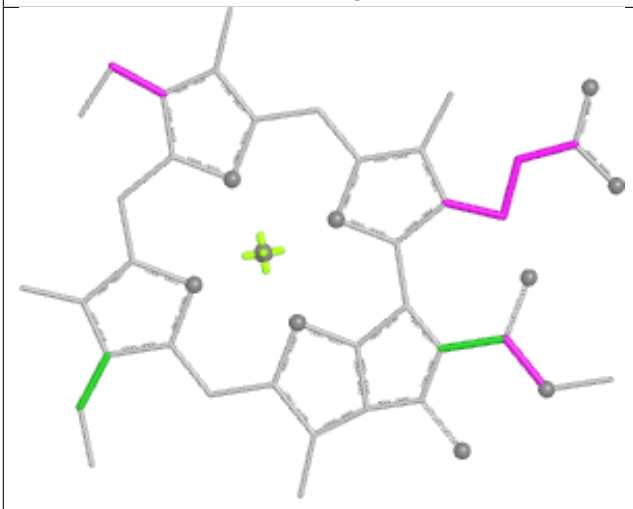

Torsions

Rings

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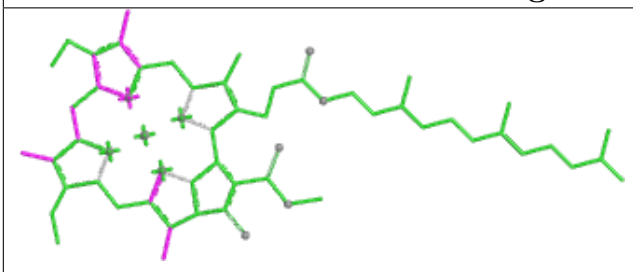

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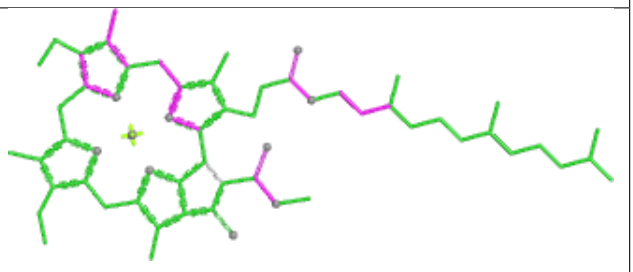

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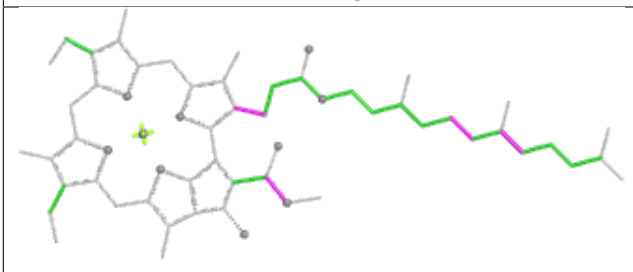

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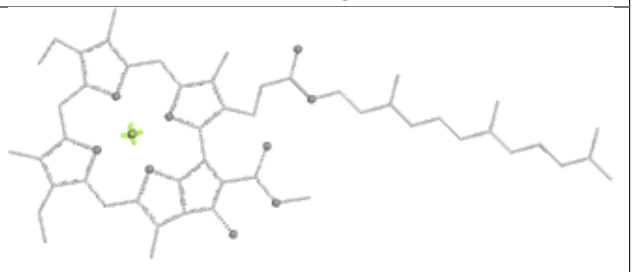
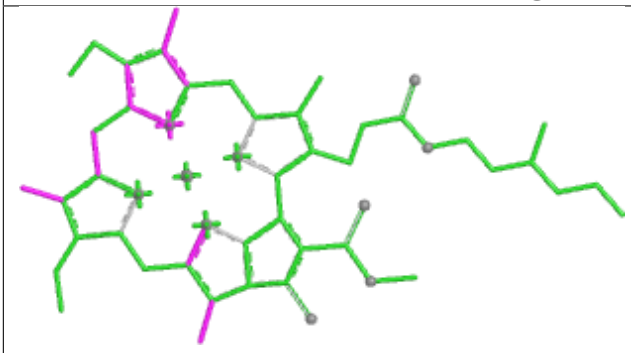


Rings

Ligand CLA 7 311



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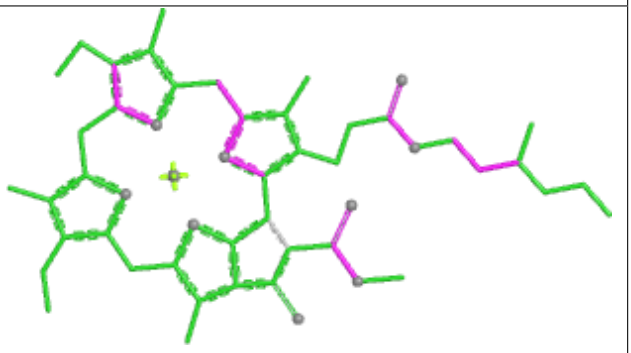

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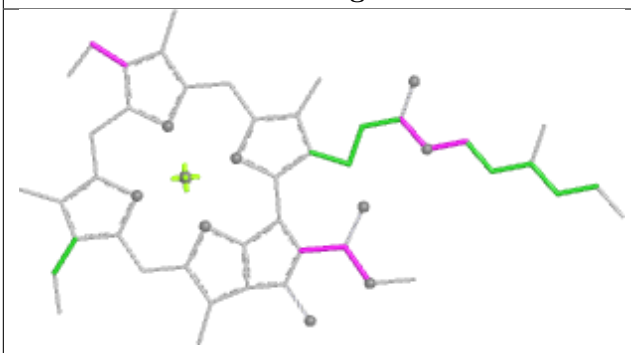

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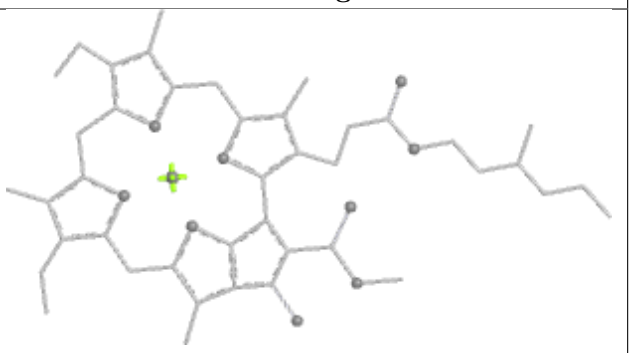
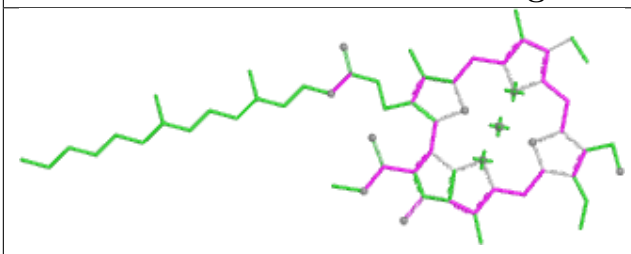


Rings

Ligand CHL 7 306



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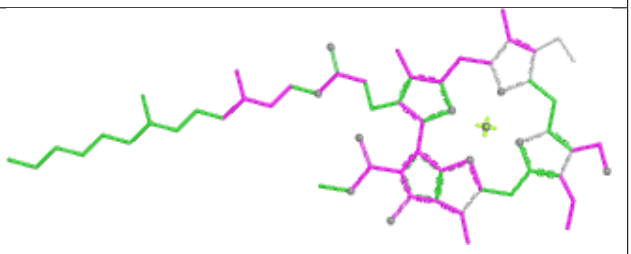

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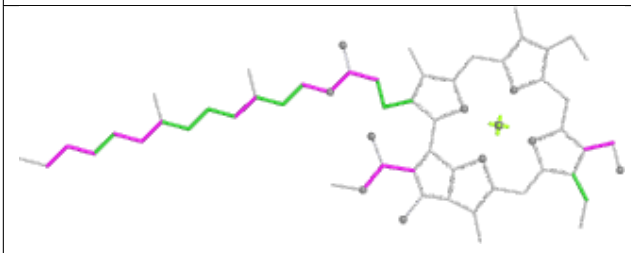

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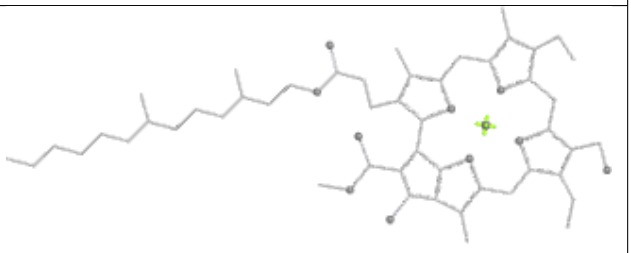

Rings

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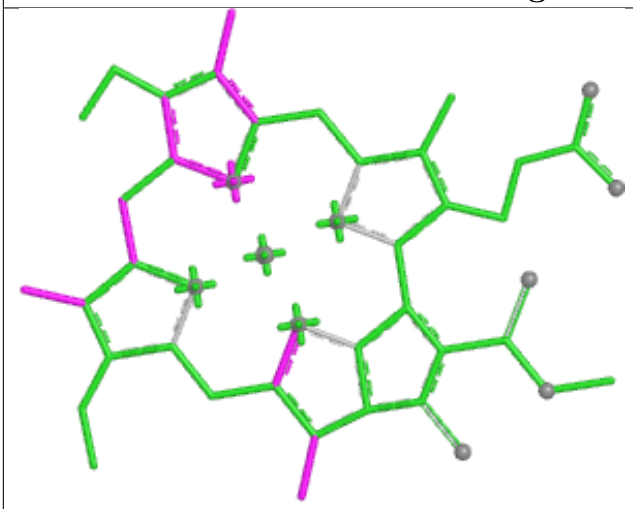

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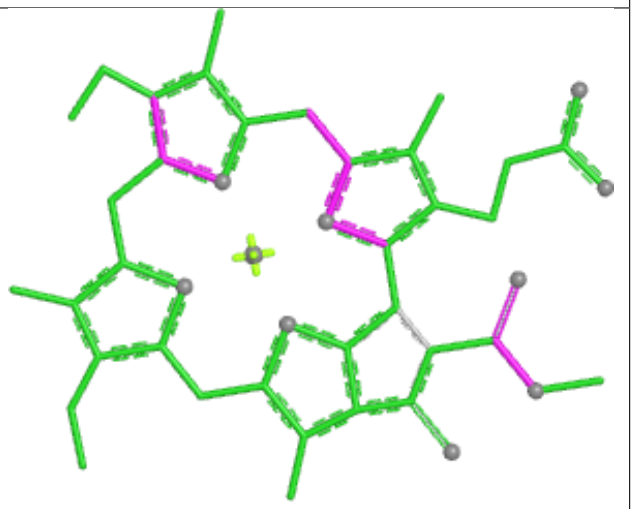
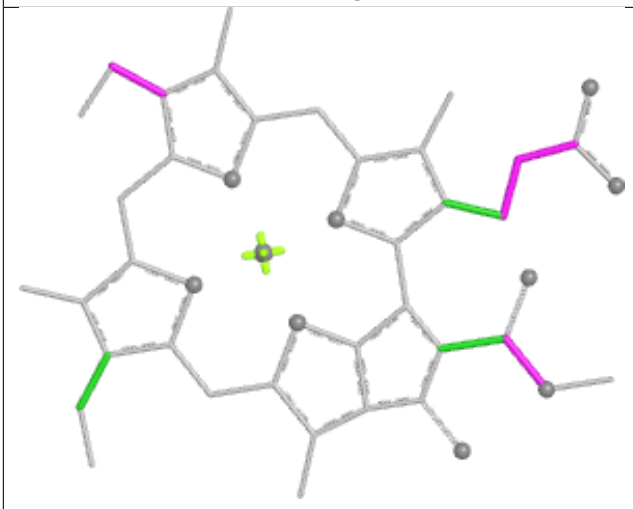


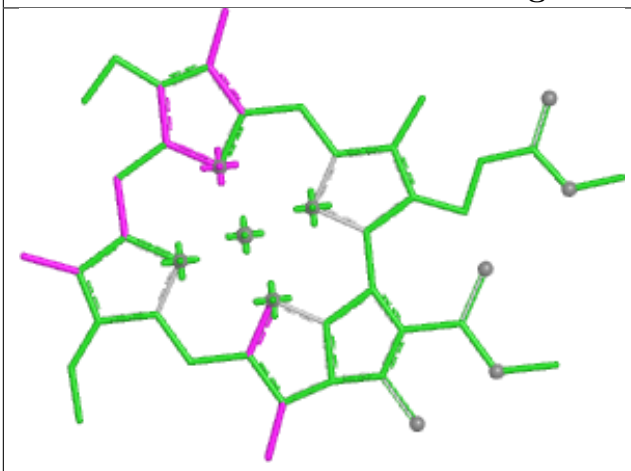
Bond angles



Torsions

Rings

Ligand CLA 8 311



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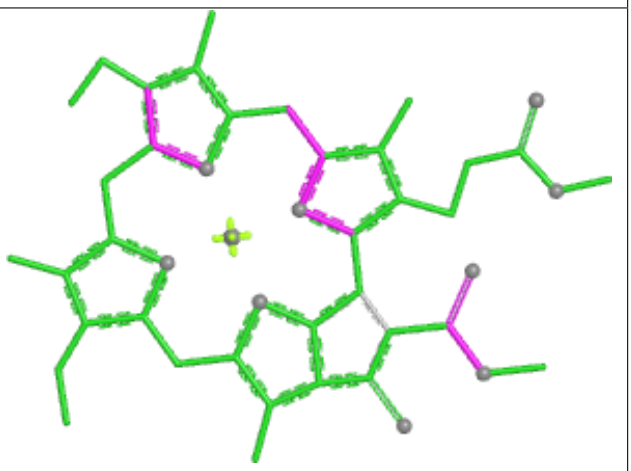

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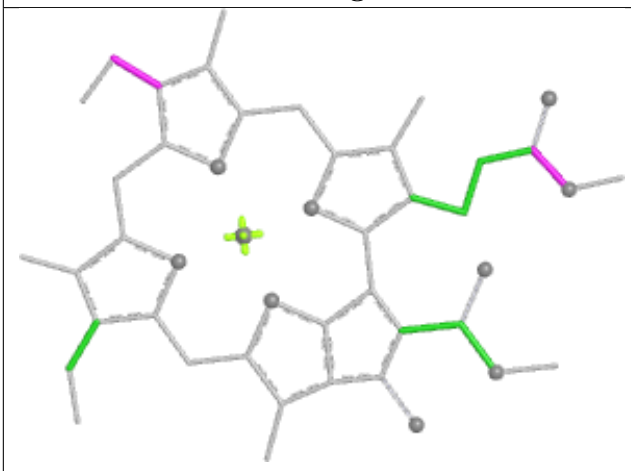

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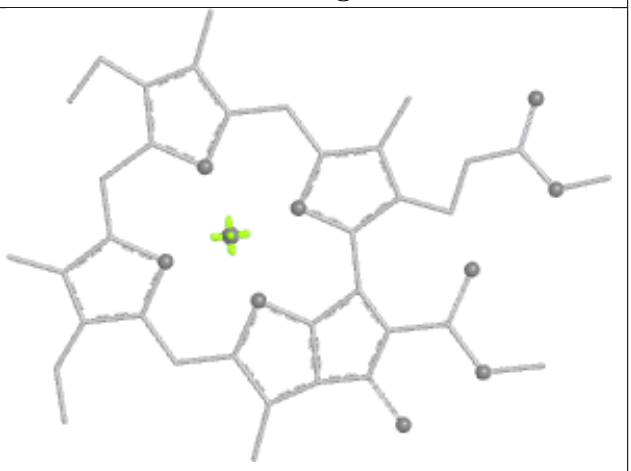
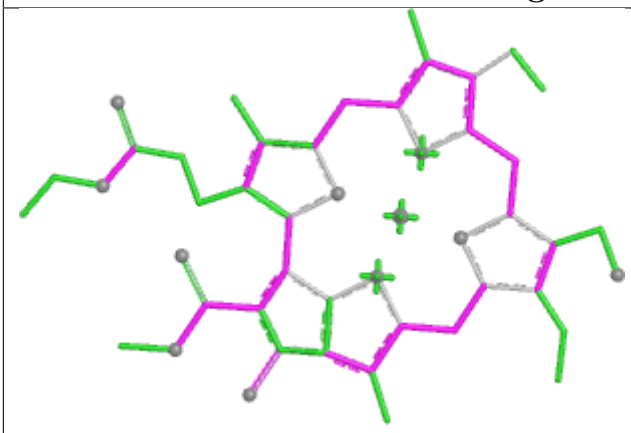


Rings

Ligand CHL 7 305



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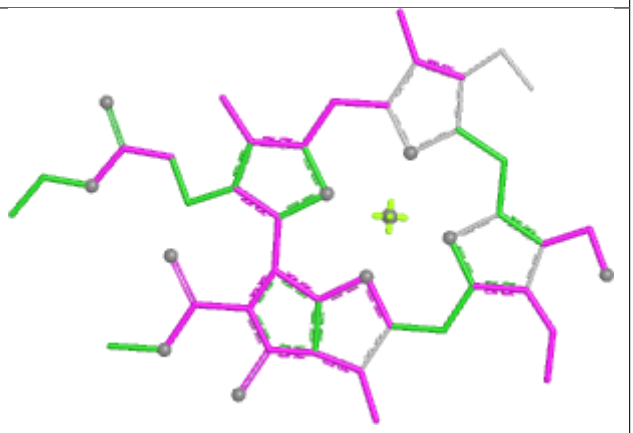
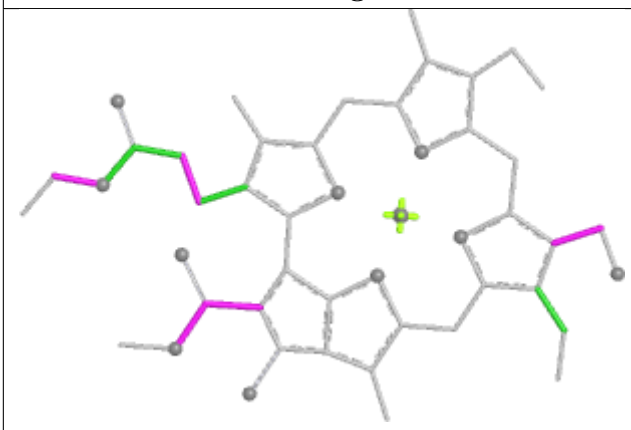


Bond angles



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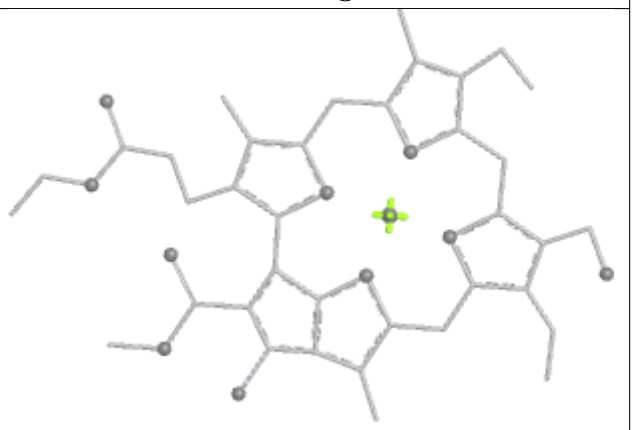
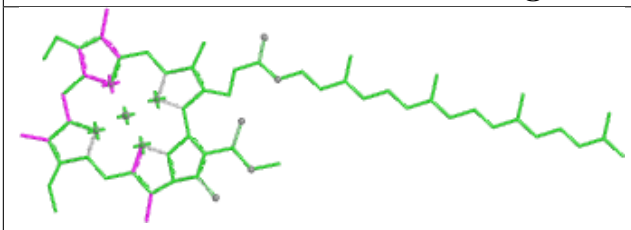


Rings

Ligand CLA B 809



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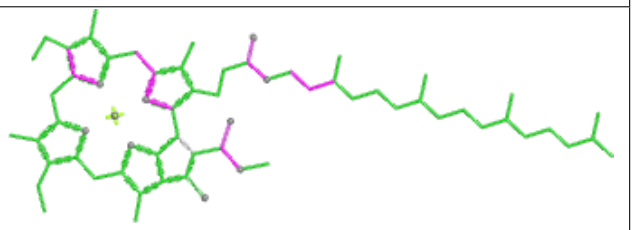
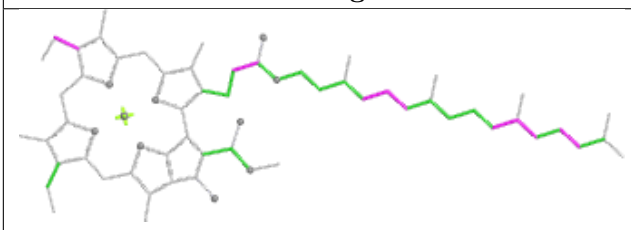


Bond angles



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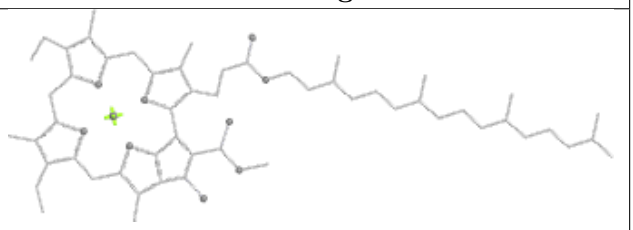
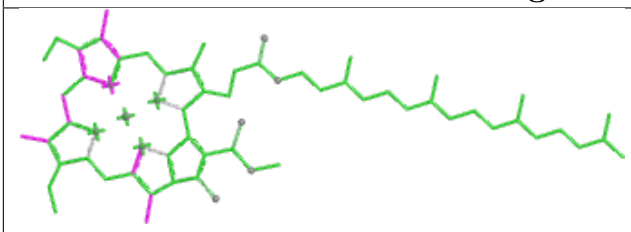
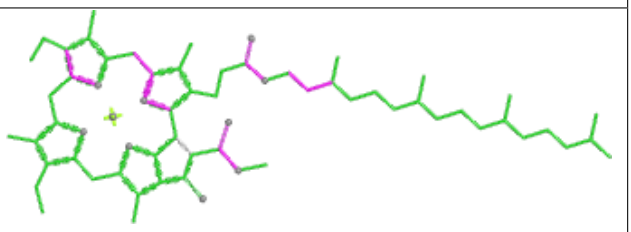
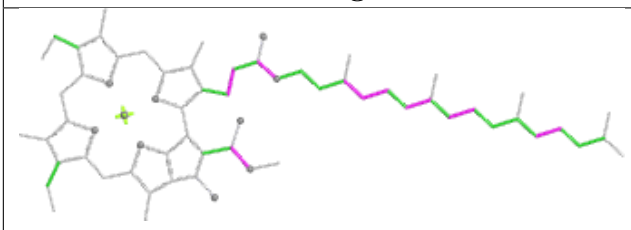
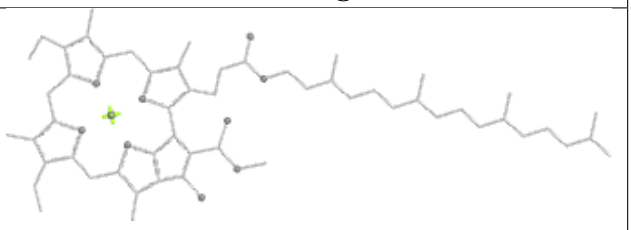
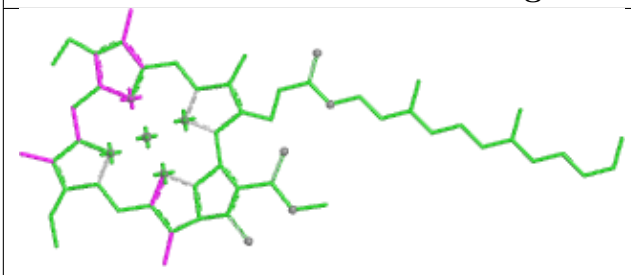
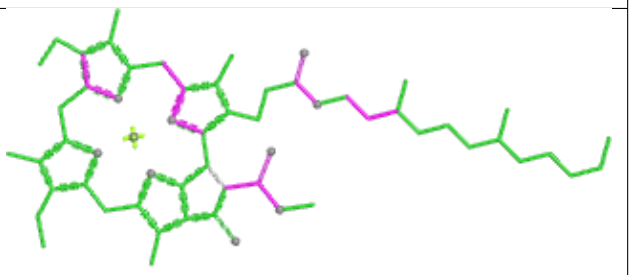
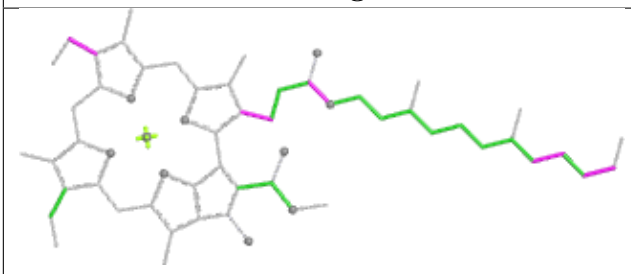
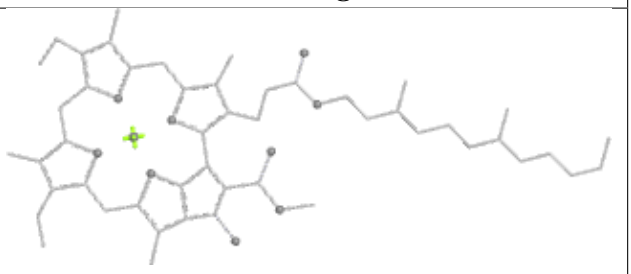
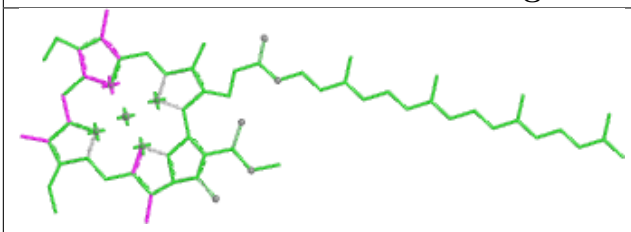


Rings

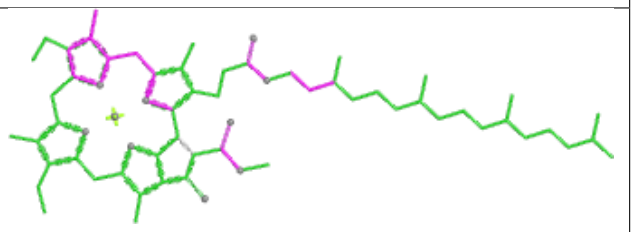
Ligand CLA 1 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

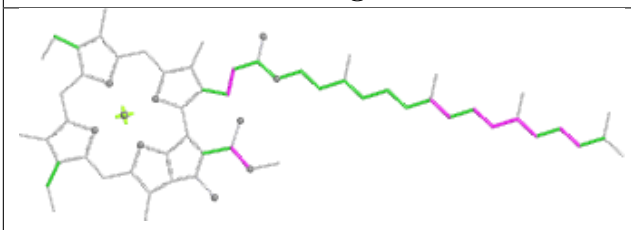
Ligand CLA A 853



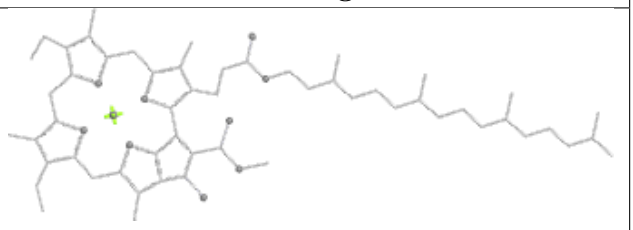
Bond lengths



Bond angles

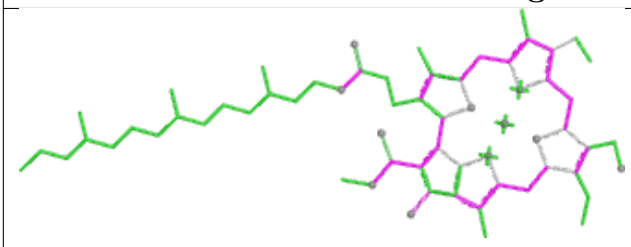


Torsions

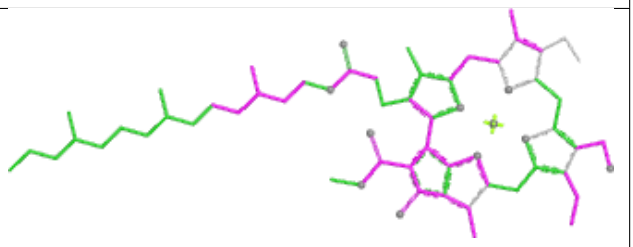


Rings

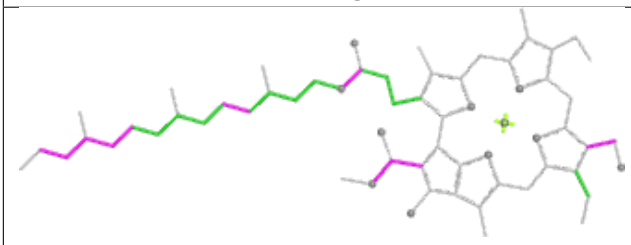
Ligand CHL 7 301



Bond lengths



Bond angles



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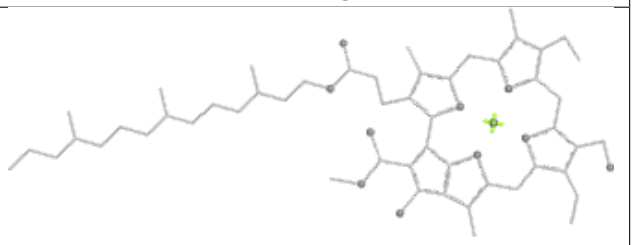
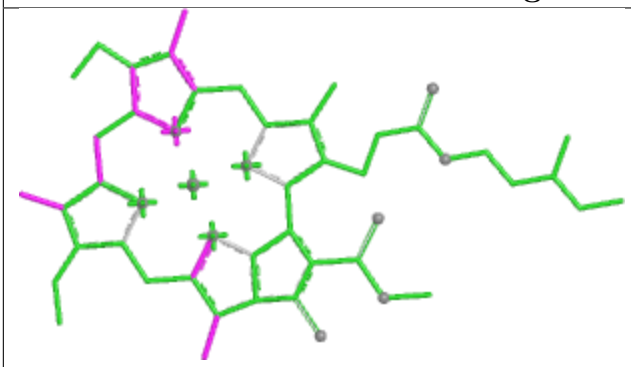


Rings

Ligand CLA A 822



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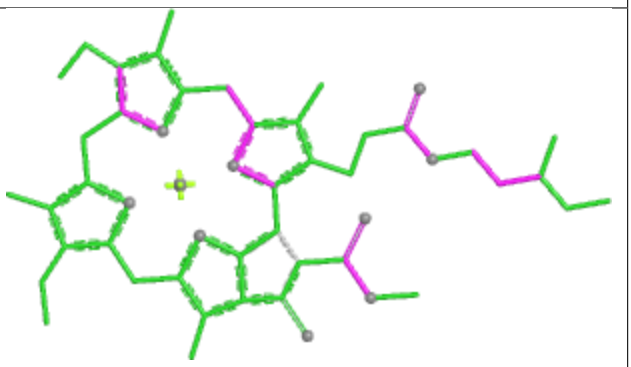
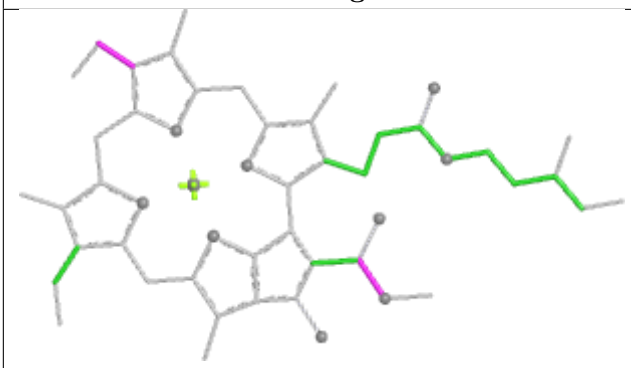


Bond angles



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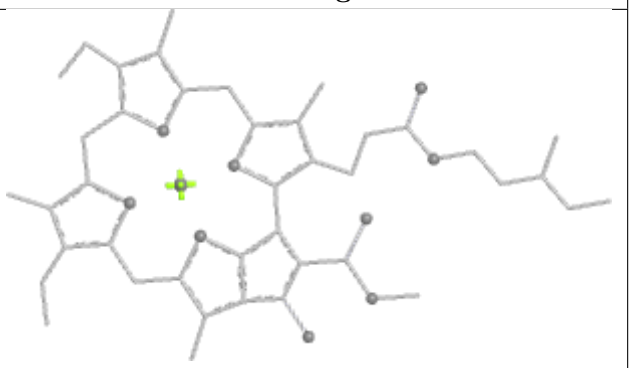
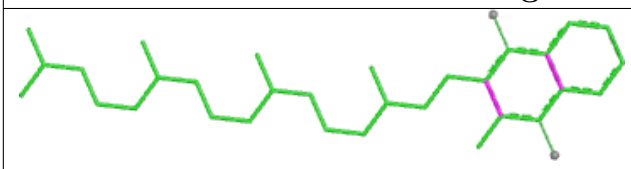


Rings

Ligand PQN A 841



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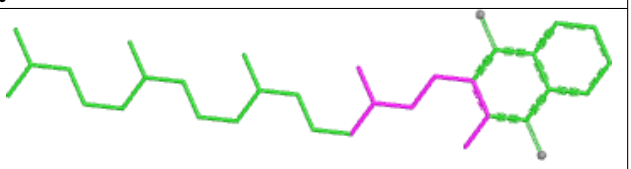
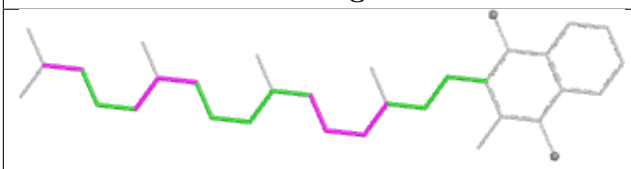


Bond angles



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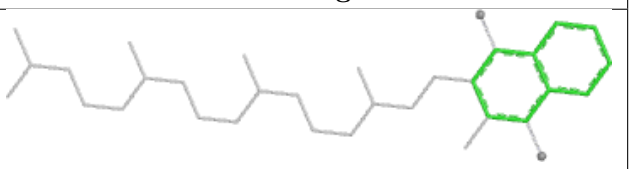
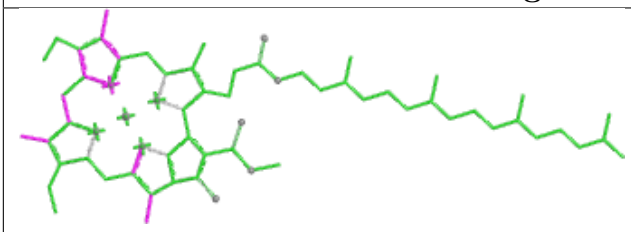


Rings

Ligand CLA A 818



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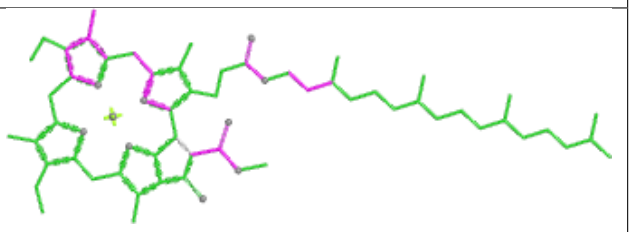
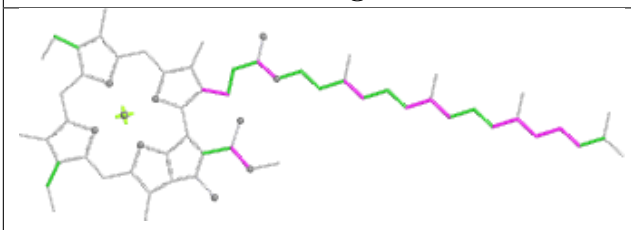


Bond angles



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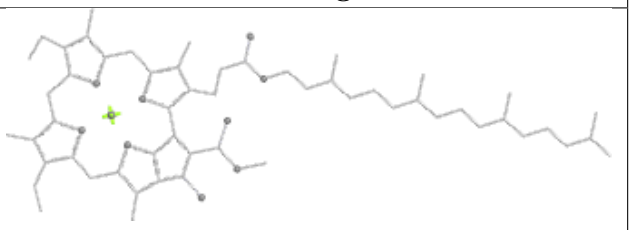
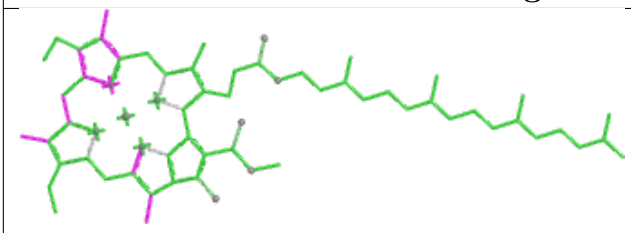


Rings

Ligand CLA A 826



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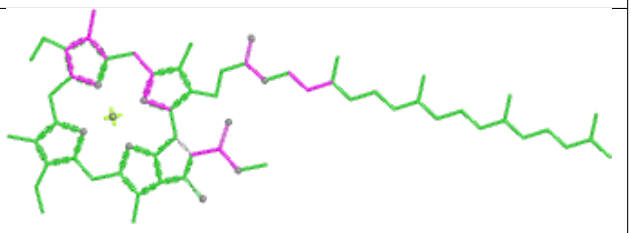
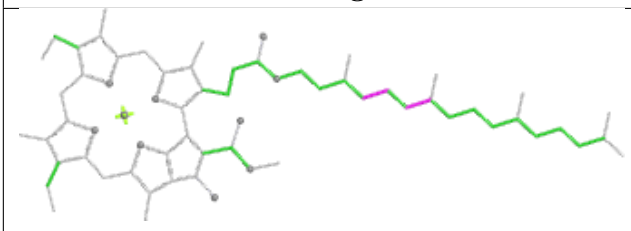


Bond angles



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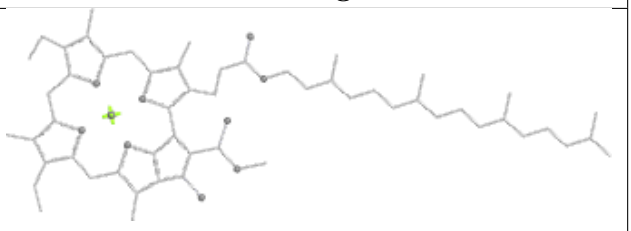
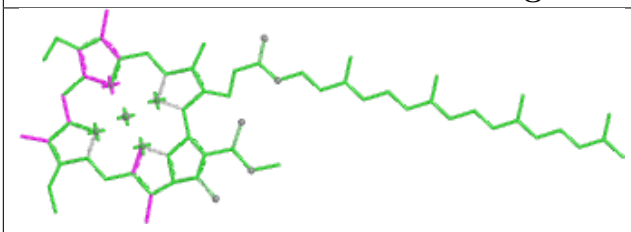


Rings

Ligand CLA B 827



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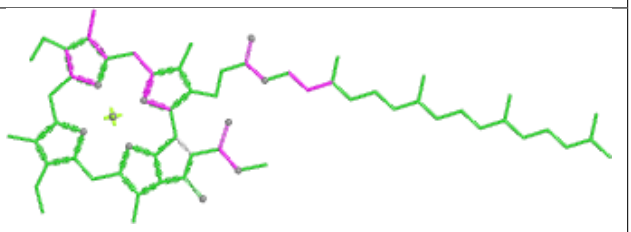
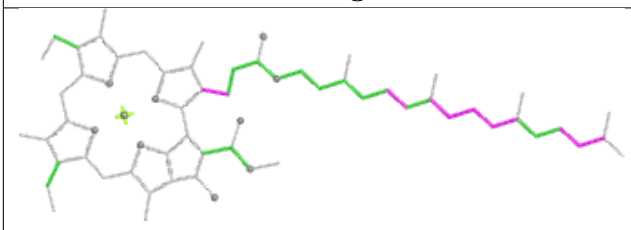


Bond angles



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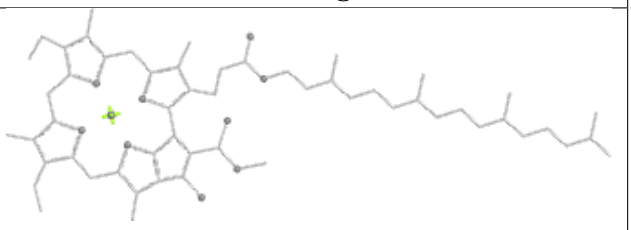
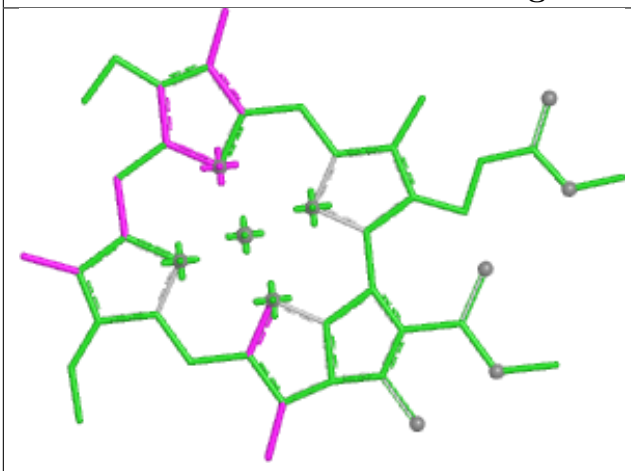


Rings

Ligand CLA 1 313



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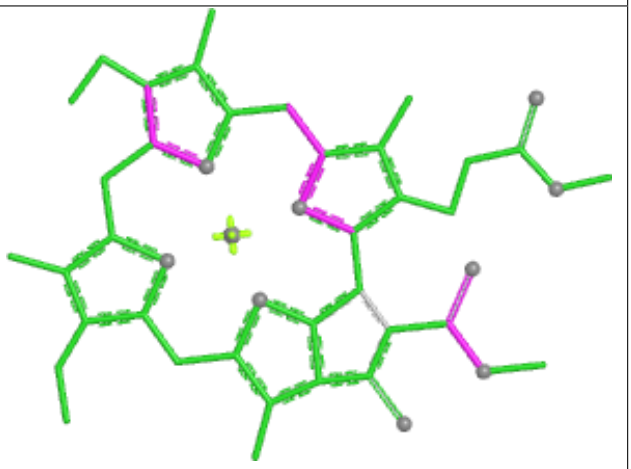

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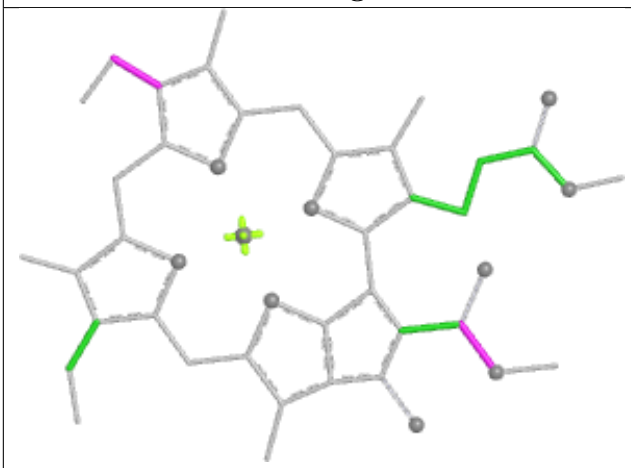

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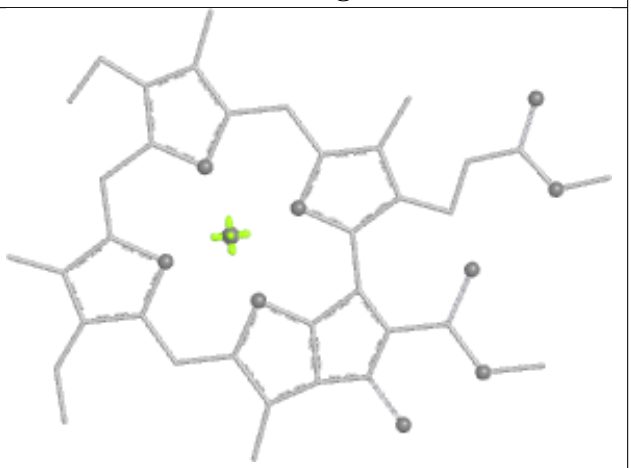
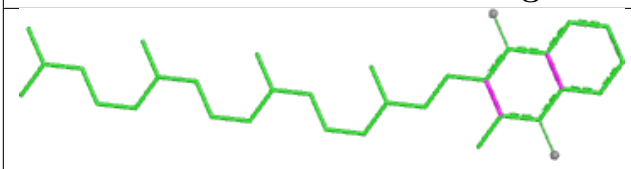
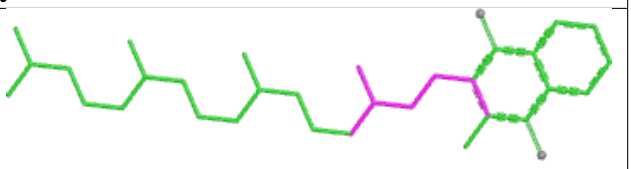


Rings

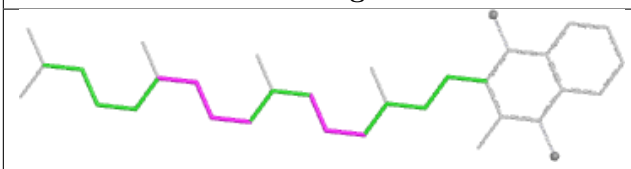
Ligand PQN B 842



Bond lengths



Bond angles



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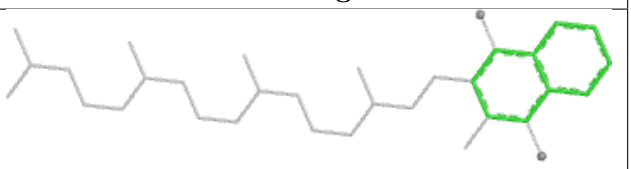
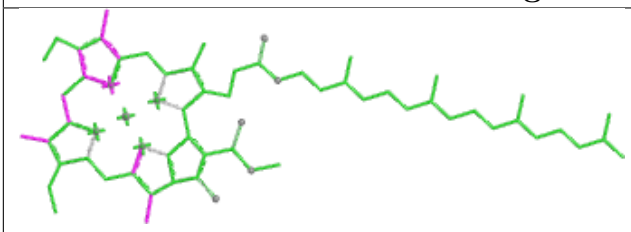


Rings

Ligand CLA A 825



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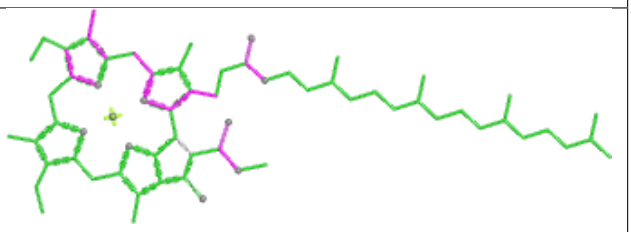
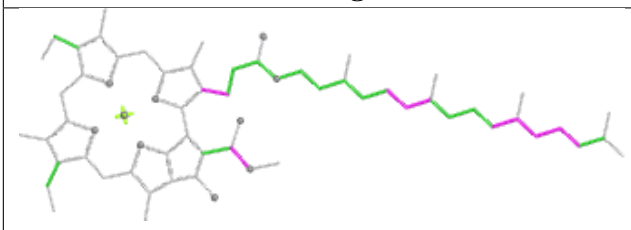


Bond angles



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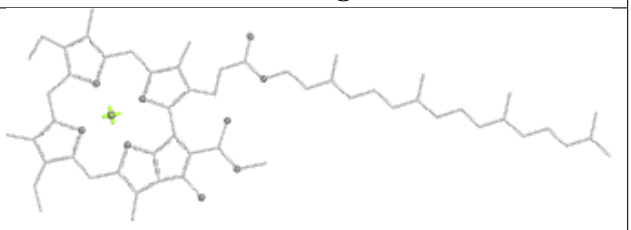
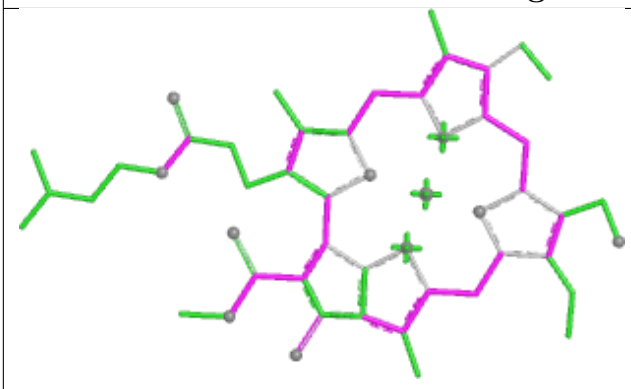


Rings

Ligand CHL 2 312



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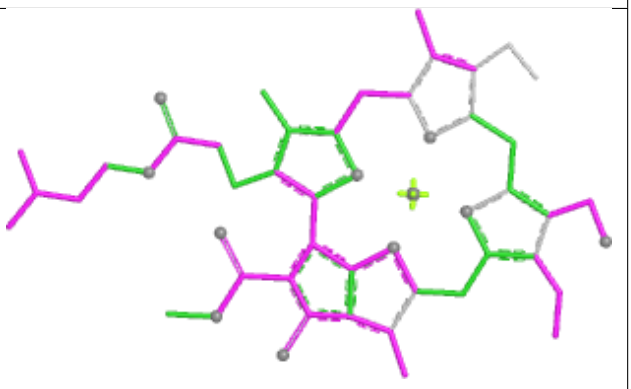
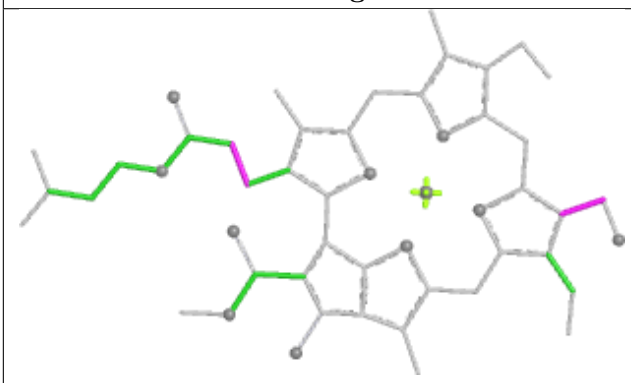


Bond angles



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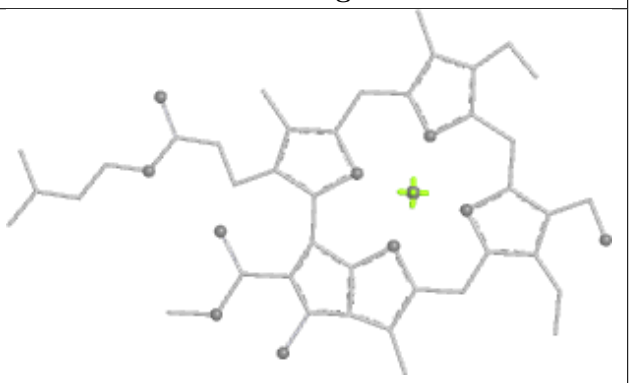
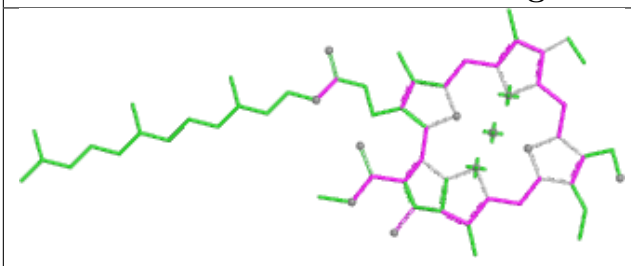
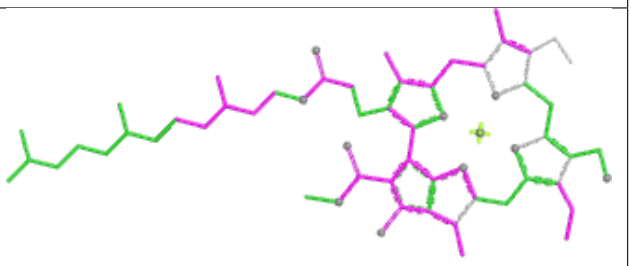
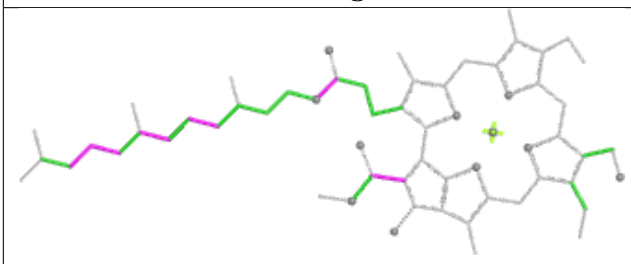
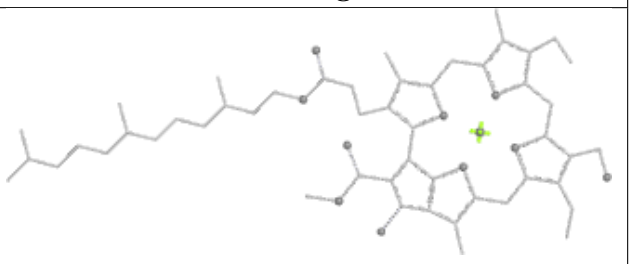
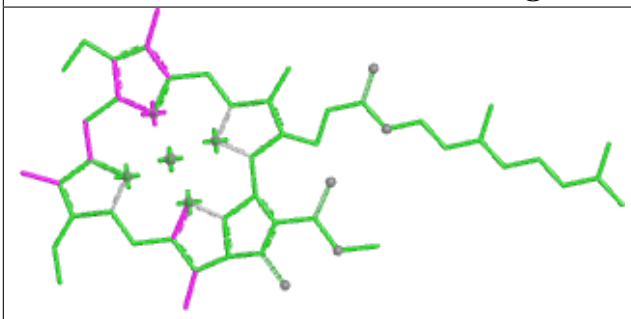
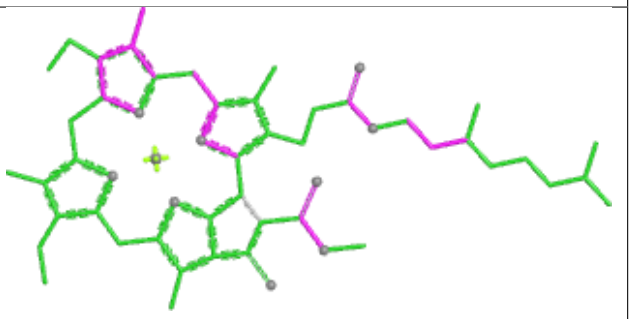
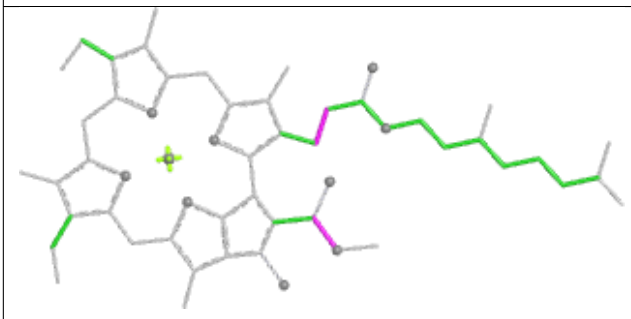
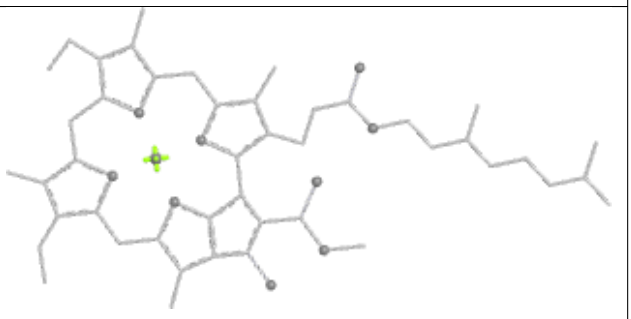
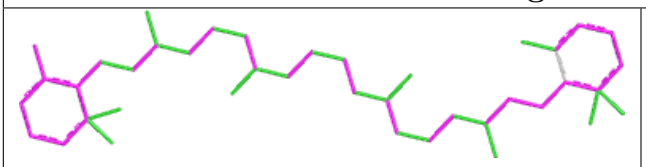


Rings

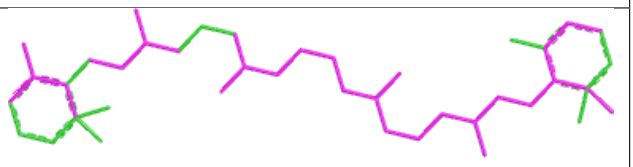
Ligand CHL 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

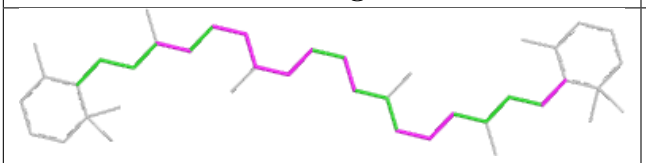
Ligand 8CT B 846



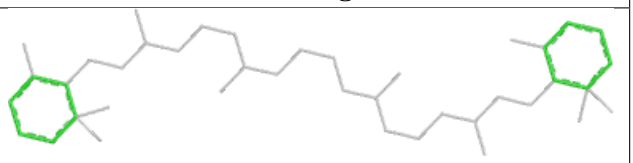
Bond lengths



Bond angles

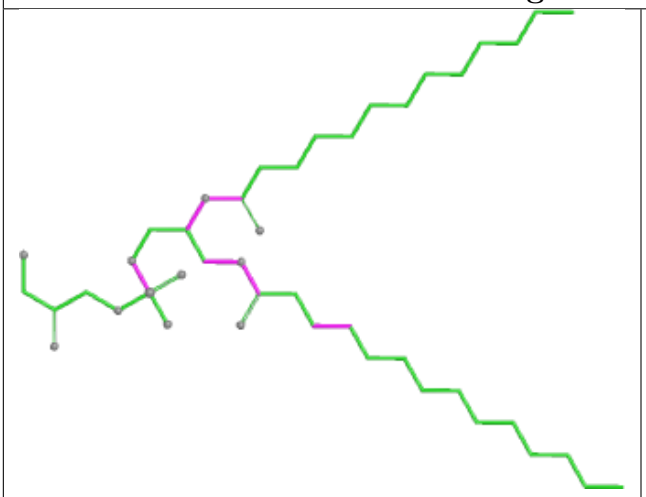


Torsions

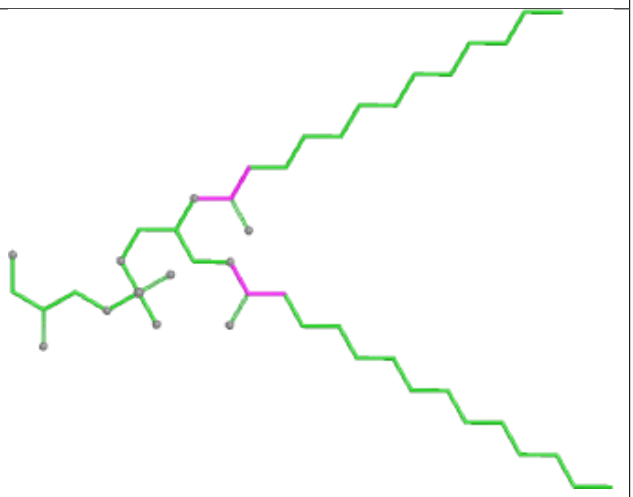


Rings

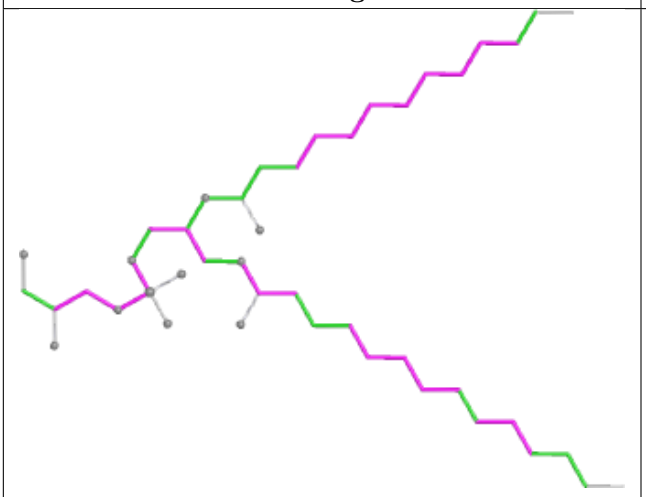
Ligand LHG 8 320



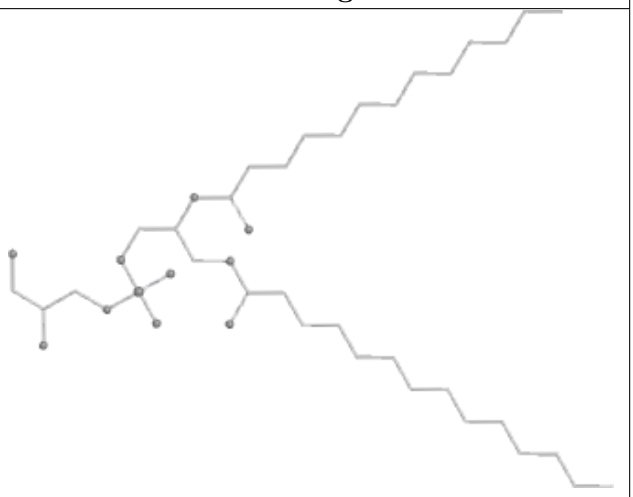
Bond lengths



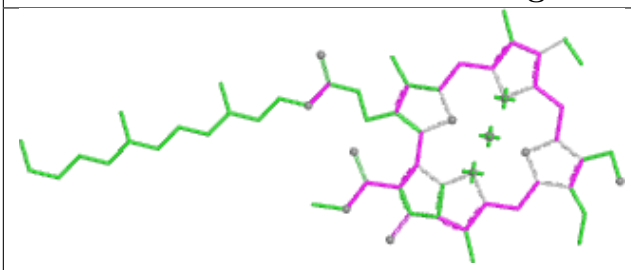
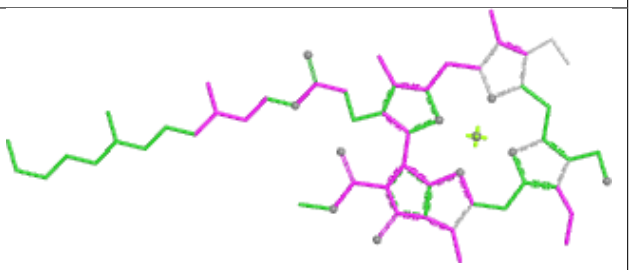
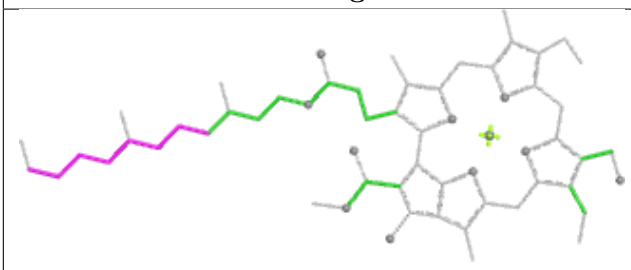
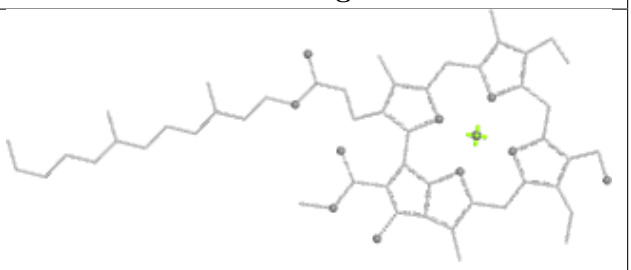
Bond angles

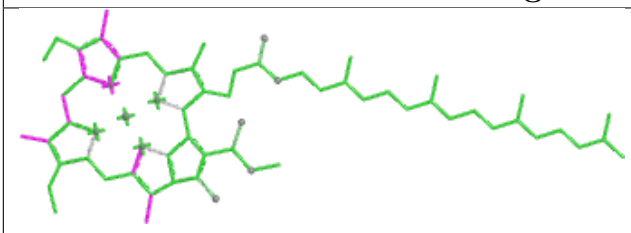
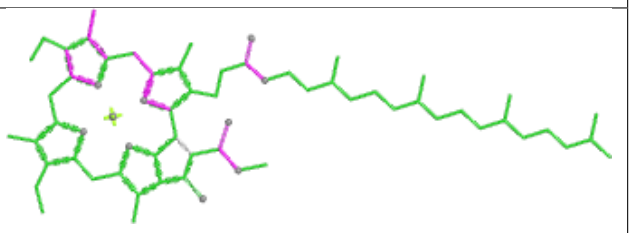
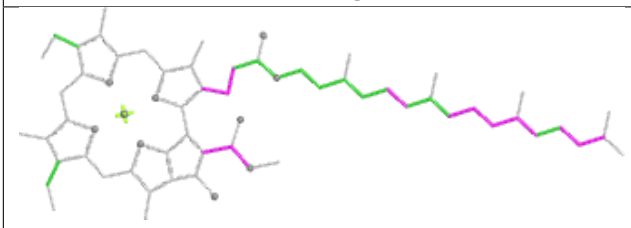
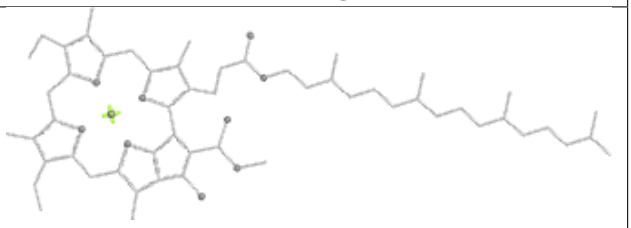


Torsions

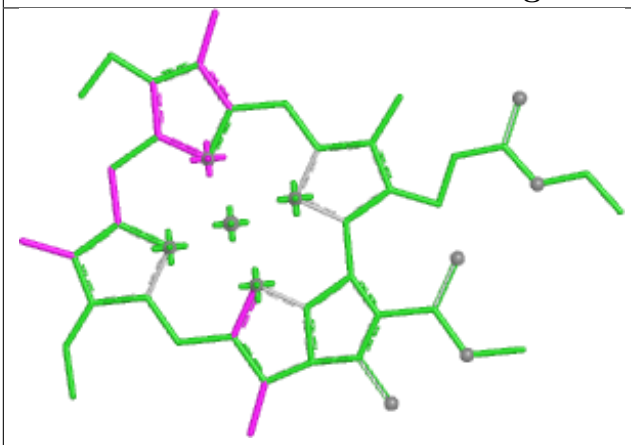


Rings

Ligand CHL 6 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 204



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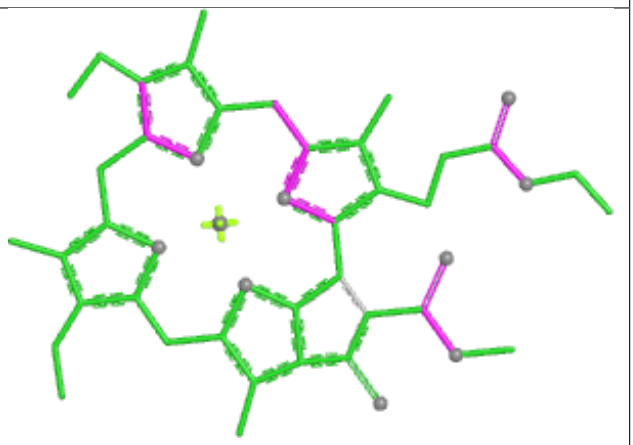
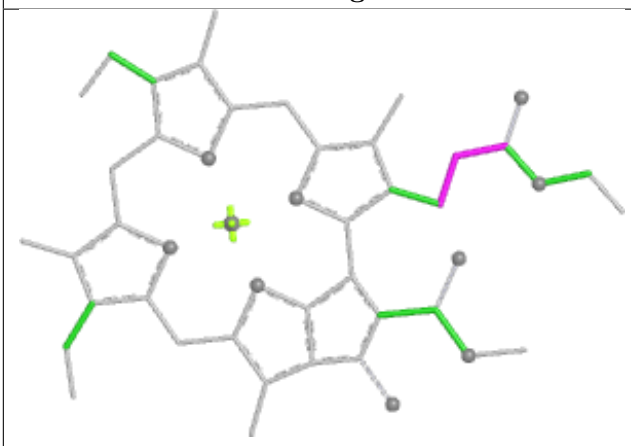


Bond angles



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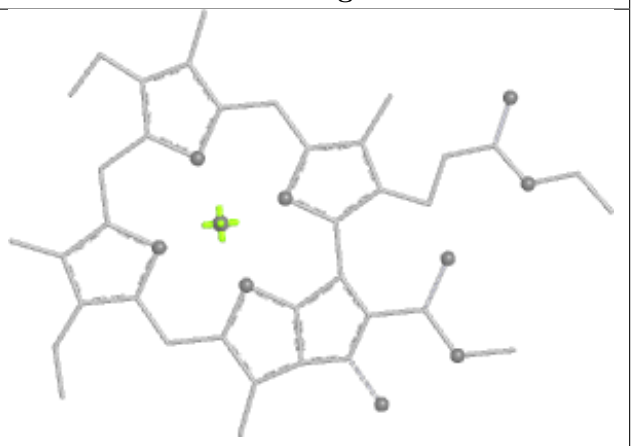
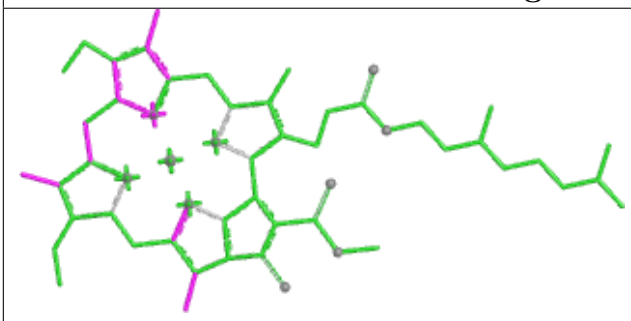
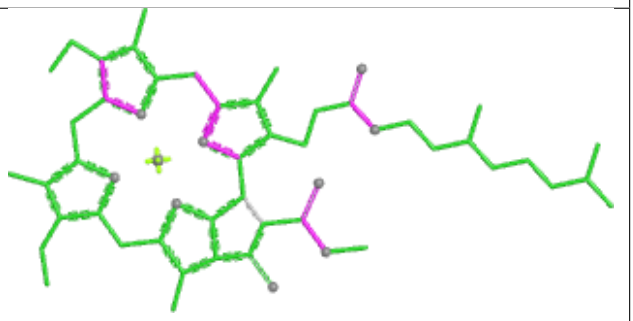


Rings

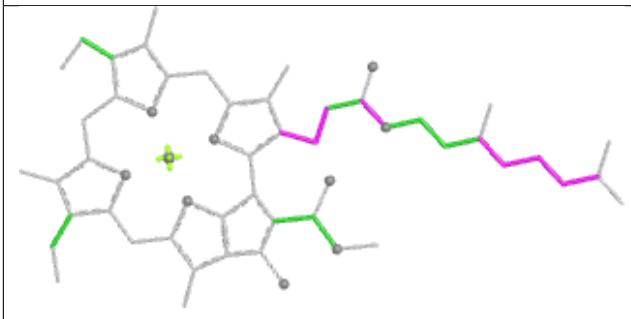
Ligand CLA B 813



Bond lengths



Bond angles



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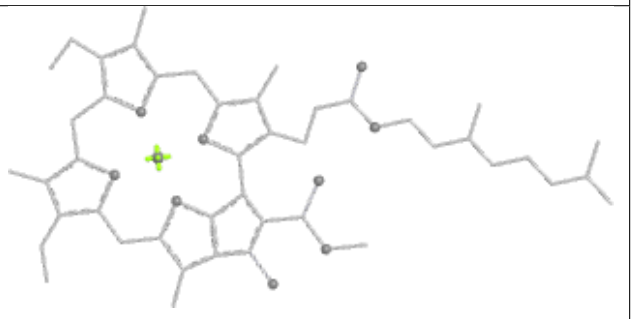
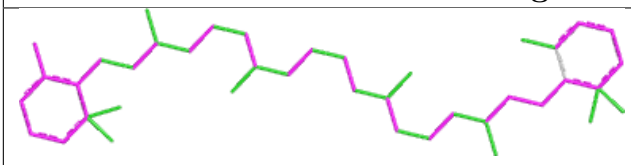


Rings

Ligand 8CT 2 314



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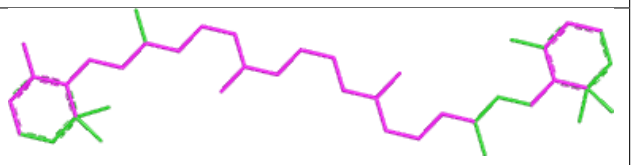
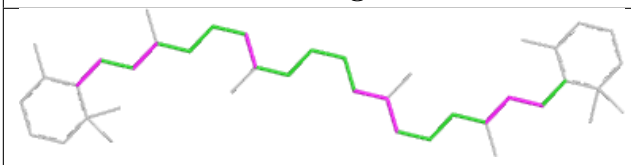


Bond angles



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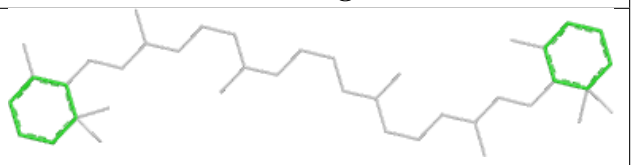
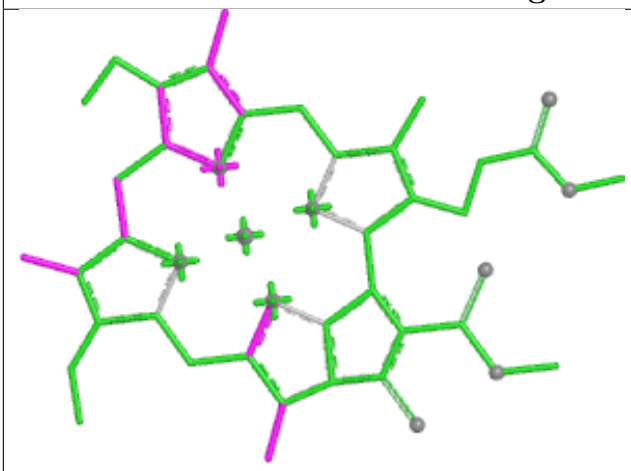


Rings

Ligand CLA 8 304



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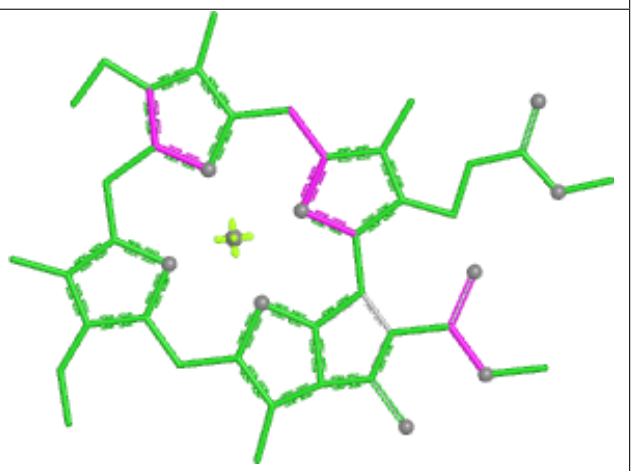
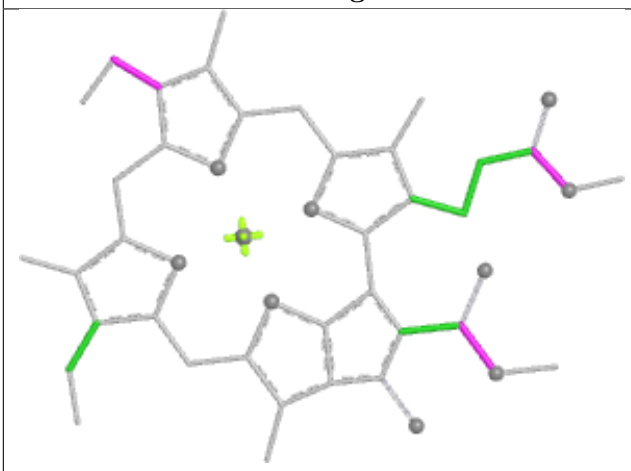


Bond angles



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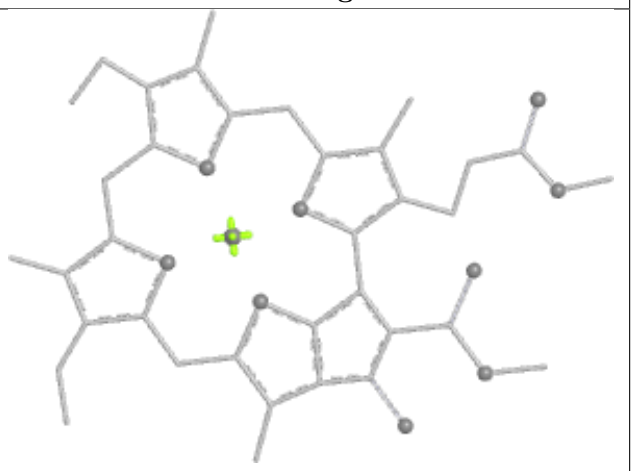
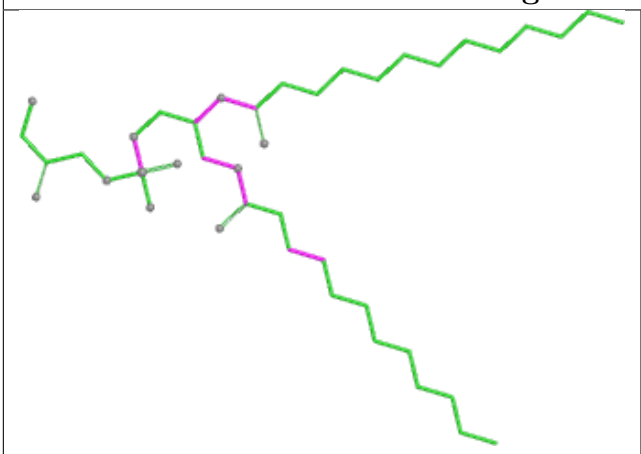


Rings

Ligand LHG A 850



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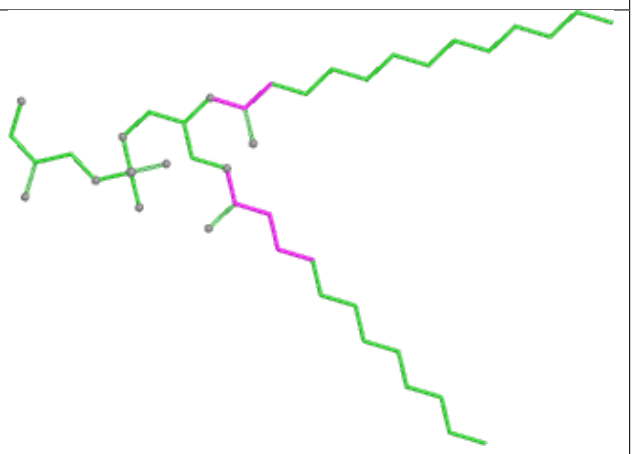
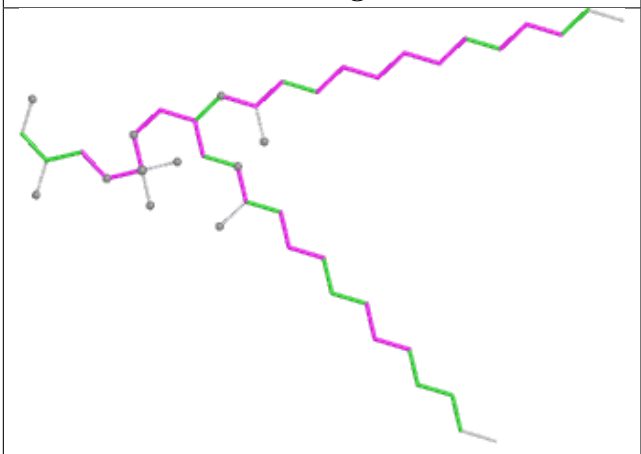


Bond angles



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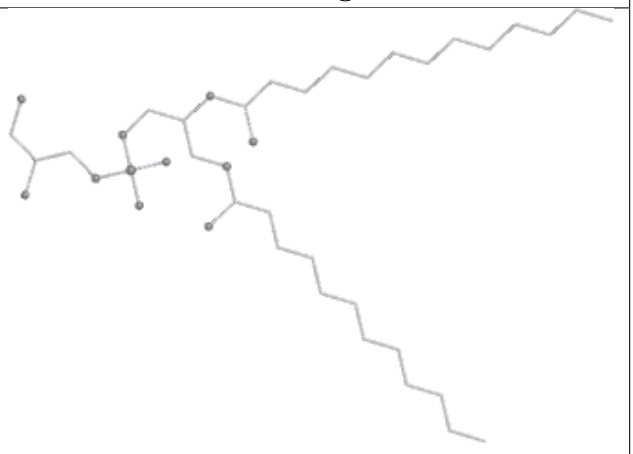
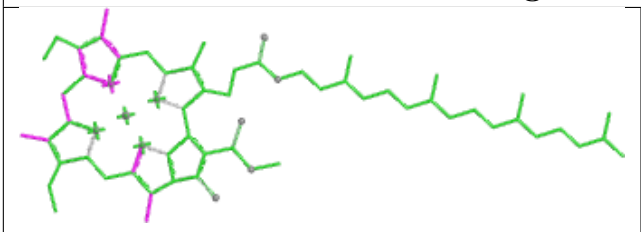


Rings

Ligand CLA A 802



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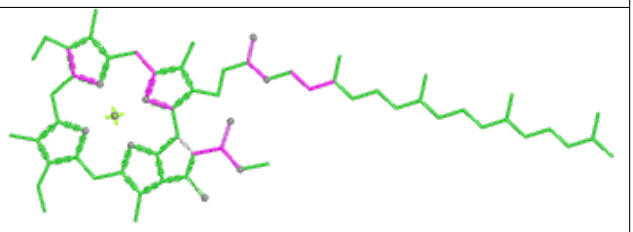
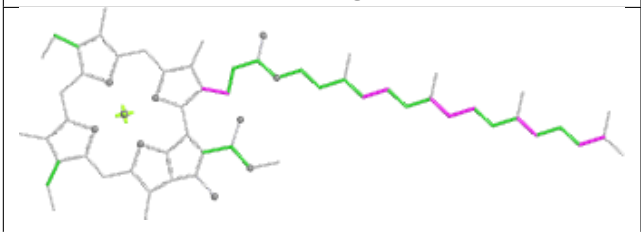
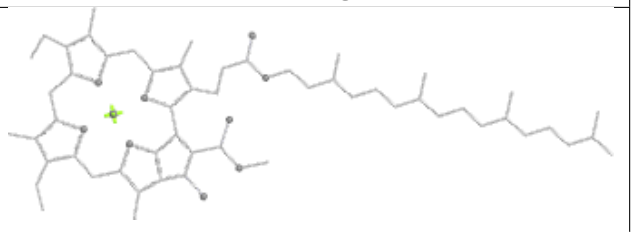


Bond angles

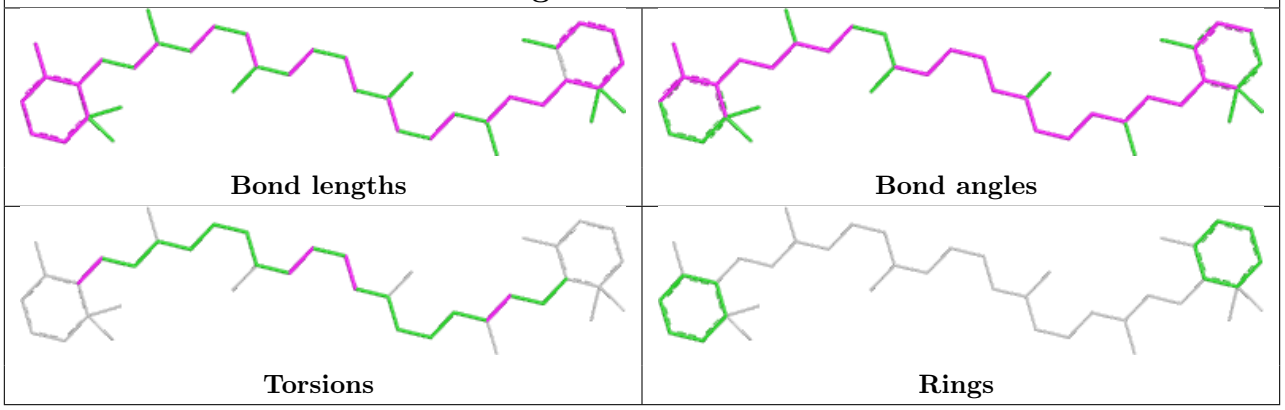


Torsions

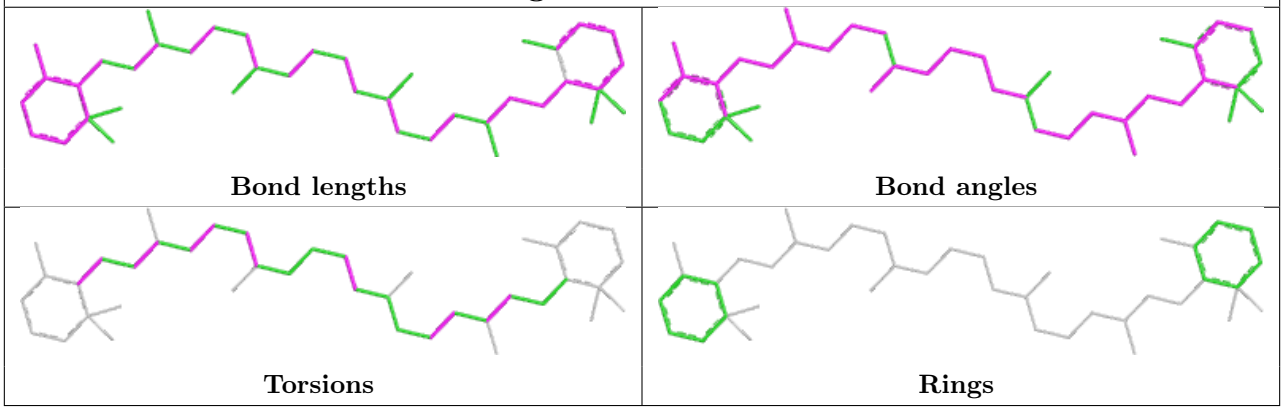


Rings

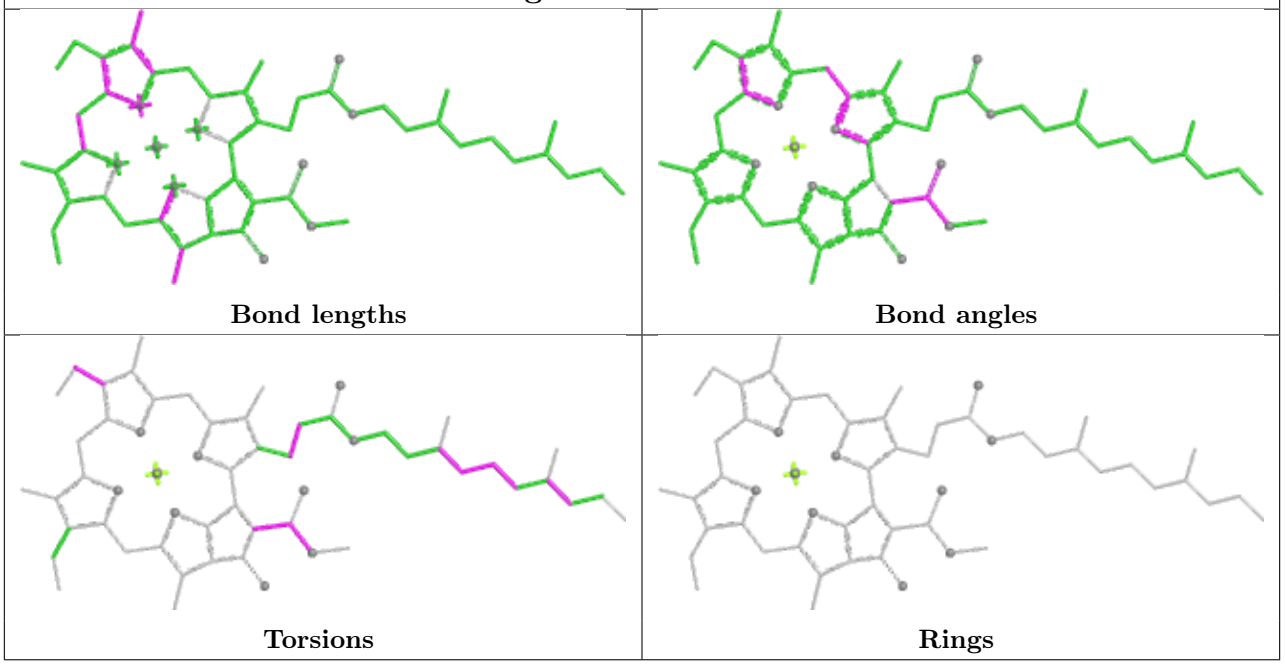
Ligand 8CT 0 314



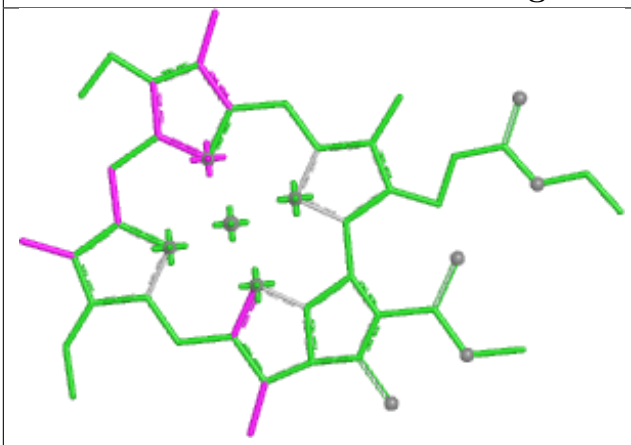
Ligand 8CT A 845



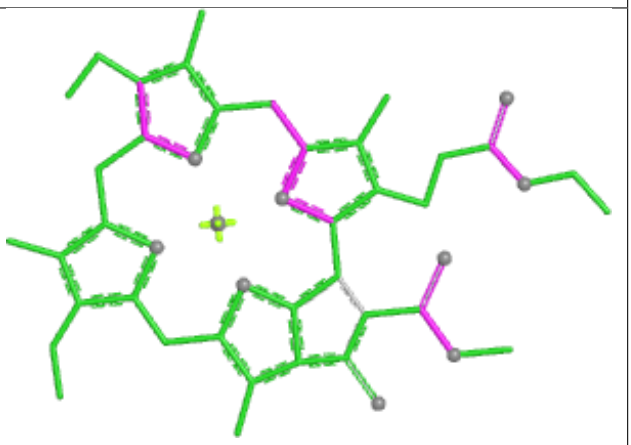
Ligand CLA A 834



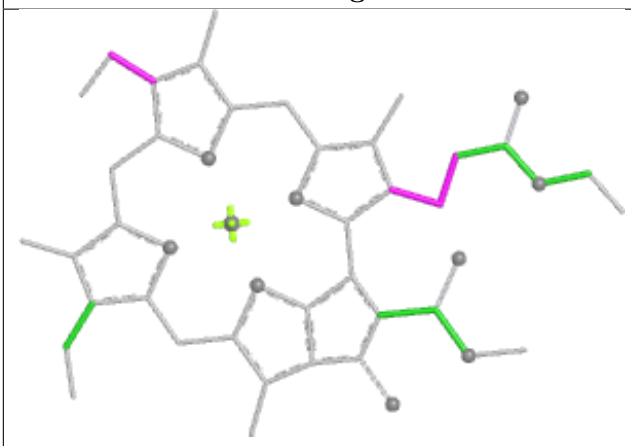
Ligand CLA 3 306



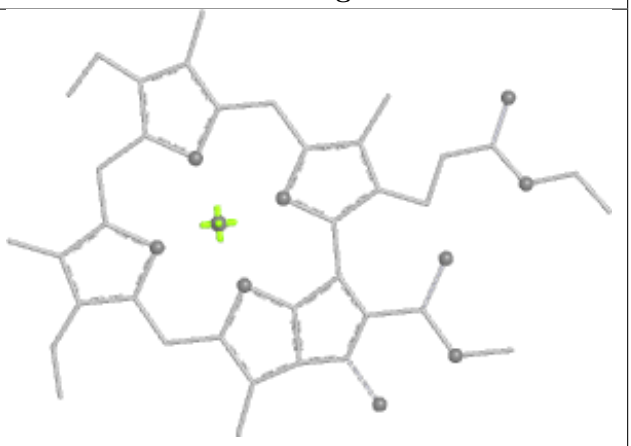
Bond lengths



Bond angles

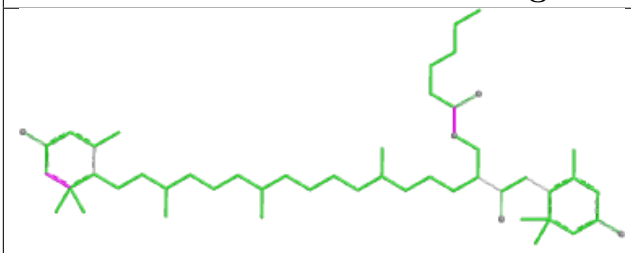


Torsions



Rings

Ligand 0UR 4 317



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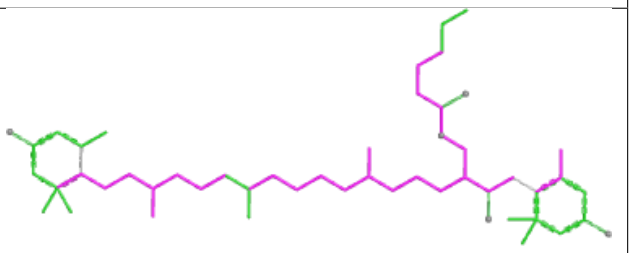
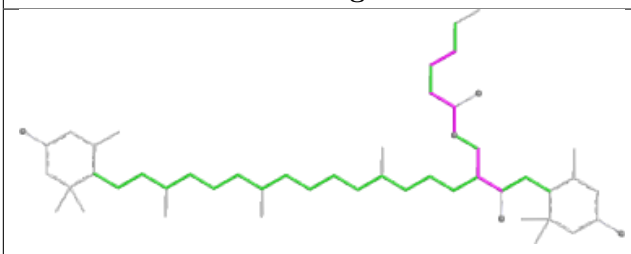


Bond angles



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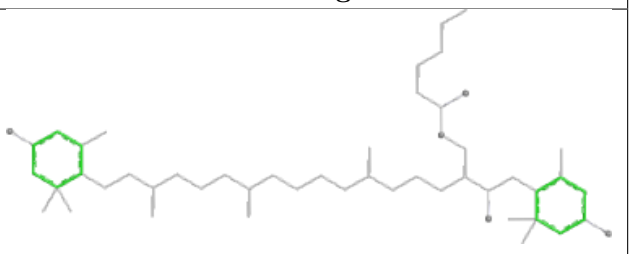
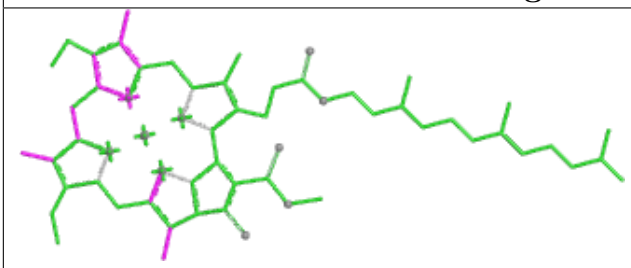


Rings

Ligand CLA B 817



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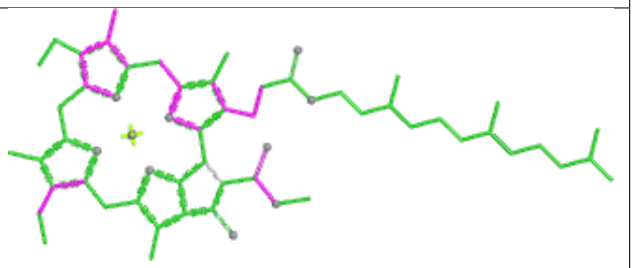
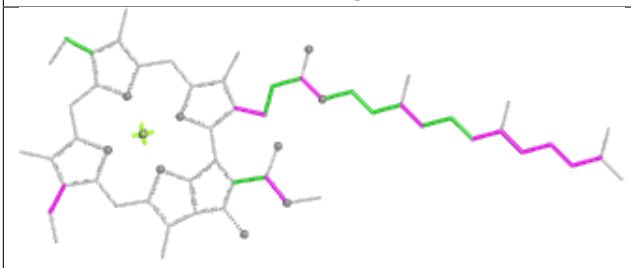
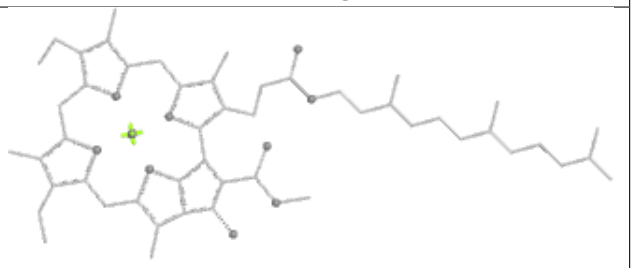


Bond angles

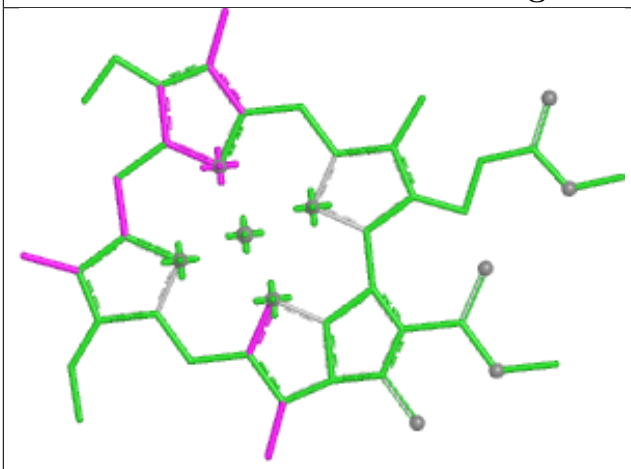


Torsions



Rings

Ligand CLA 0 319



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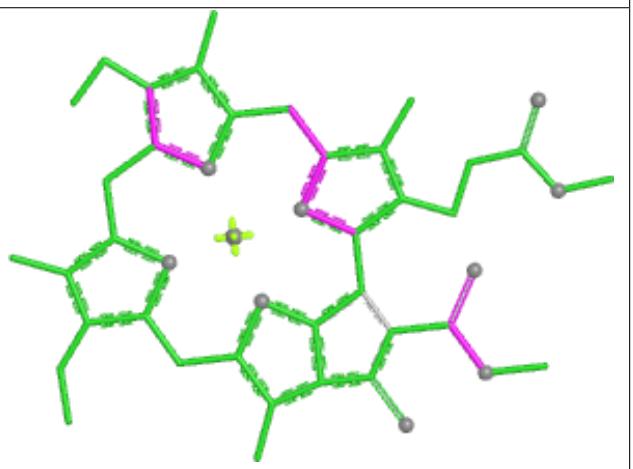
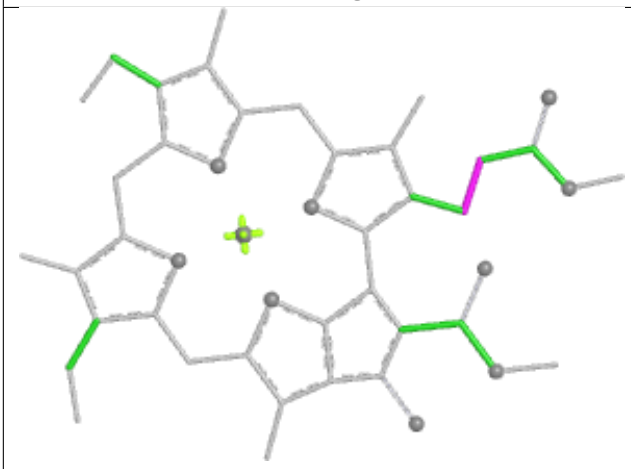
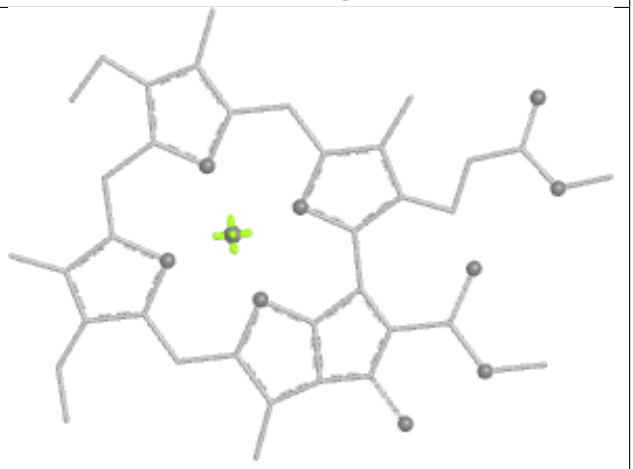


Bond angles

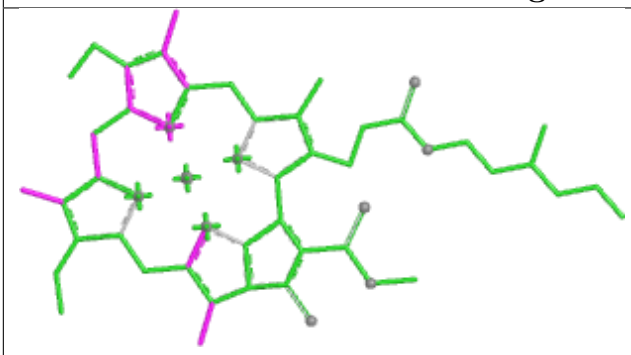


Torsions

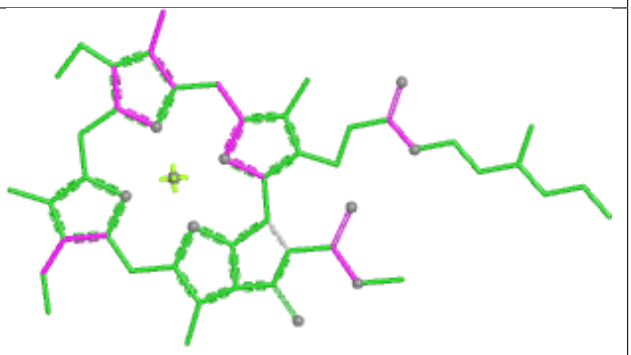


Rings

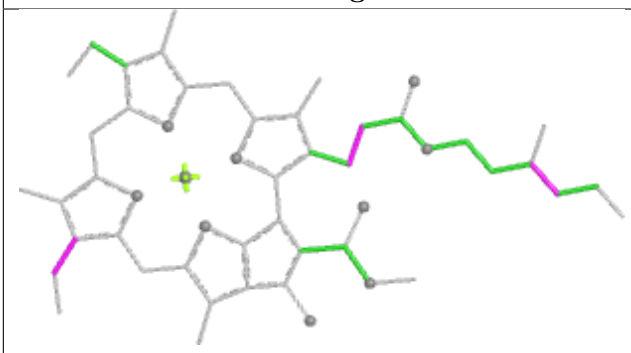
Ligand CLA 3 315



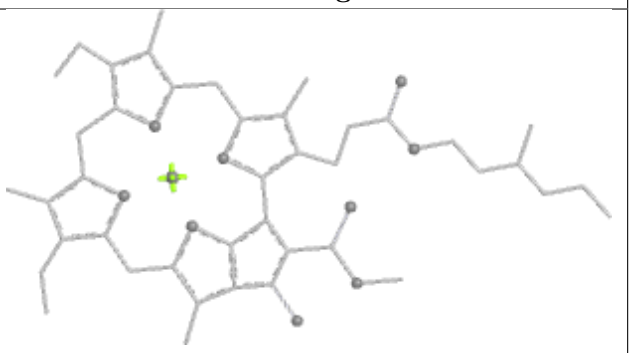
Bond lengths



Bond angles

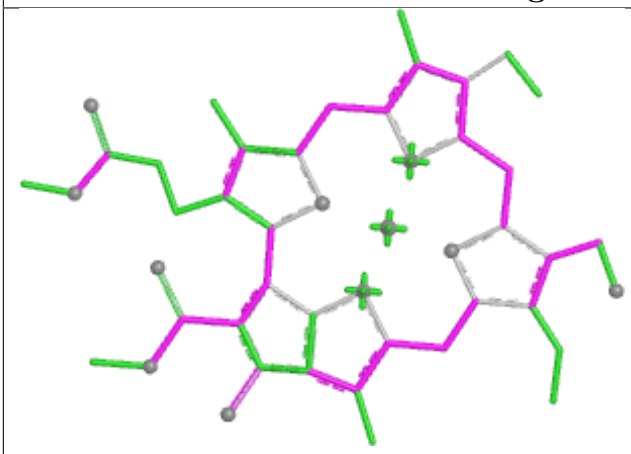


Torsions



Rings

Ligand CHL 5 306



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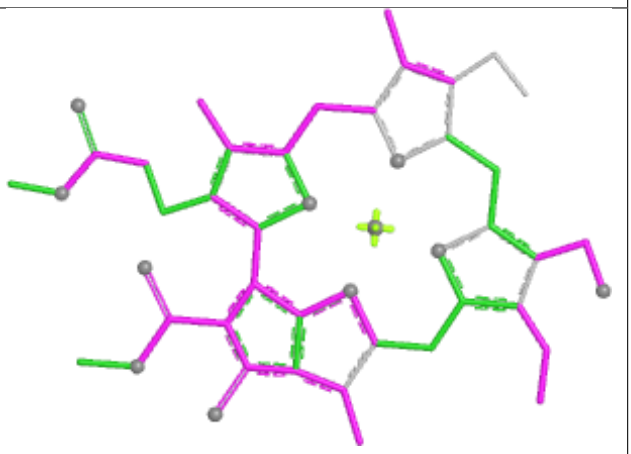

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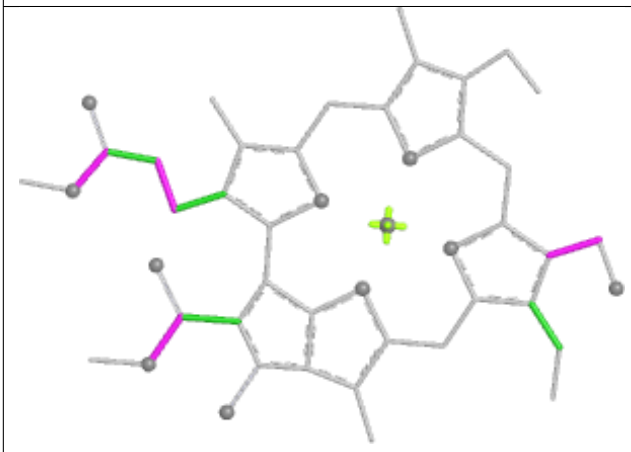
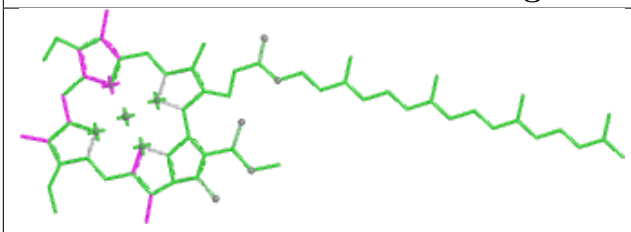


Torsions

Rings

Ligand CLA A 820



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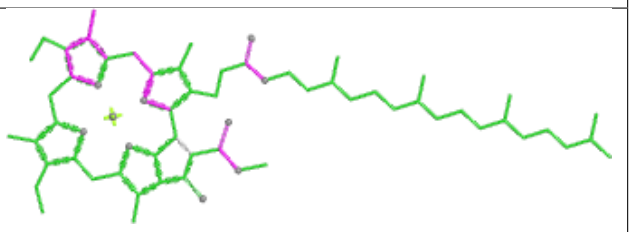

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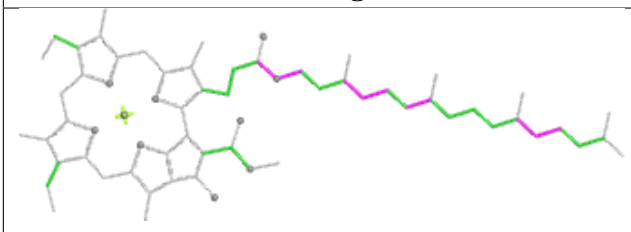

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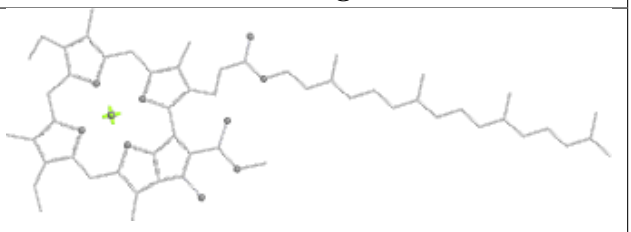
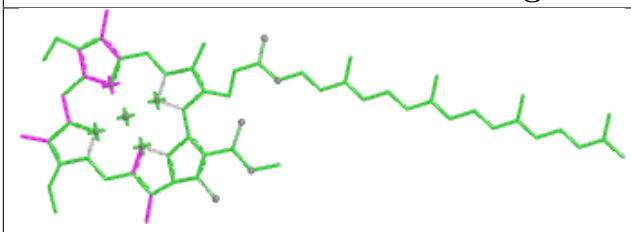


Rings

Ligand CLA A 828



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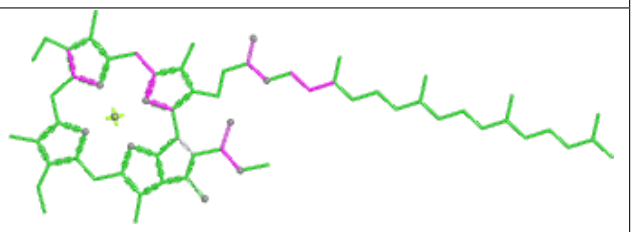

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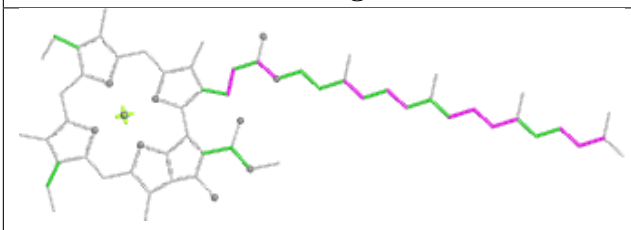

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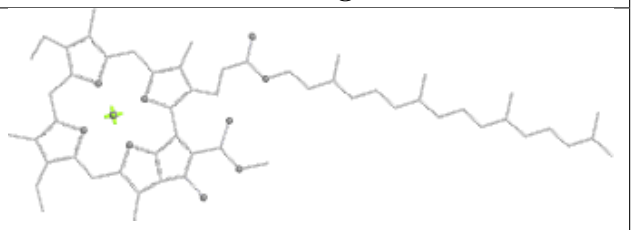
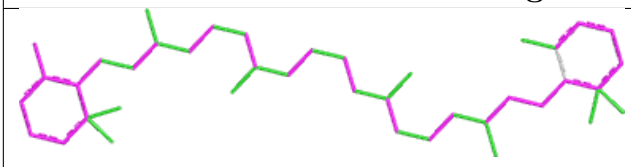


Rings

Ligand 8CT K 105



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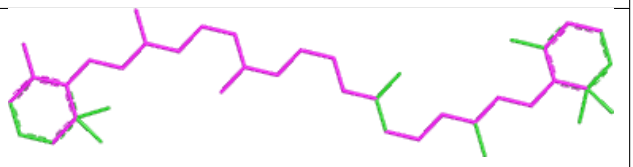
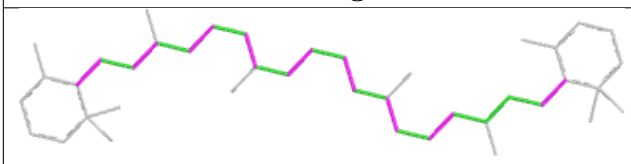


Bond angles



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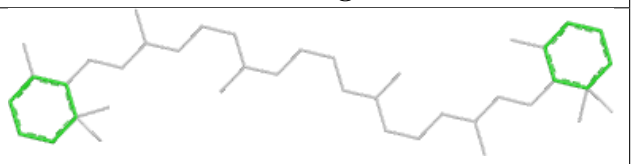
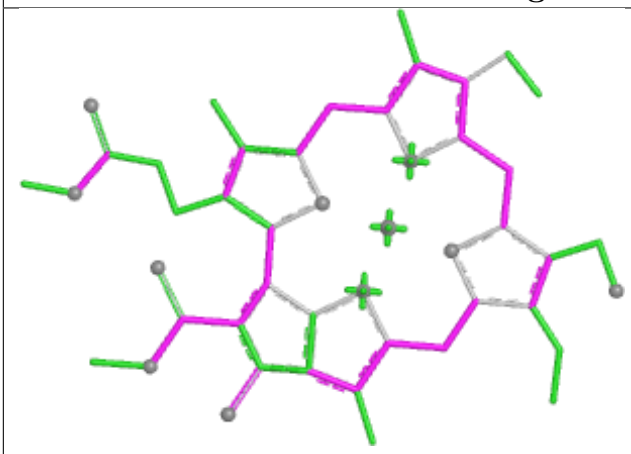


Rings

Ligand CHL 8 309



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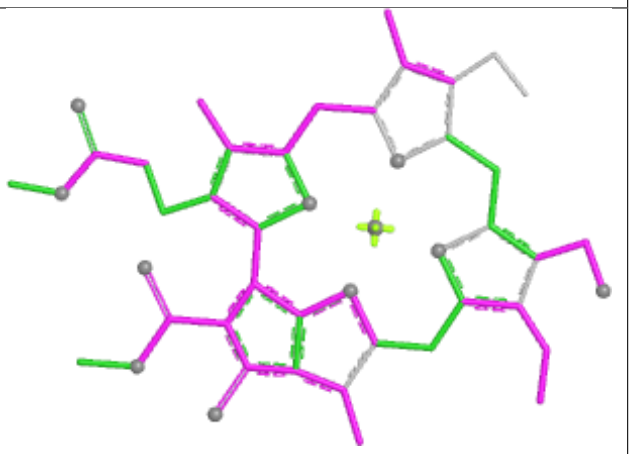

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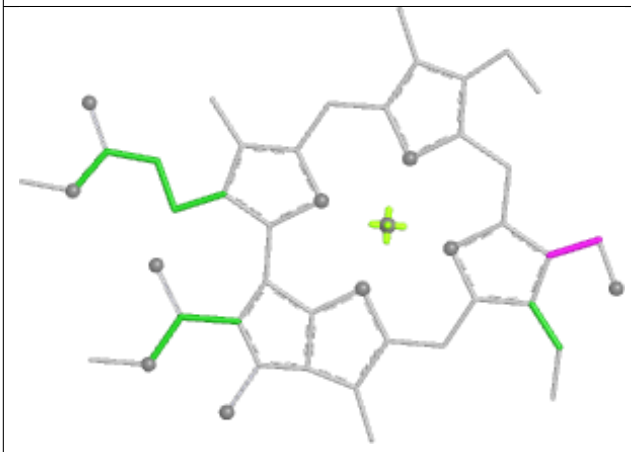
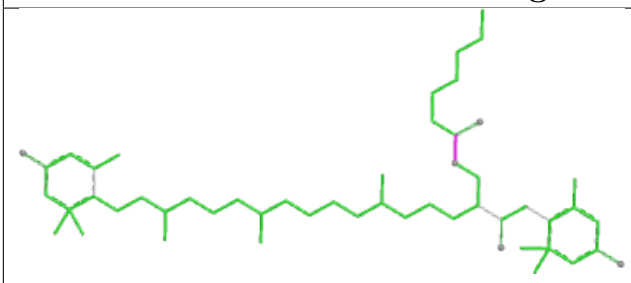


Torsions

Rings

Ligand 0UR 1 315



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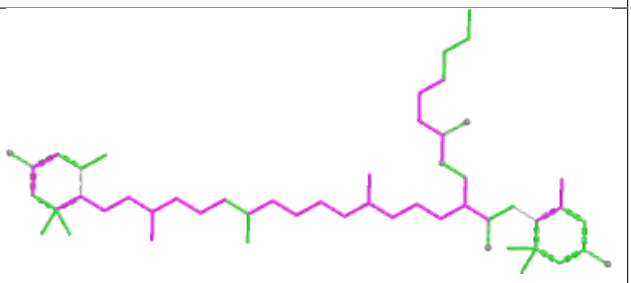
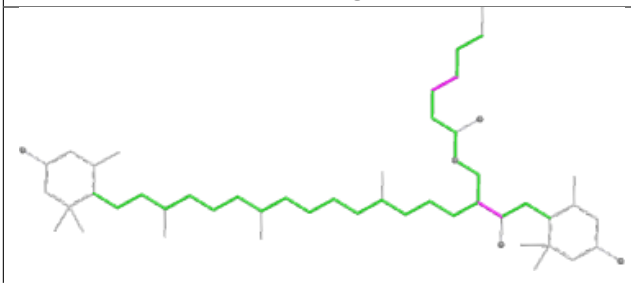


Bond angles



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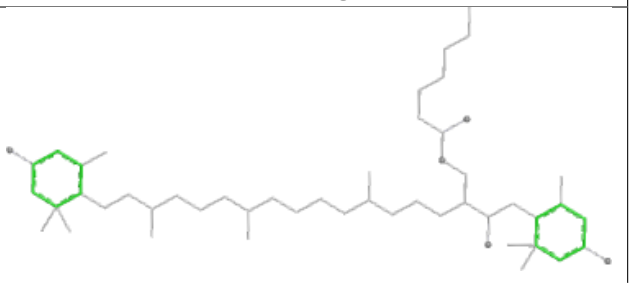
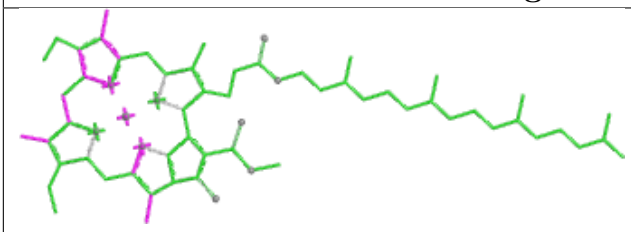


Rings

Ligand CLA B 806



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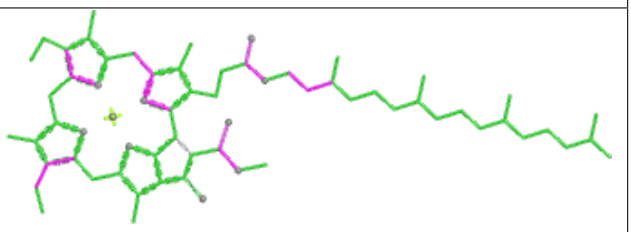

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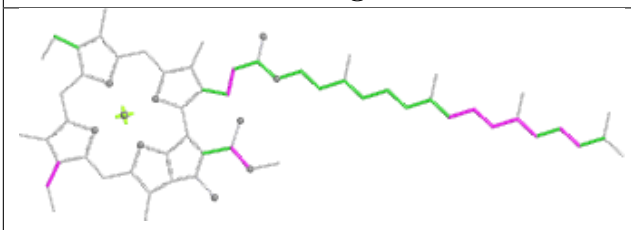

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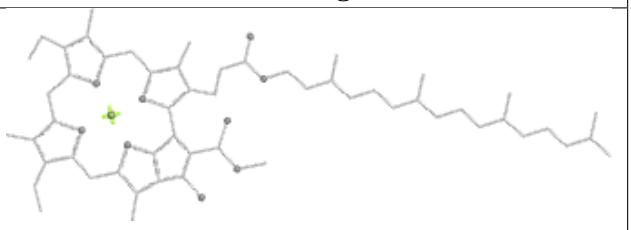
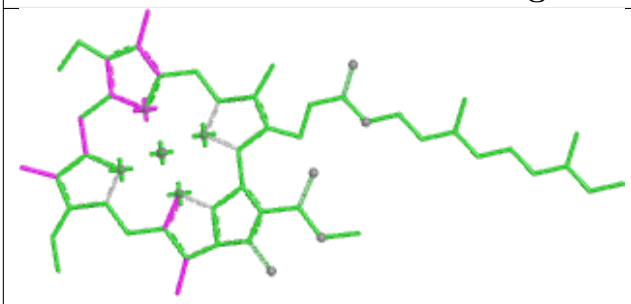


Rings

Ligand CLA 1 302



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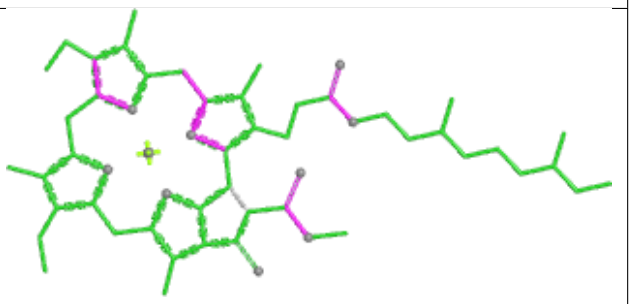
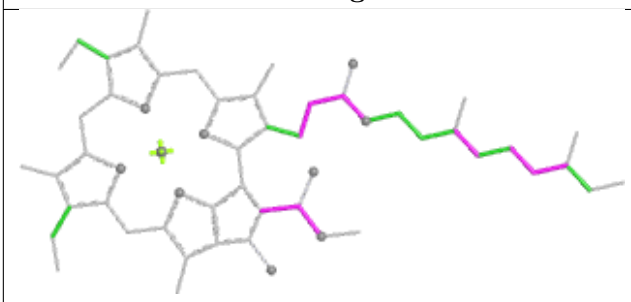


Bond angles



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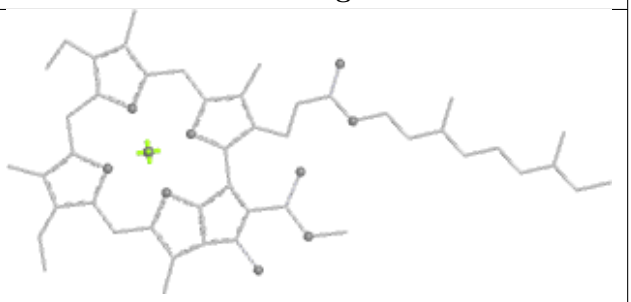
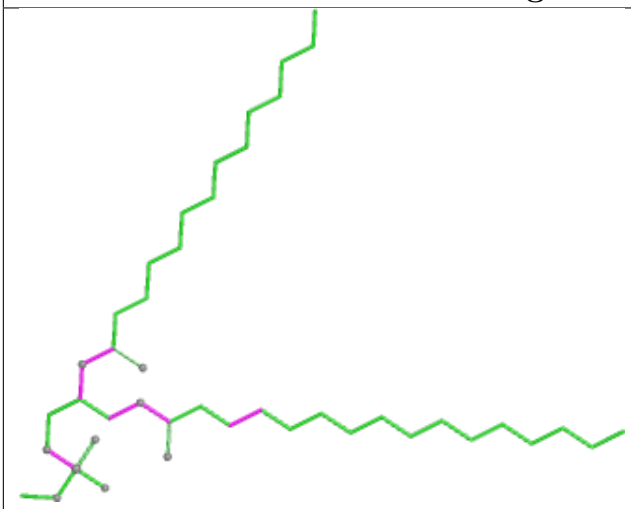


Rings

Ligand LHG 3 324



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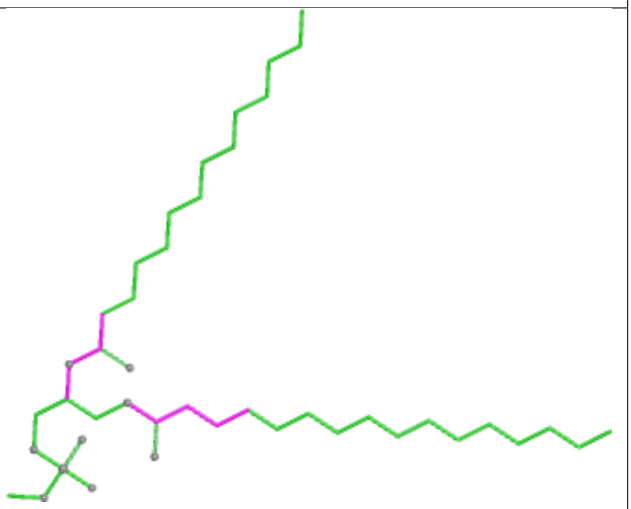
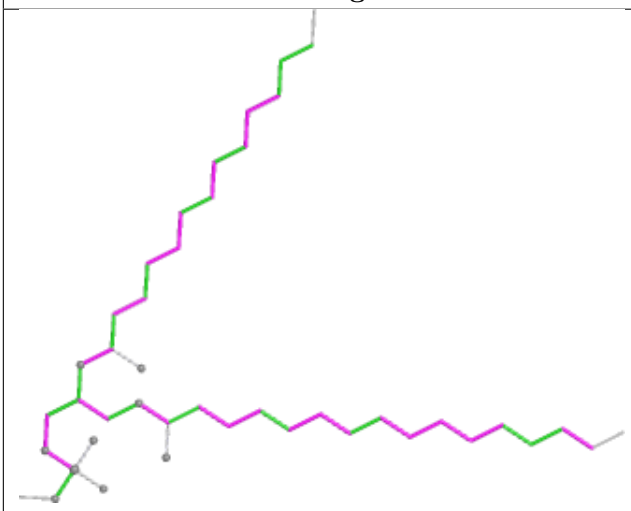


Bond angles



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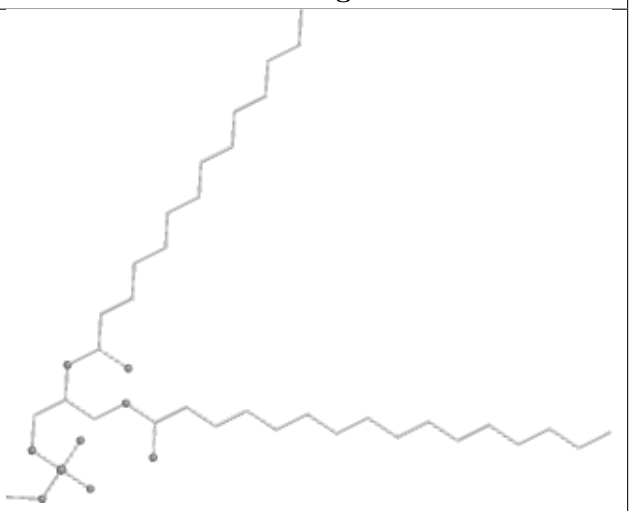
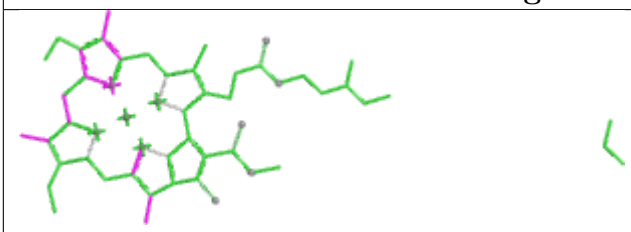


Rings

Ligand CLA A 806



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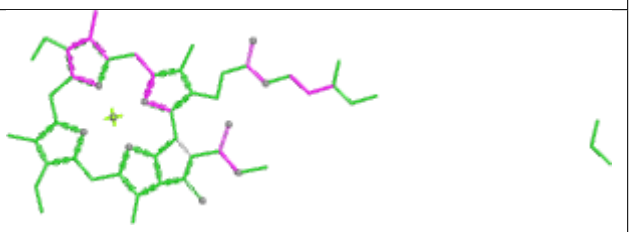
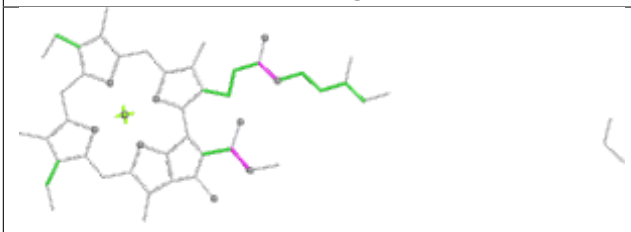


Bond angles



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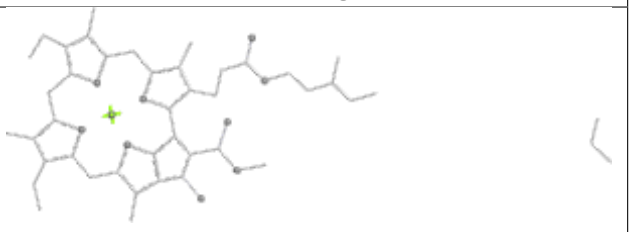
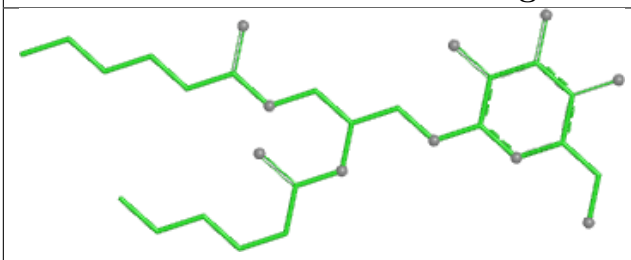


Rings

Ligand LMG O 203



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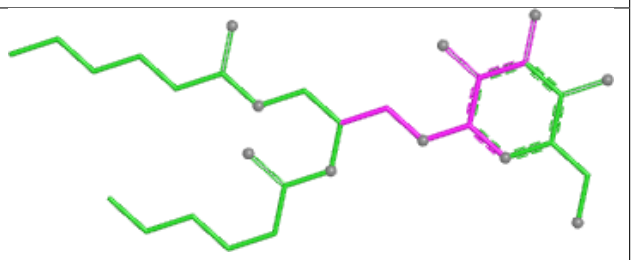
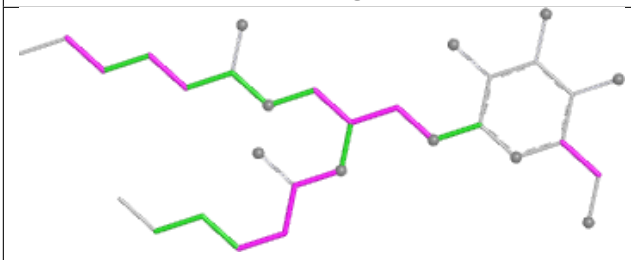
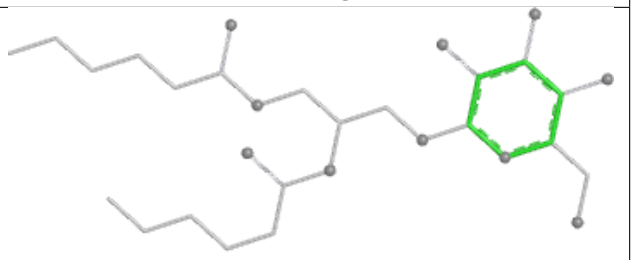


Bond angles

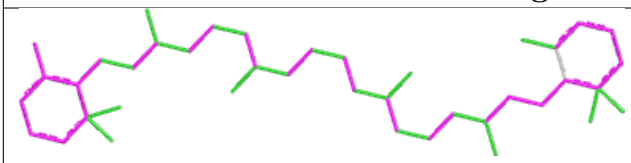


Torsions



Rings

Ligand 8CT 4 316



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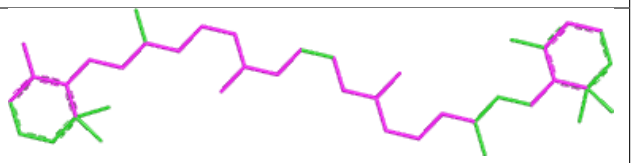

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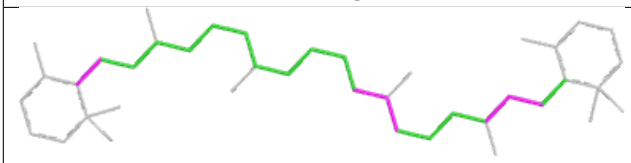

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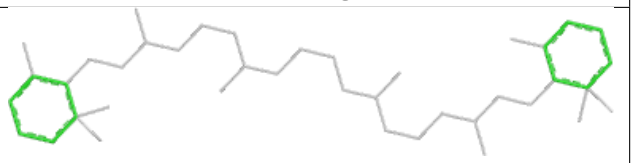
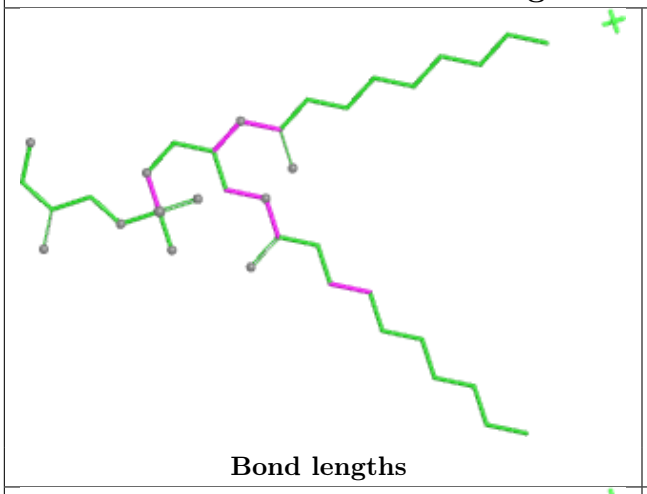


Rings

Ligand LHG 3 322



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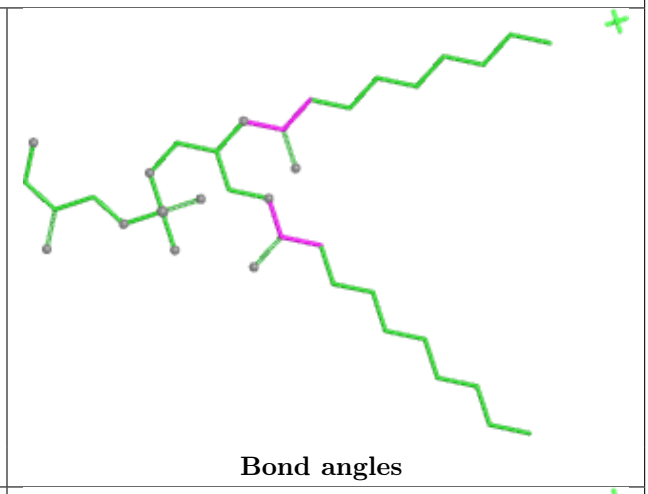
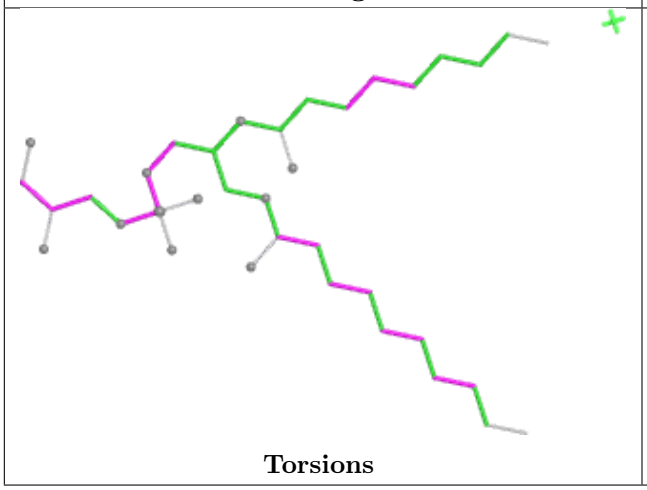


Bond angles



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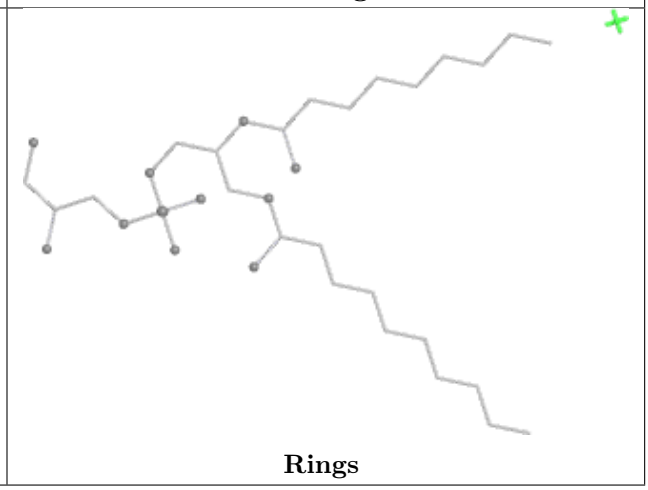
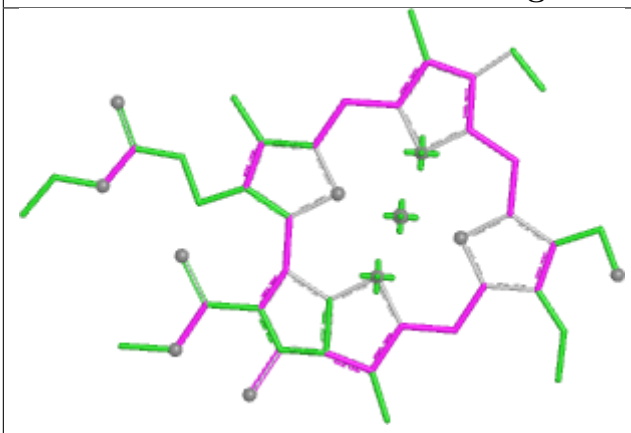
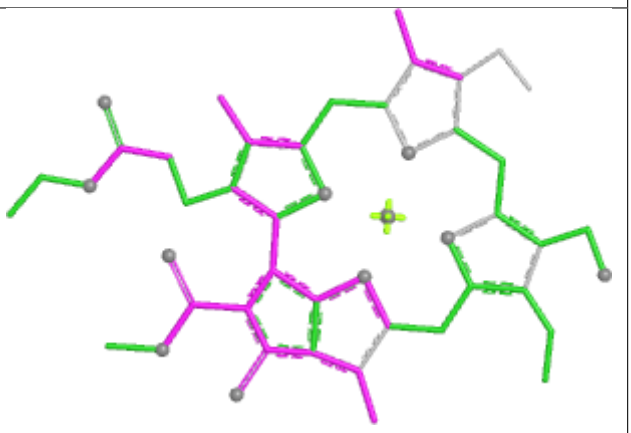


Rings

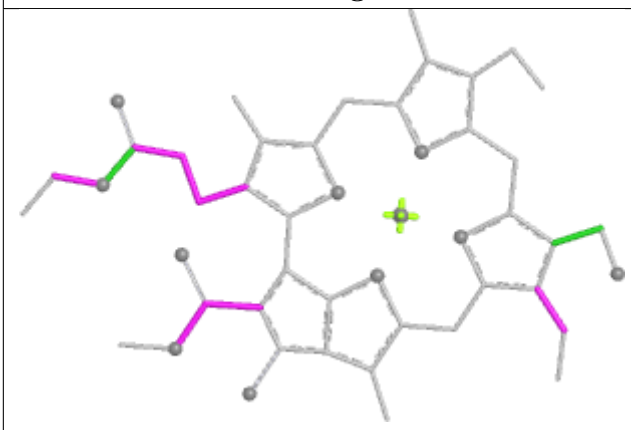
Ligand CHL 5 305



Bond lengths



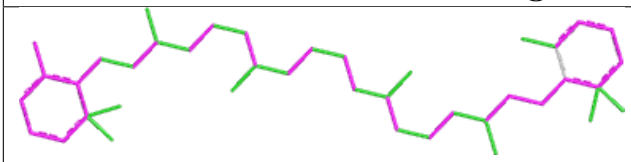
Bond angles



Torsions

Rings

Ligand 8CT B 843



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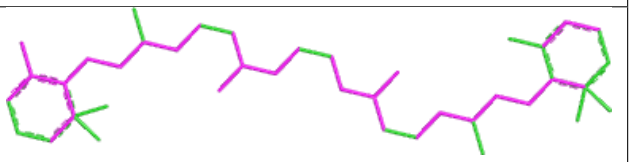
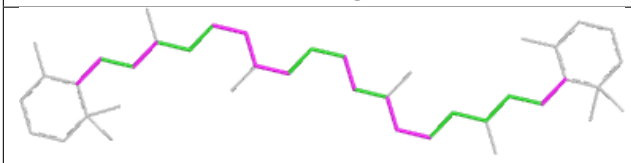
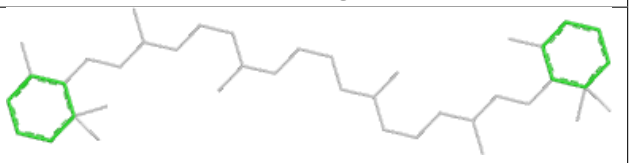


Bond angles

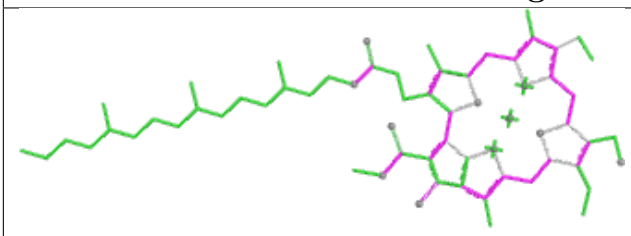


Torsions



Rings

Ligand CHL 6 302



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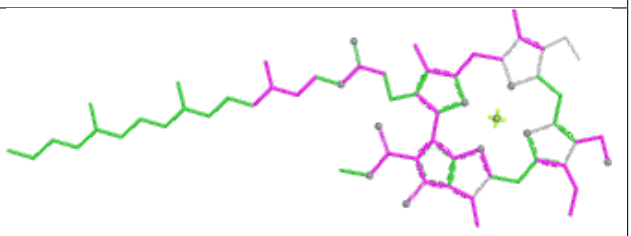
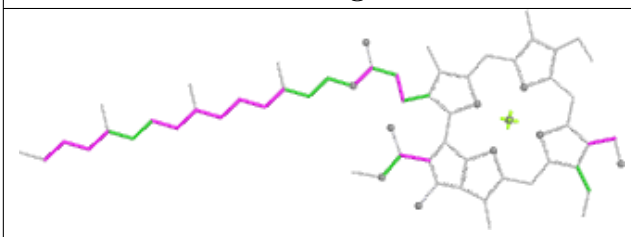
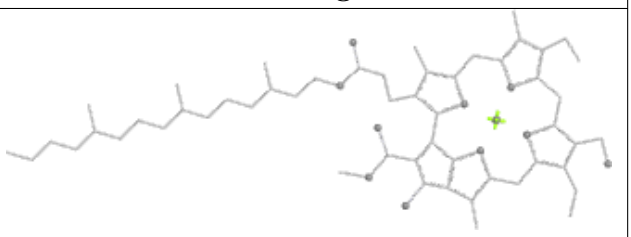


Bond angles

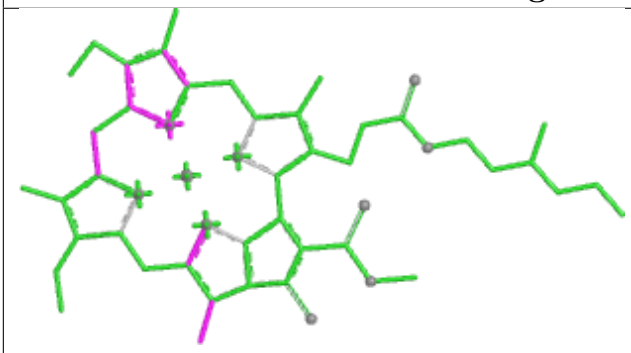


Torsions



Rings

Ligand CLA 5 303



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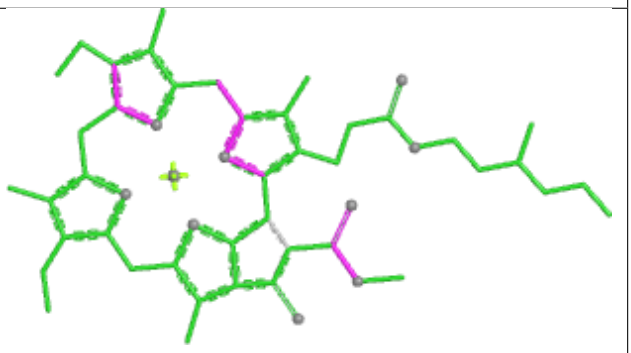
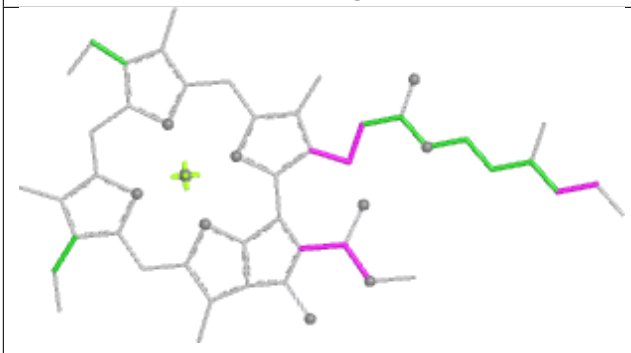
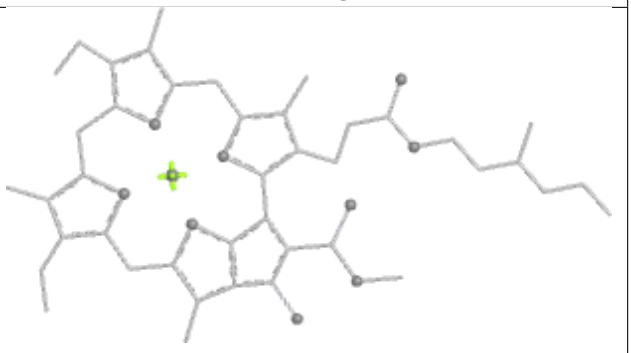


Bond angles

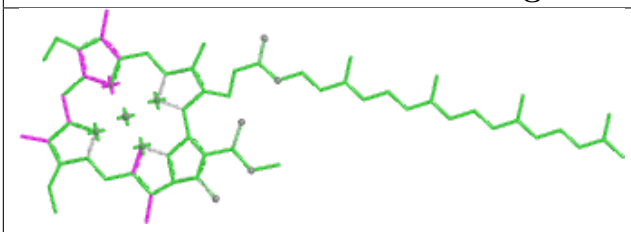


Torsions



Rings

Ligand CLA A 812



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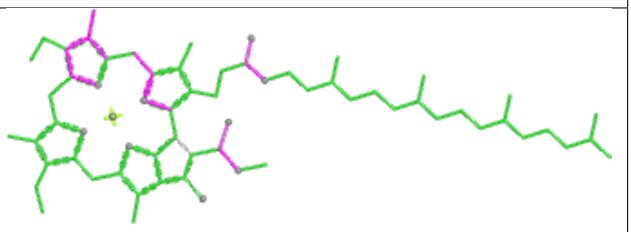
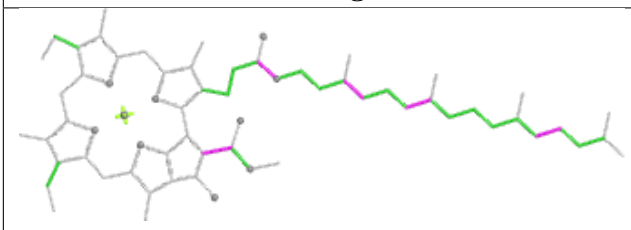
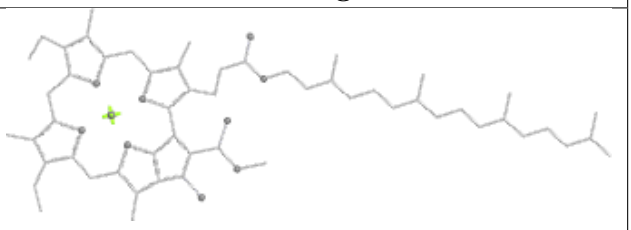


Bond angles

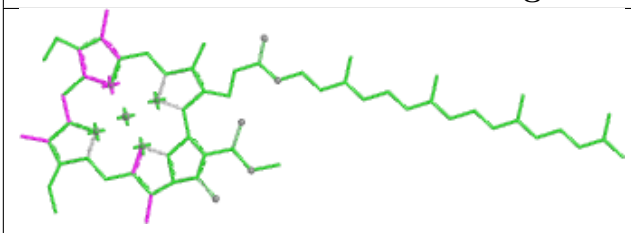


Torsions



Rings

Ligand CLA A 824



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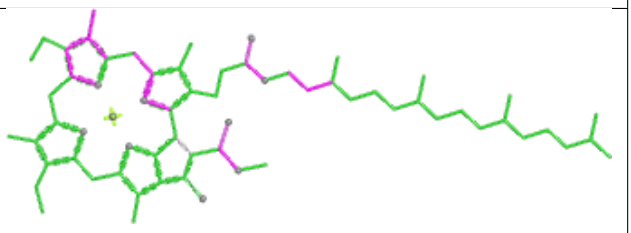
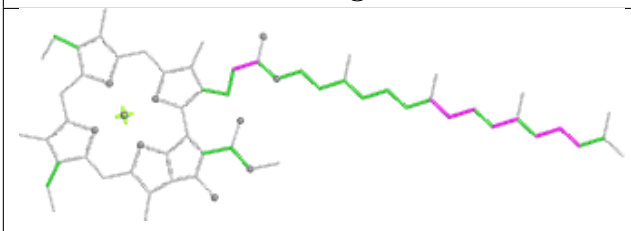


Bond angles



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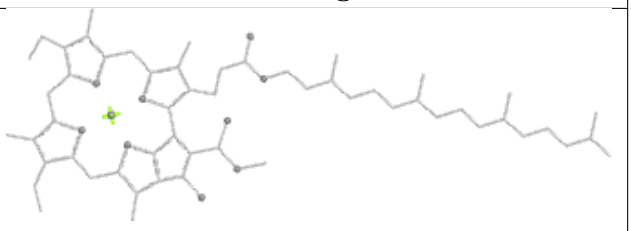
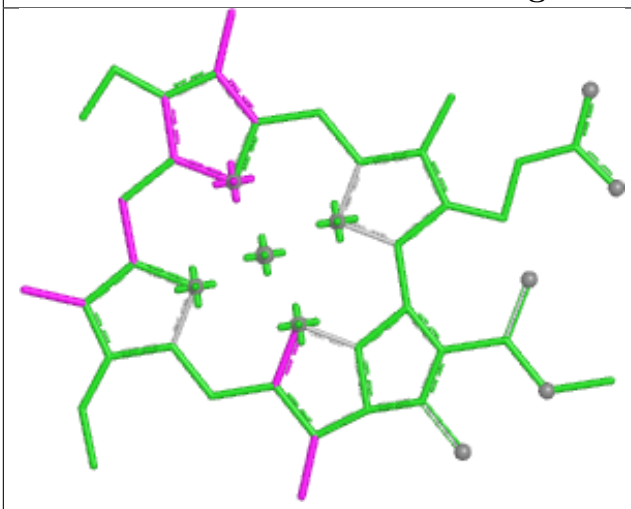


Rings

Ligand CLA 4 303



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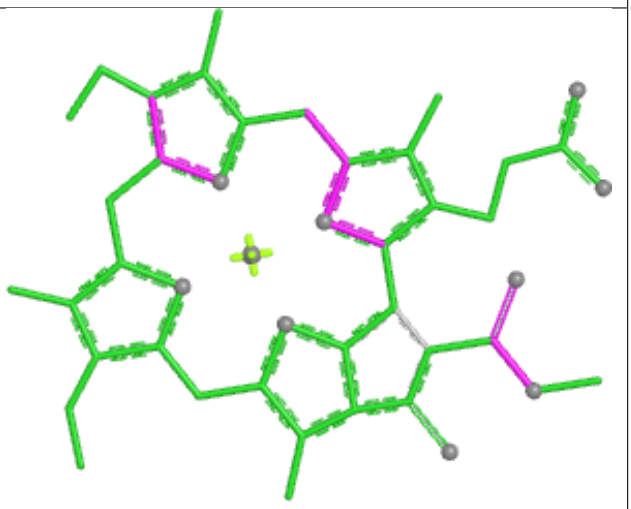

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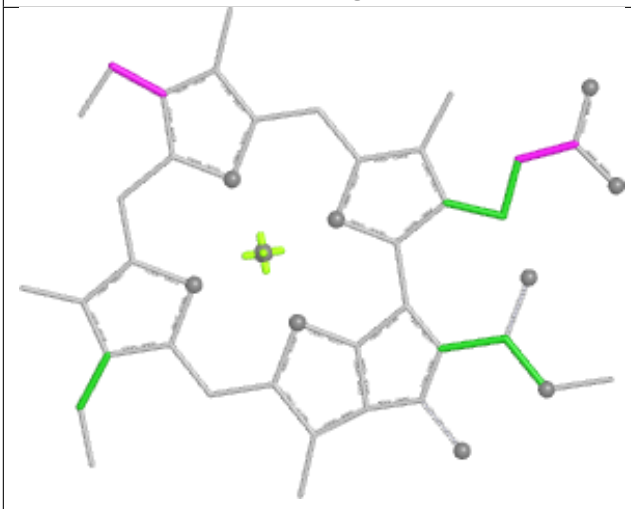
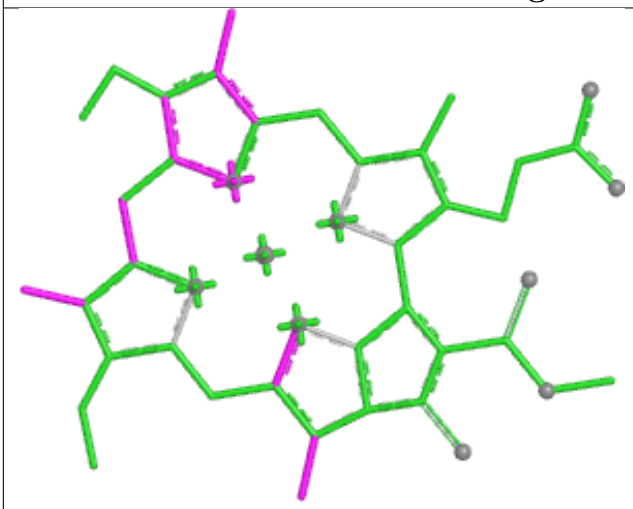


Torsions

Rings

Ligand CLA 6 314



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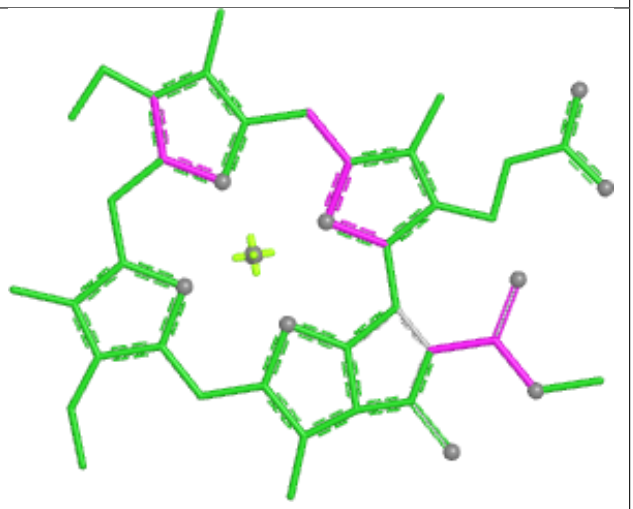

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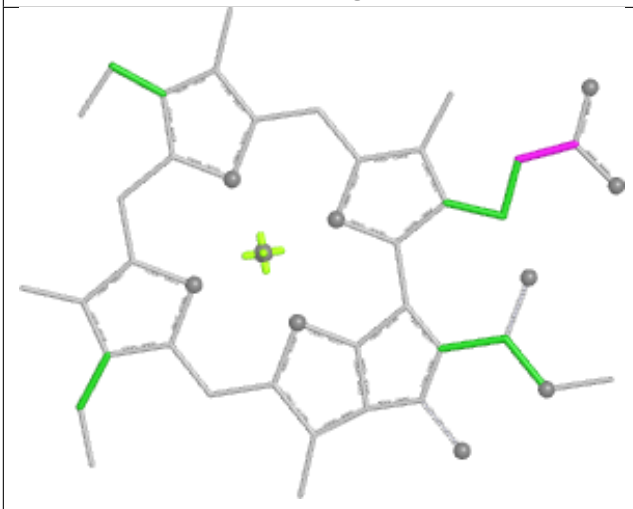
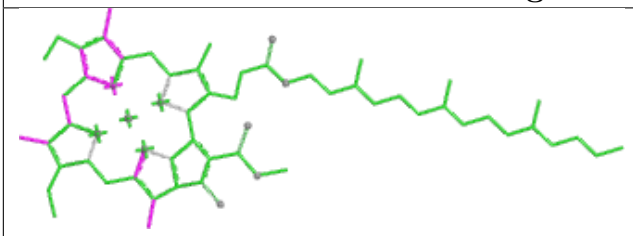


Torsions

Rings

Ligand CLA L 202



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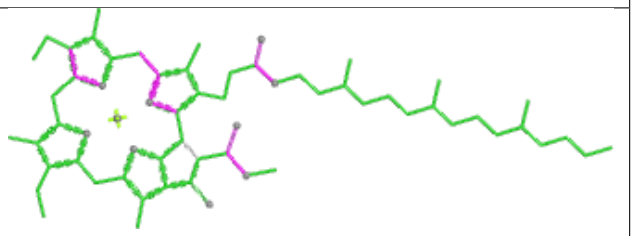
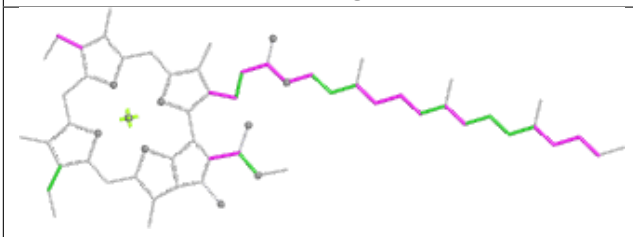
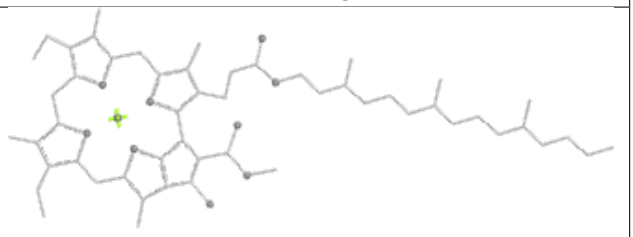


Bond angles

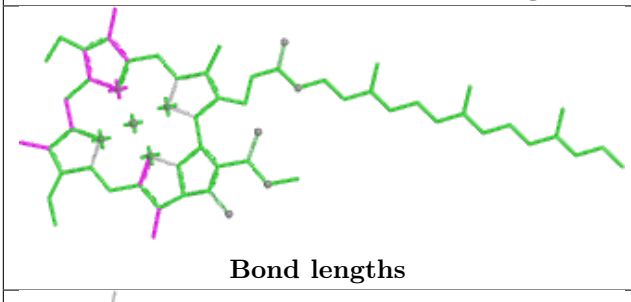


Torsions



Rings

Ligand CLA B 810



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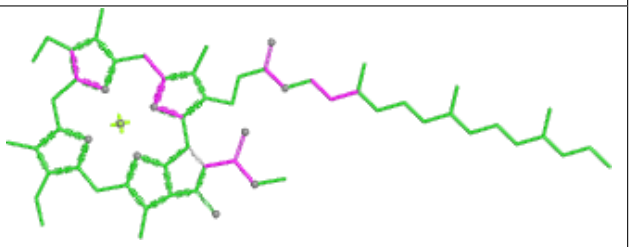
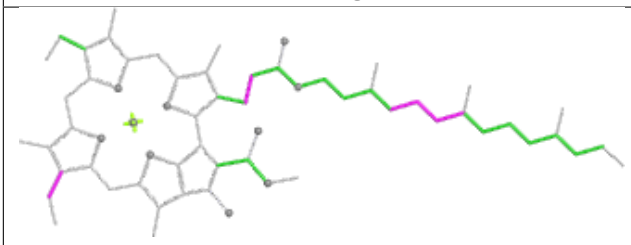
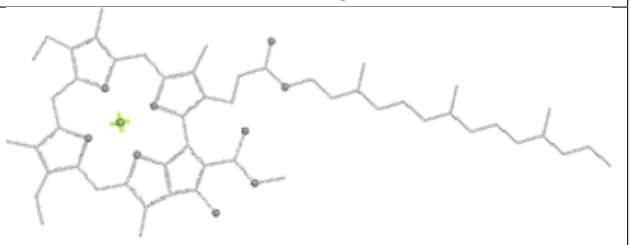


Bond angles

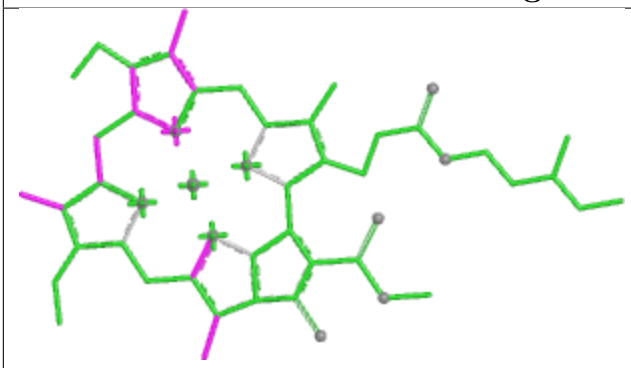


Torsions



Rings

Ligand CLA O 209



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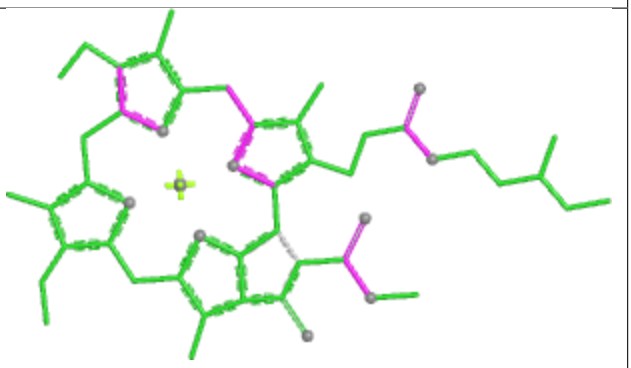
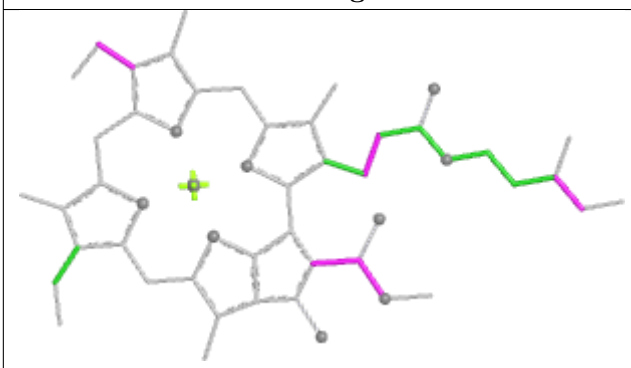
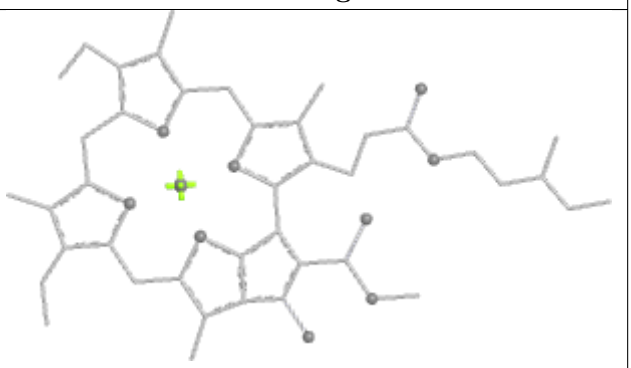


Bond angles

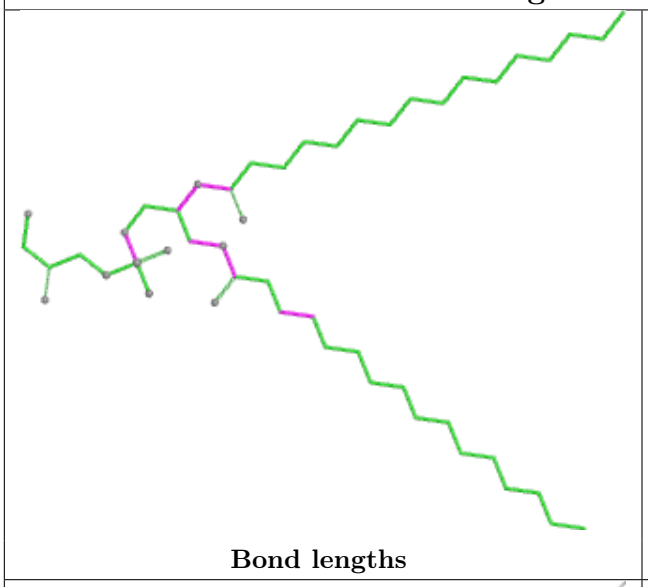


Torsions



Rings

Ligand LHG 0 317



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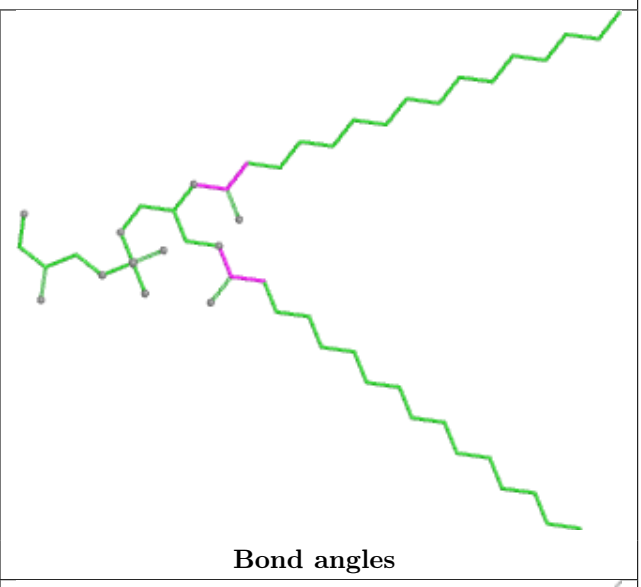
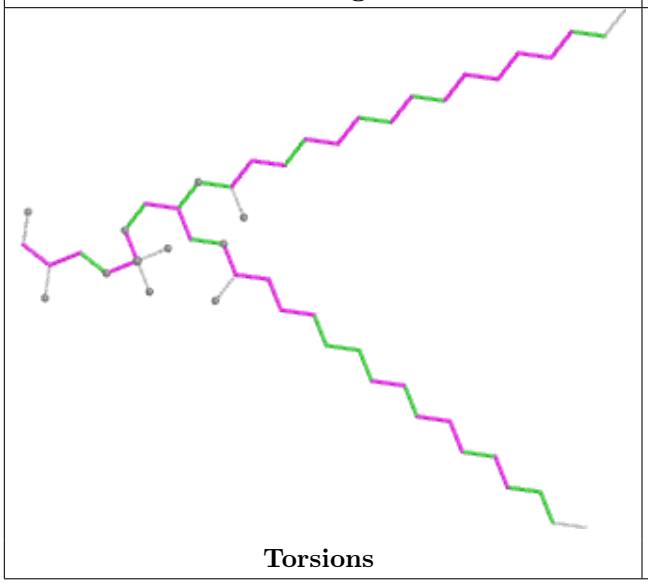


Bond angles



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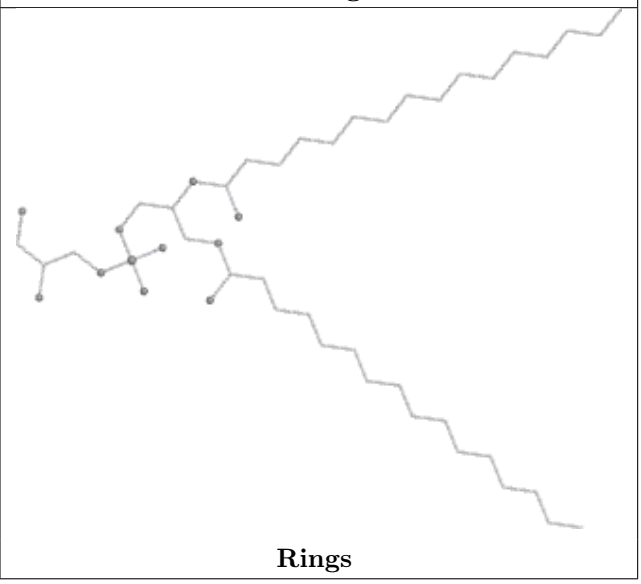
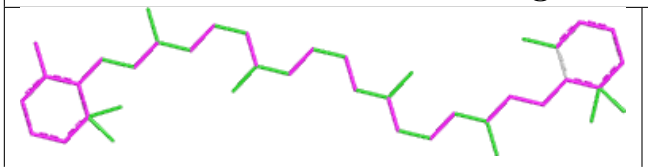


Rings

Ligand 8CT J 104



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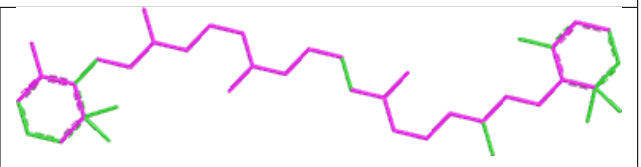
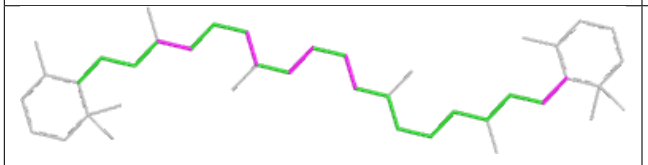


Bond angles



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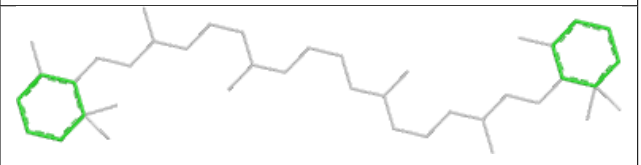
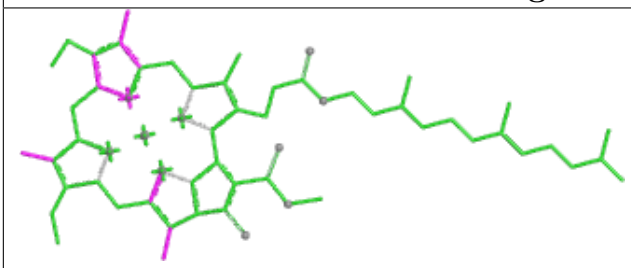


Rings

Ligand CLA 4 304



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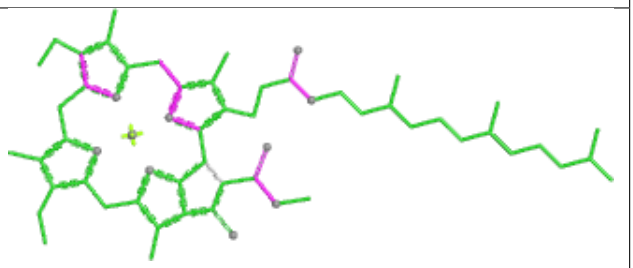
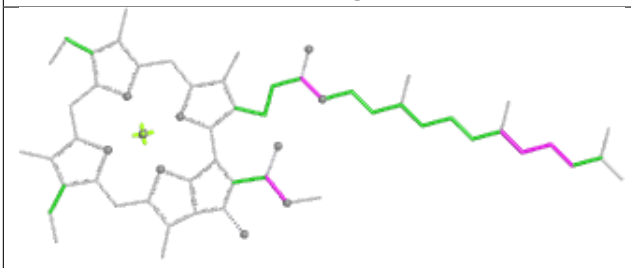


Bond angles



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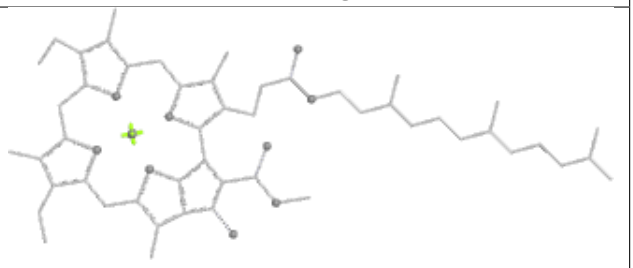
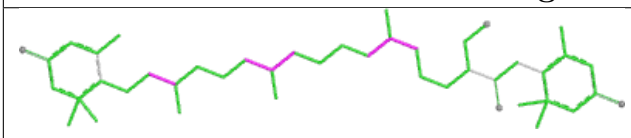
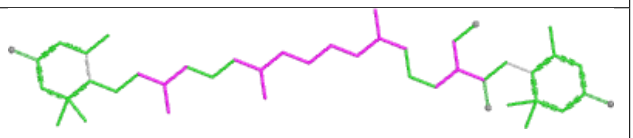


Rings

Ligand 0IE 7 321

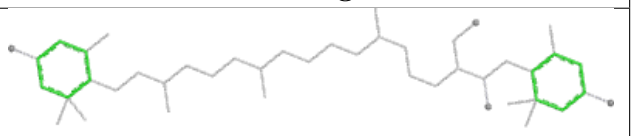


Bond lengths

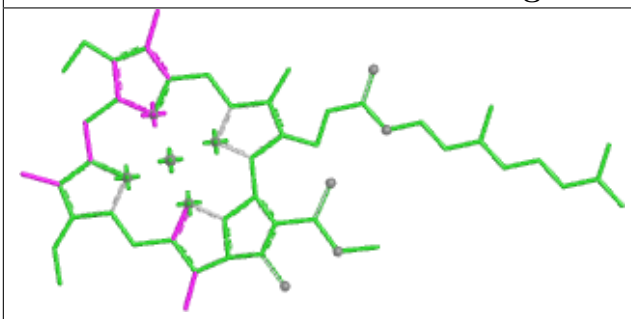
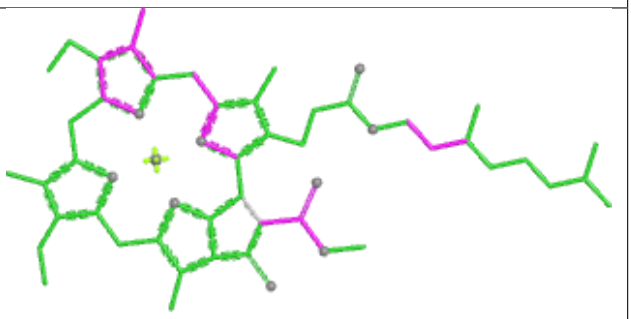
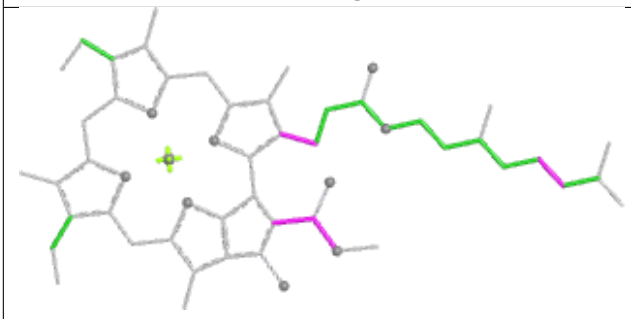
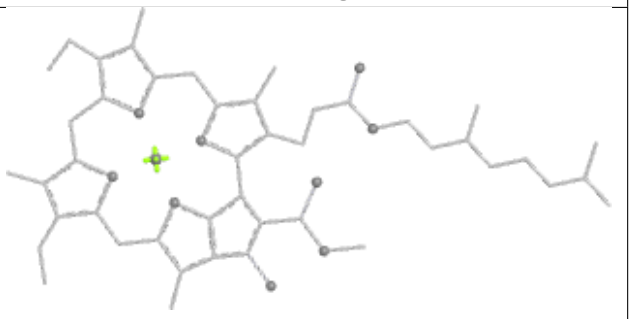


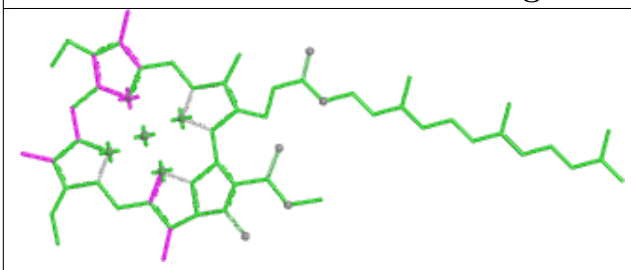
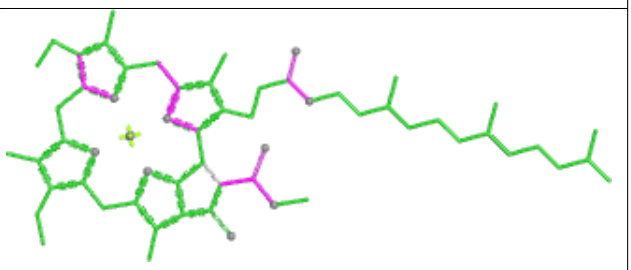
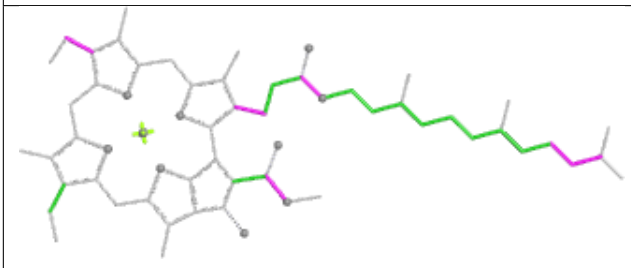
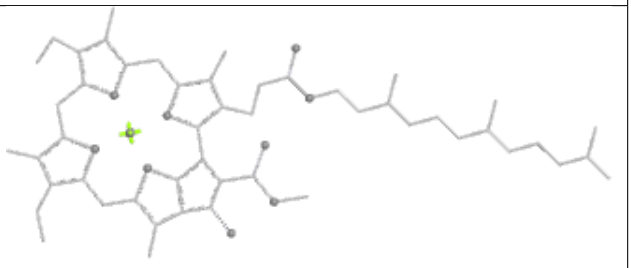
Bond angles

Torsions

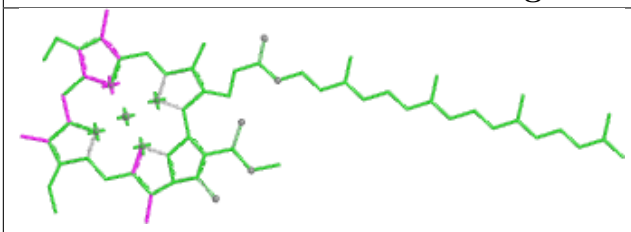


Rings

Ligand CLA H 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 829



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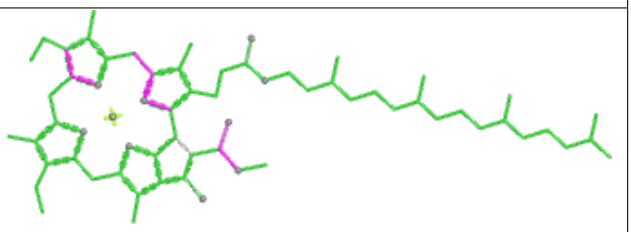
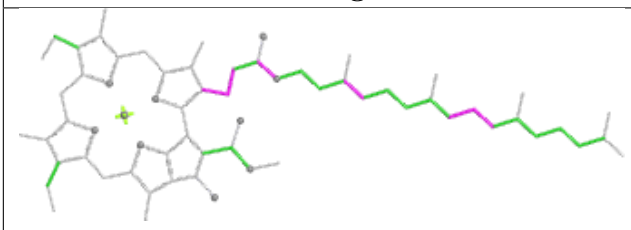
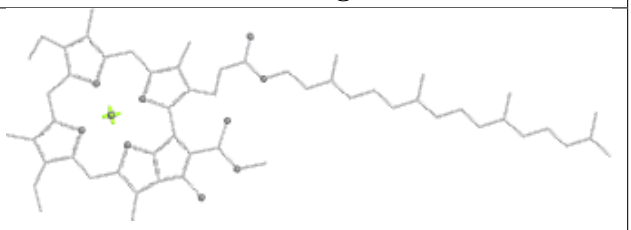


Bond angles

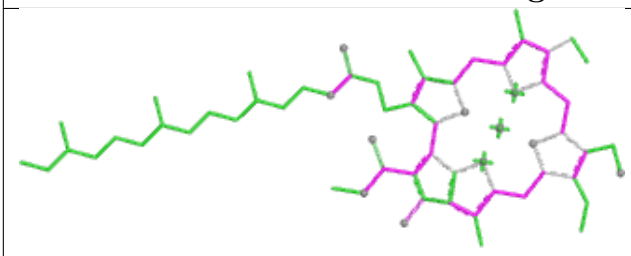


Torsions



Rings

Ligand CHL 3 302



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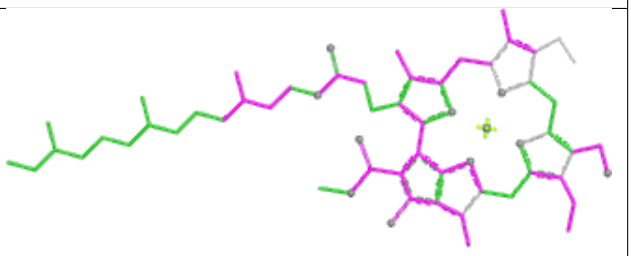
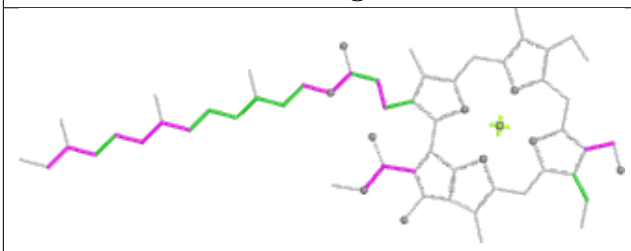


Bond angles



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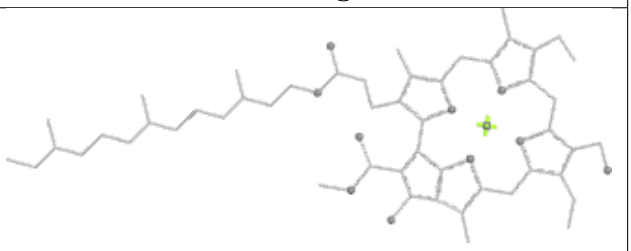
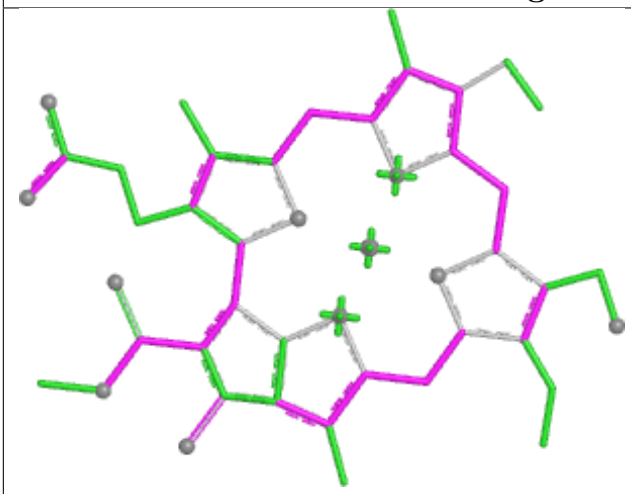


Rings

Ligand CHL 5 304



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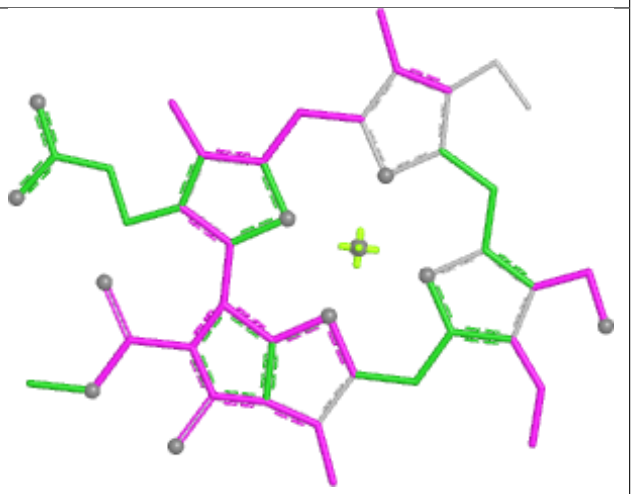
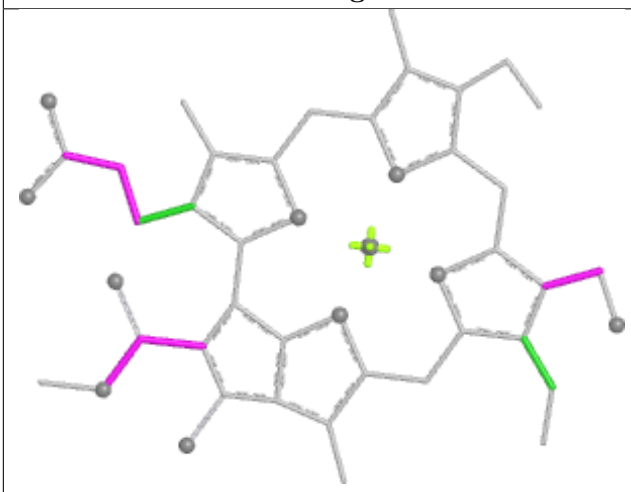


Bond angles



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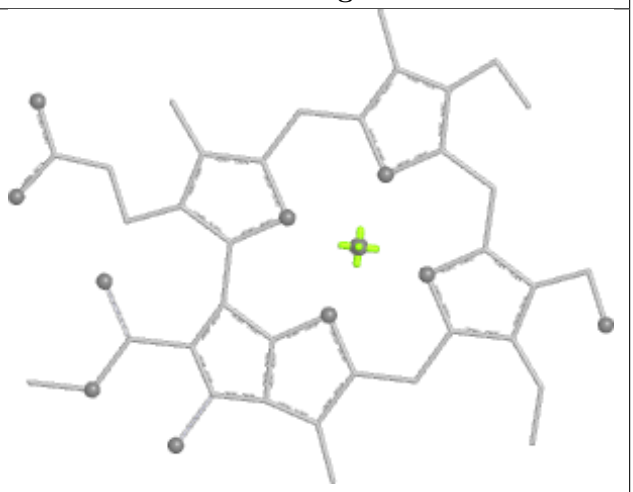
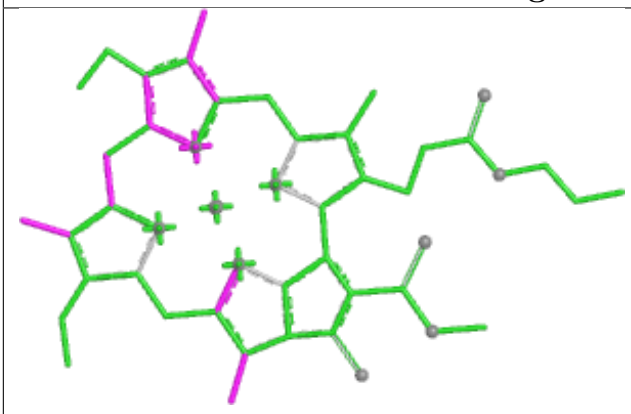


Rings

Ligand CLA 4 311



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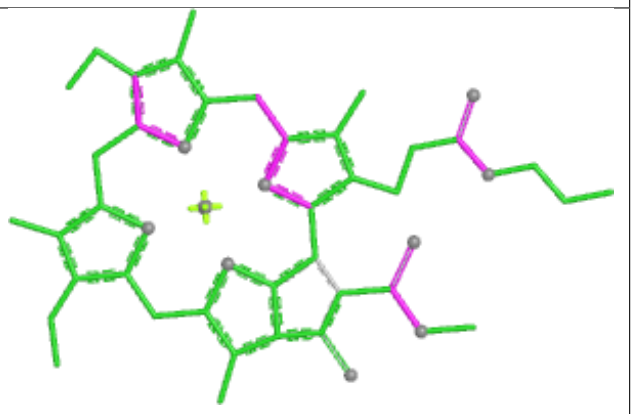
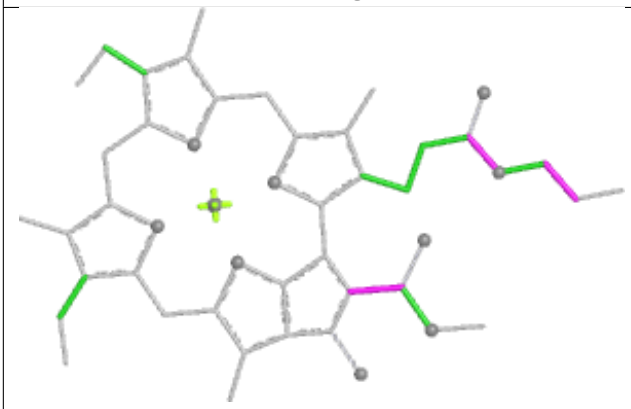


Bond angles



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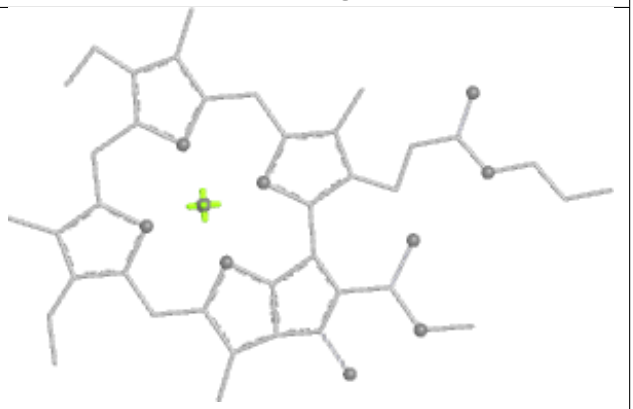
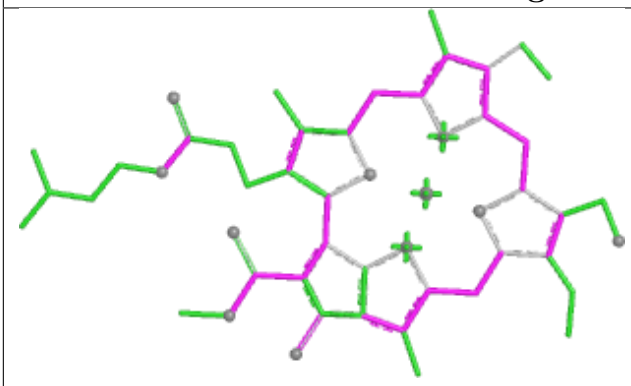


Rings

Ligand CHL 4 307



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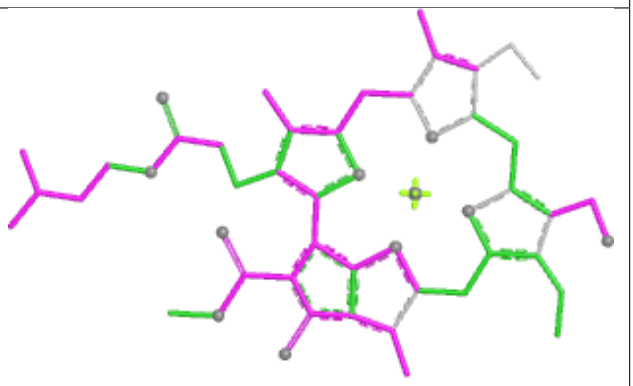
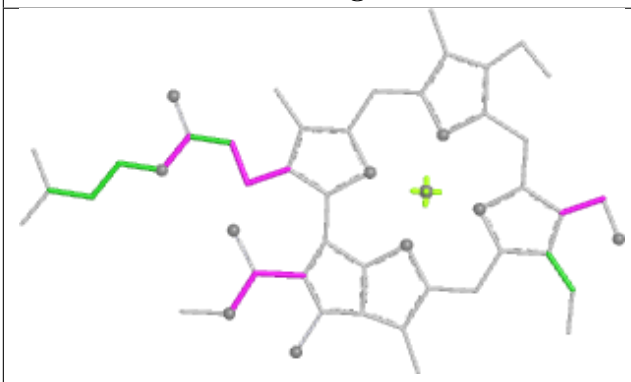


Bond angles



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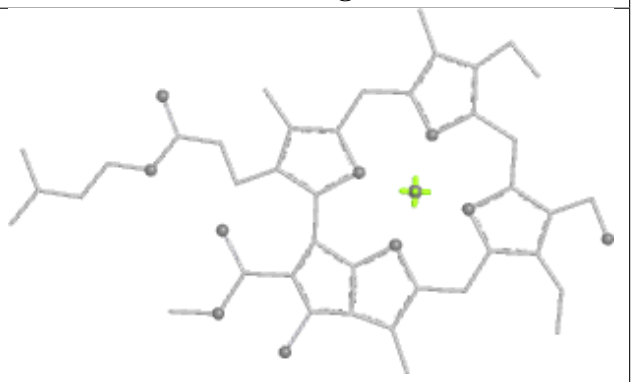
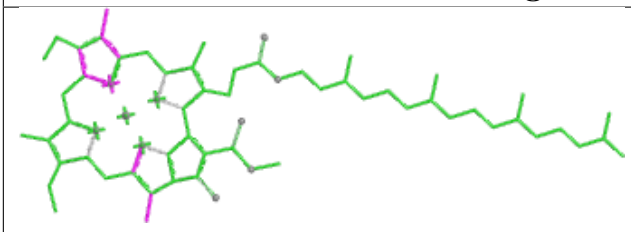


Rings

Ligand CLA B 840



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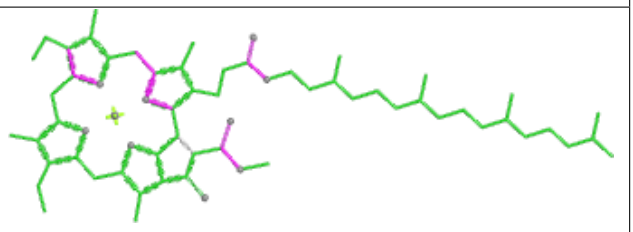
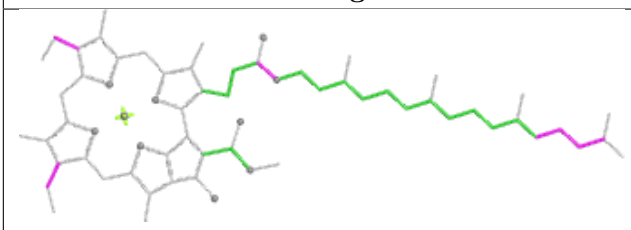


Bond angles



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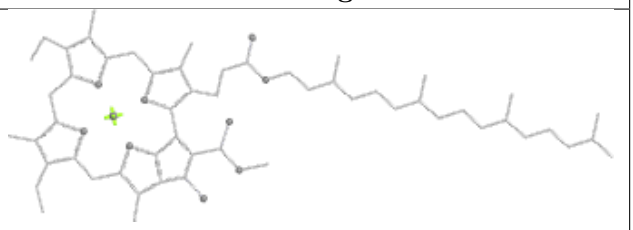
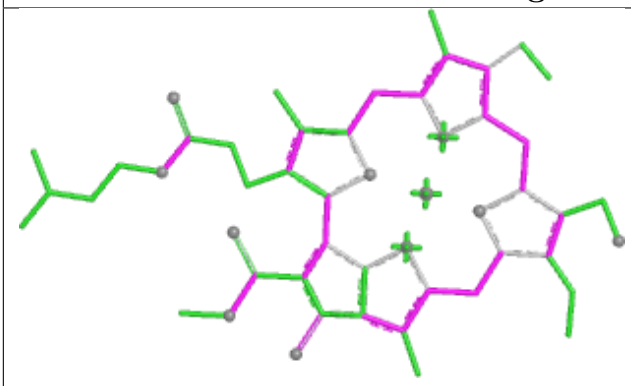


Rings

Ligand CHL 8 307



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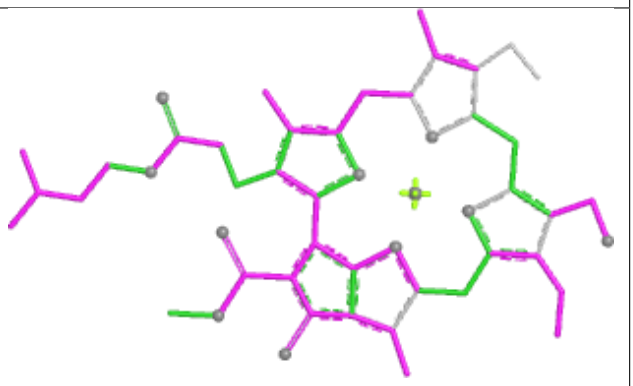
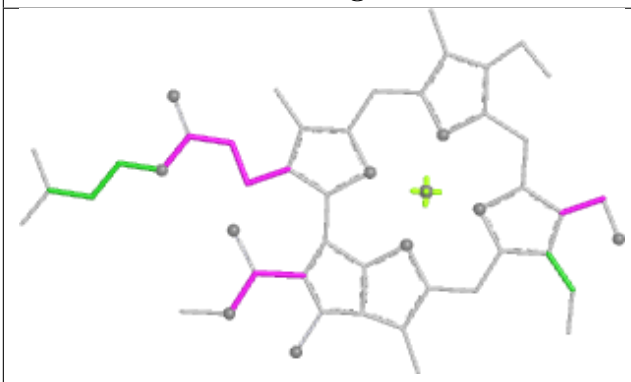


Bond angles



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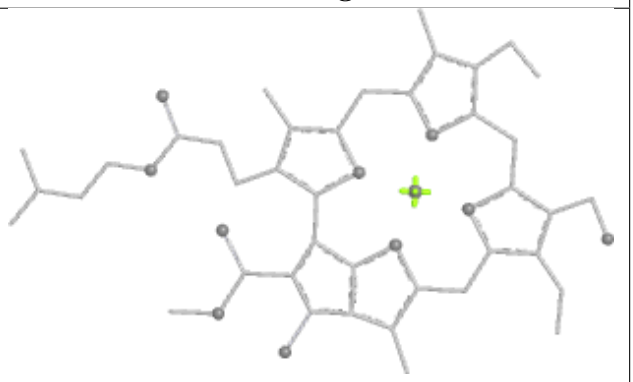
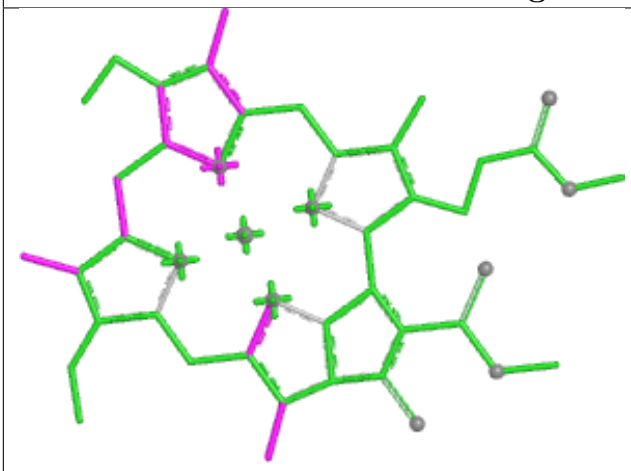


Rings

Ligand CLA 5 307



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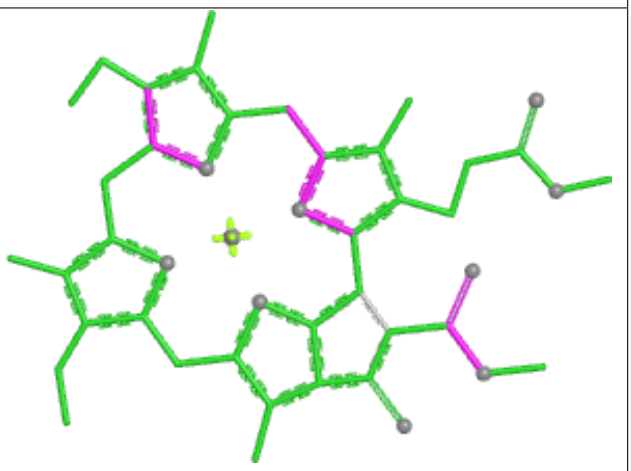

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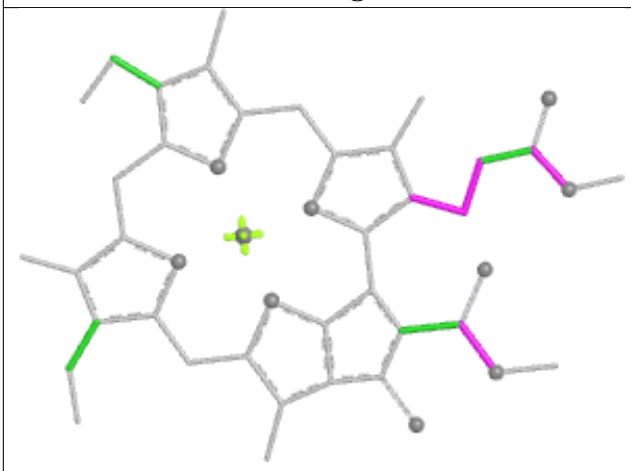

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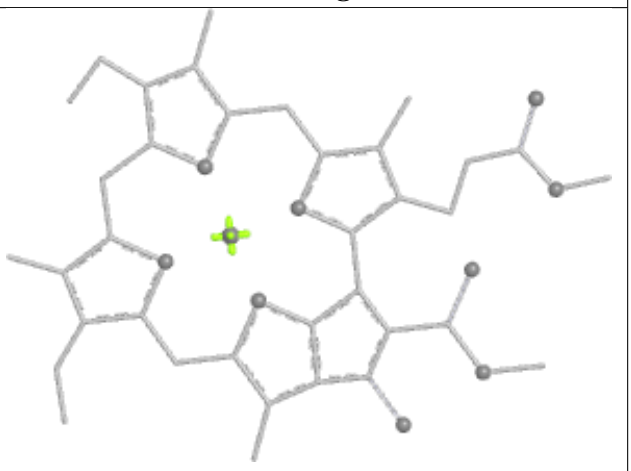
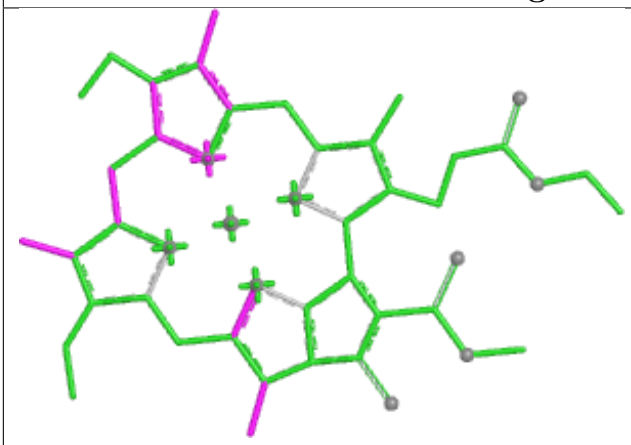


Rings

Ligand CLA 0 310



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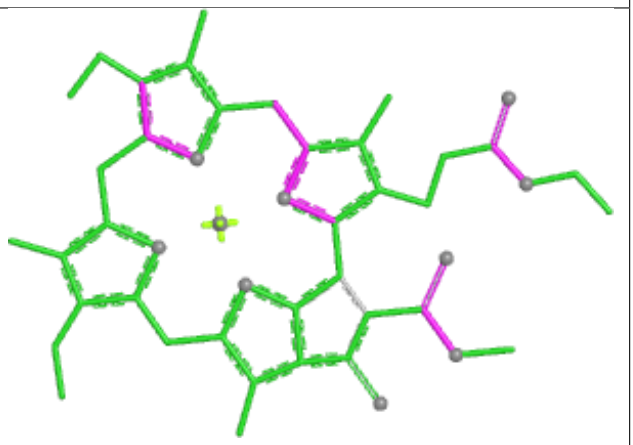
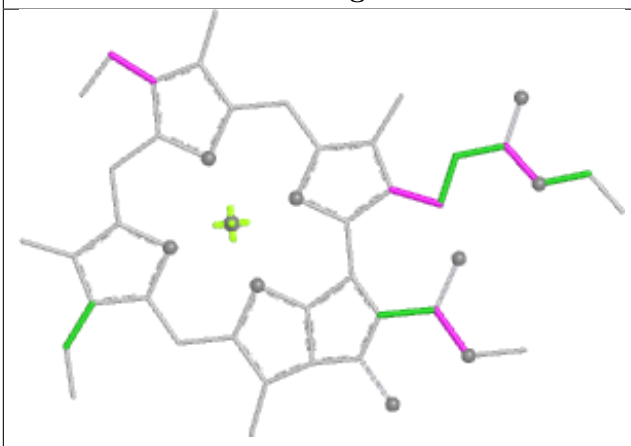


Bond angles



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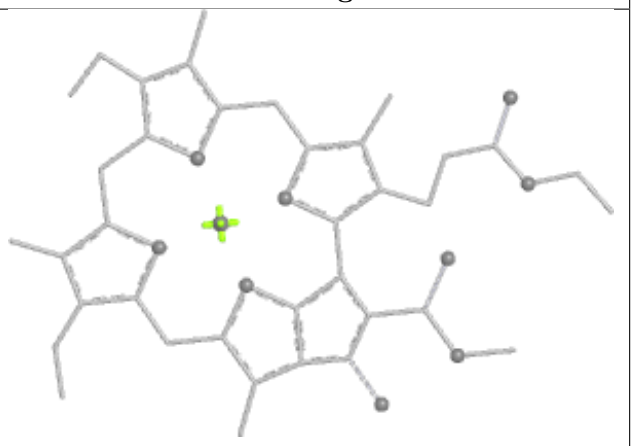
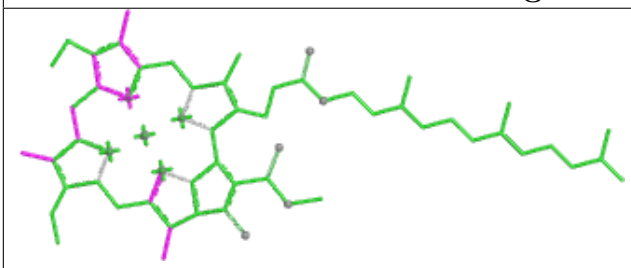


Rings

Ligand CLA B 819



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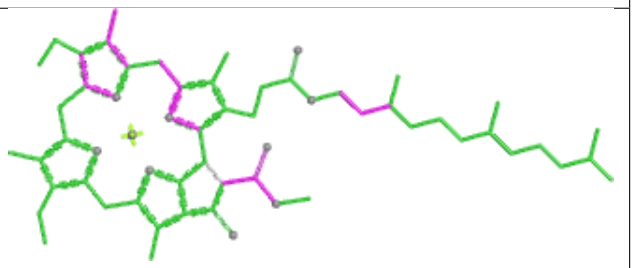
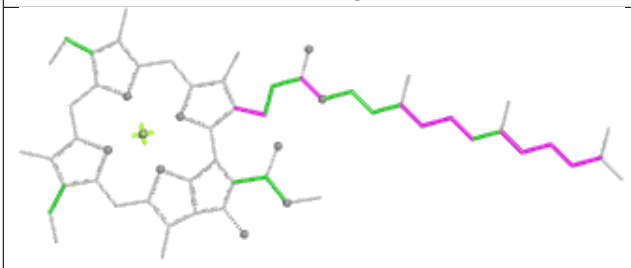


Bond angles



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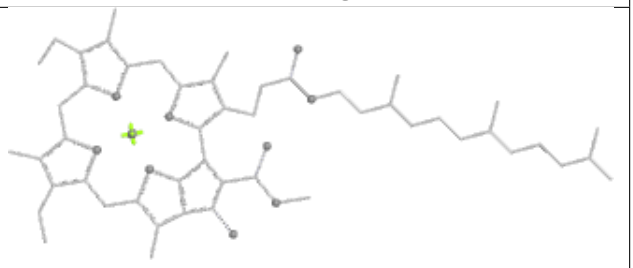
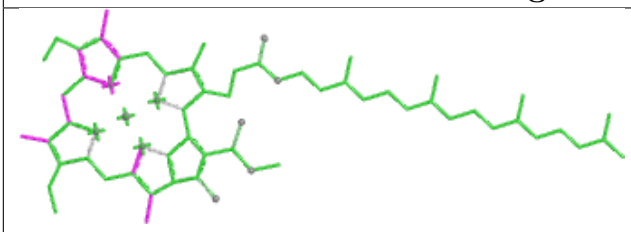


Rings

Ligand CLA 3 304



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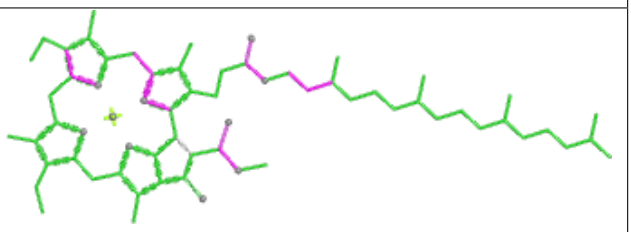
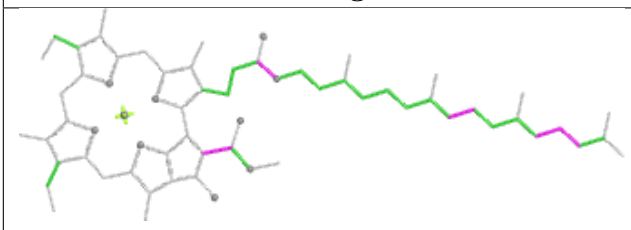


Bond angles



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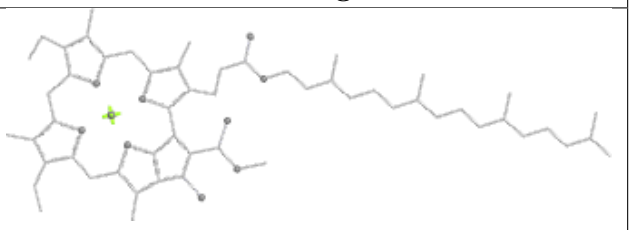
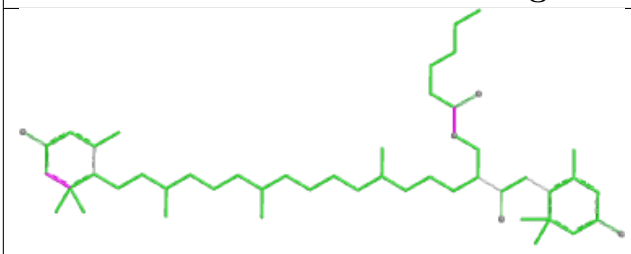


Rings

Ligand 0UR 2 315



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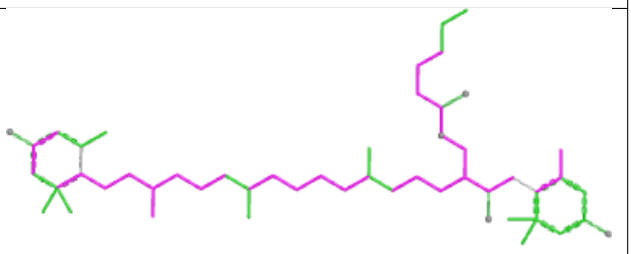
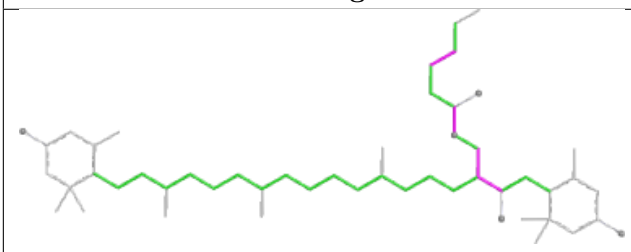
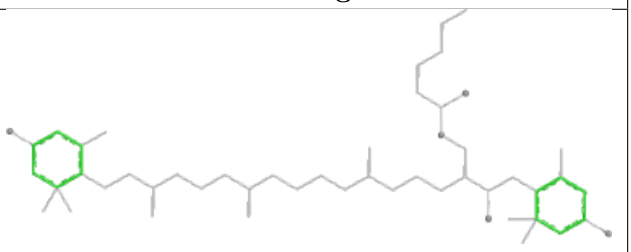


Bond angles

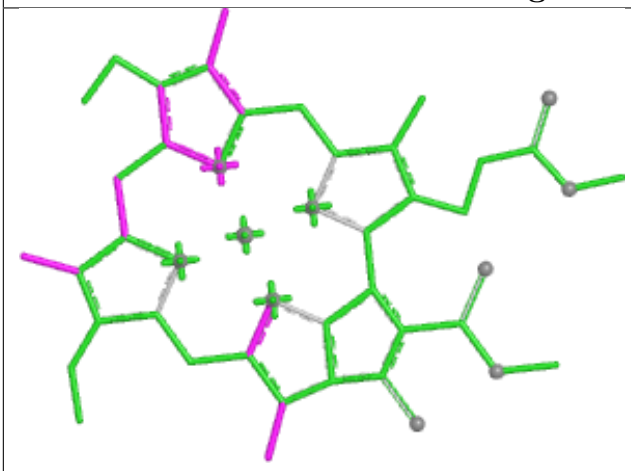


Torsions

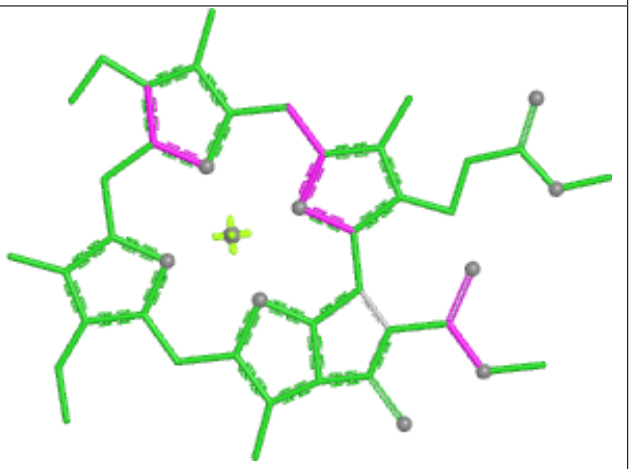


Rings

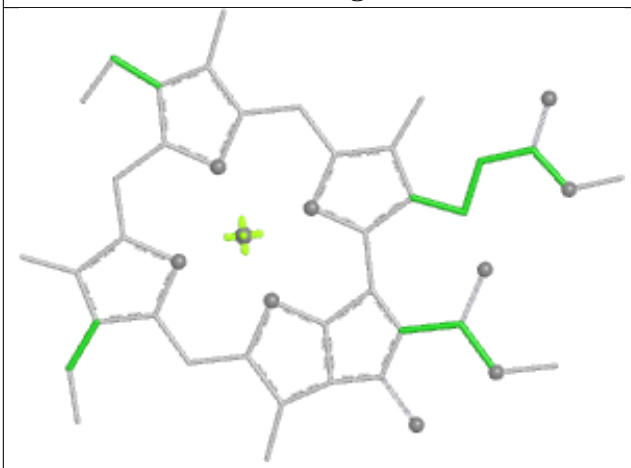
Ligand CLA 3 314



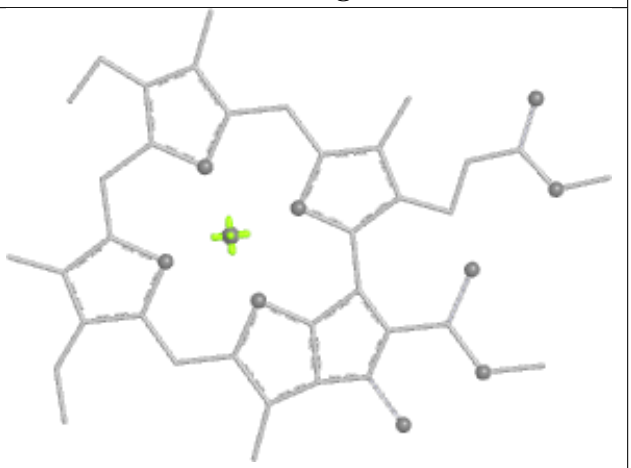
Bond lengths



Bond angles

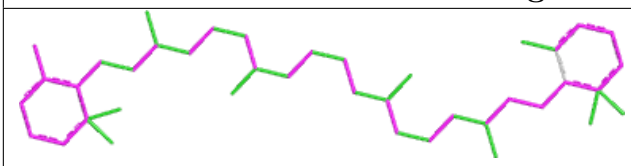


Torsions



Rings

Ligand 8CT B 848



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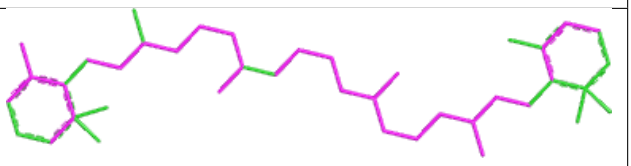

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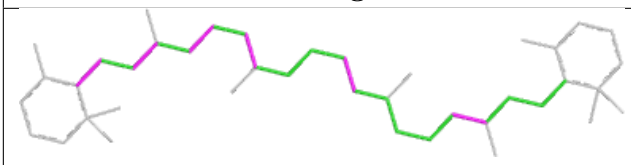
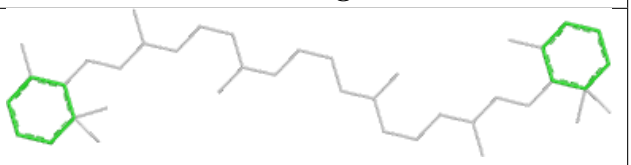
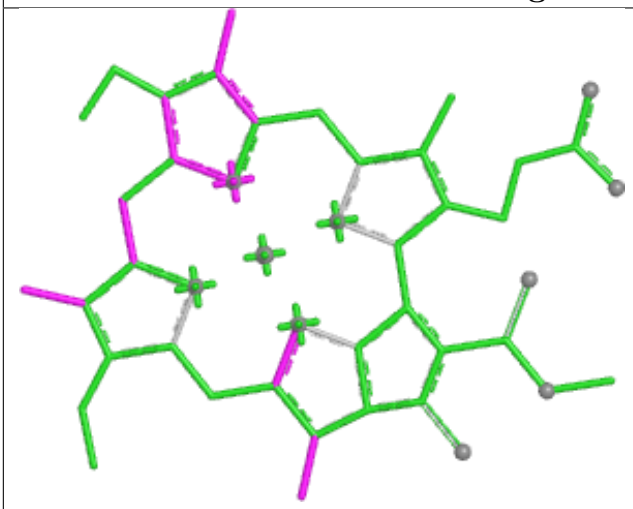


Torsions



Rings

Ligand CLA 4 314



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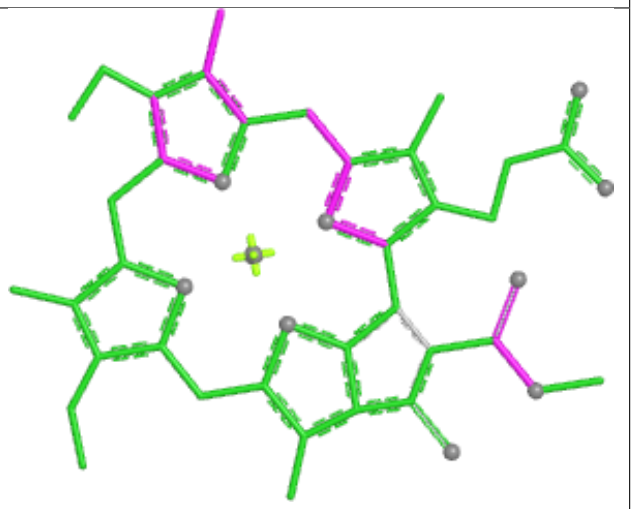

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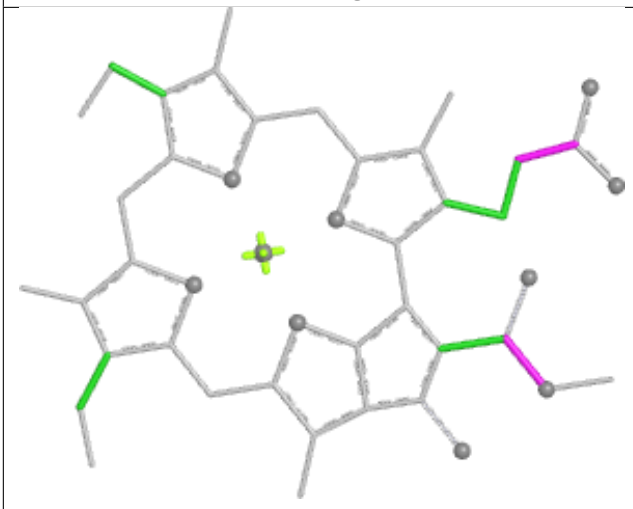
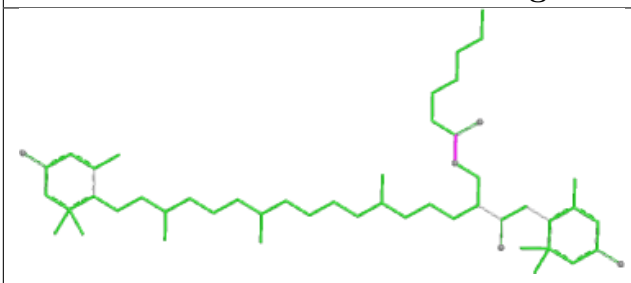


Torsions

Rings

Ligand 0UR 1 316



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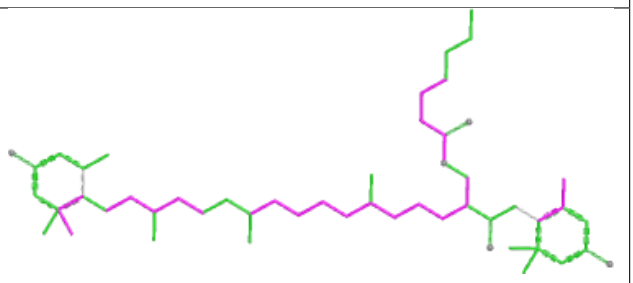

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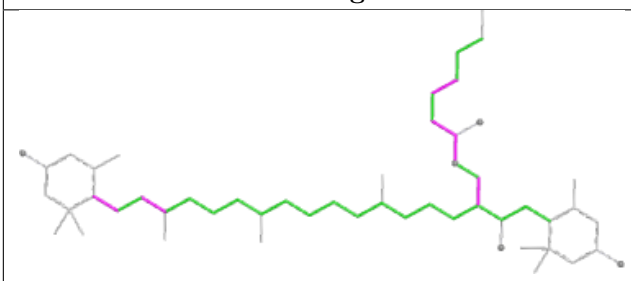
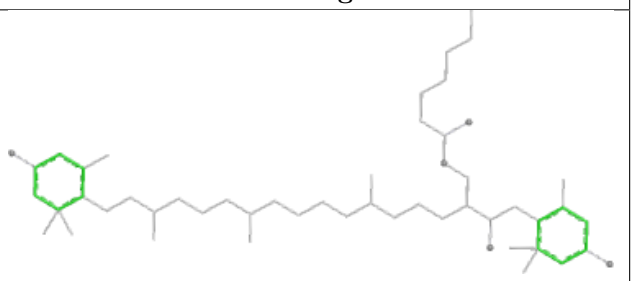
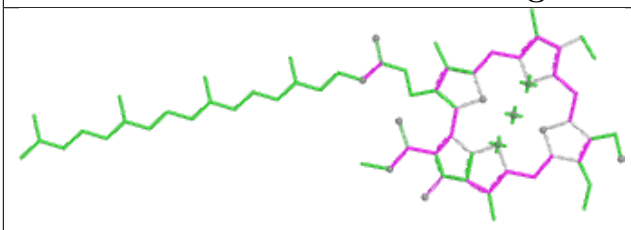


Torsions



Rings

Ligand CHL 3 307



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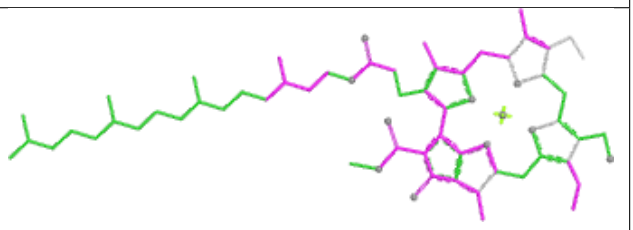

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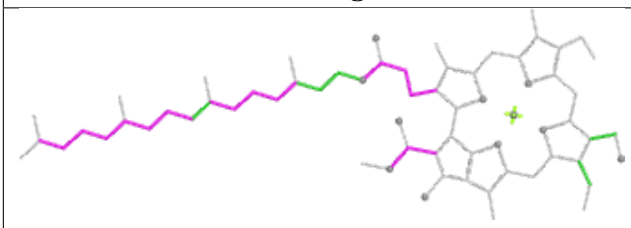

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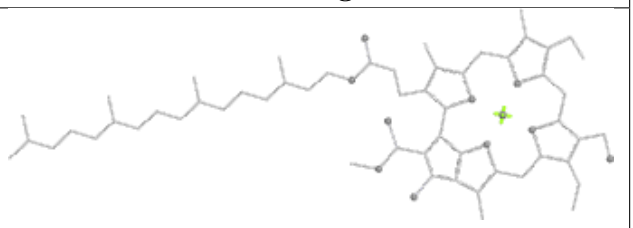
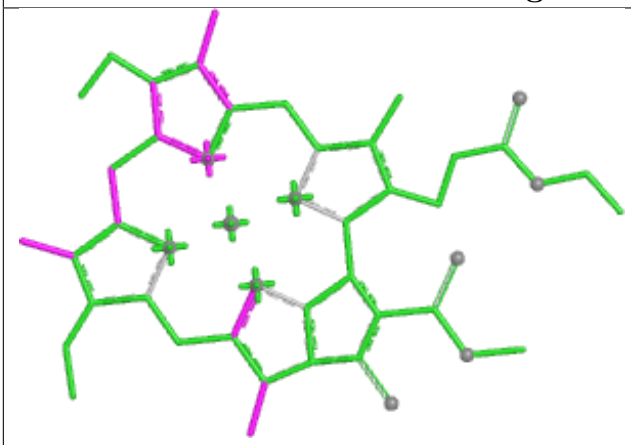


Rings

Ligand CLA F 302



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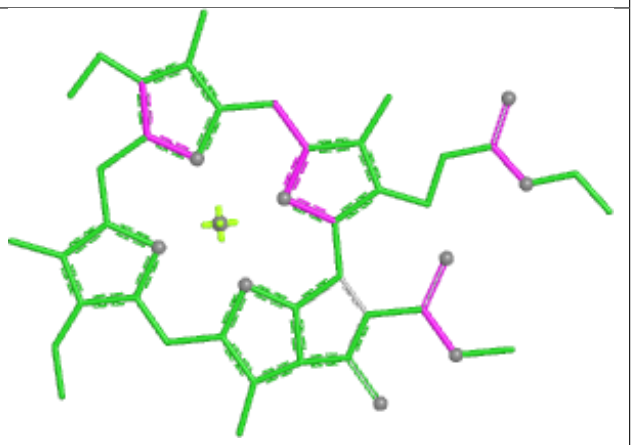

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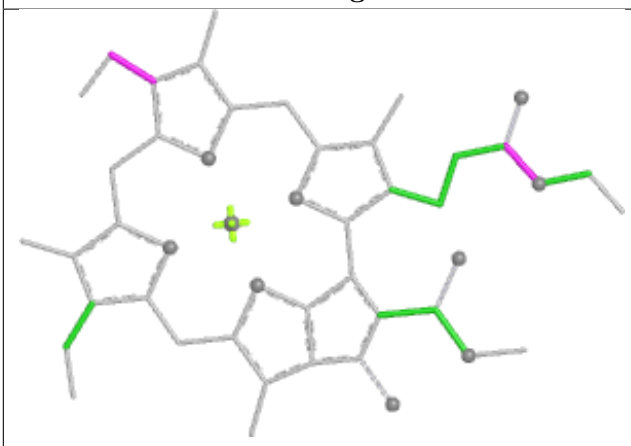

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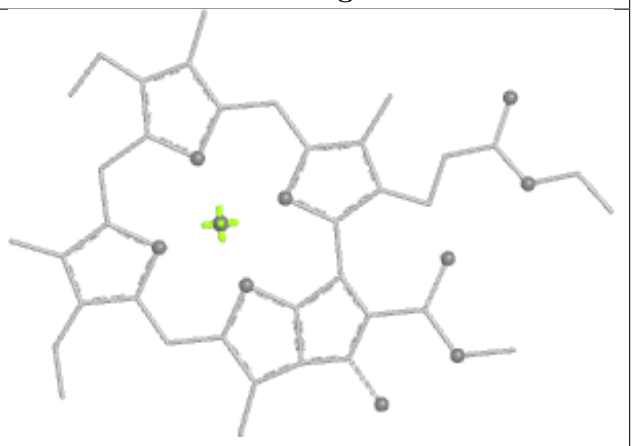
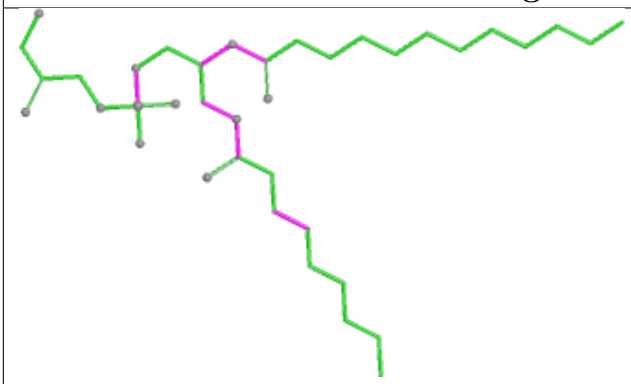


Rings

Ligand LHG B 852



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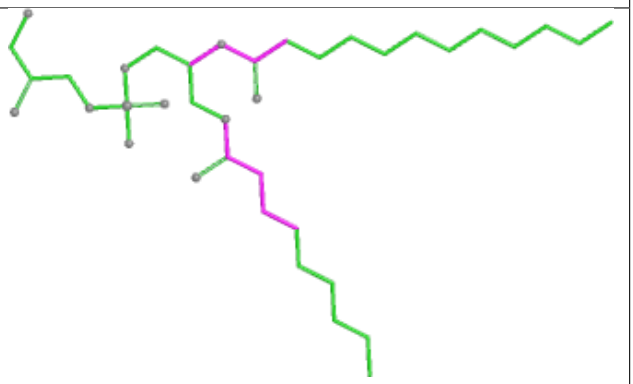

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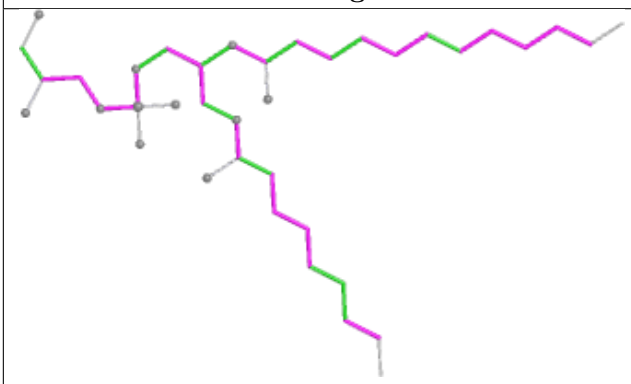

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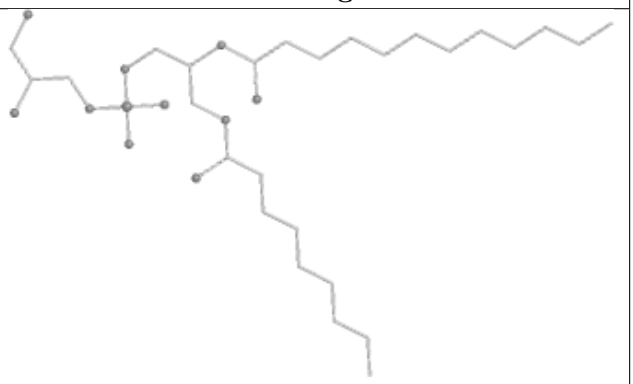
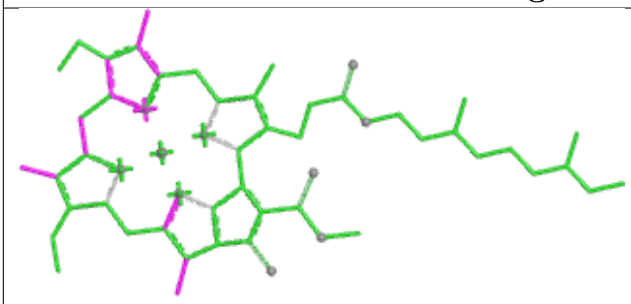


Rings

Ligand CLA 5 311



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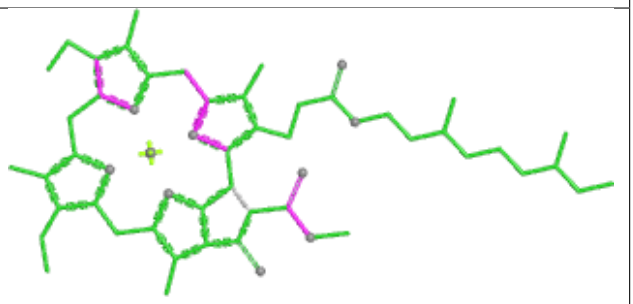

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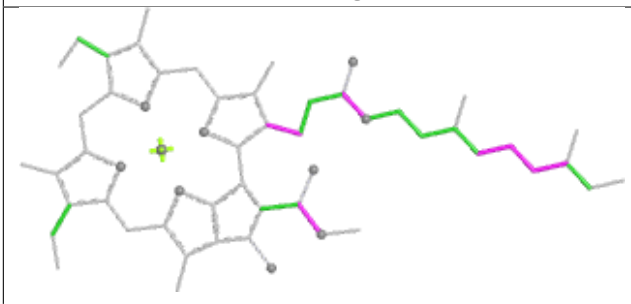

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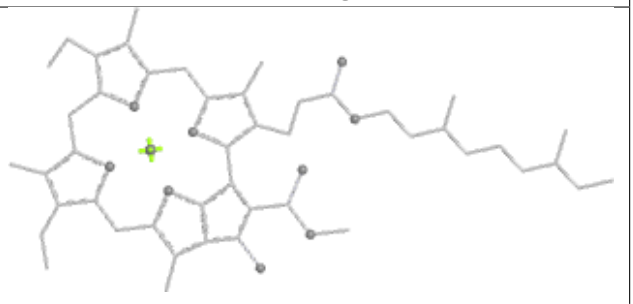
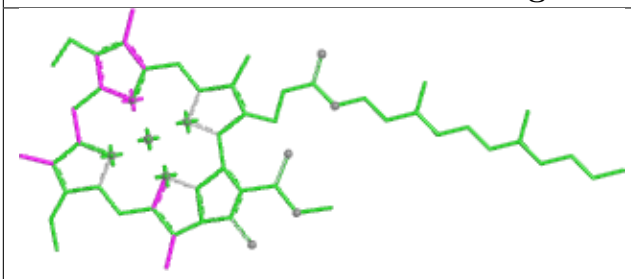


Rings

Ligand CLA 6 309



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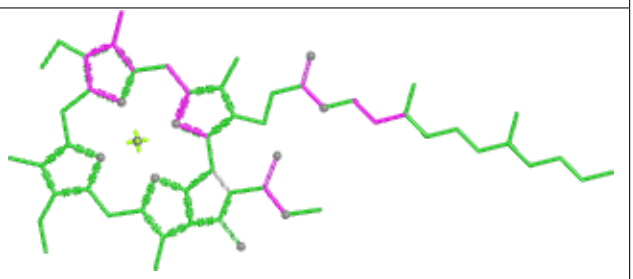

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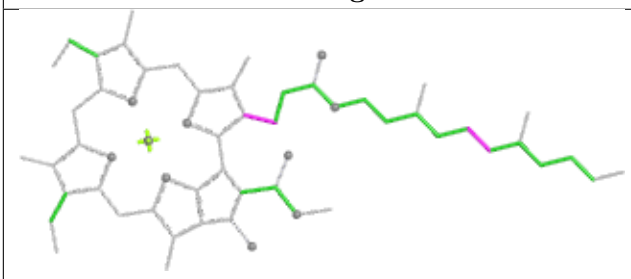

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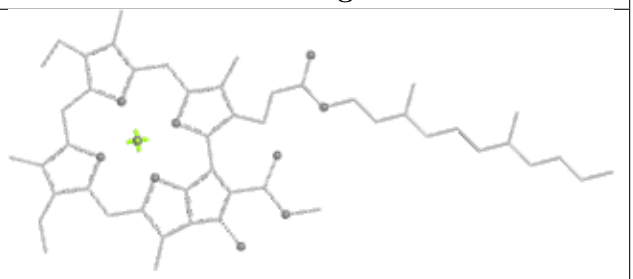
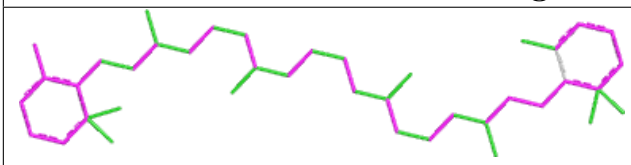


Rings

Ligand 8CT J 101



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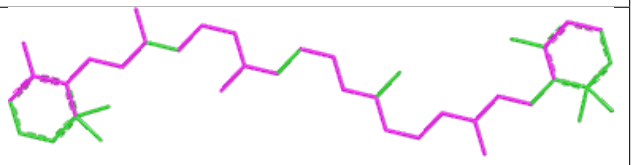
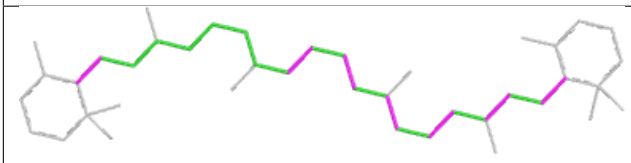


Bond angles



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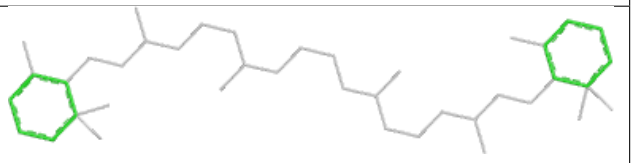
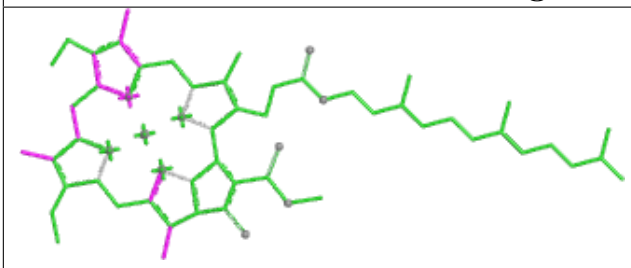


Rings

Ligand CLA 5 308



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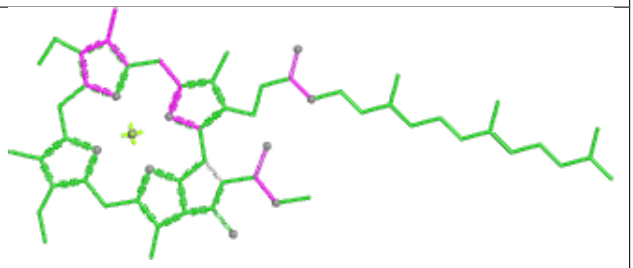
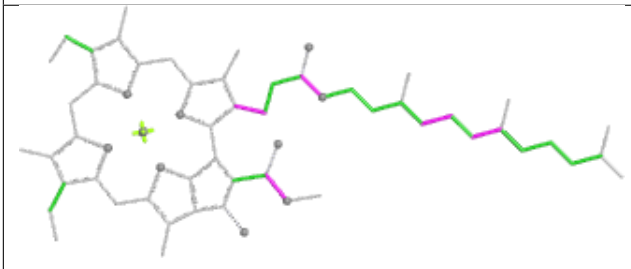


Bond angles



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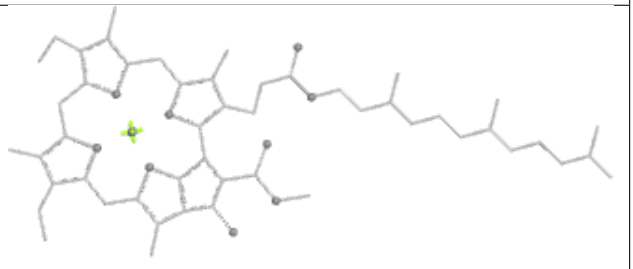
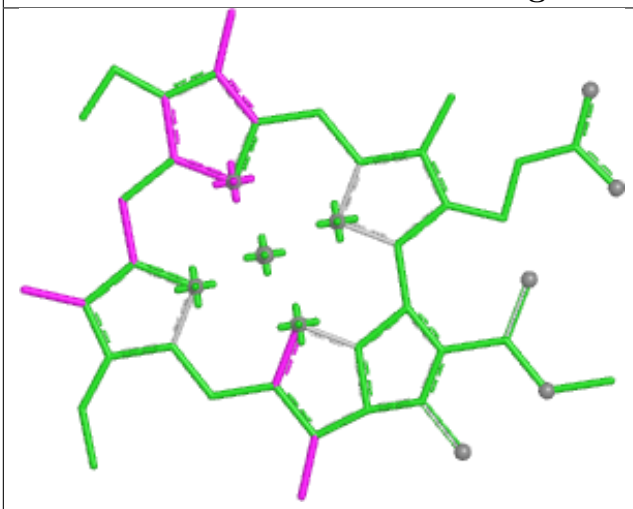


Rings

Ligand CLA 5 309



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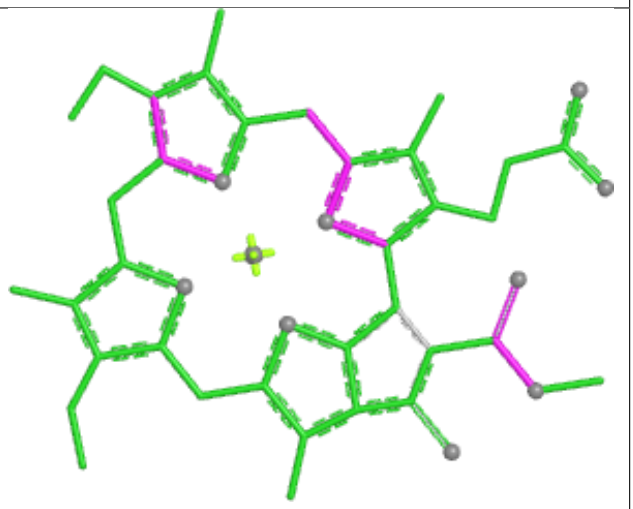
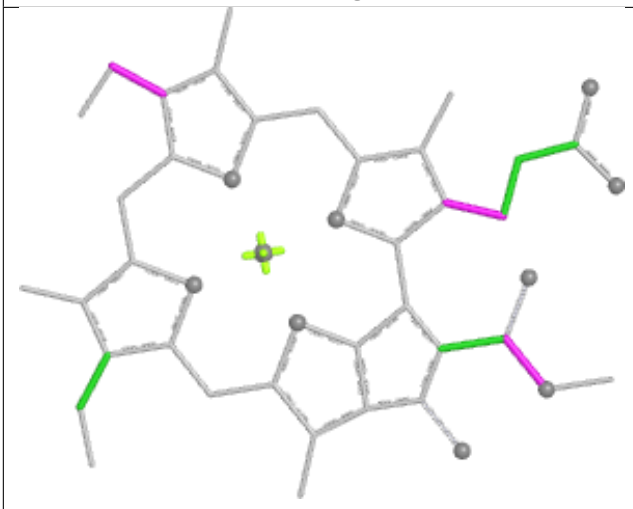


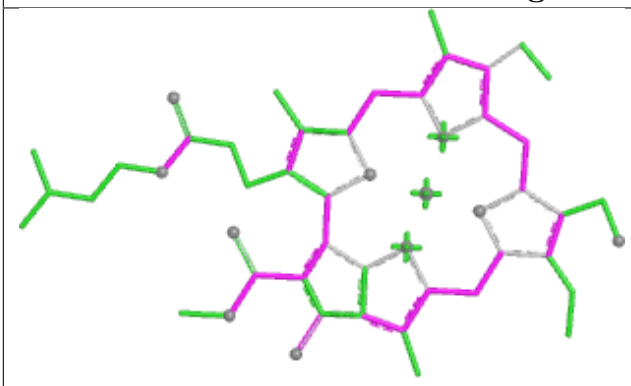
Bond angles



Torsions

Rings

Ligand CHL 6 306



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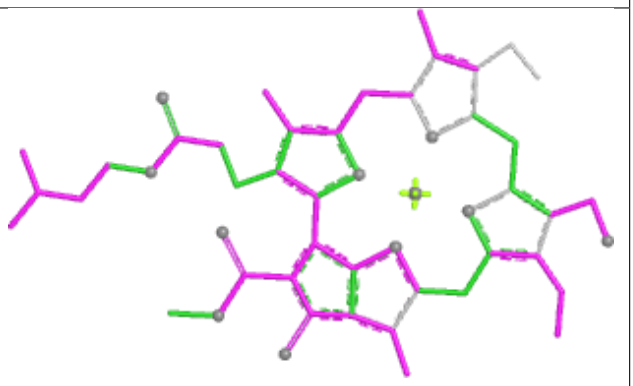
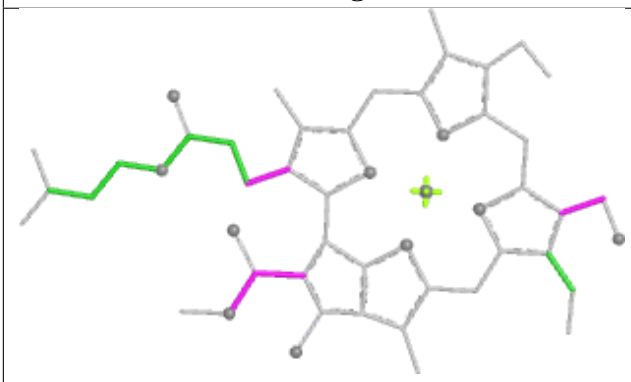


Bond angles



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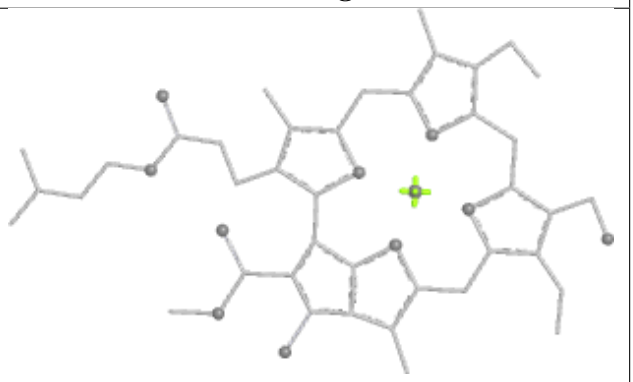
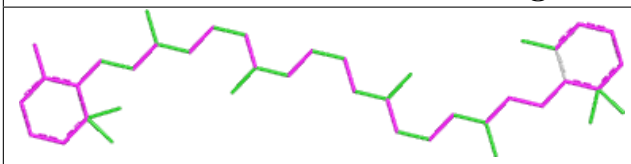


Rings

Ligand 8CT L 207



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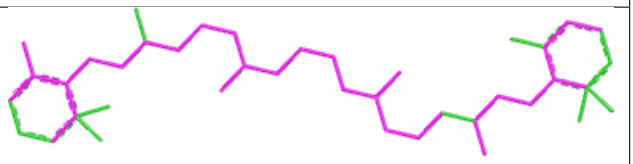
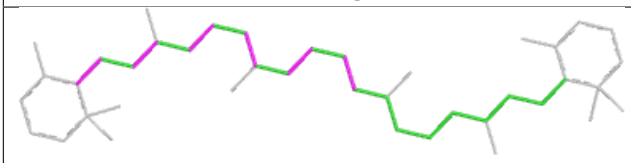


Bond angles



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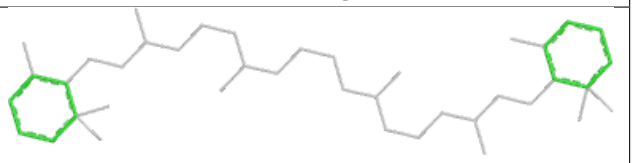
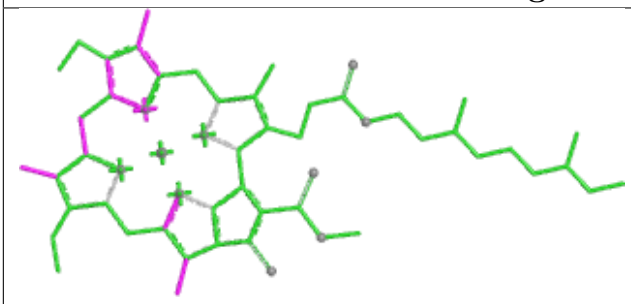
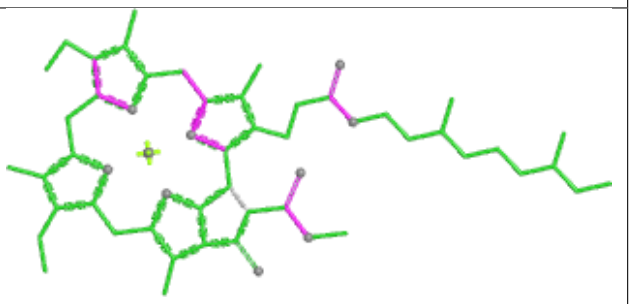
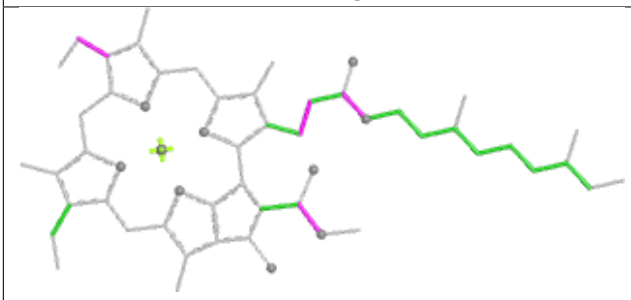
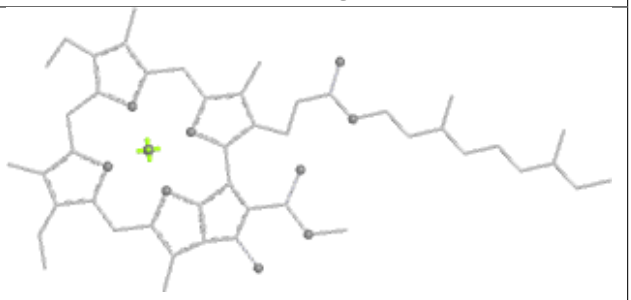
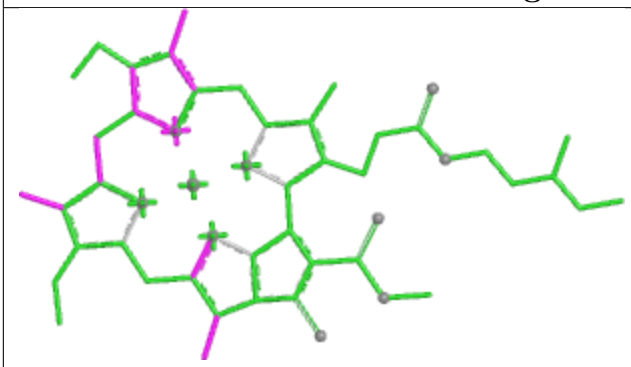
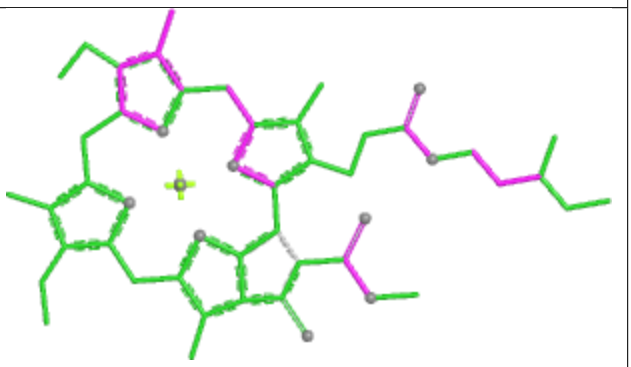
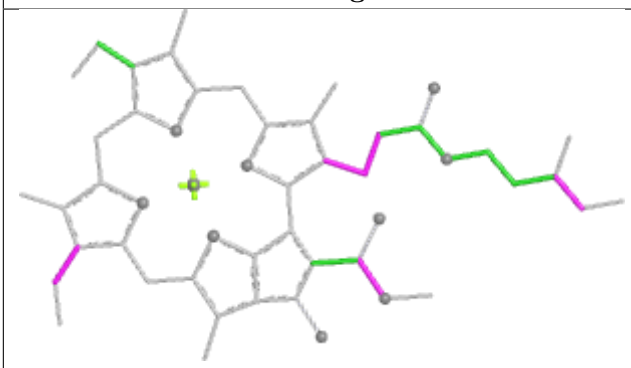
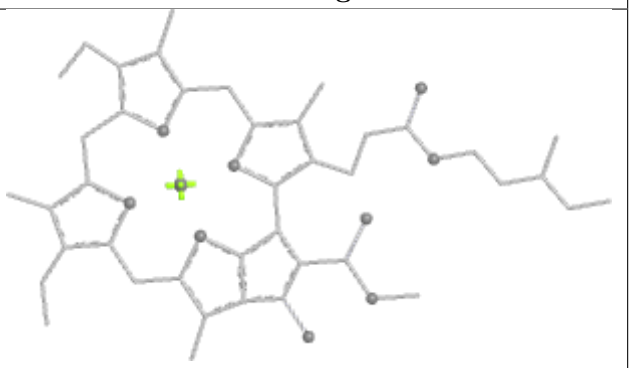
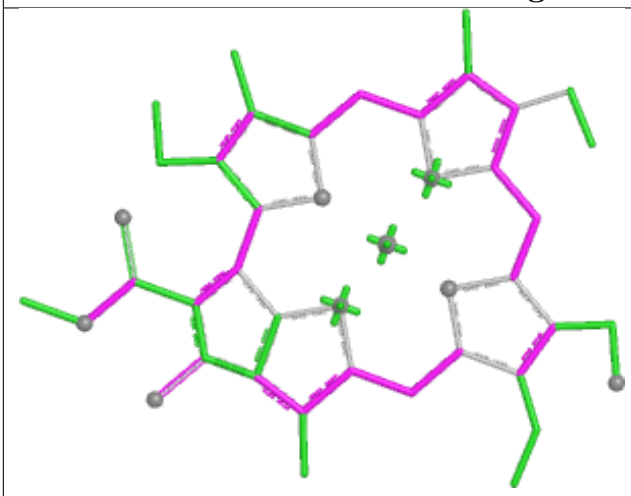


Rings

Ligand CLA 6 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 6 315



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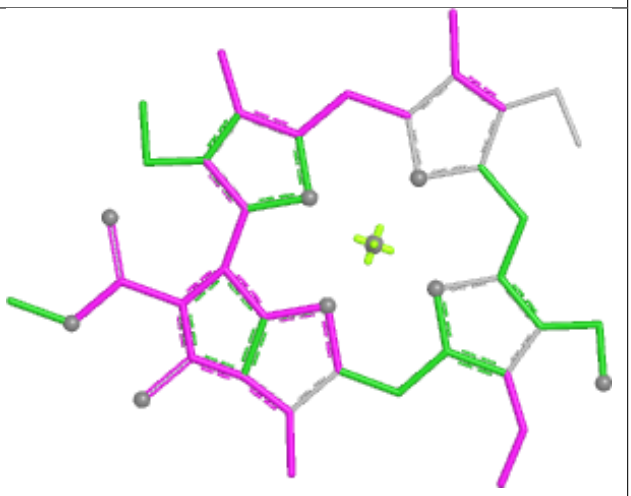

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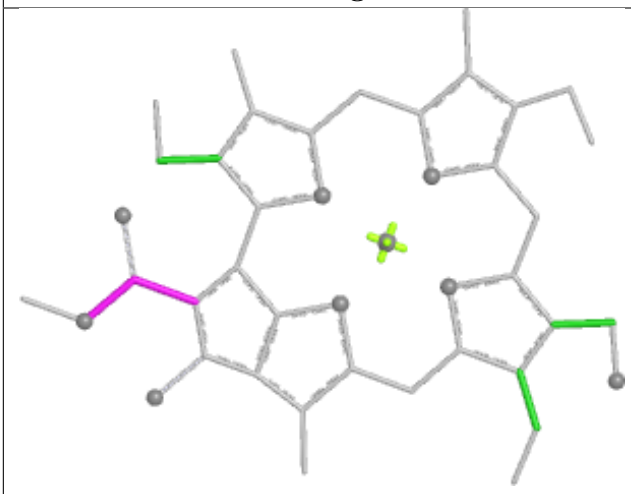
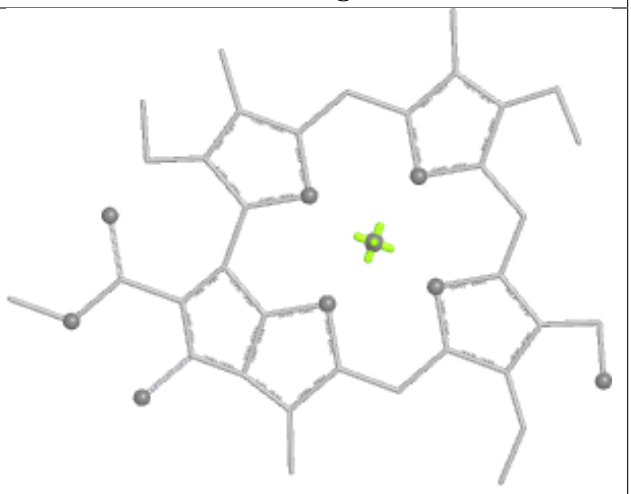
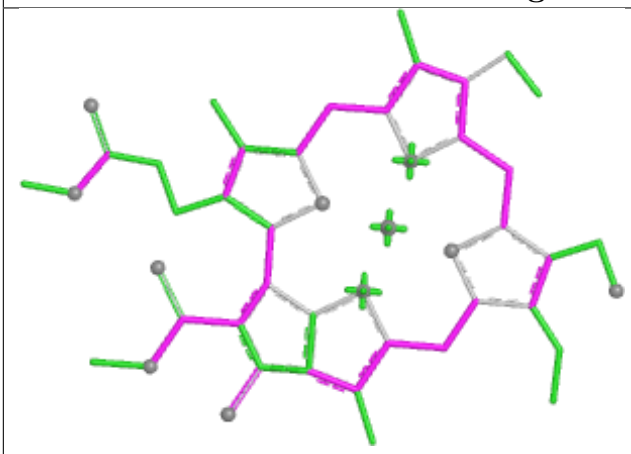


Torsions



Rings

Ligand CHL 2 307



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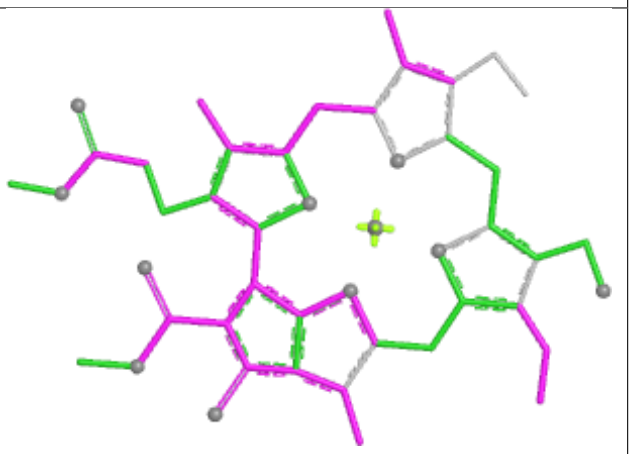

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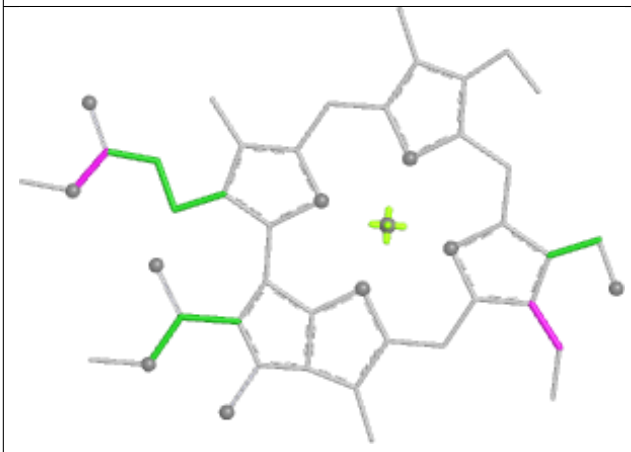
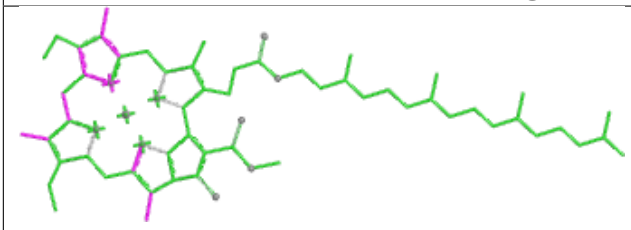


Torsions

Rings

Ligand CLA A 805



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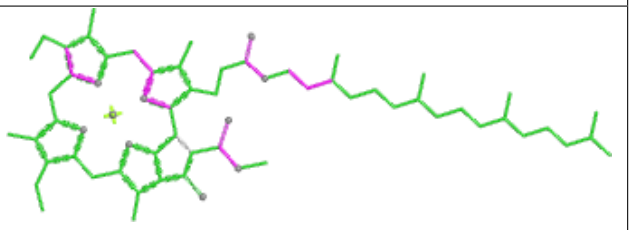
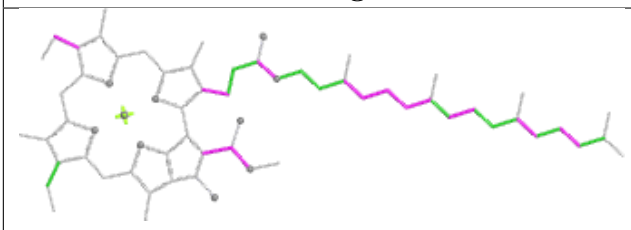
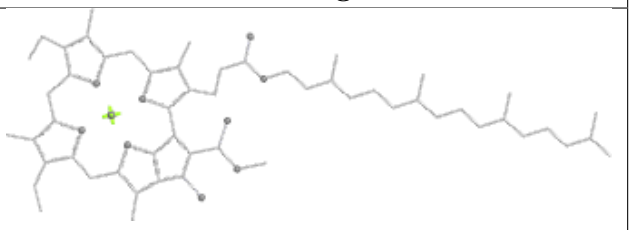


Bond angles

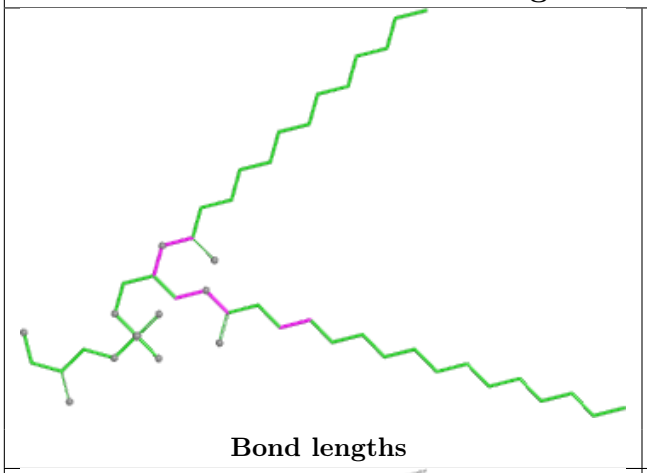


Torsions



Rings

Ligand LHG I 102



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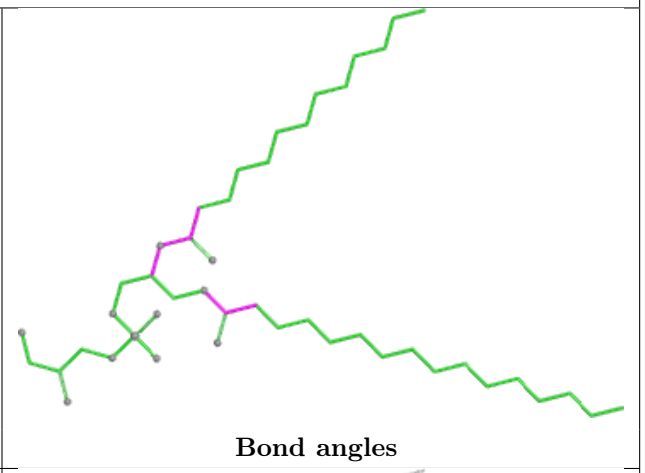
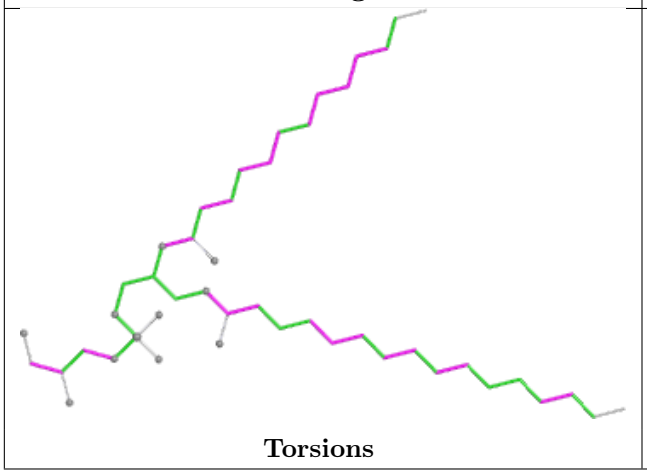


Bond angles



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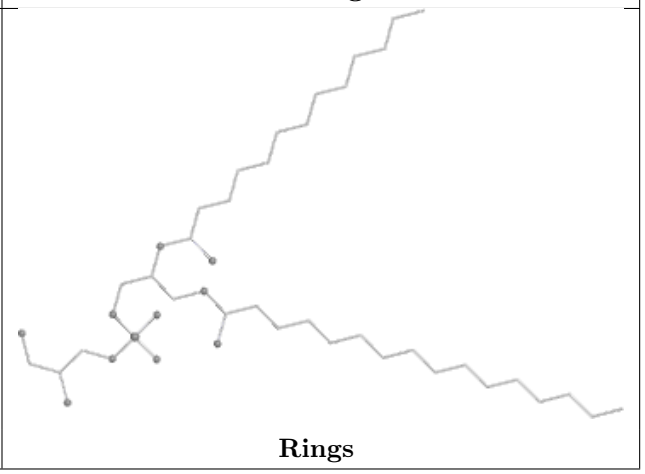
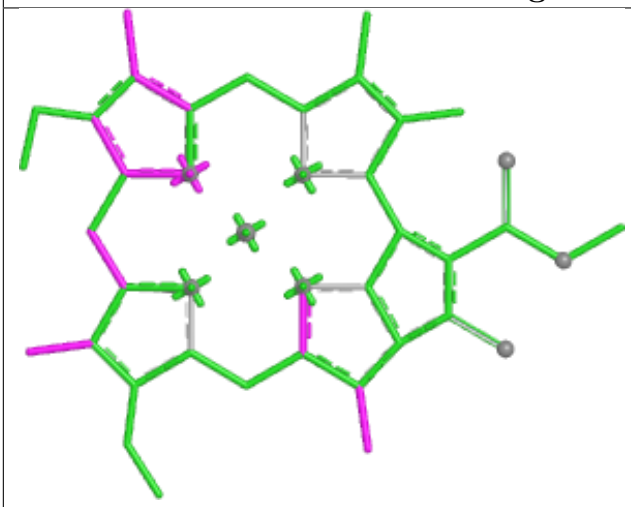


Rings

Ligand CLA 0 309



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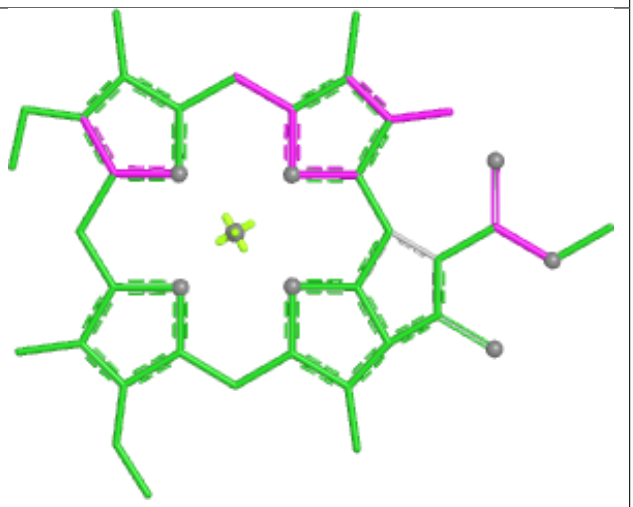

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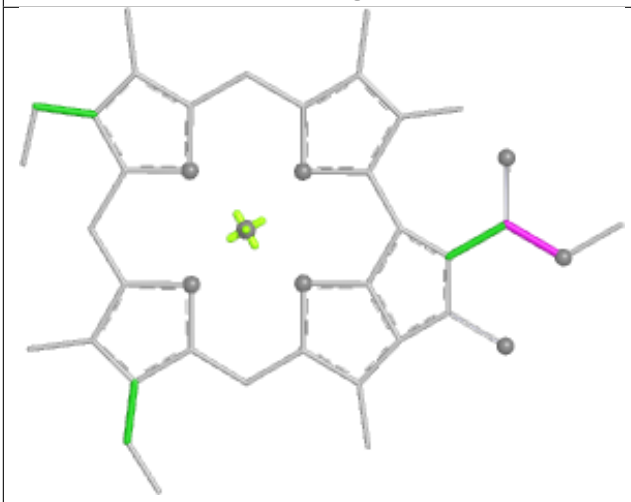

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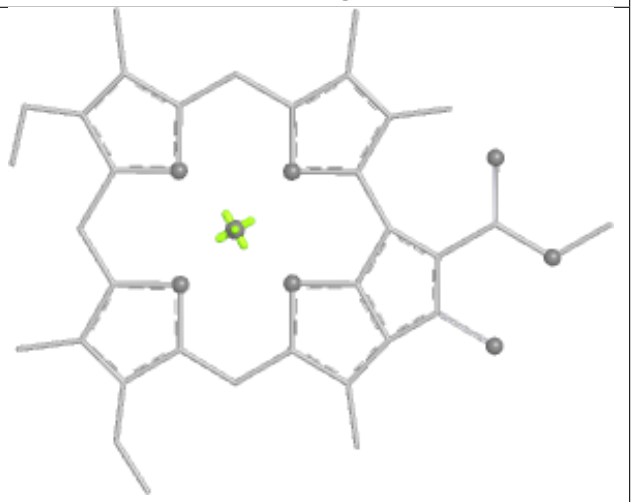
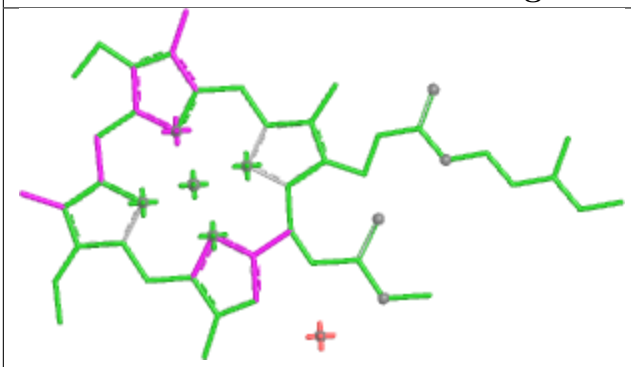


Rings

Ligand CLA B 826



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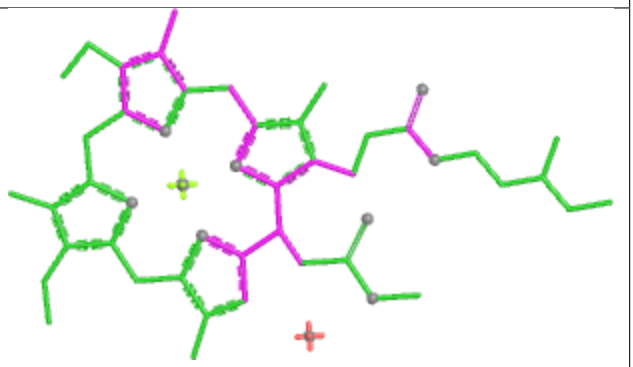
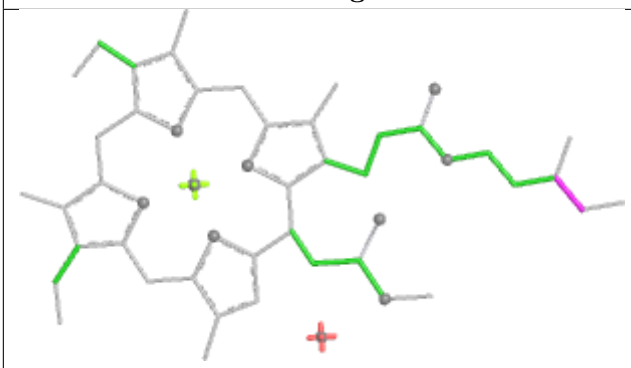


Bond angles



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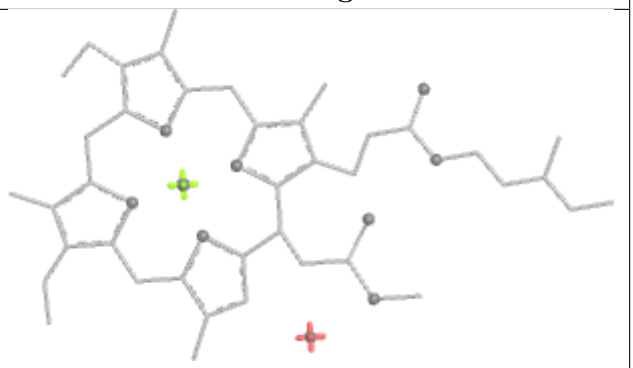
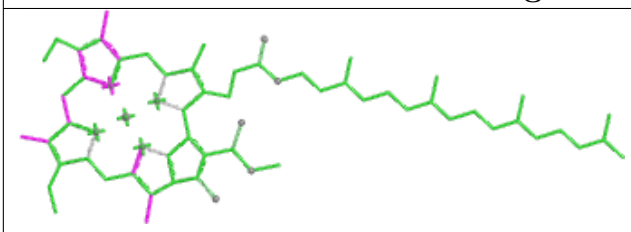


Rings

Ligand CLA B 811



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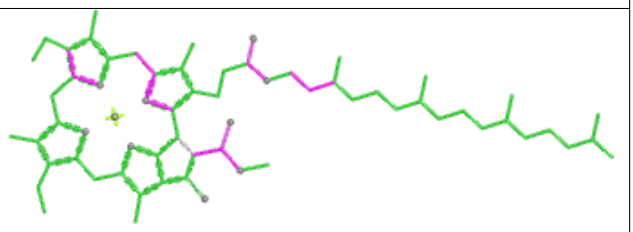
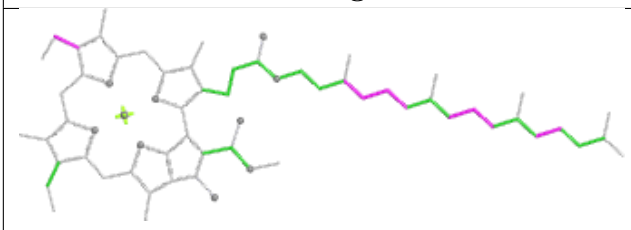


Bond angles



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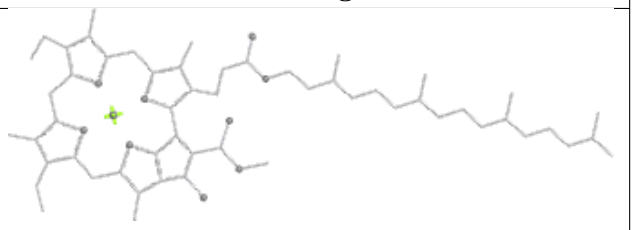
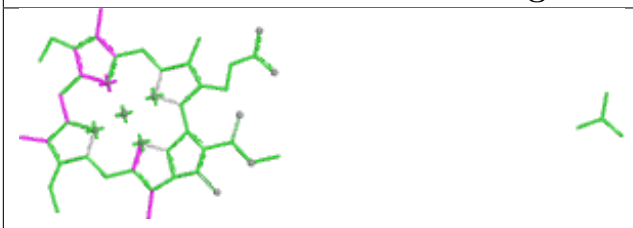


Rings

Ligand CLA 7 315



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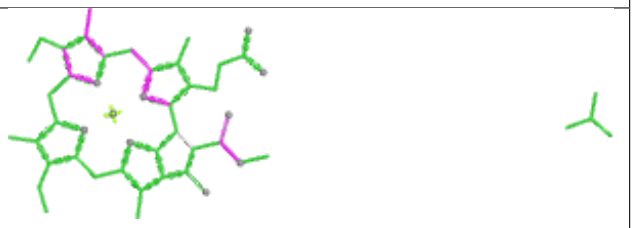

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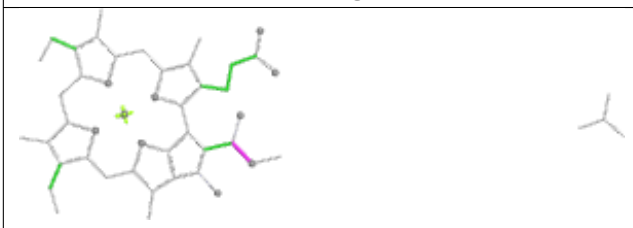

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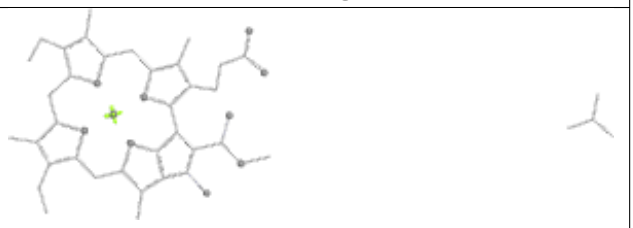
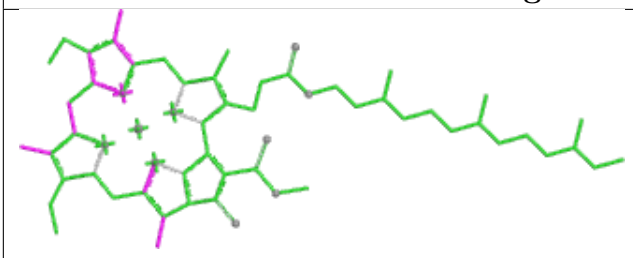


Rings

Ligand CLA A 816



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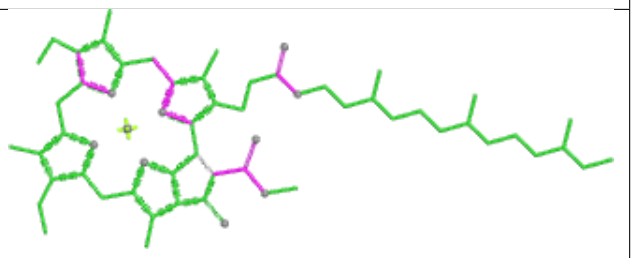
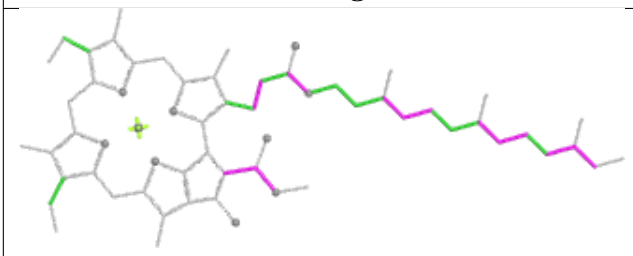


Bond angles



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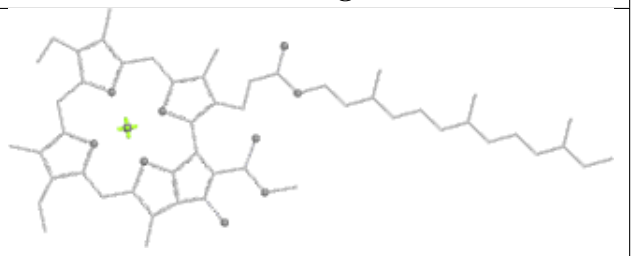
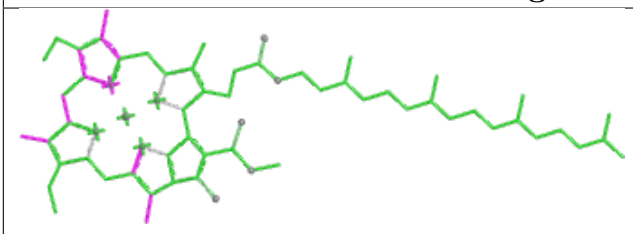


Rings

Ligand CLA 3 309



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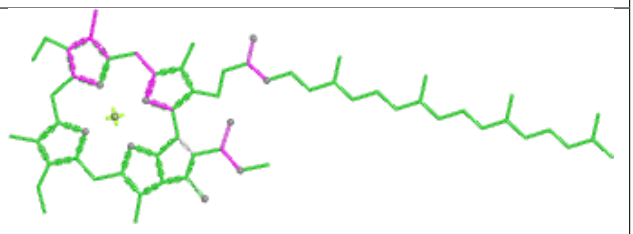
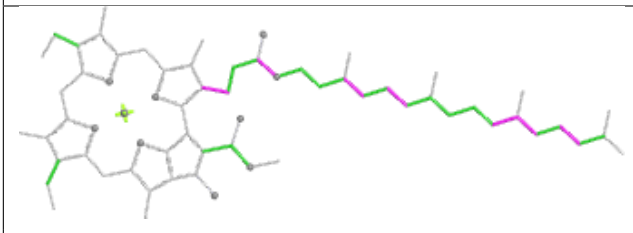
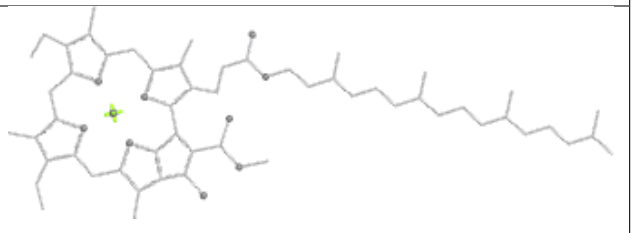


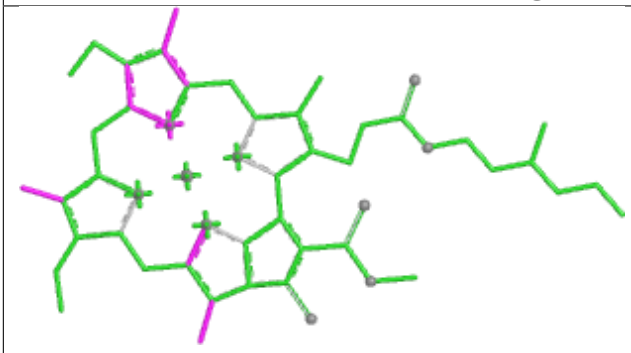
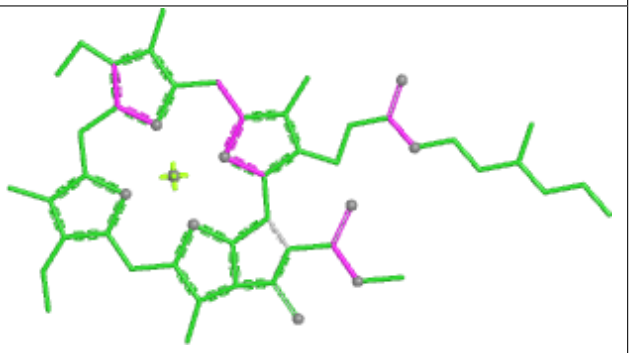
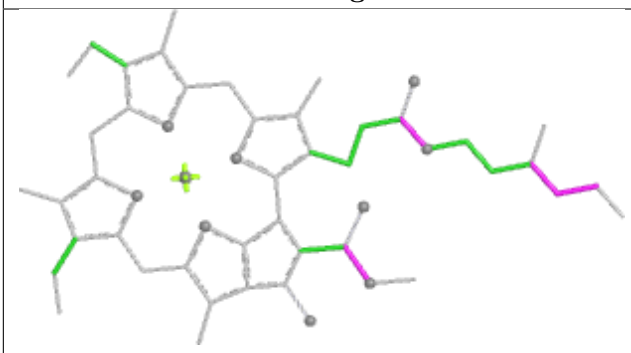
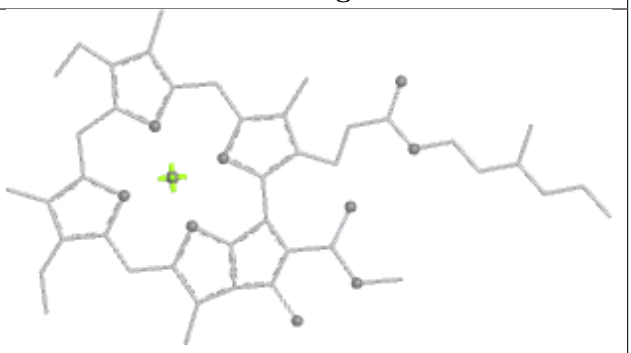
Bond angles

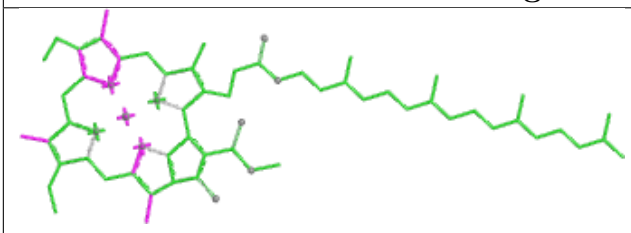
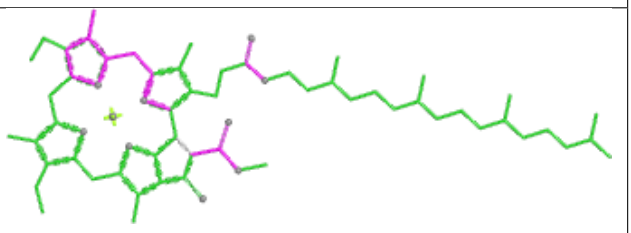
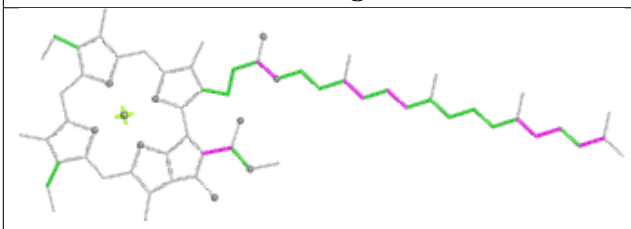
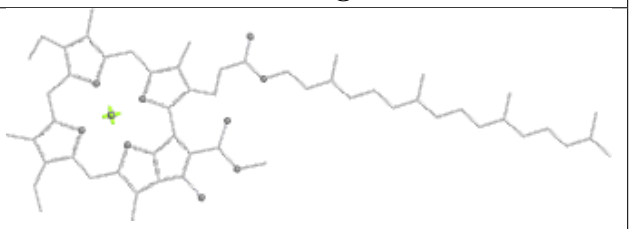


Torsions

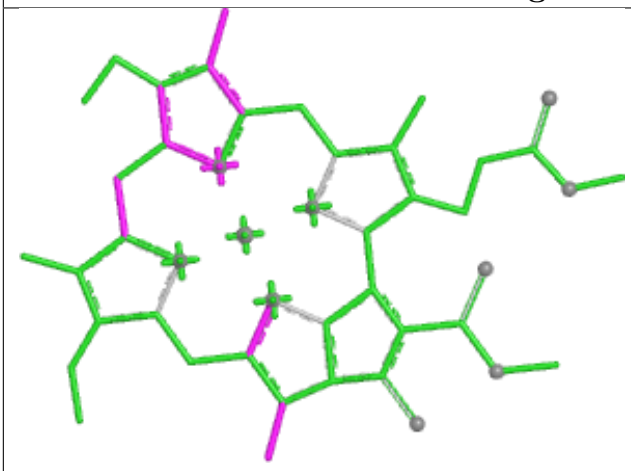


Rings

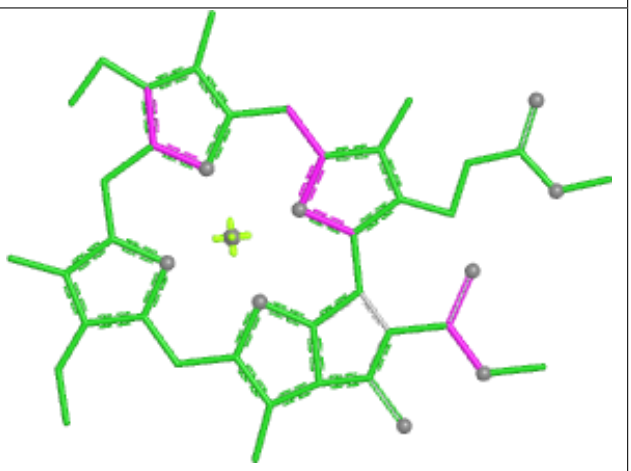
Ligand CLA 6 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

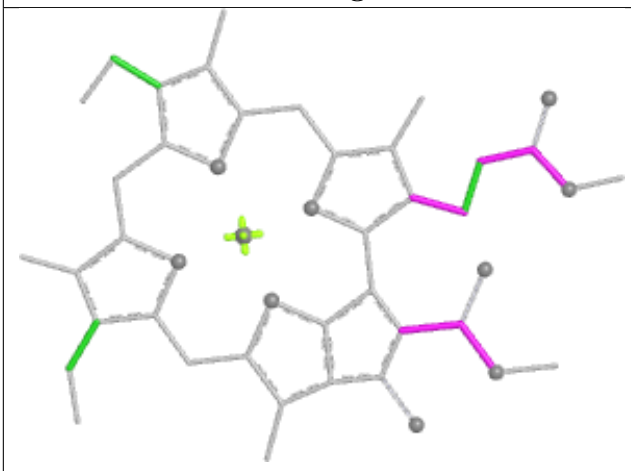
Ligand CLA 0 312



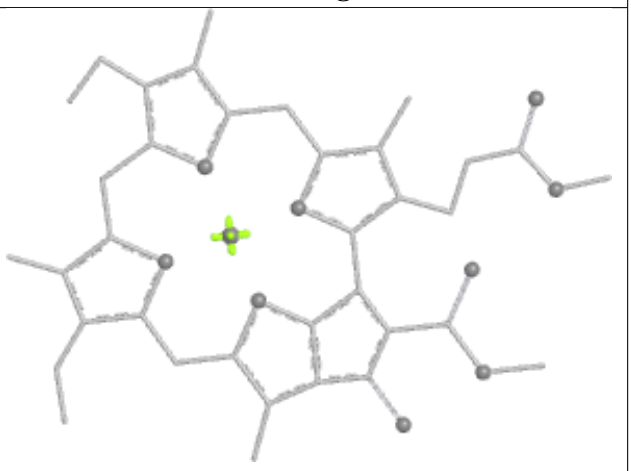
Bond lengths



Bond angles

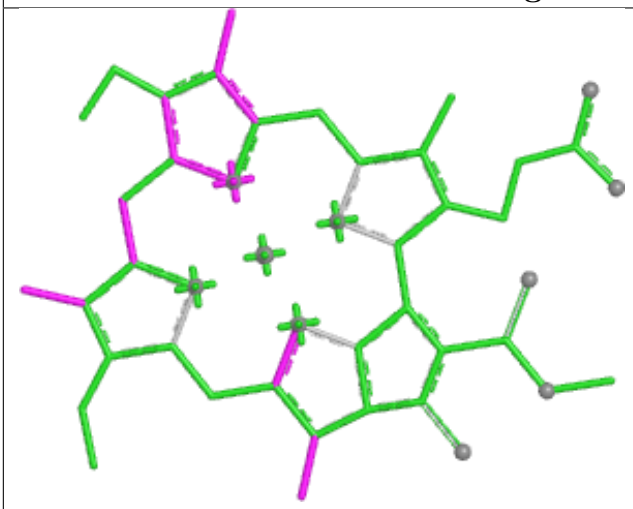


Torsions



Rings

Ligand CLA B 835



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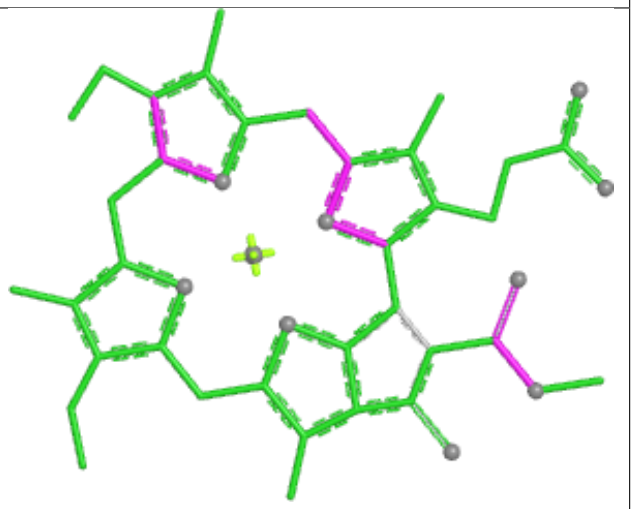
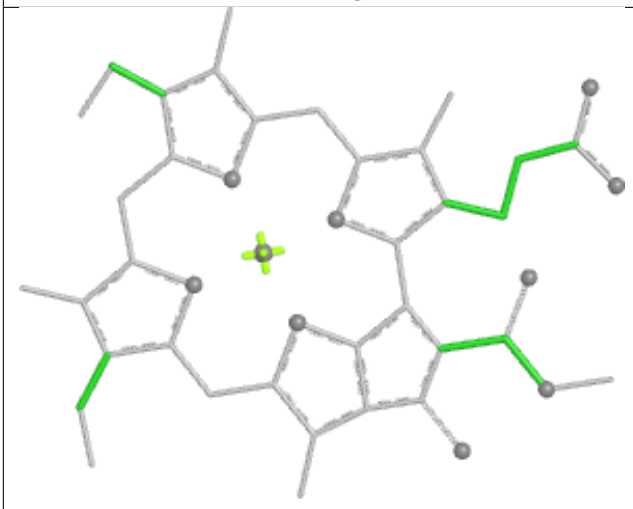


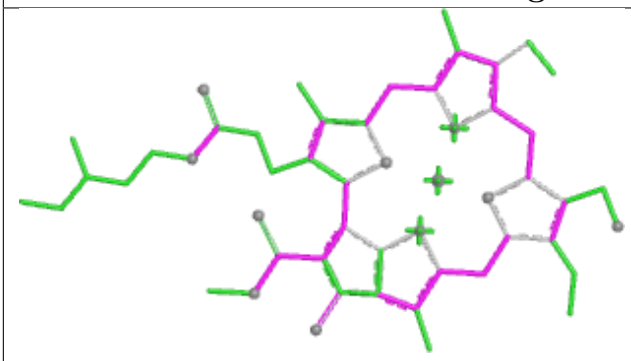
Bond angles



Torsions

Rings

Ligand CHL 8 301



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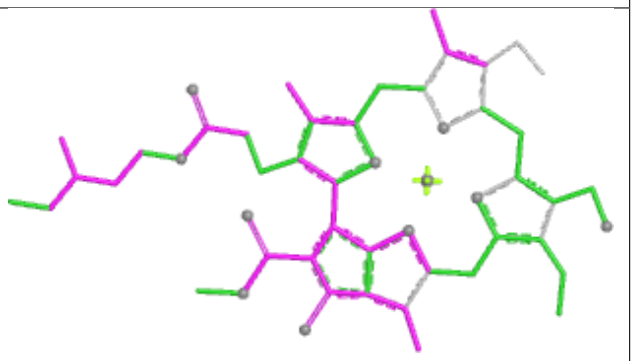

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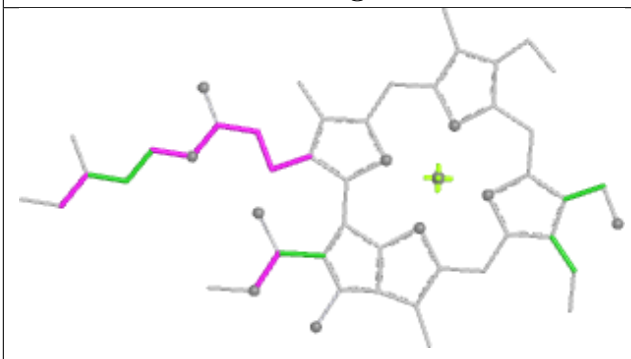

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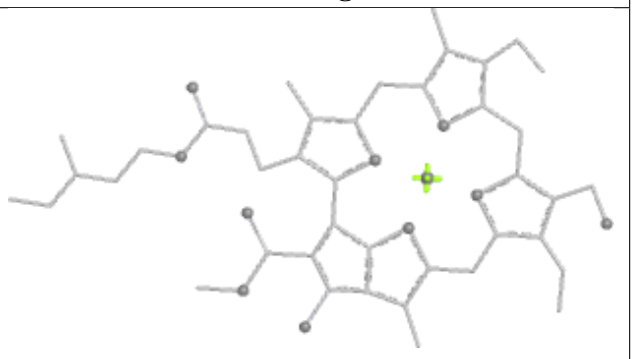
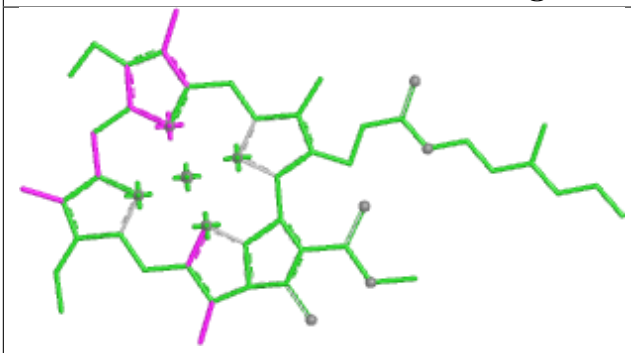


Rings

Ligand CLA 9 310



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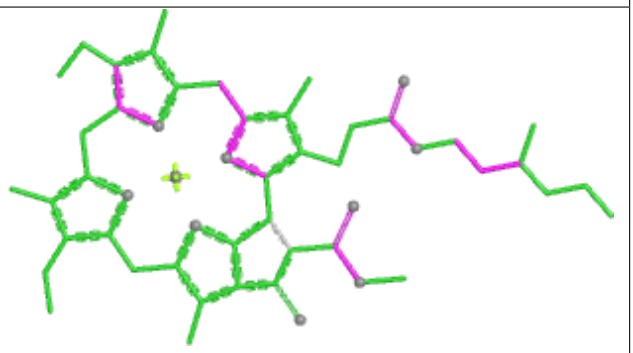

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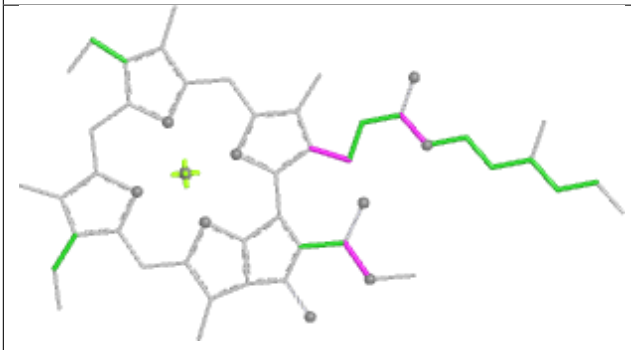
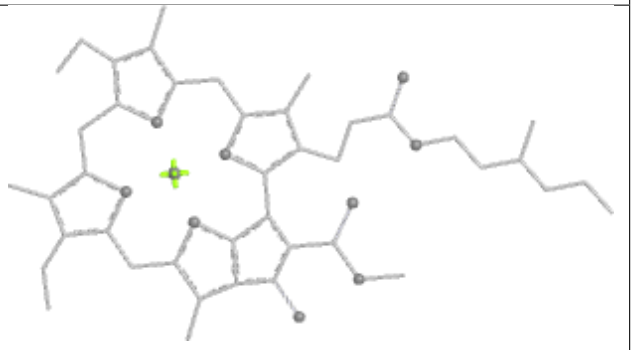
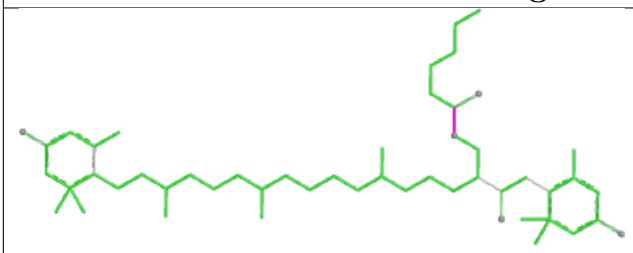


Torsions



Rings

Ligand 0UR 5 314



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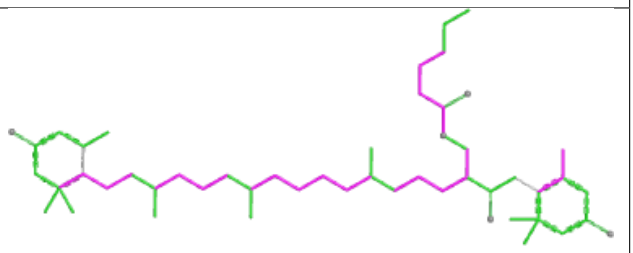
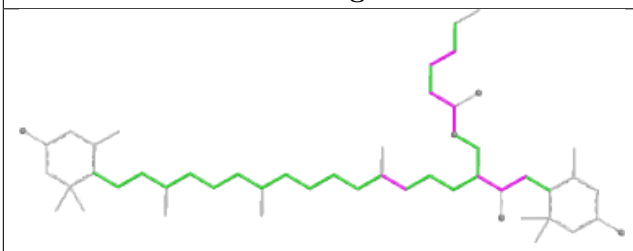


Bond angles



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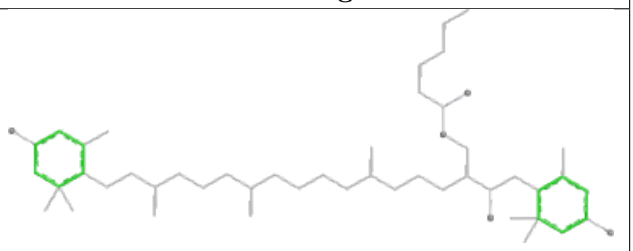
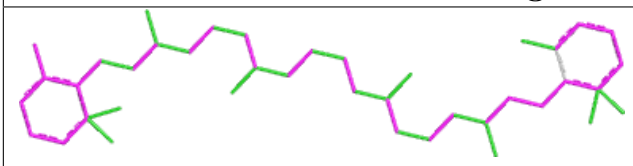


Rings

Ligand 8CT A 847



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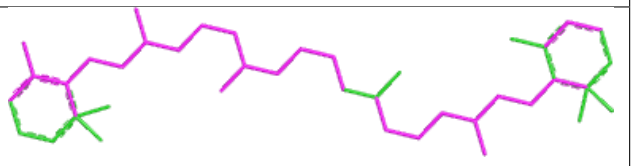
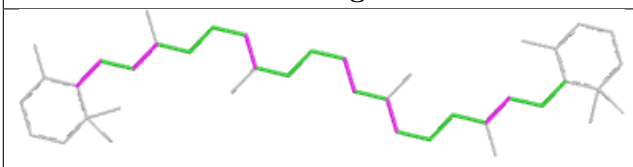


Bond angles



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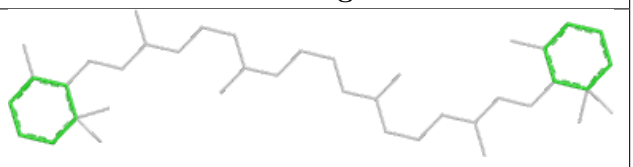
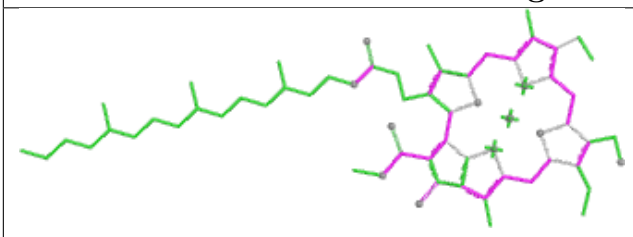


Rings

Ligand CHL 1 301



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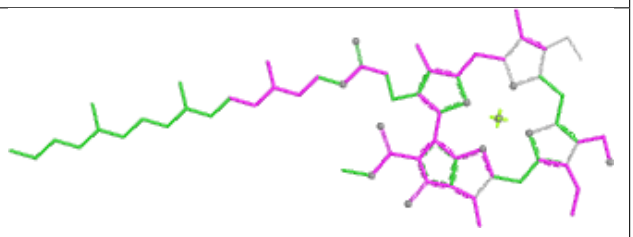
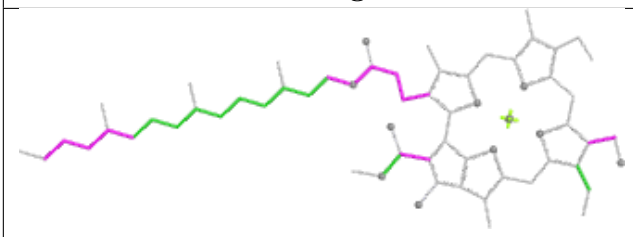


Bond angles



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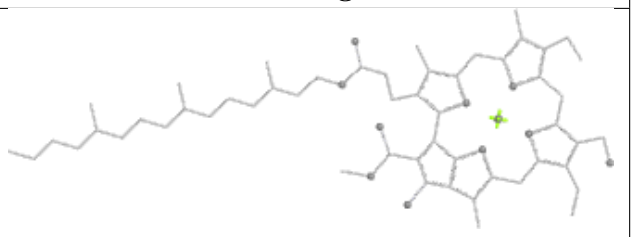
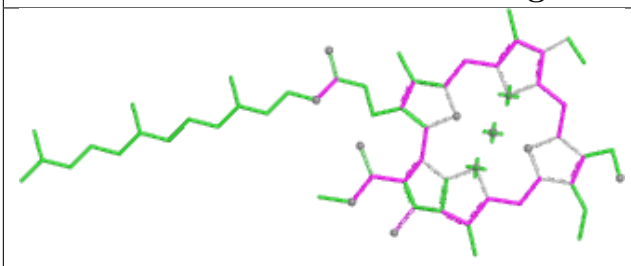


Rings

Ligand CHL 6 301



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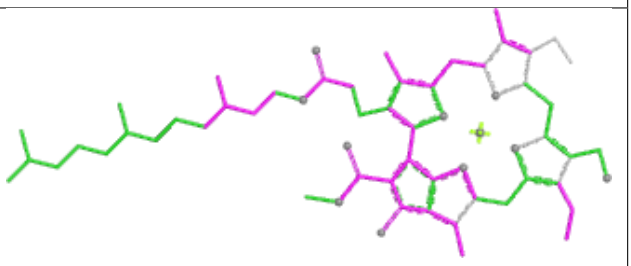
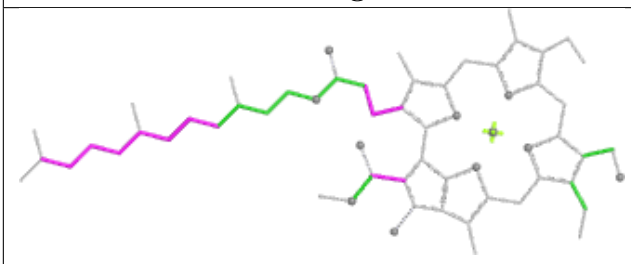


Bond angles



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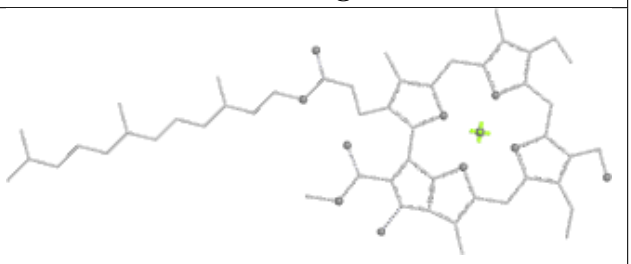
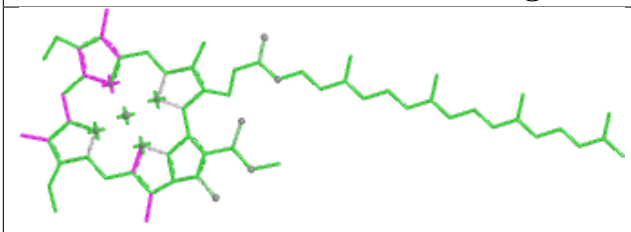


Rings

Ligand CLA A 808



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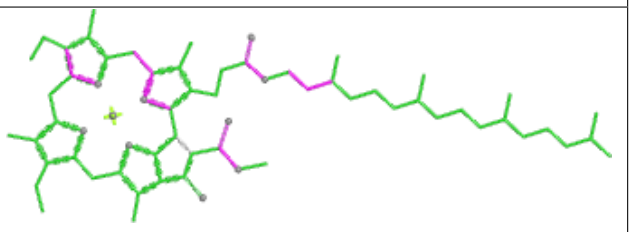
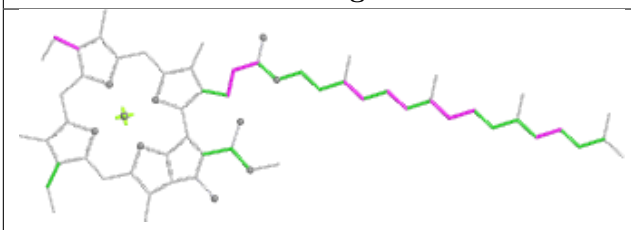
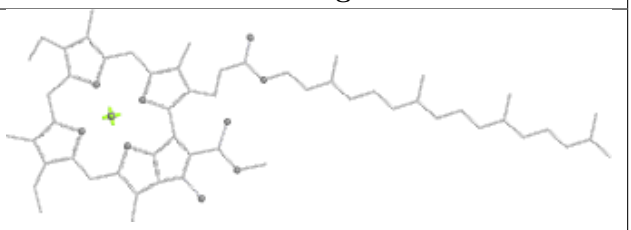


Bond angles

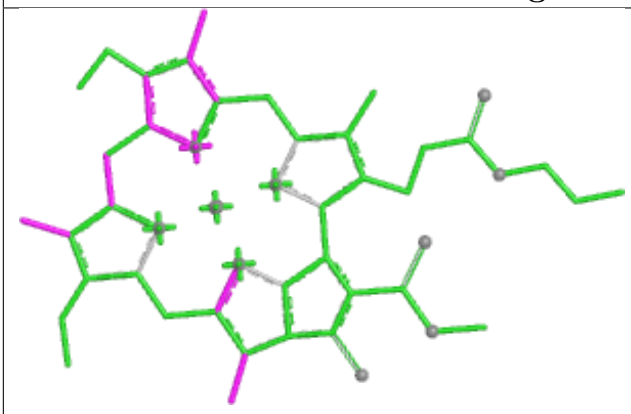


Torsions



Rings

Ligand CLA 6 311



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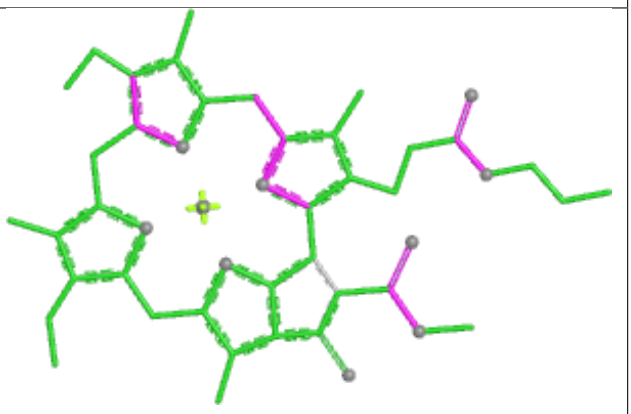
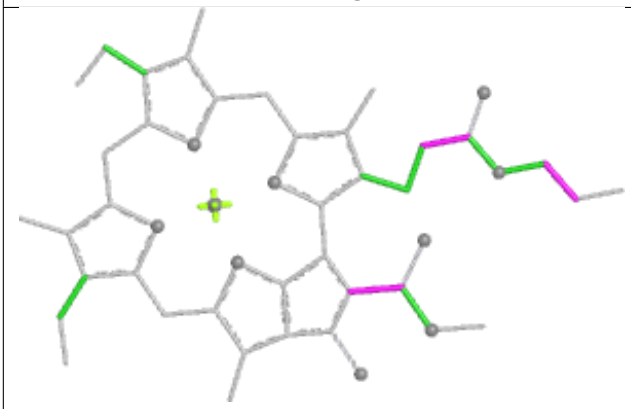
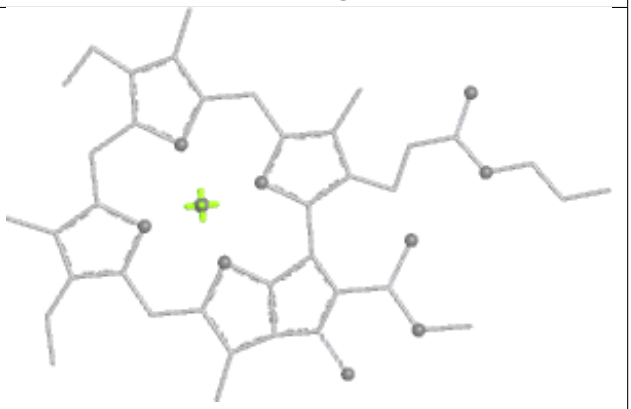


Bond angles

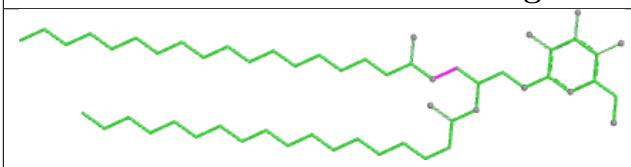


Torsions



Rings

Ligand LMG 9 317



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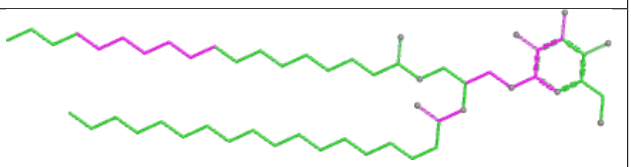
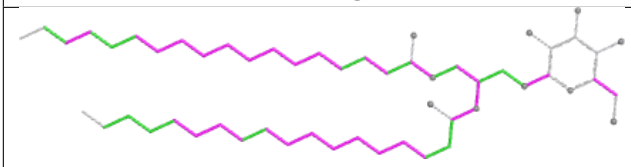


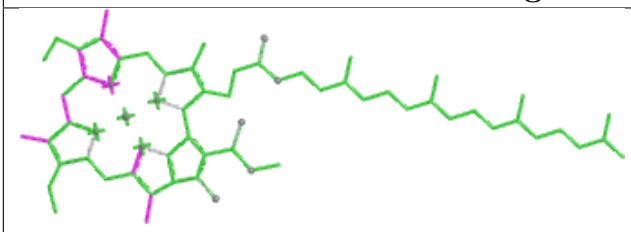
Bond angles



Torsions

Rings

Ligand CLA B 837



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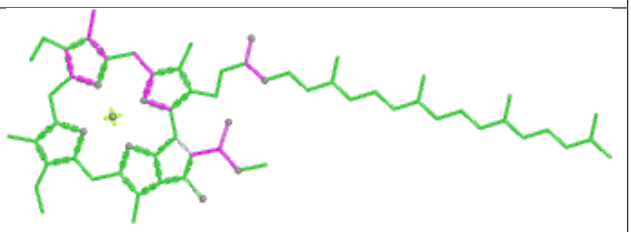
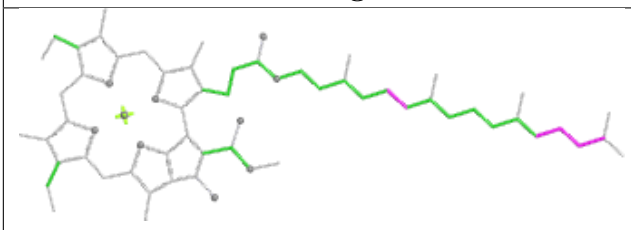


Bond angles



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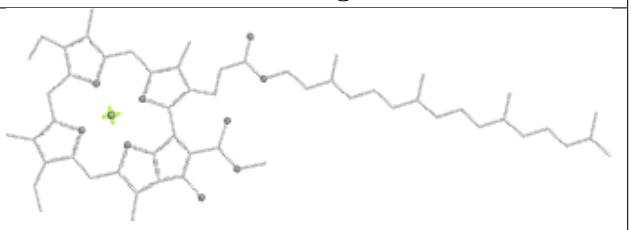
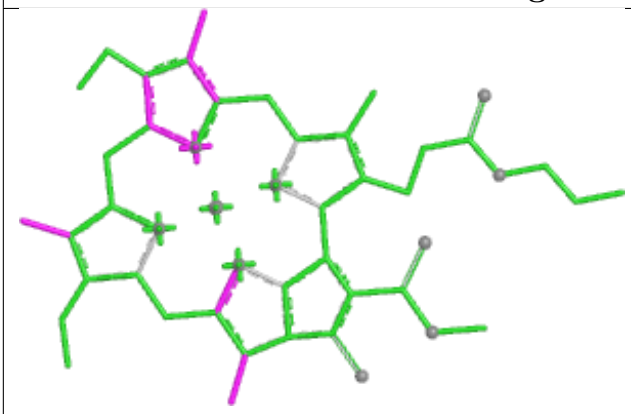


Rings

Ligand CLA 2 310



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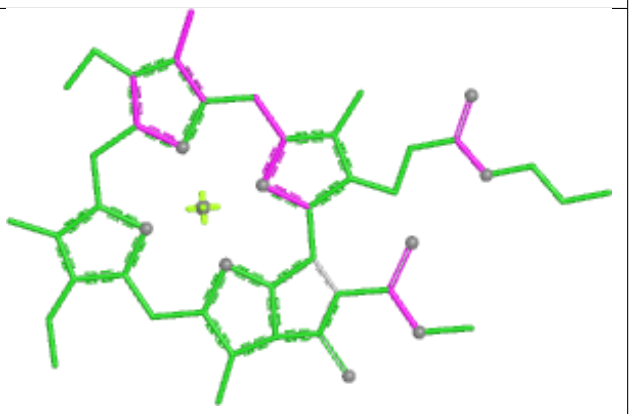
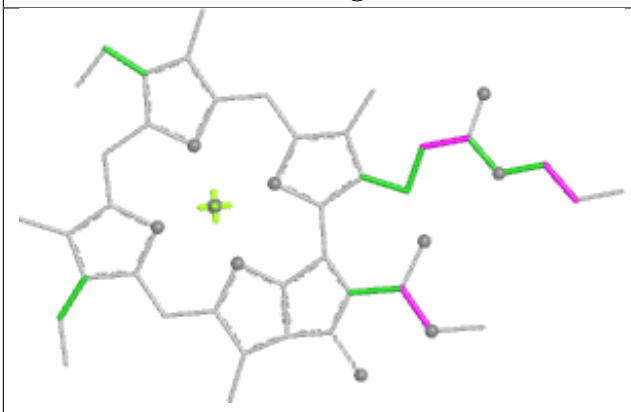


Bond angles



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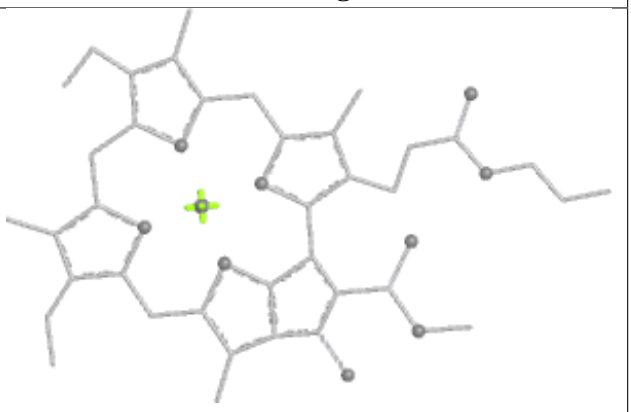
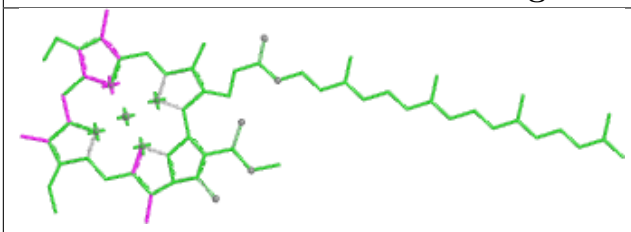


Rings

Ligand CLA 6 316



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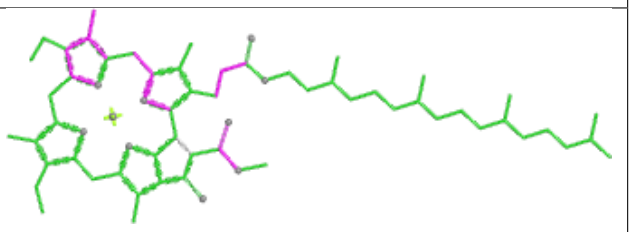
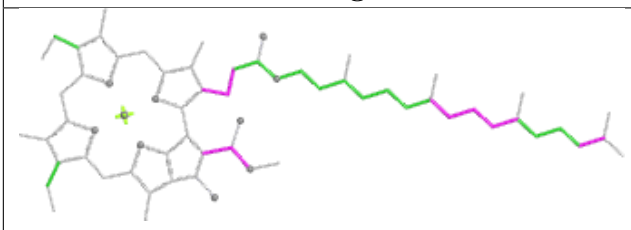


Bond angles



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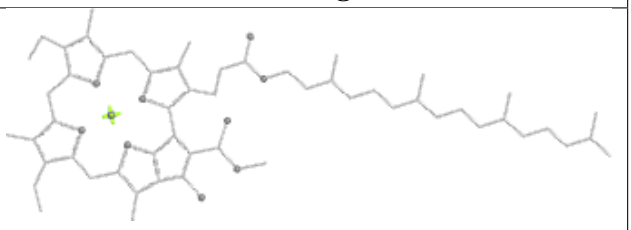
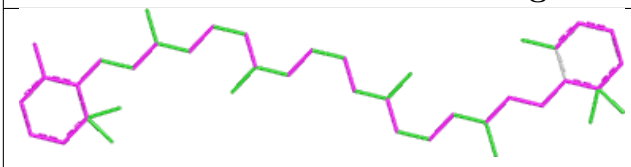


Rings

Ligand 8CT L 204



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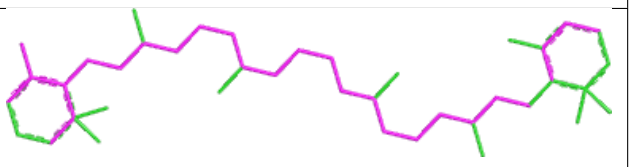
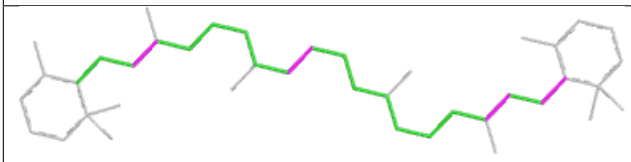
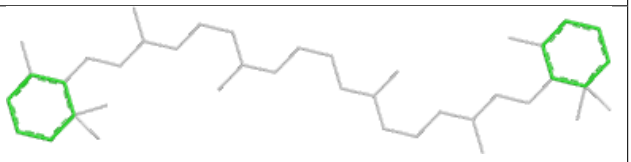


Bond angles

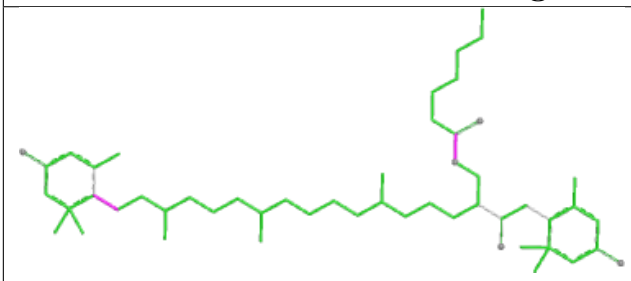


Torsions

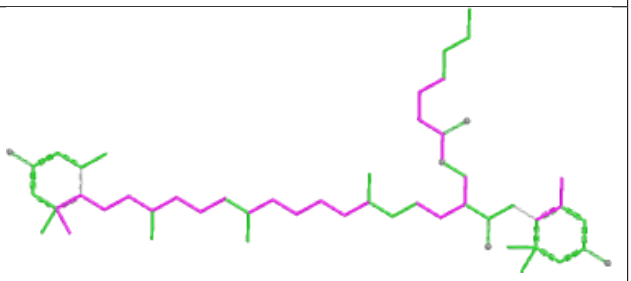


Rings

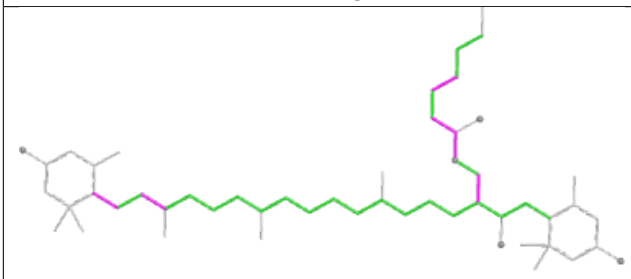
Ligand 0UR 6 321



Bond lengths



Bond angles



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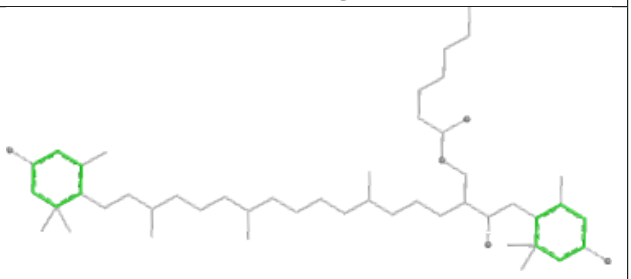
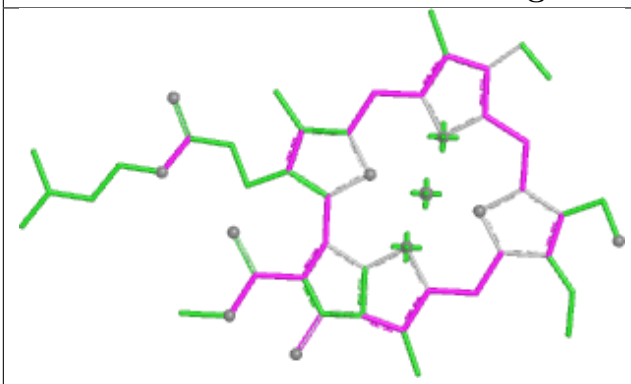


Rings

Ligand CHL 3 305



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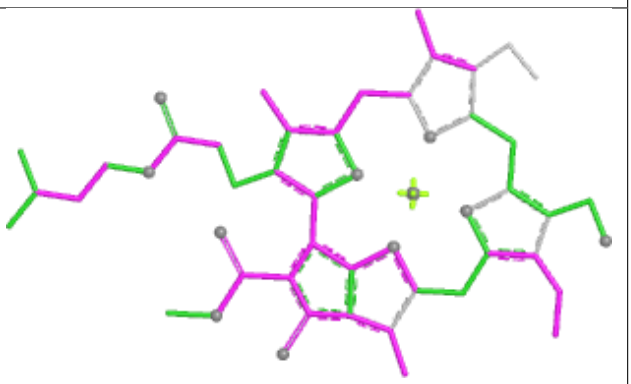
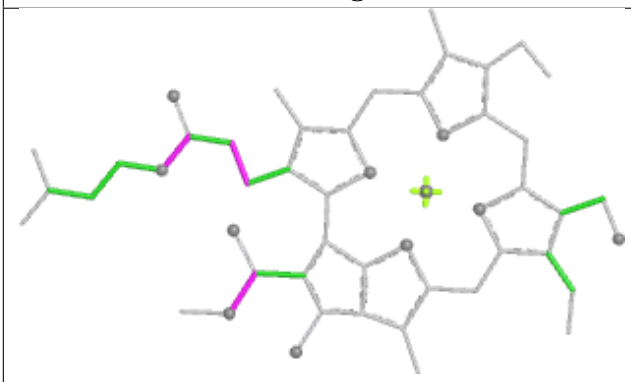
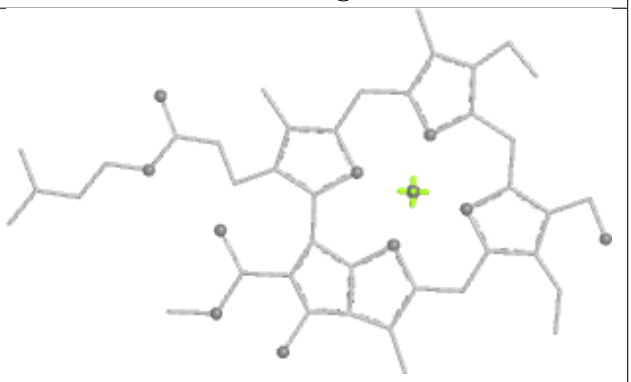


Bond angles

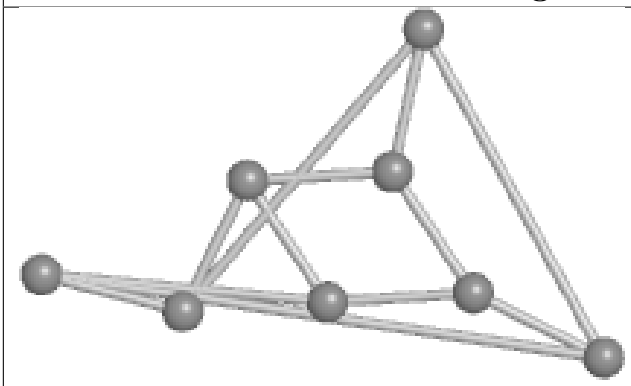


Torsions



Rings

Ligand SF4 C 102



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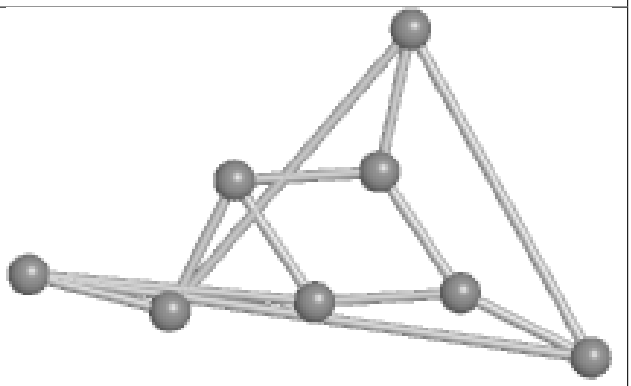
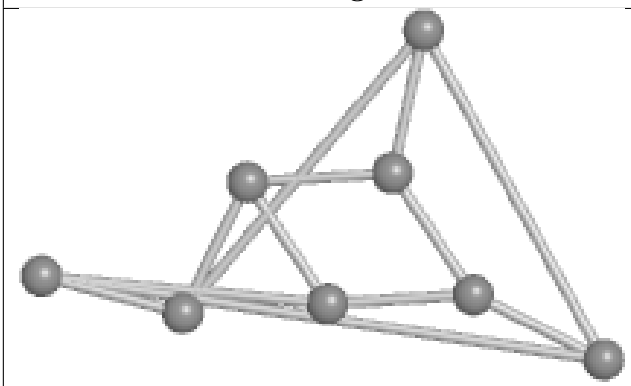
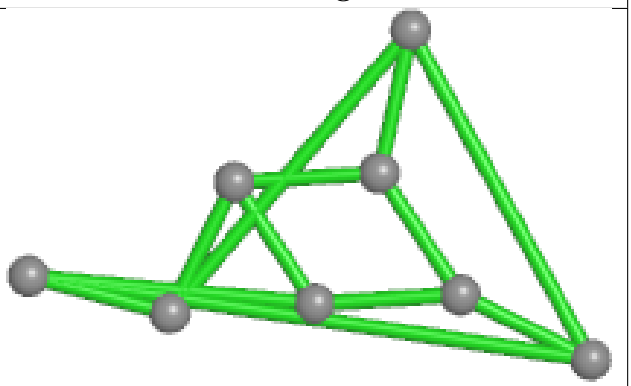


Bond angles

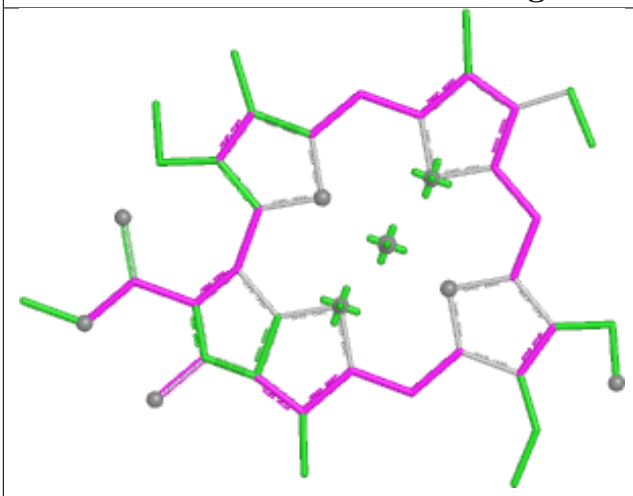


Torsions



Rings

Ligand CHL 2 304



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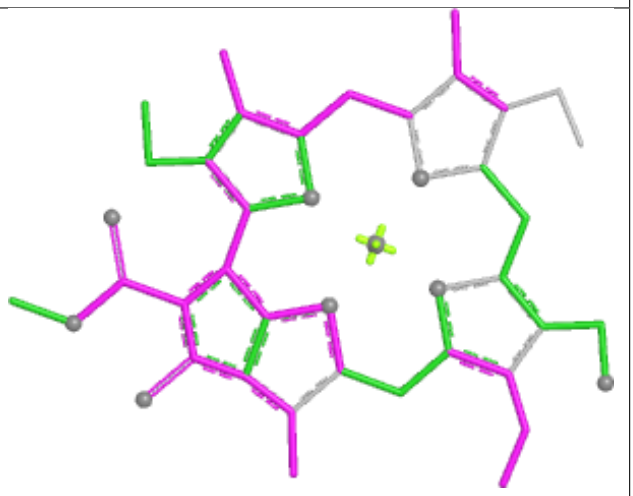
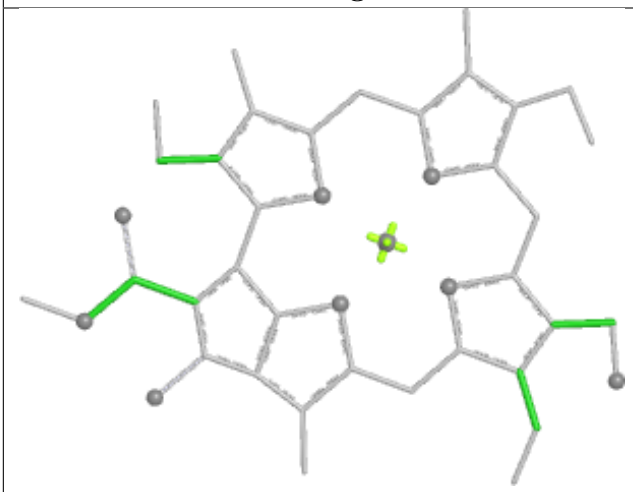


Bond angles



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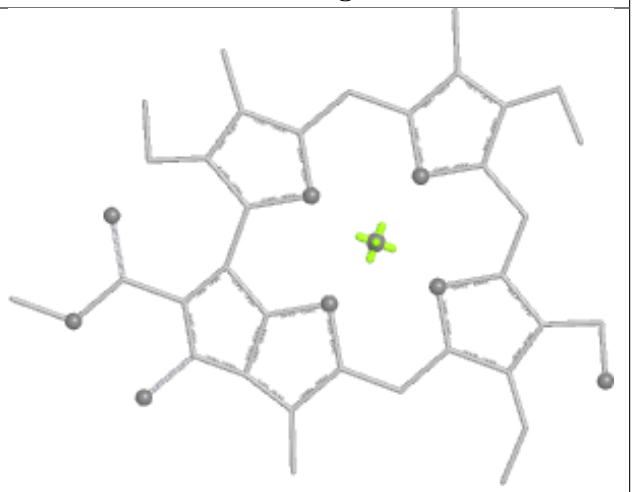
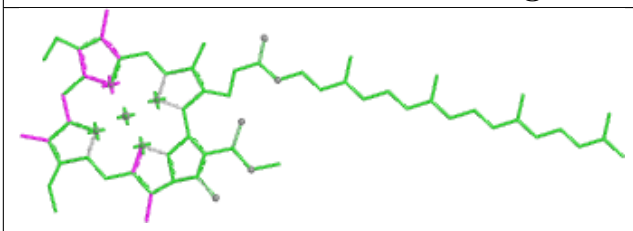


Rings

Ligand CLA A 838



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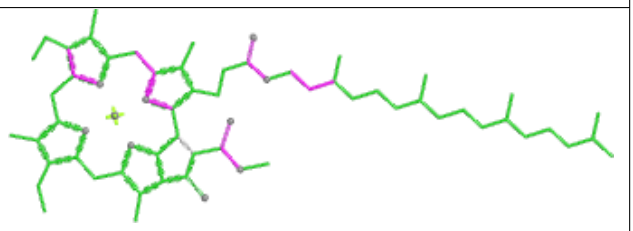
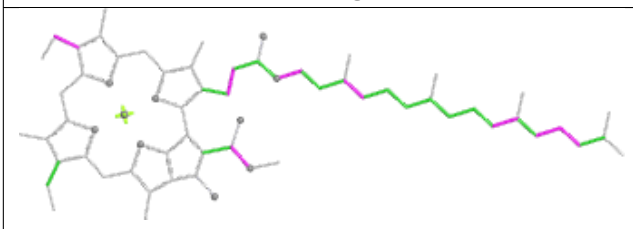


Bond angles



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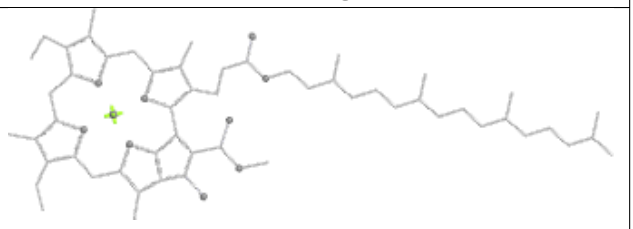
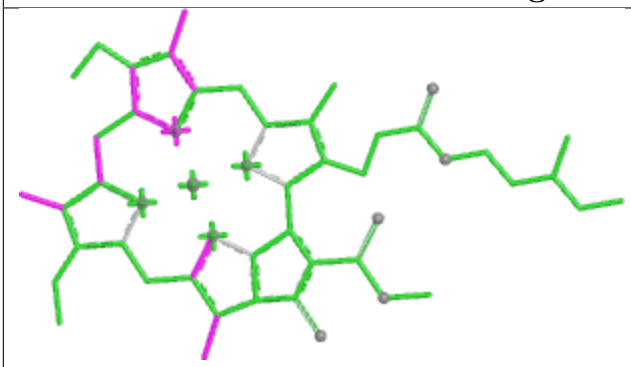


Rings

Ligand CLA 6 318



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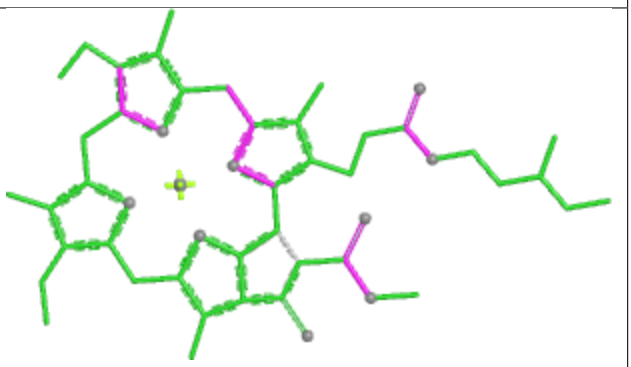
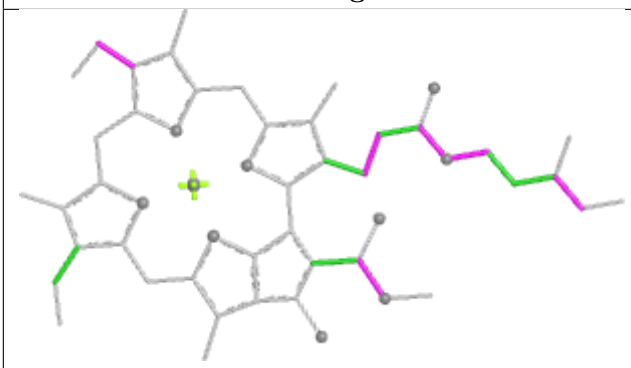


Bond angles



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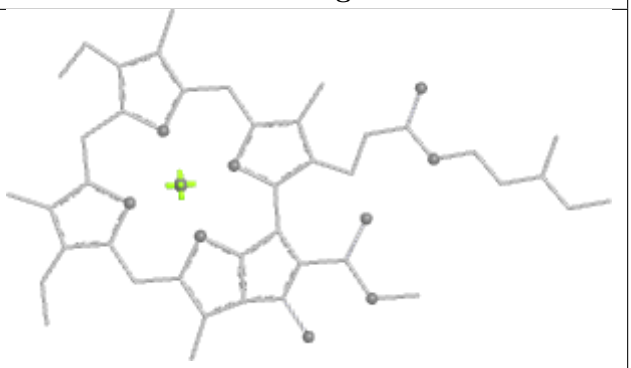
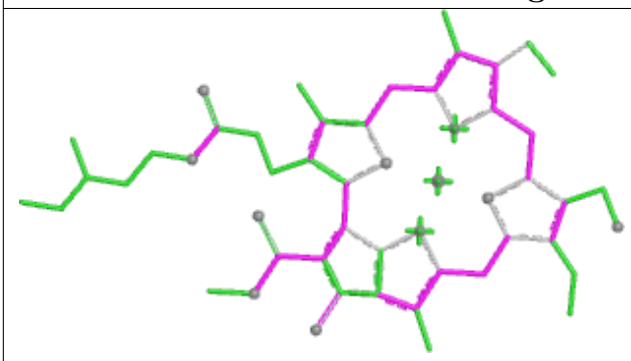


Rings

Ligand CHL 0 301



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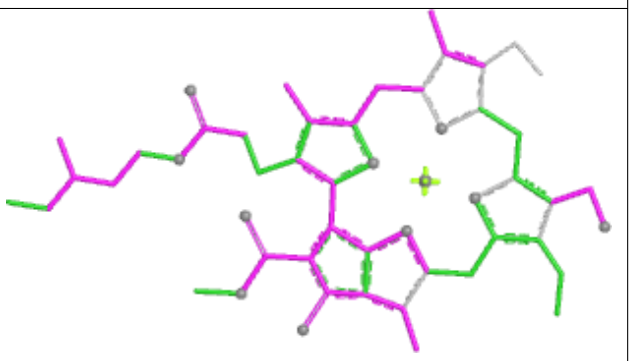
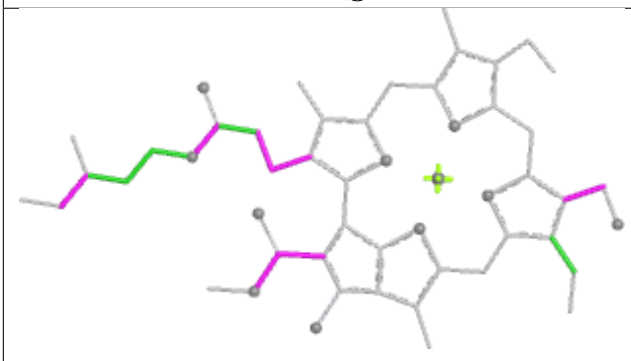


Bond angles



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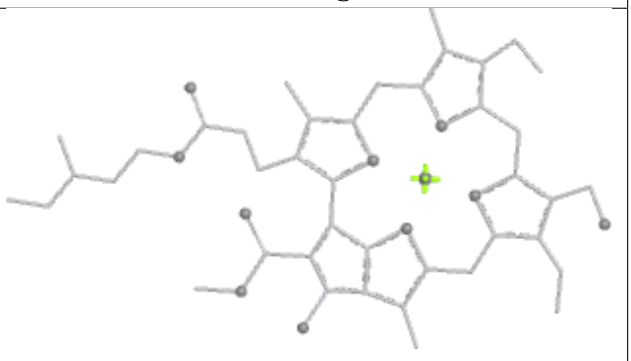
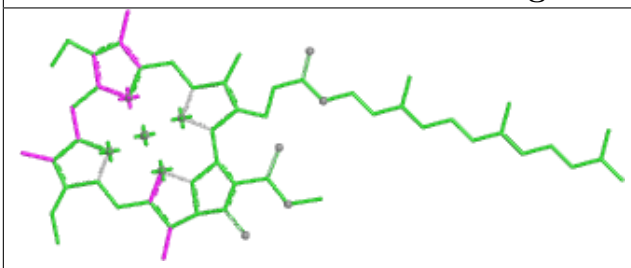
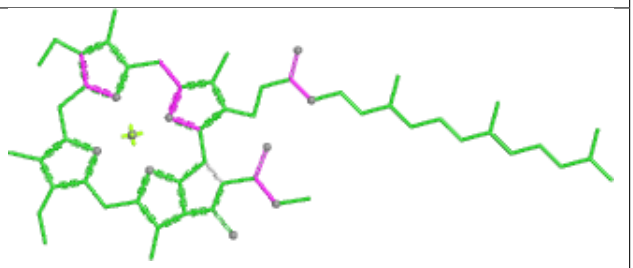
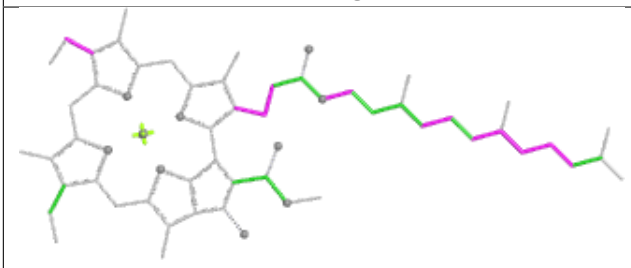
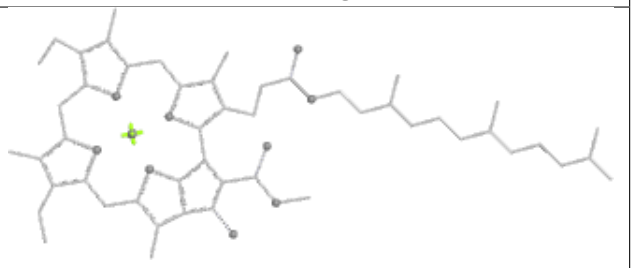
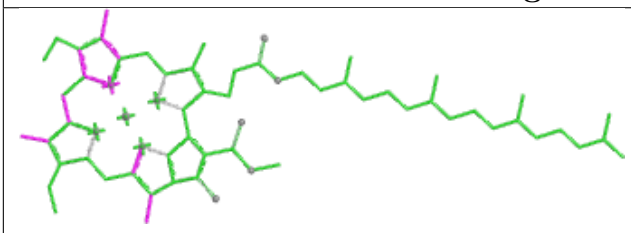
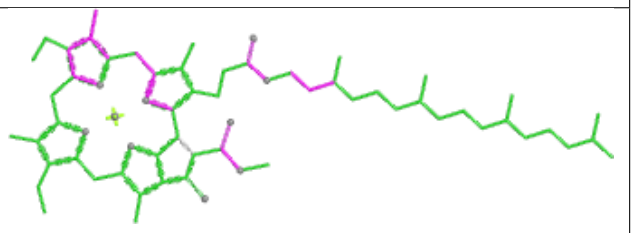
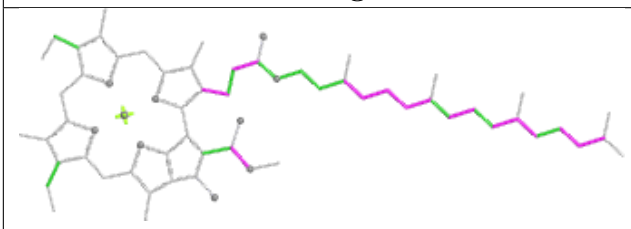
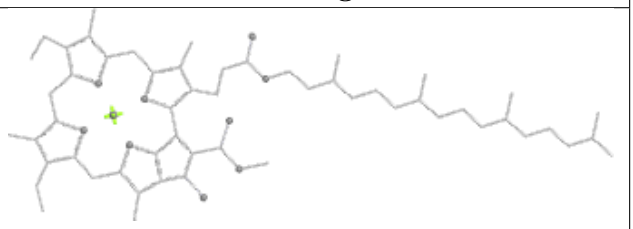
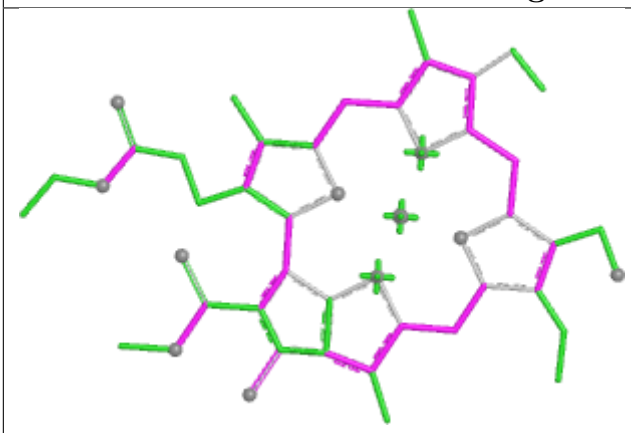


Rings

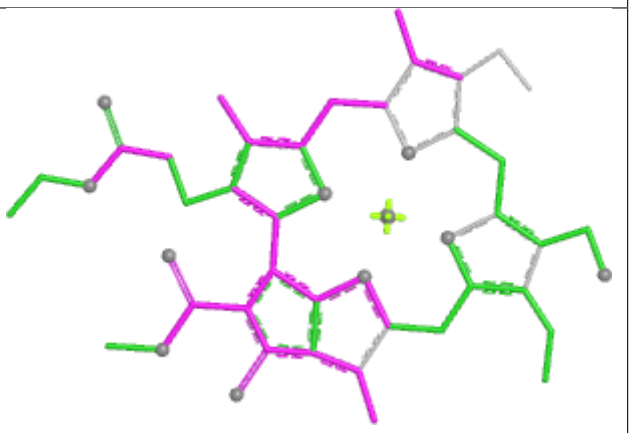
Ligand CLA 0 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

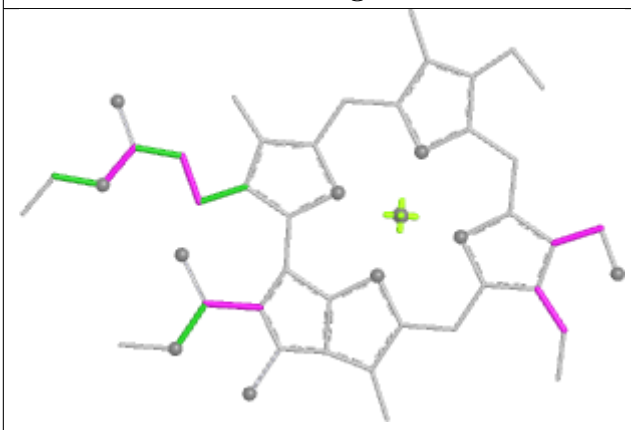
Ligand CHL 0 306



Bond lengths



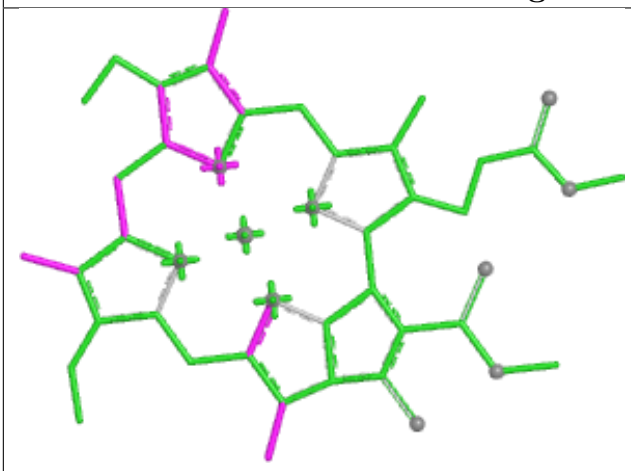
Bond angles



Torsions

Rings

Ligand CLA 3 311



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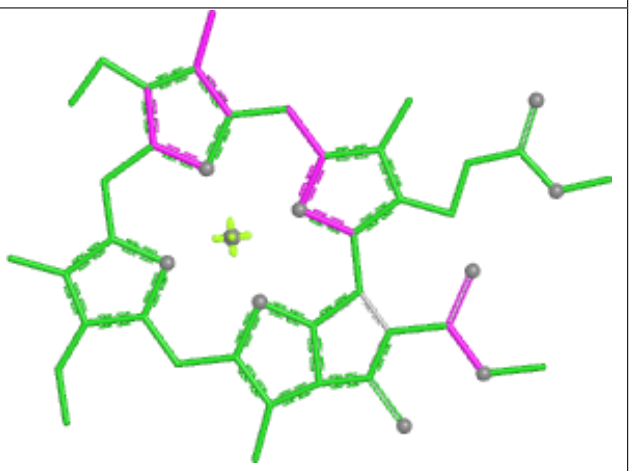
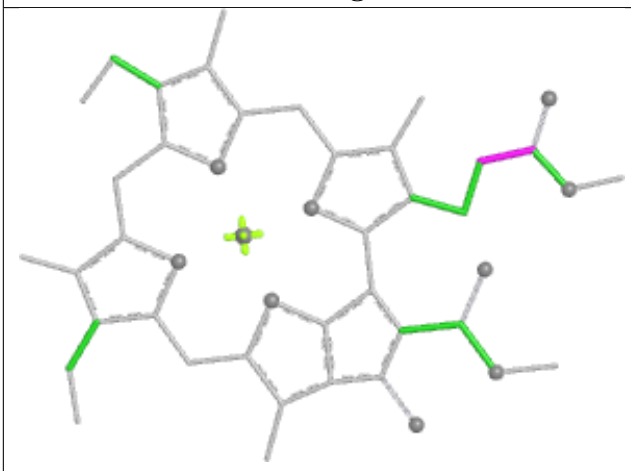
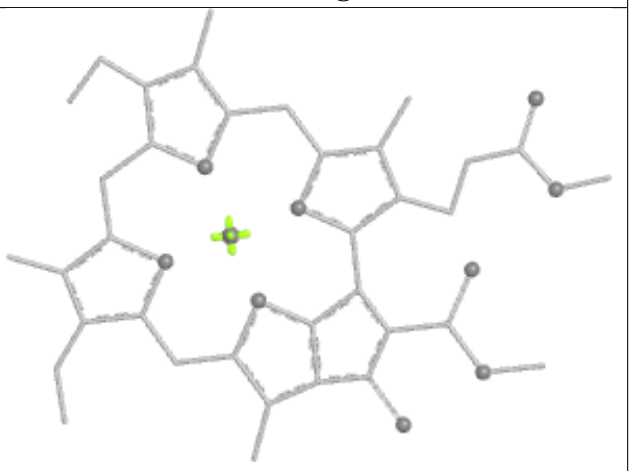


Bond angles

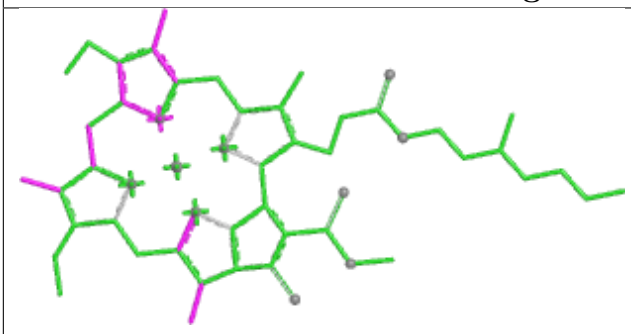


Torsions



Rings

Ligand CLA K 102



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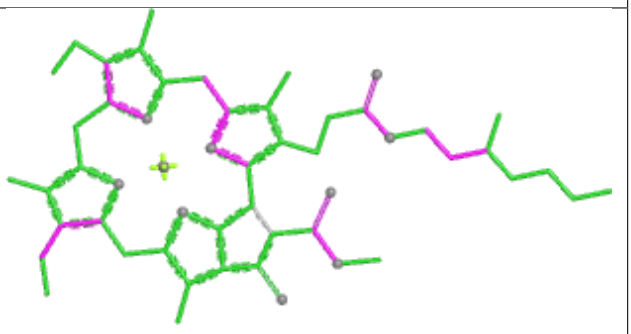
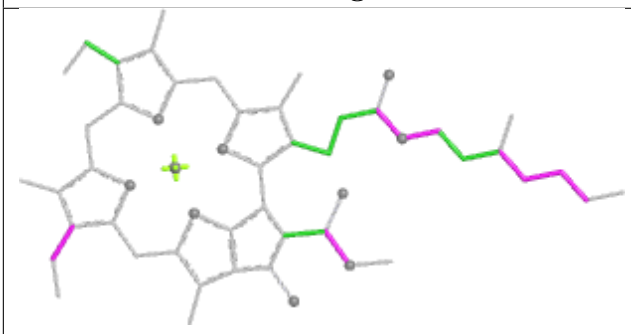


Bond angles



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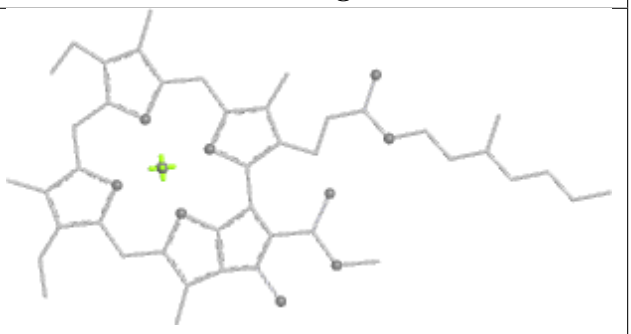
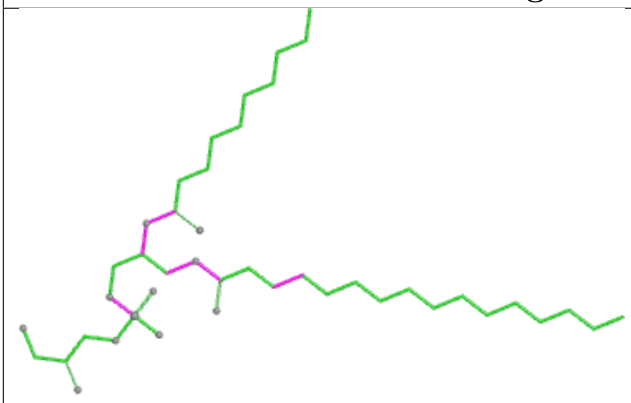


Rings

Ligand LHG 1 318



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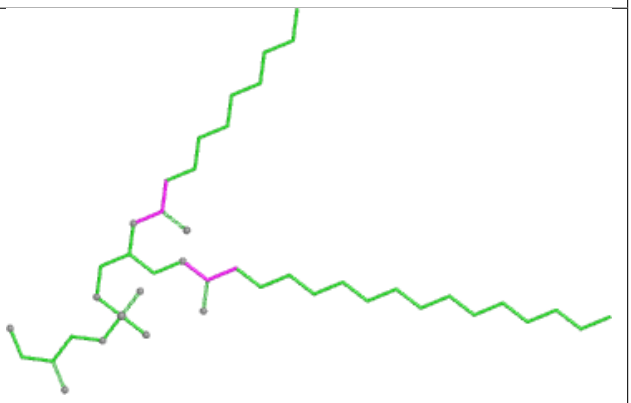
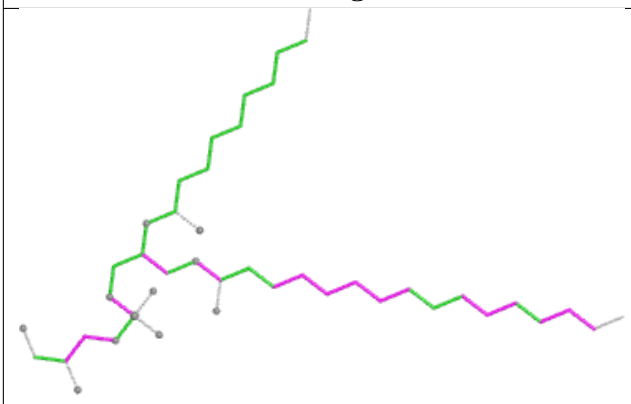
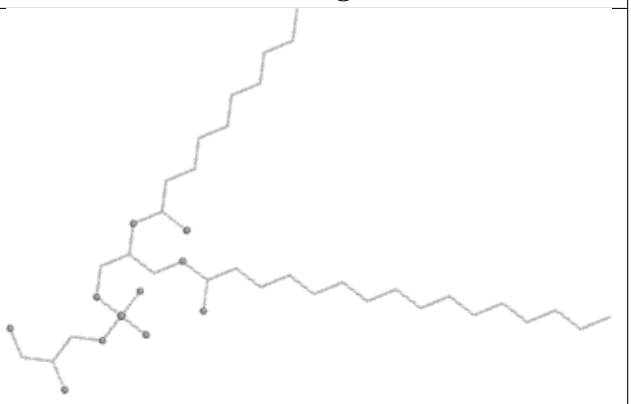


Bond angles

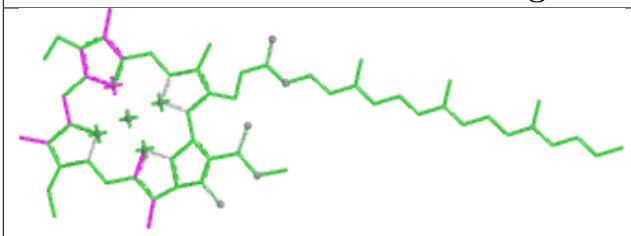


Torsions



Rings

Ligand CLA 1 309



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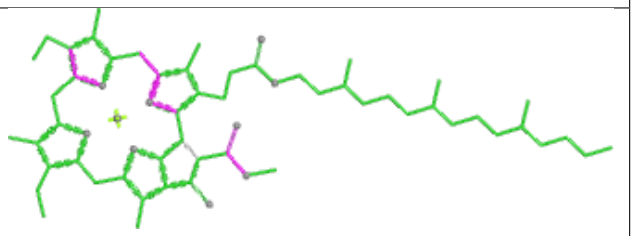
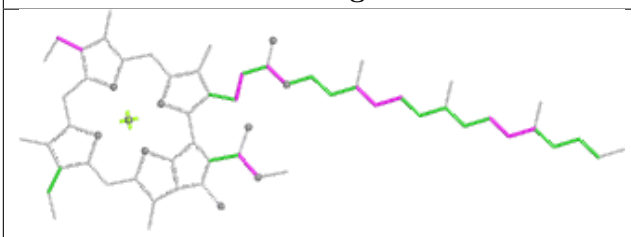
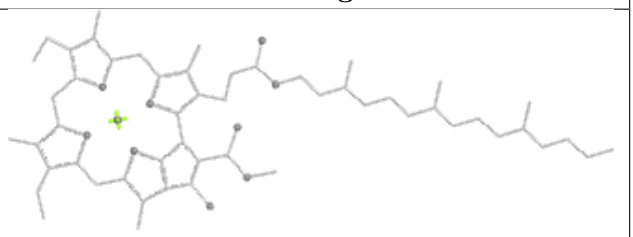


Bond angles

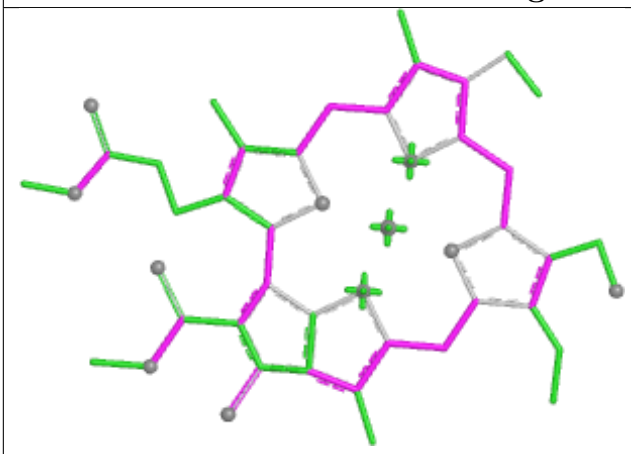


Torsions

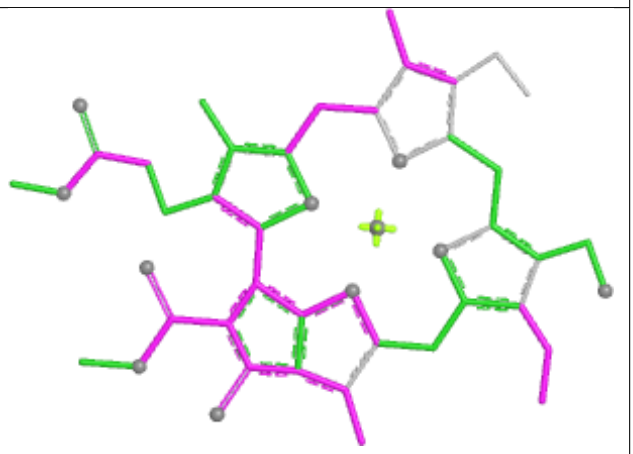


Rings

Ligand CHL 5 312



Bond lengths

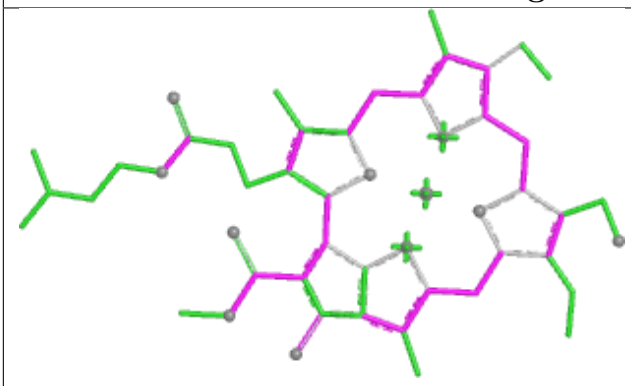


Bond angles

Torsions

Rings

Ligand CHL 8 308



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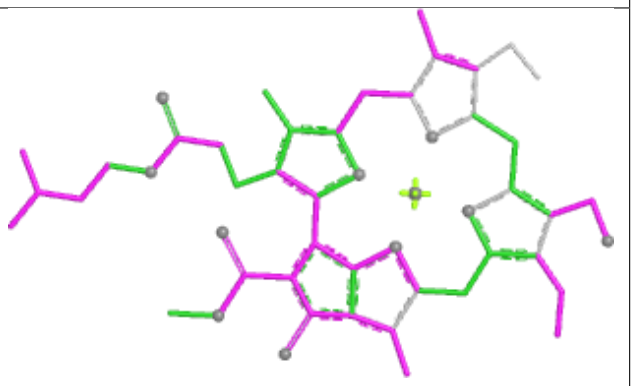
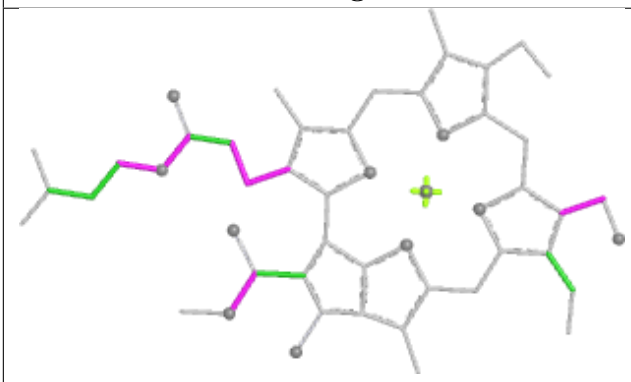
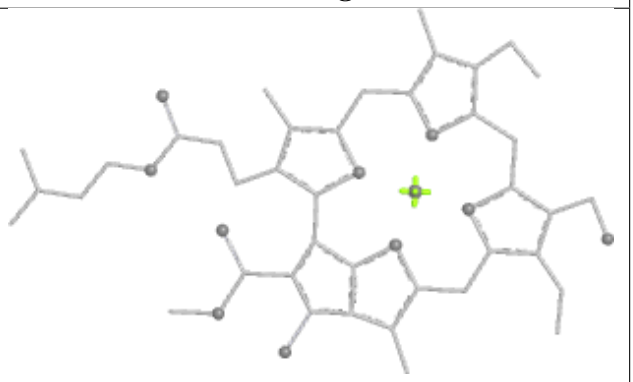


Bond angles

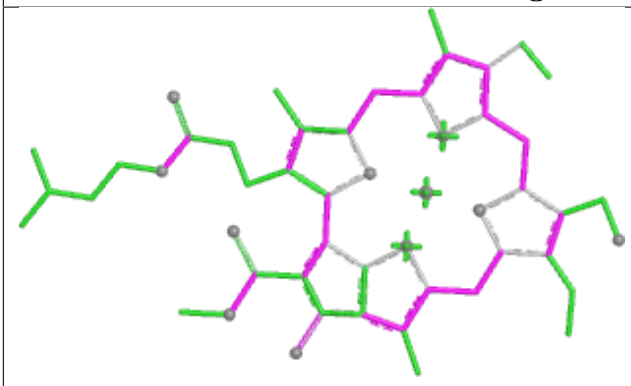


Torsions



Rings

Ligand CHL 0 305



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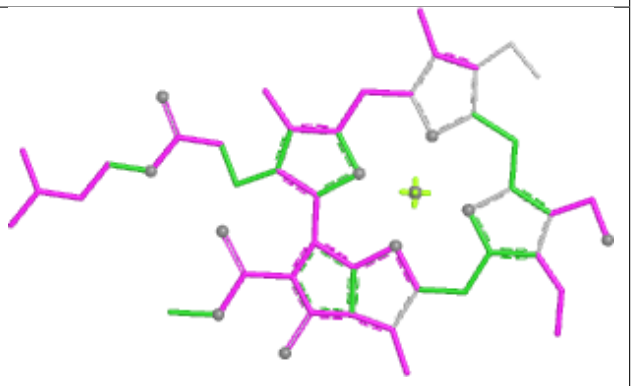
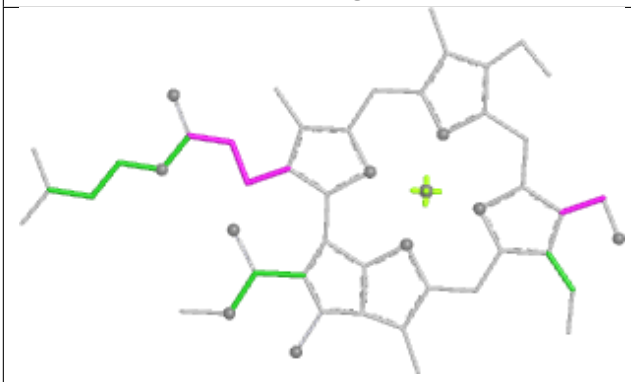


Bond angles



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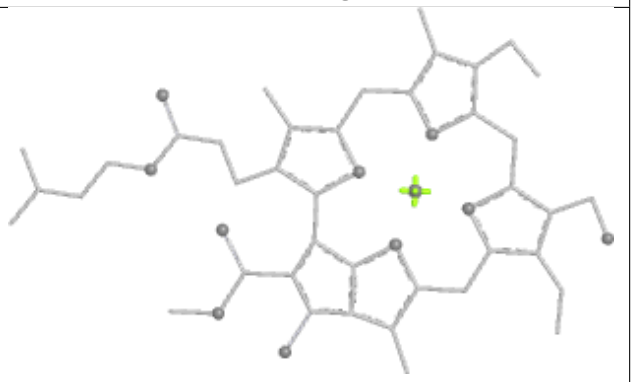
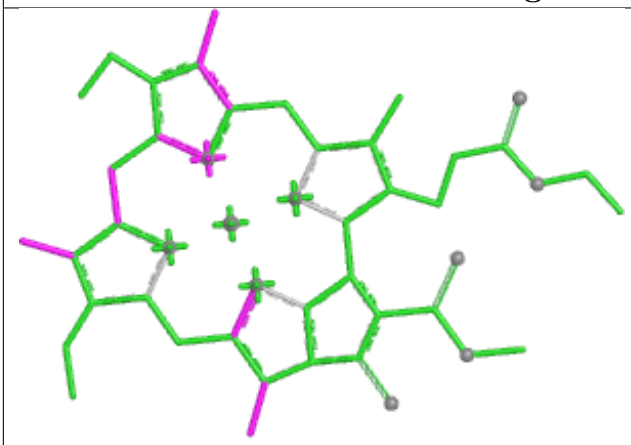


Rings

Ligand CLA B 838



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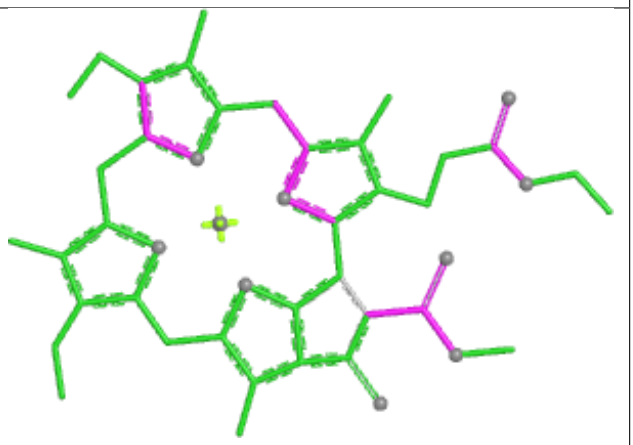
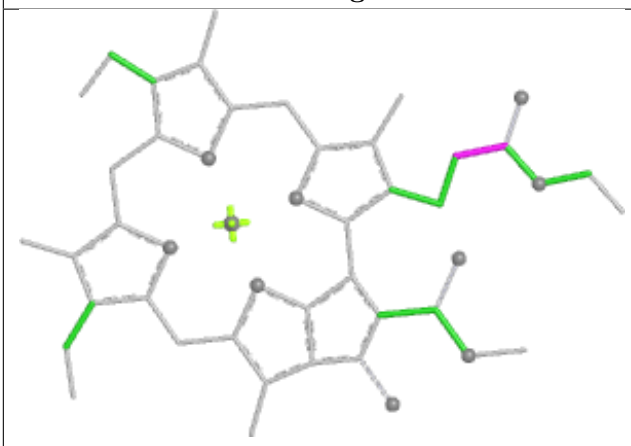
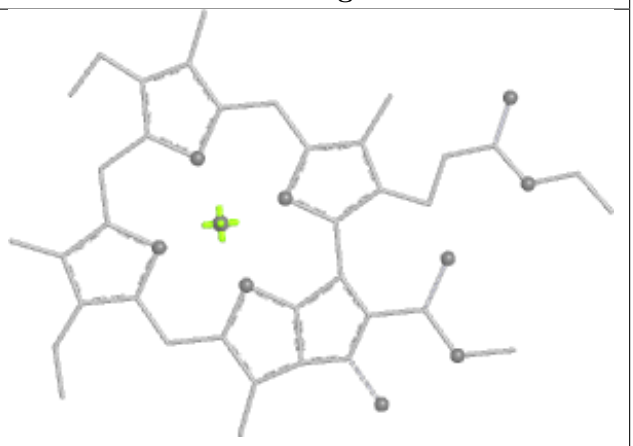


Bond angles

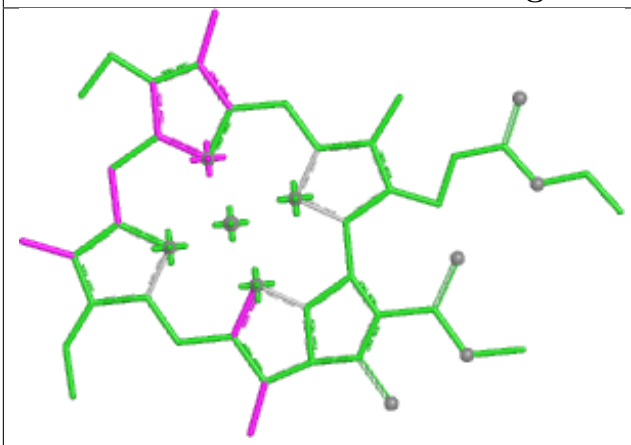


Torsions



Rings

Ligand CLA L 206



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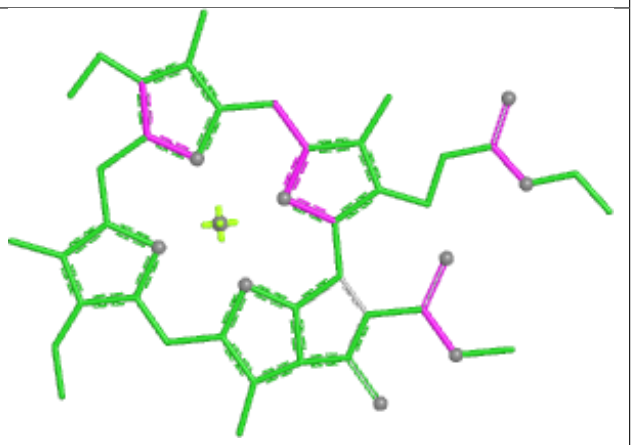
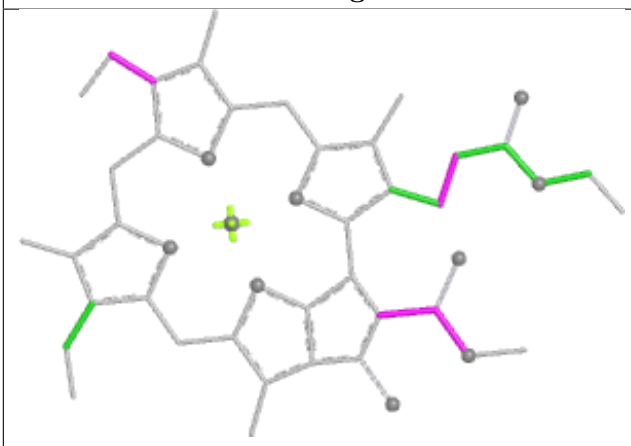


Bond angles



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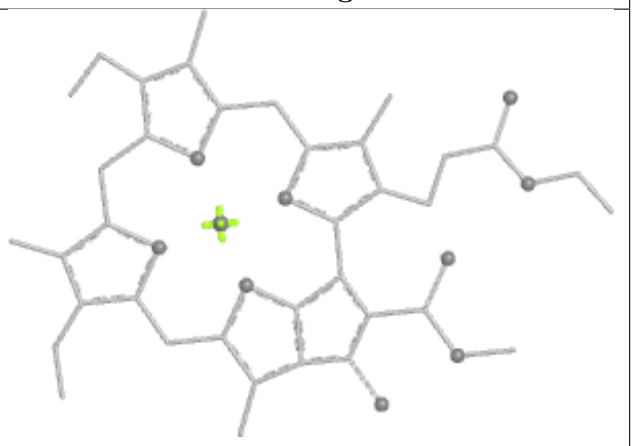
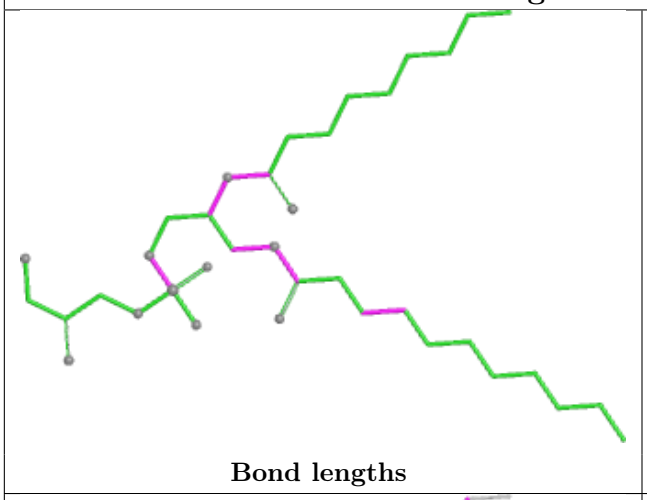


Rings

Ligand LHG 5 316



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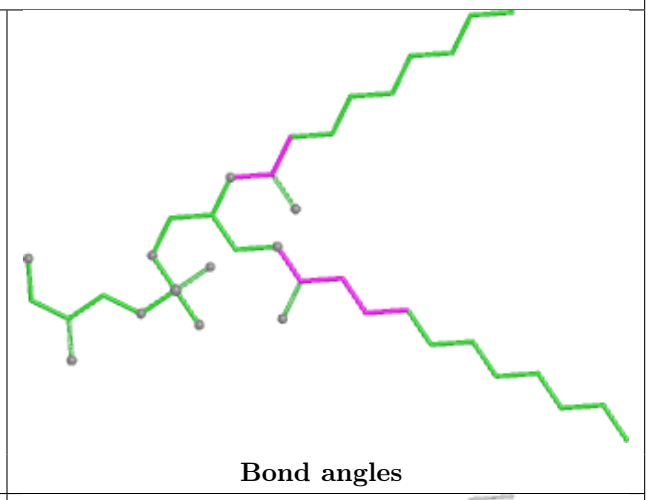
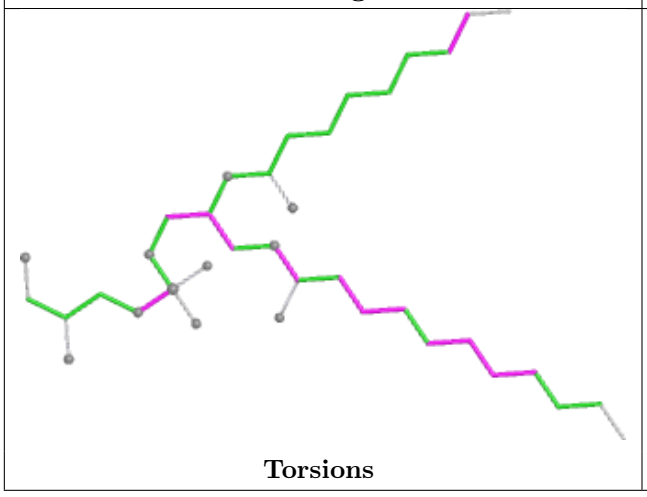
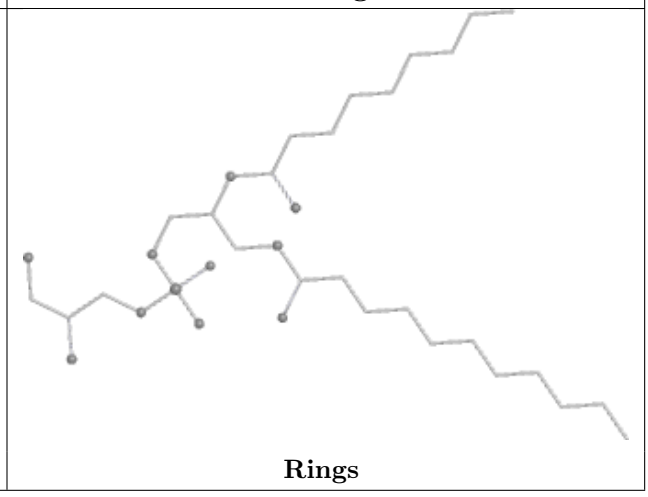


Bond angles

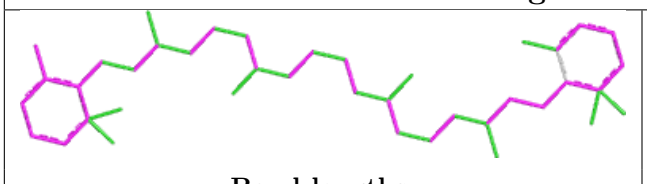


Torsions



Rings

Ligand 8CT B 845



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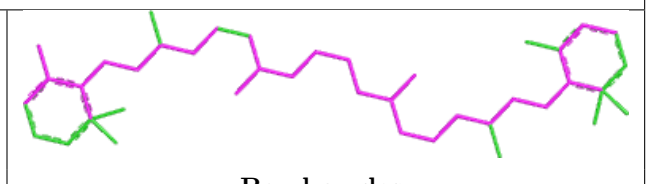
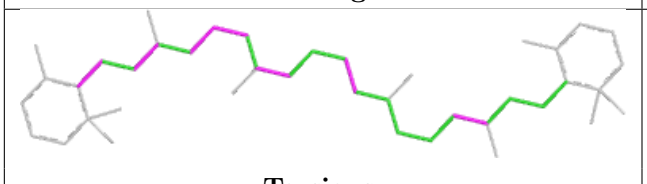


Bond angles



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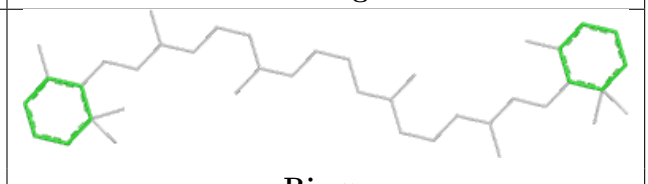
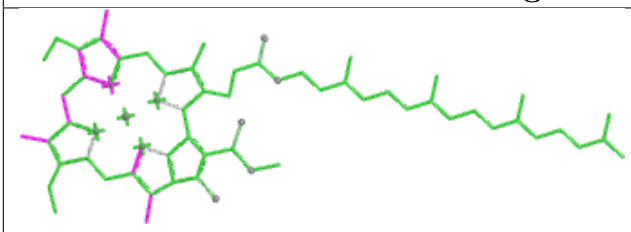


Rings

Ligand CLA A 814



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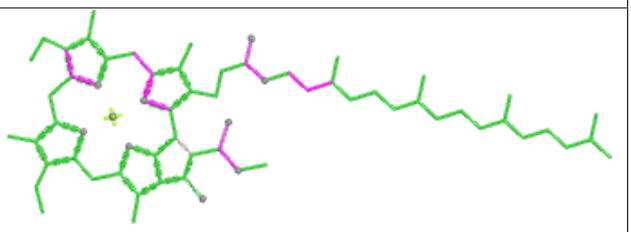
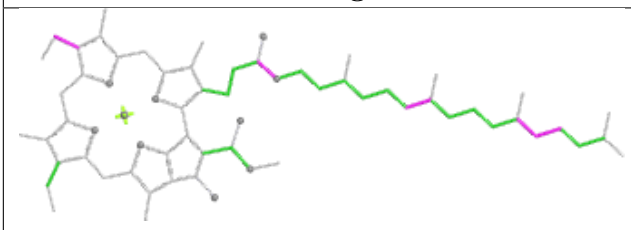


Bond angles



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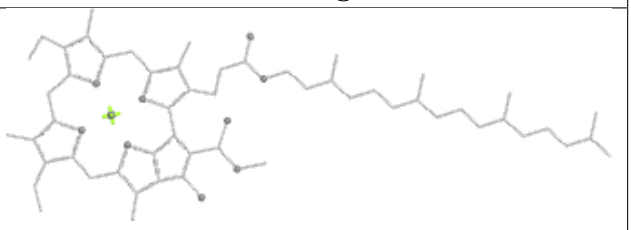
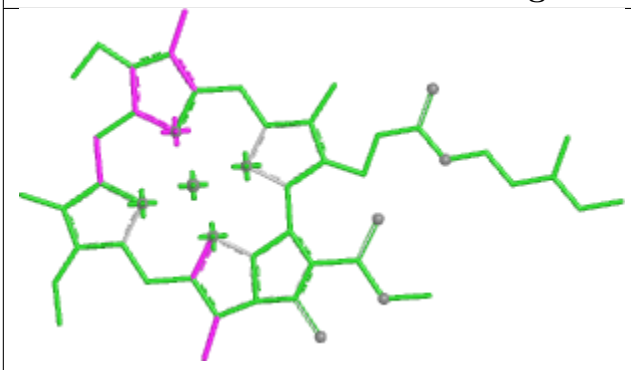


Rings

Ligand CLA 9 304



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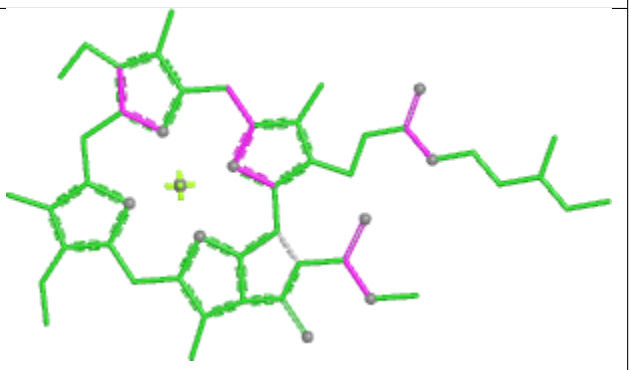
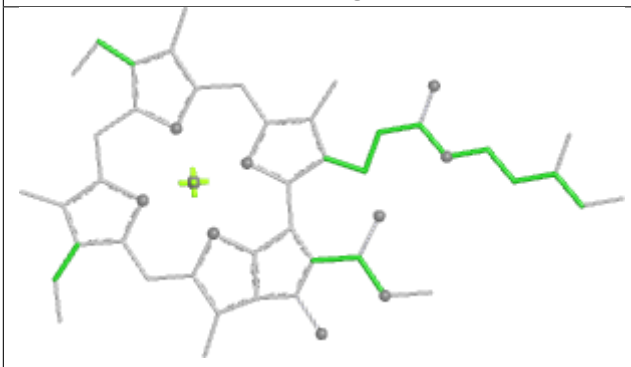


Bond angles



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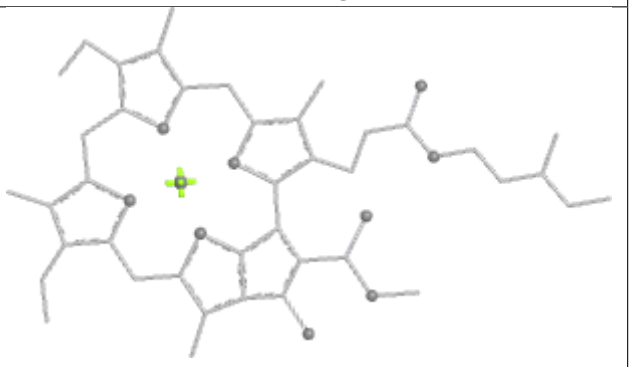
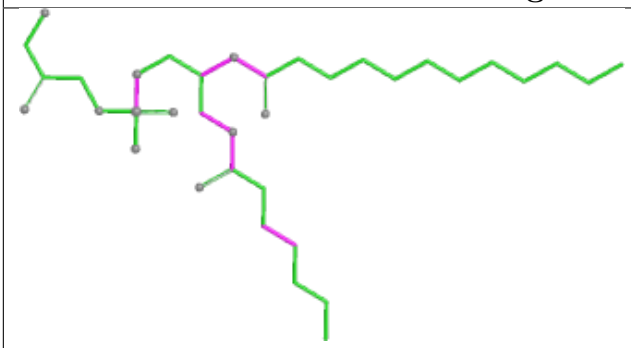


Rings

Ligand LHG 3 320



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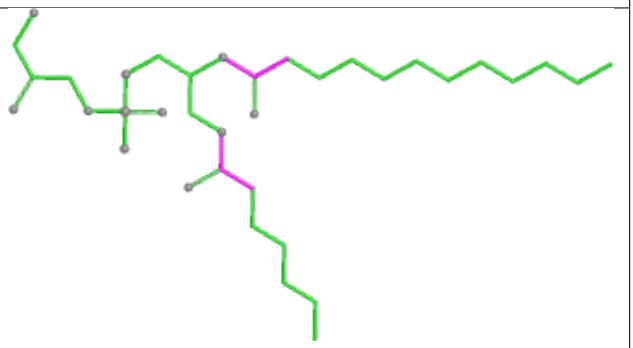
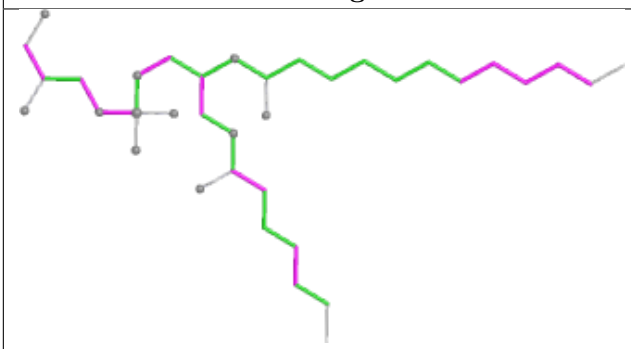


Bond angles



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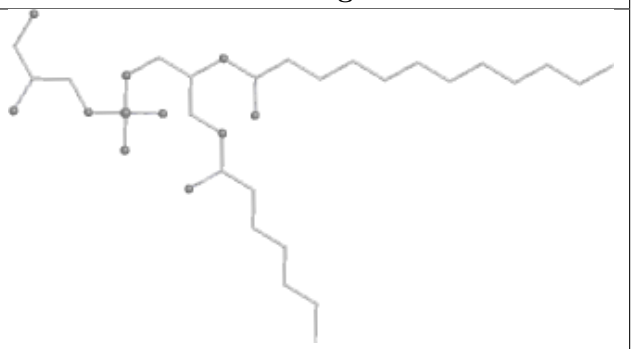
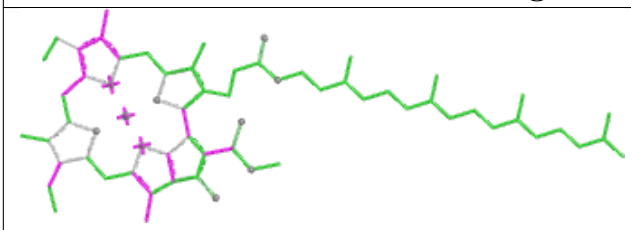


Rings

Ligand CL0 A 852



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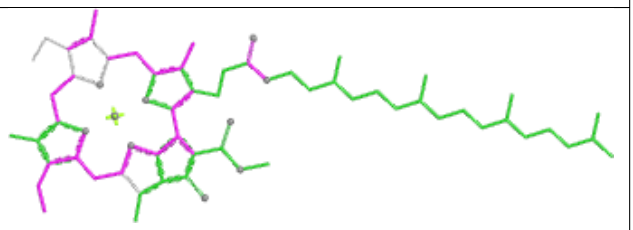
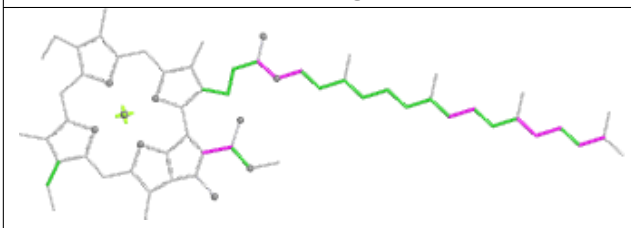


Bond angles



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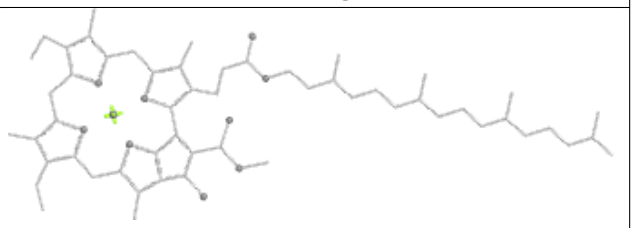
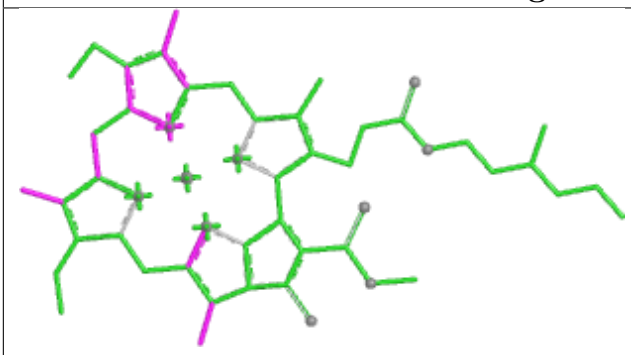


Rings

Ligand CLA 1 303



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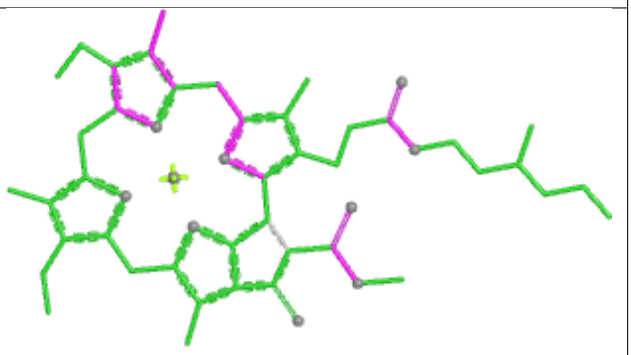
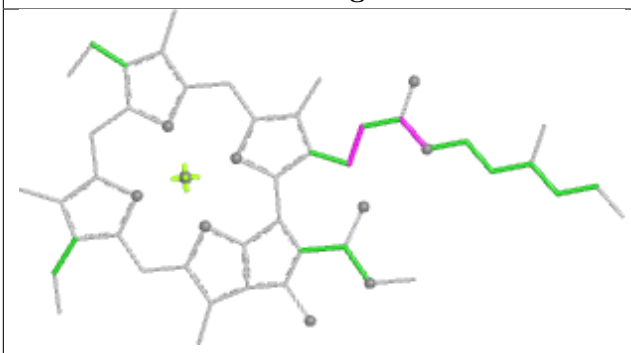


Bond angles



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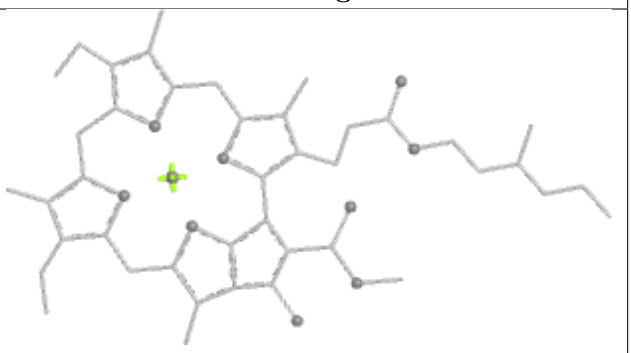
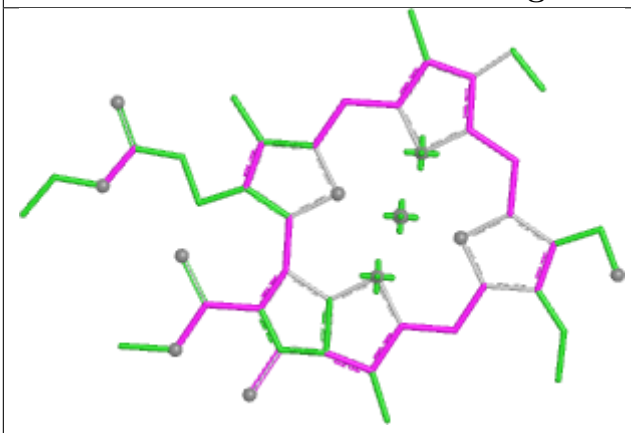
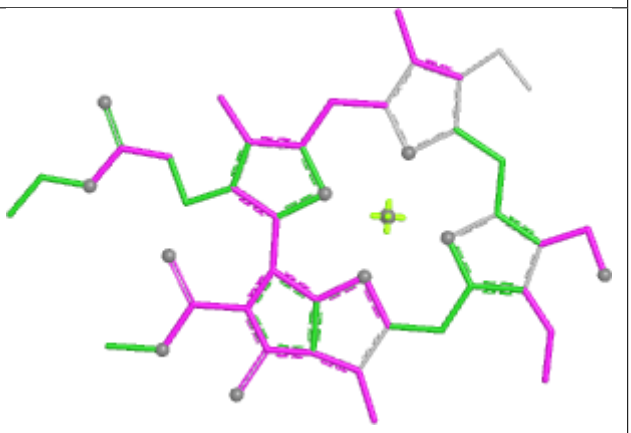


Rings

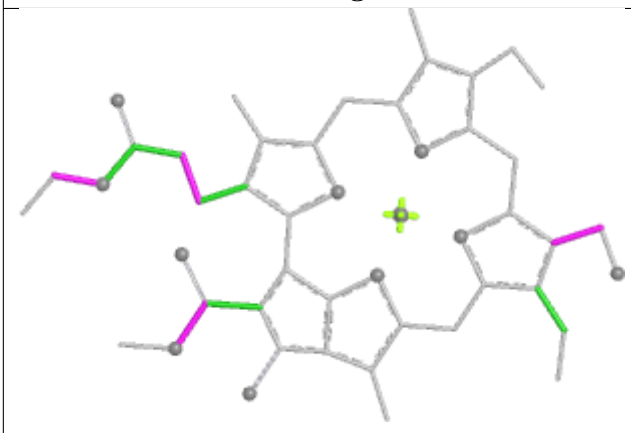
Ligand CHL 4 306



Bond lengths



Bond angles



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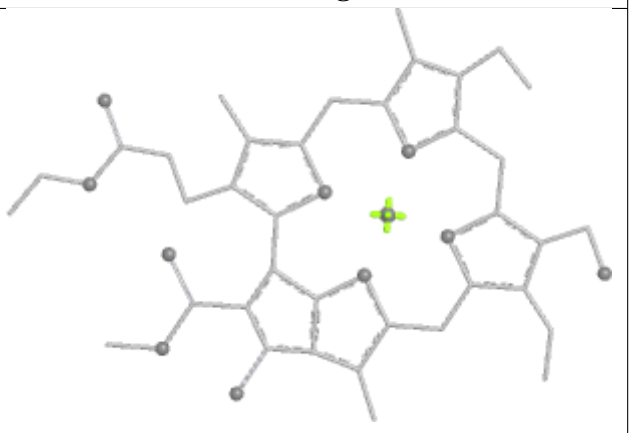
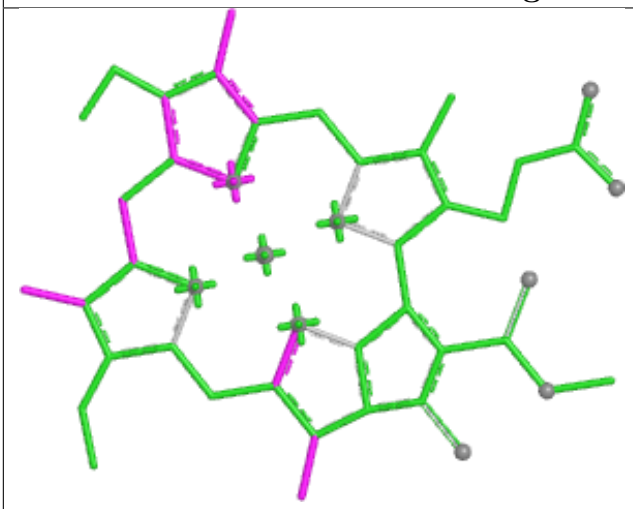


Rings

Ligand CLA G 102



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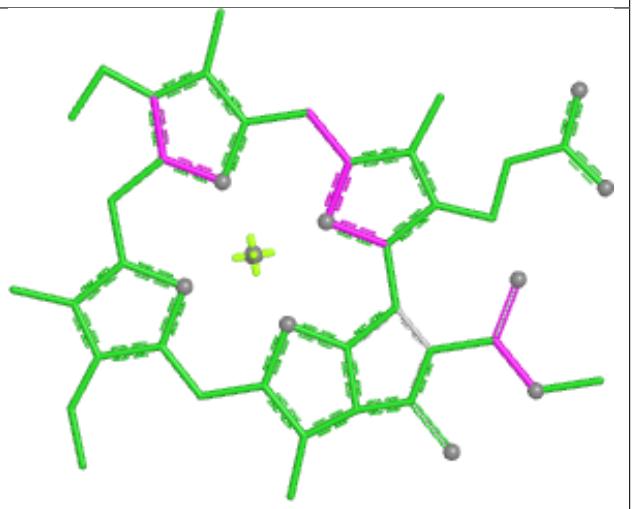
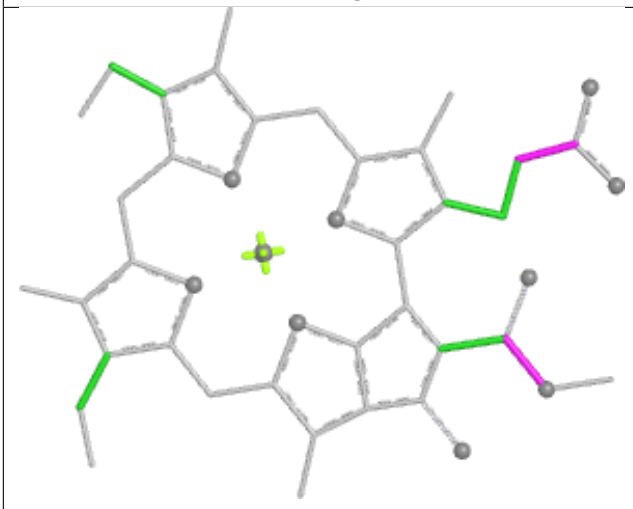


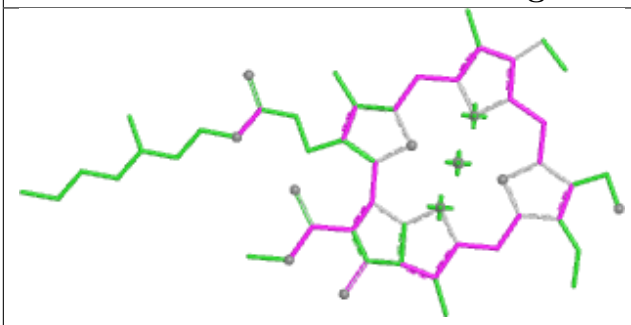
Bond angles



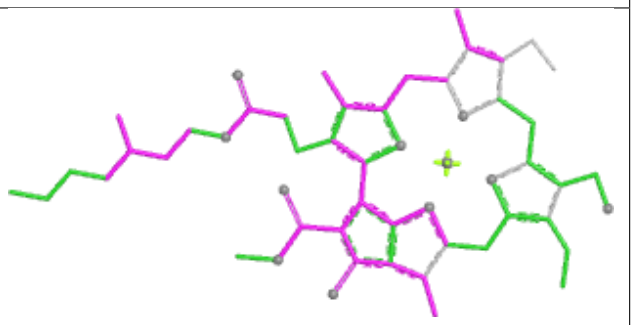
Torsions

Rings

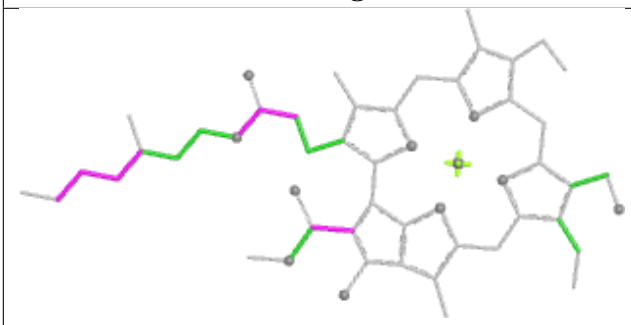
Ligand CHL 4 315



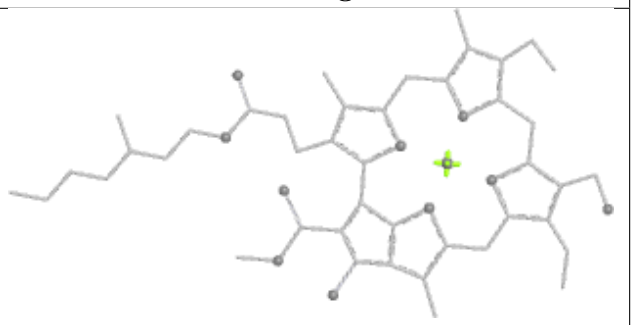
Bond lengths



Bond angles

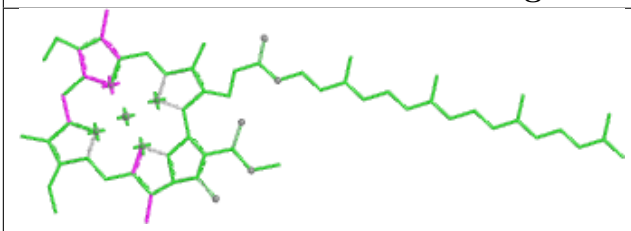


Torsions



Rings

Ligand CLA B 841



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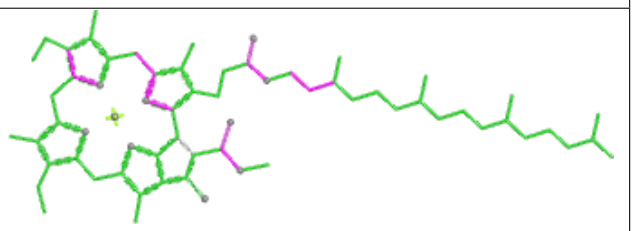
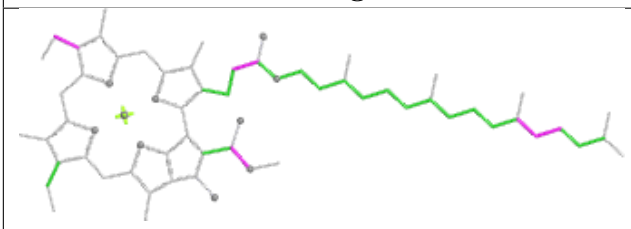


Bond angles



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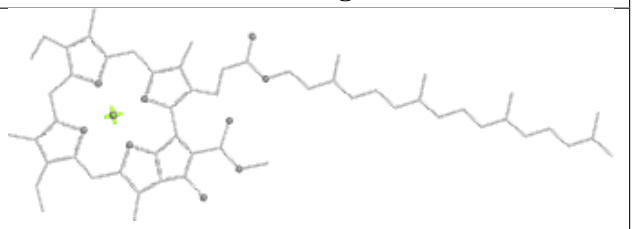
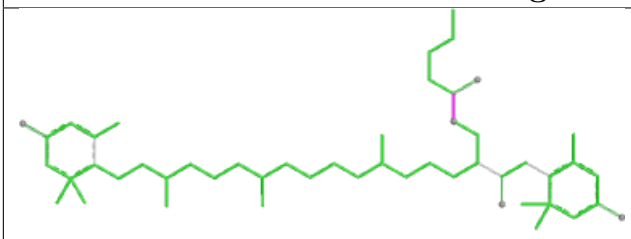


Rings

Ligand 0UR 2 316



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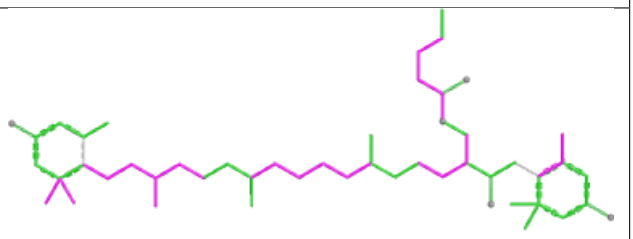
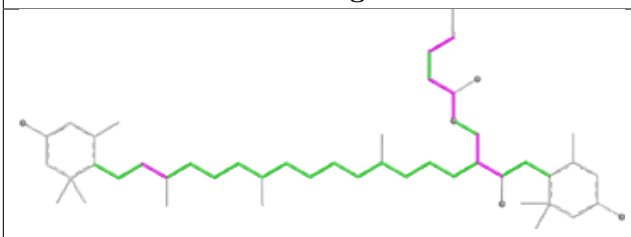


Bond angles



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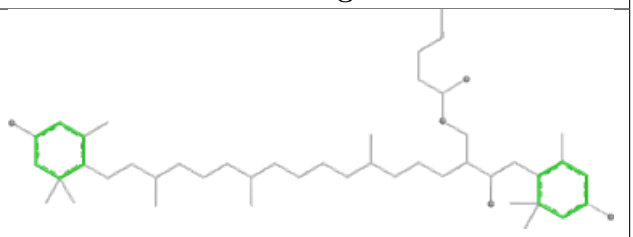
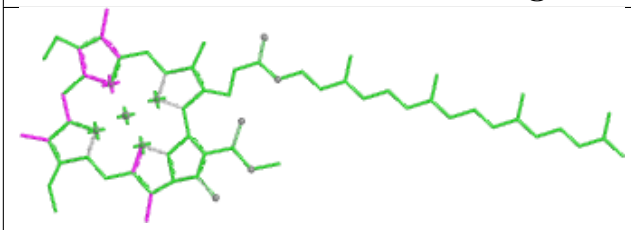


Rings

Ligand CLA 0 311



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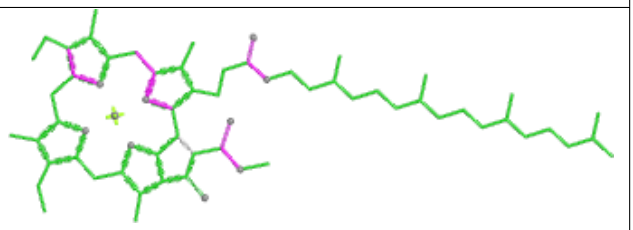

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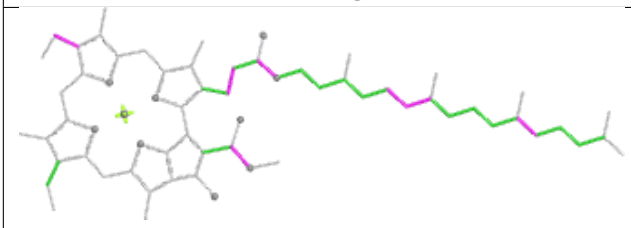

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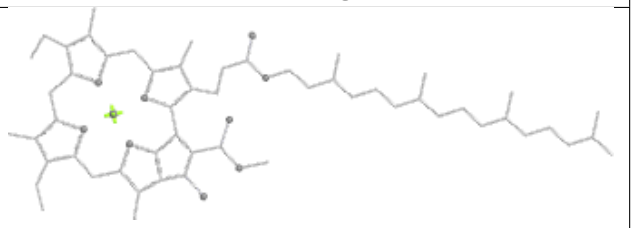
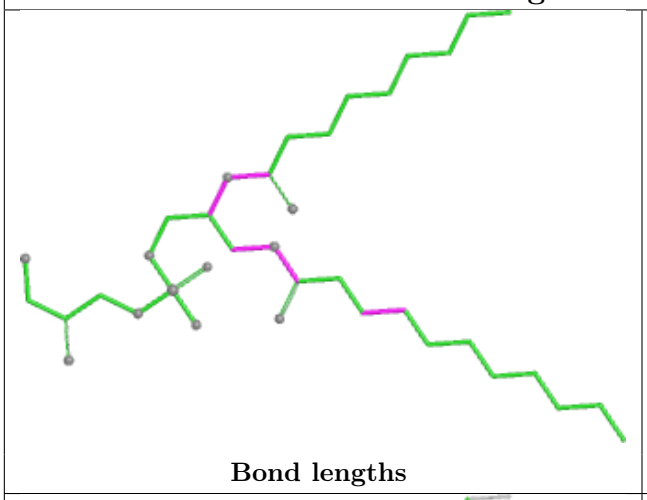


Rings

Ligand LHG 6 322



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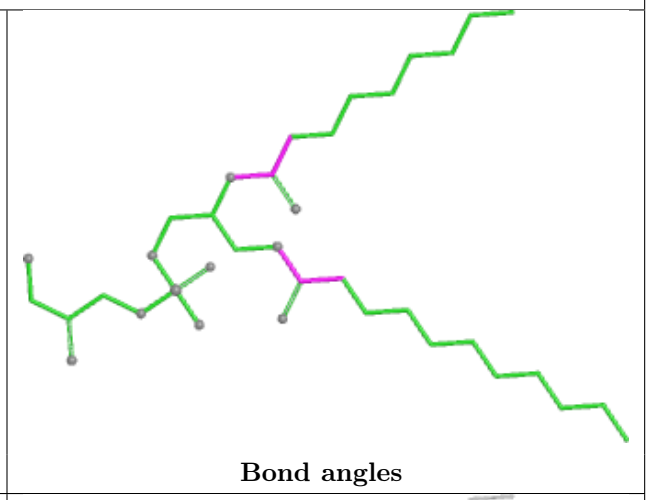
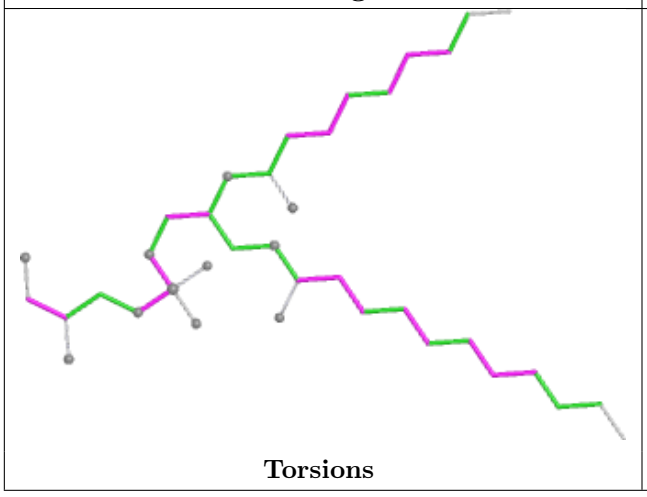


Bond angles



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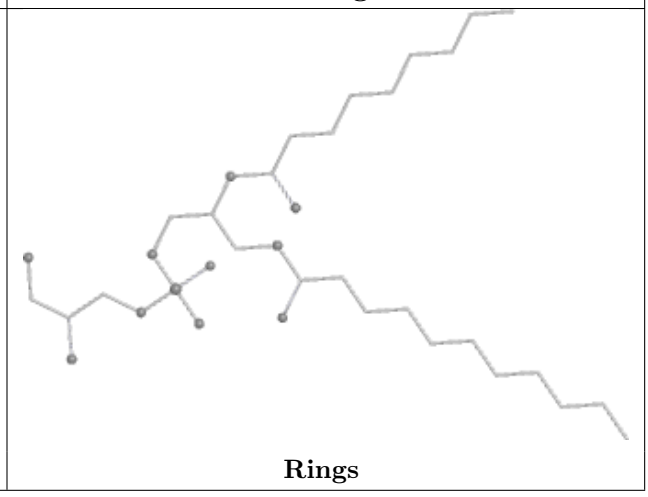
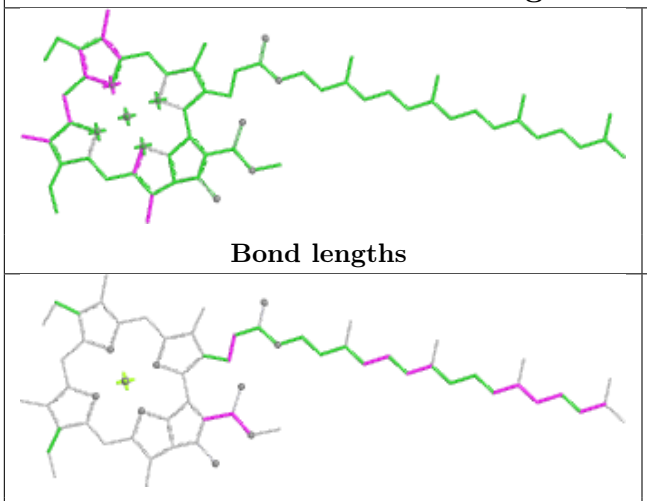


Rings

Ligand CLA B 804



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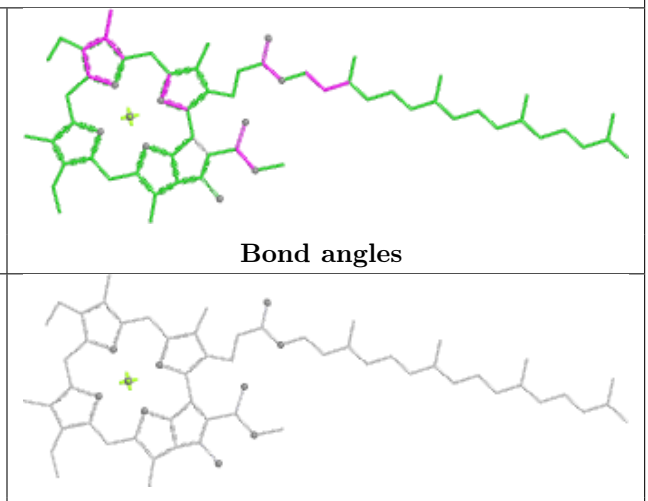
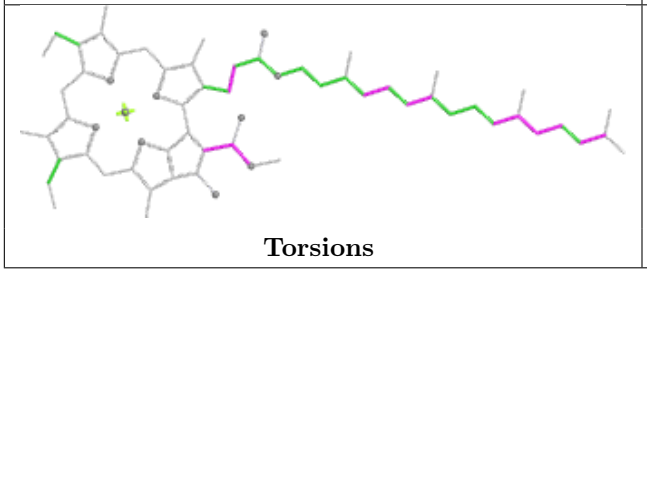
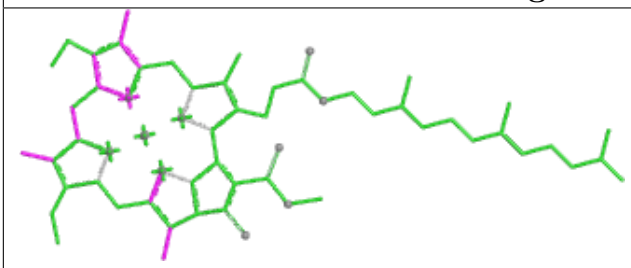
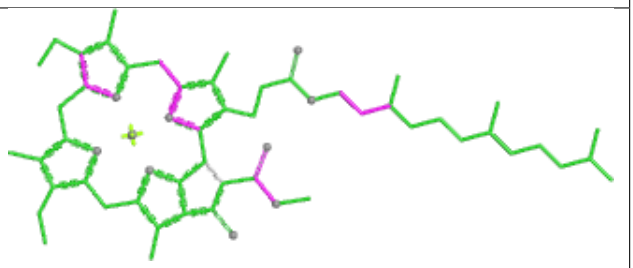
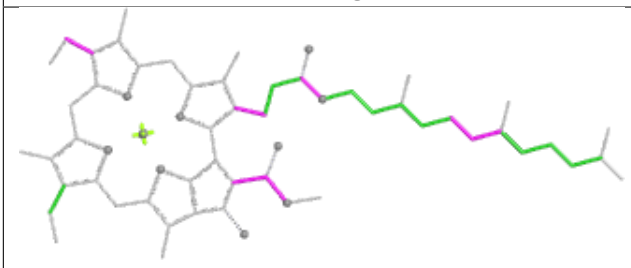
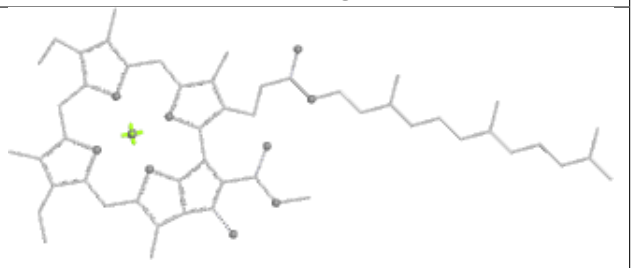


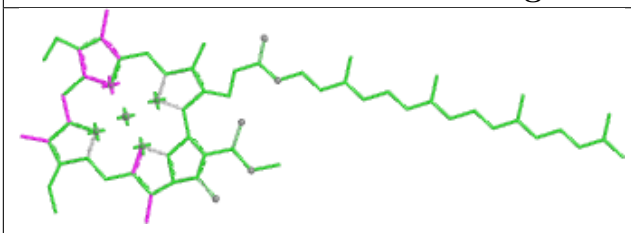
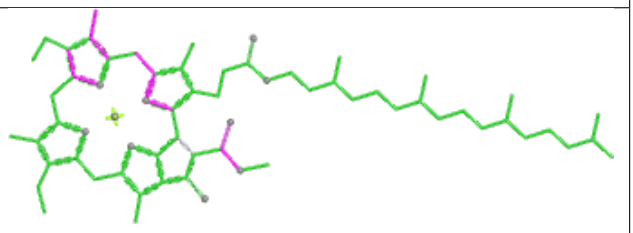
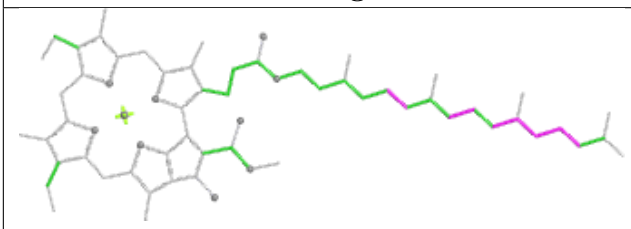
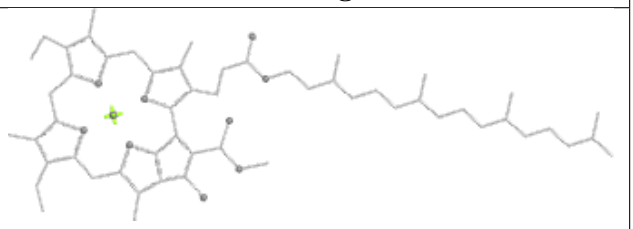
Bond angles



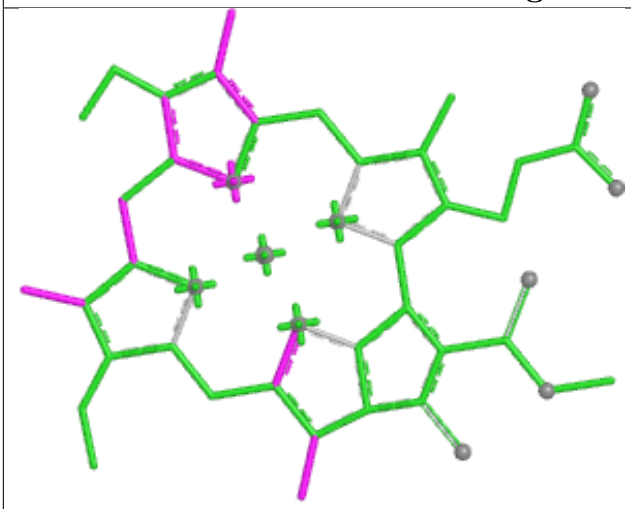
Torsions

Rings

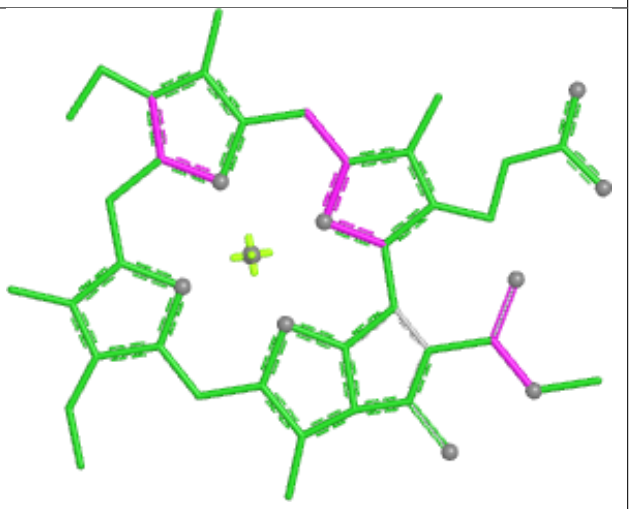
Ligand CLA 6 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

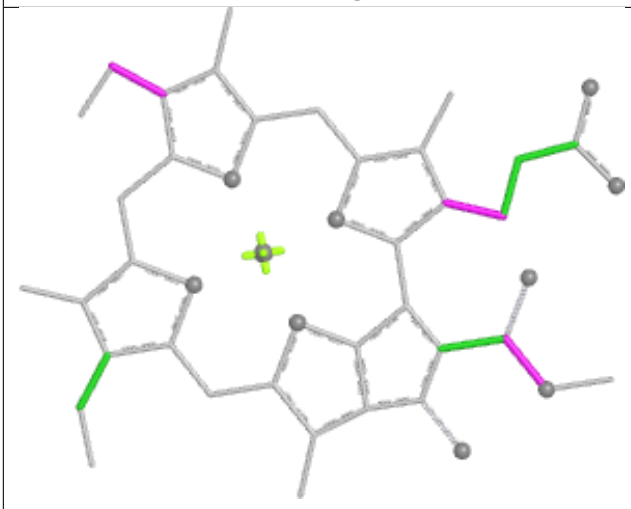
Ligand CLA F 303



Bond lengths



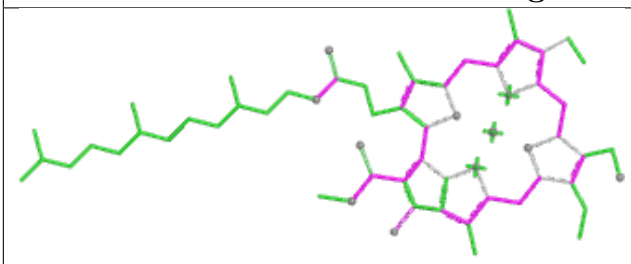
Bond angles



Torsions

Rings

Ligand CHL 6 323



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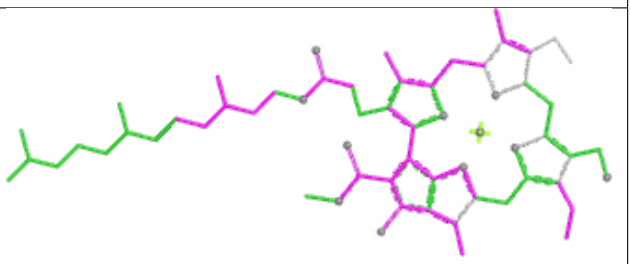

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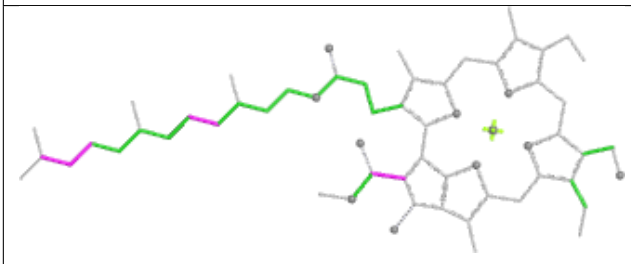

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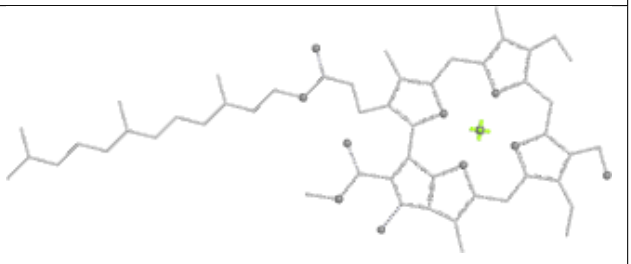
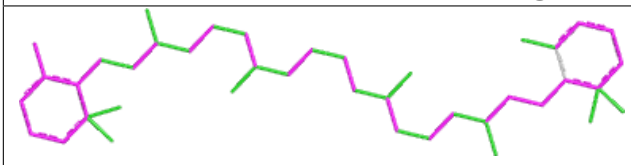


Rings

Ligand 8CT 3 323



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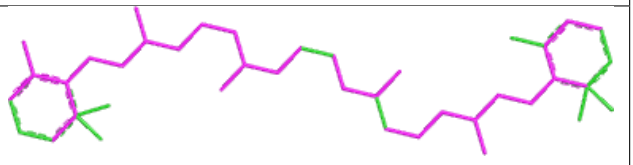
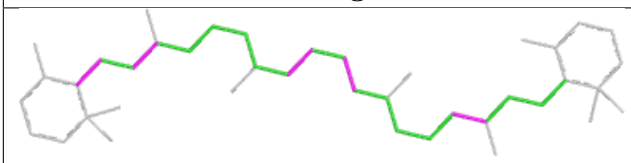


Bond angles



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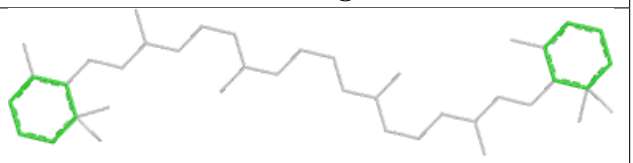
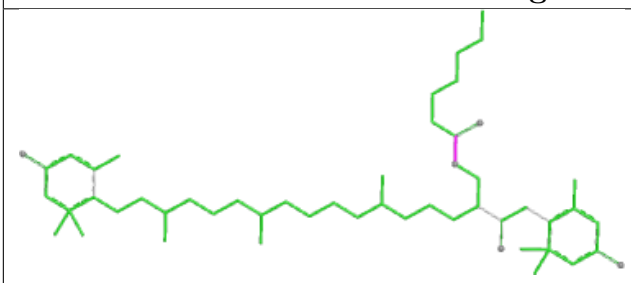


Rings

Ligand 0UR 0 316



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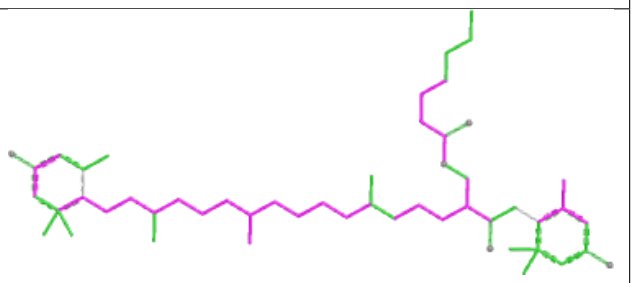
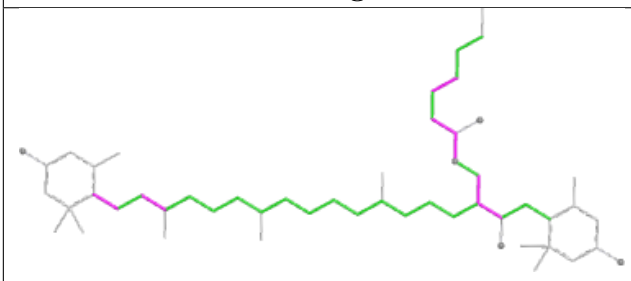


Bond angles



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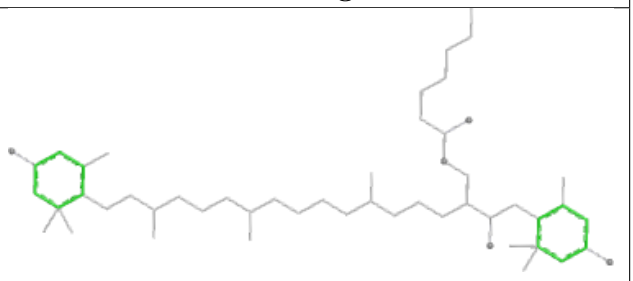
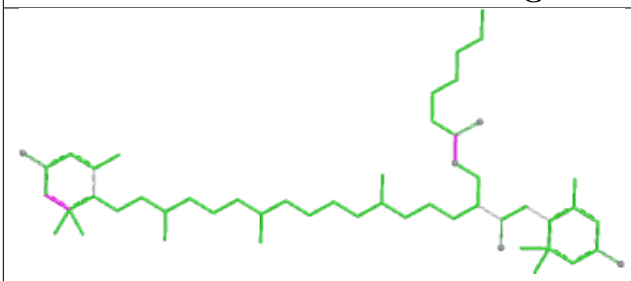


Rings

Ligand 0UR O 207



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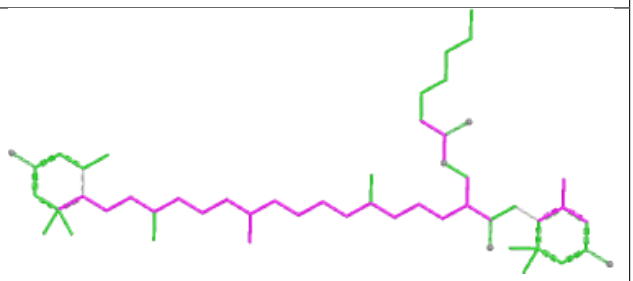
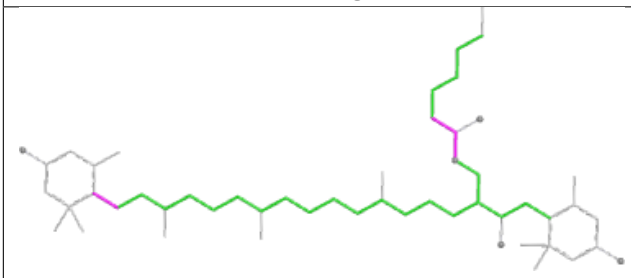


Bond angles



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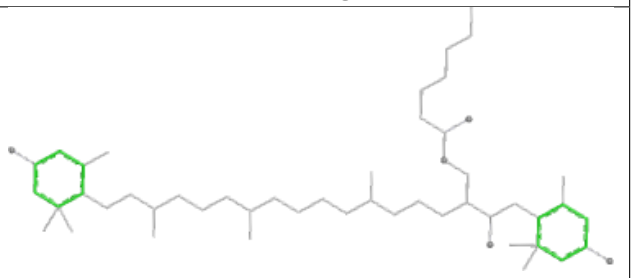
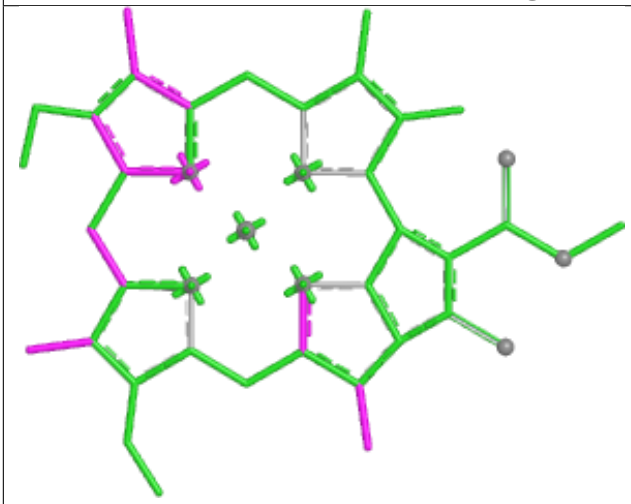


Rings

Ligand CLA O 204



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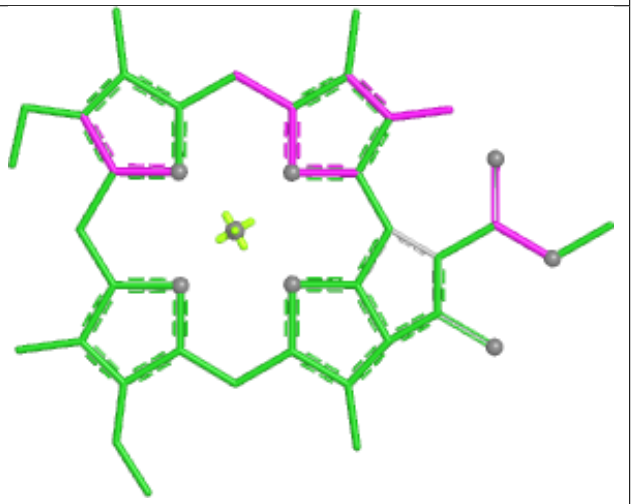
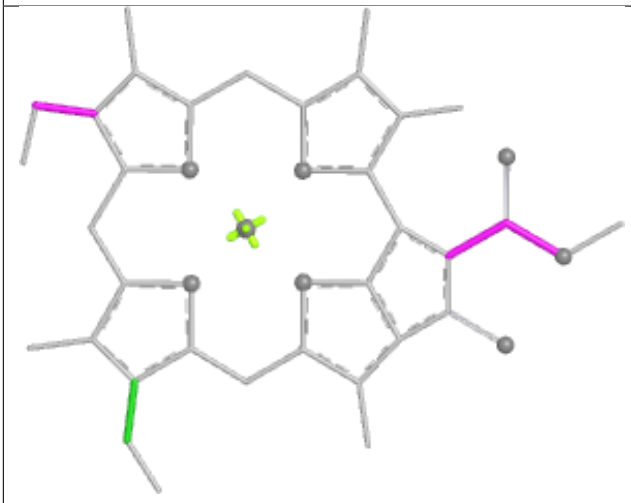
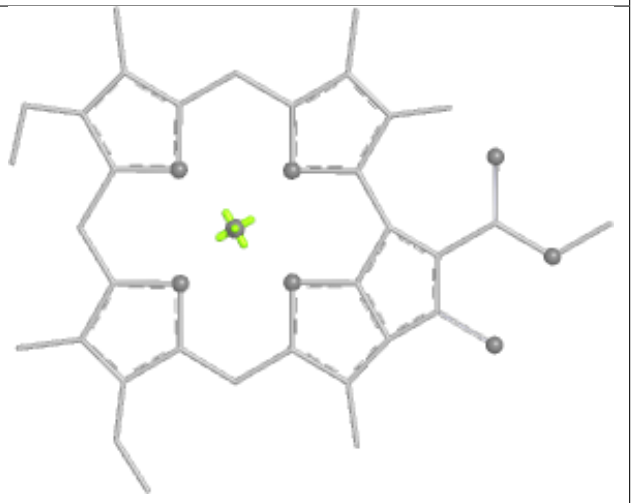


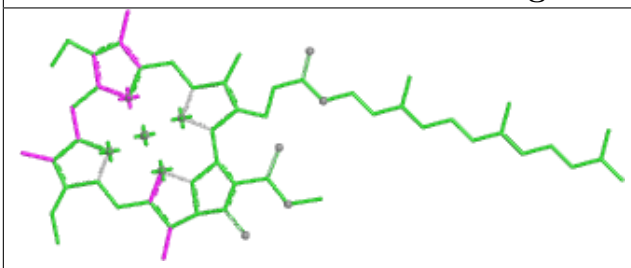
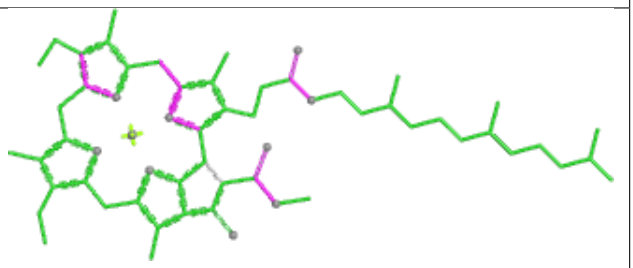
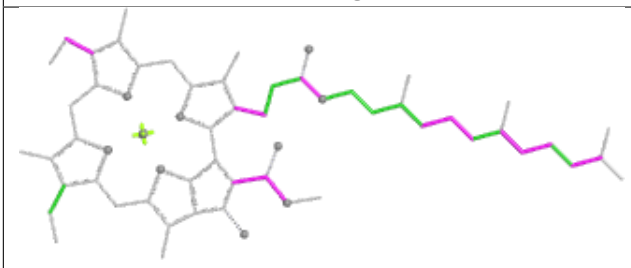
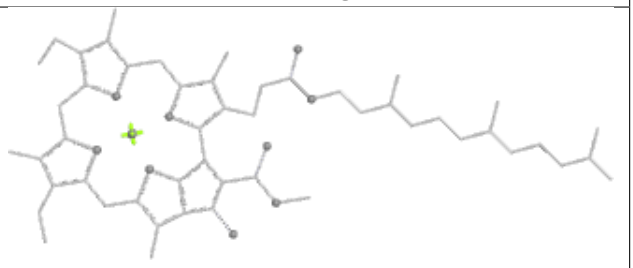
Bond angles

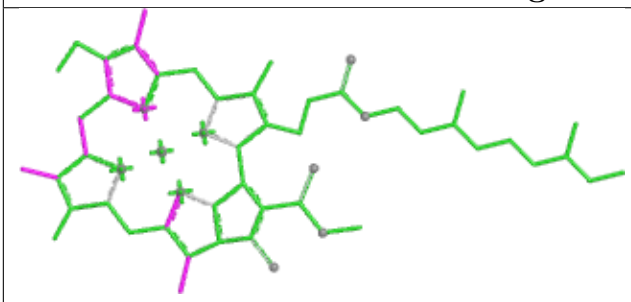
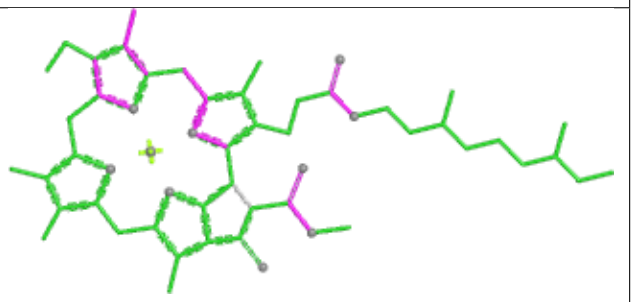
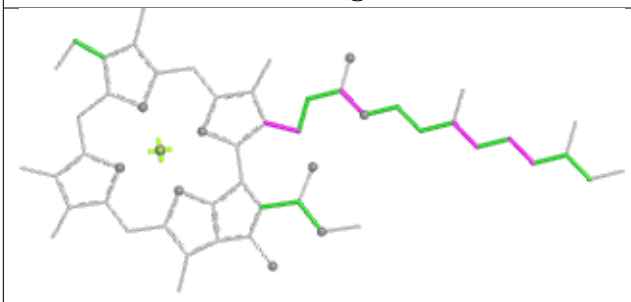
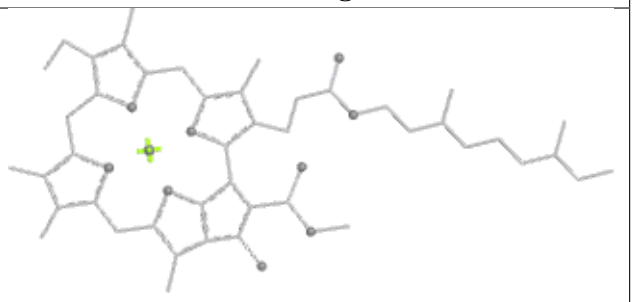


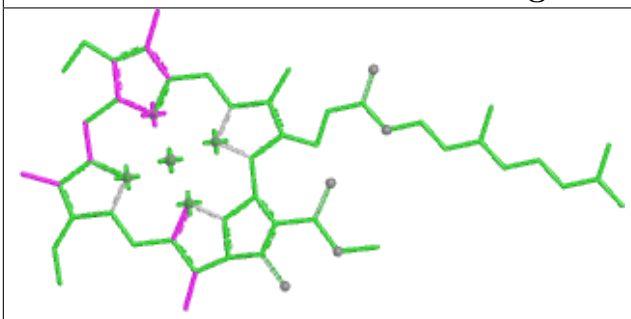
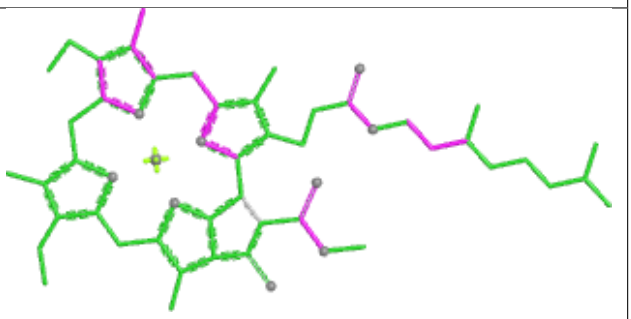
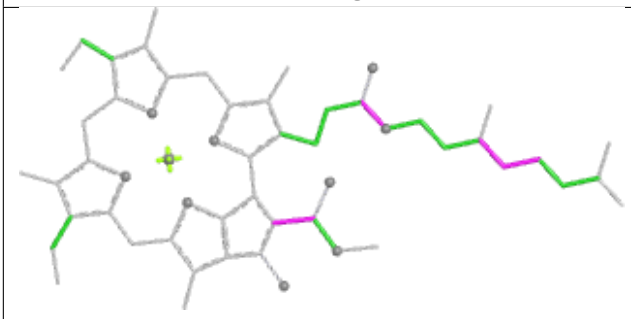
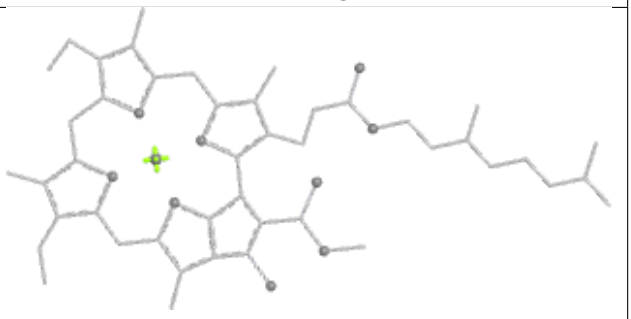
Torsions



Rings

Ligand CLA 4 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

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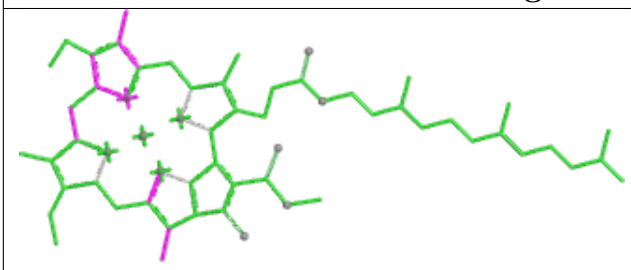
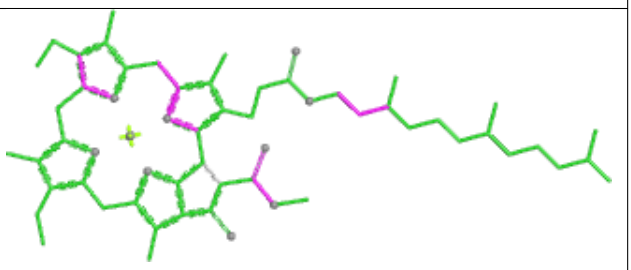
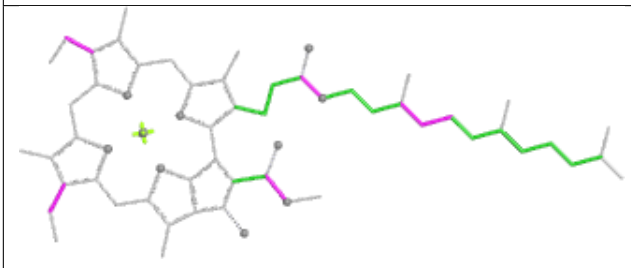
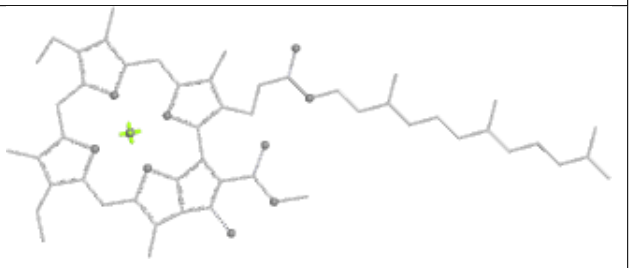
 Bond lengths	 Bond angles
 Torsions	 Rings

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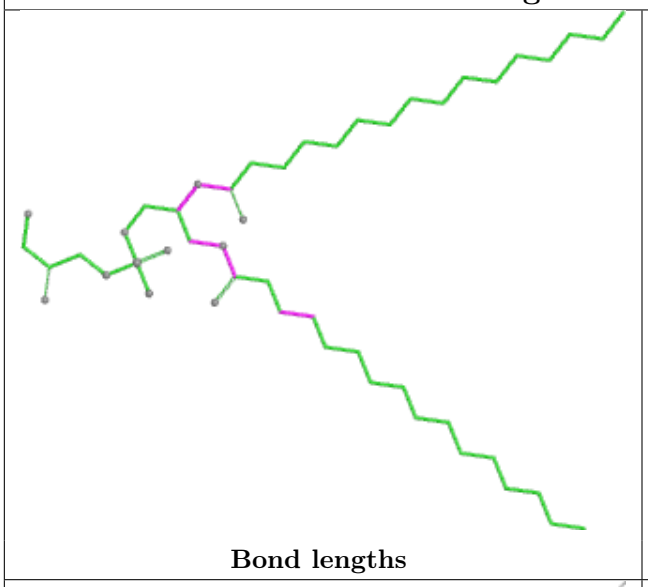
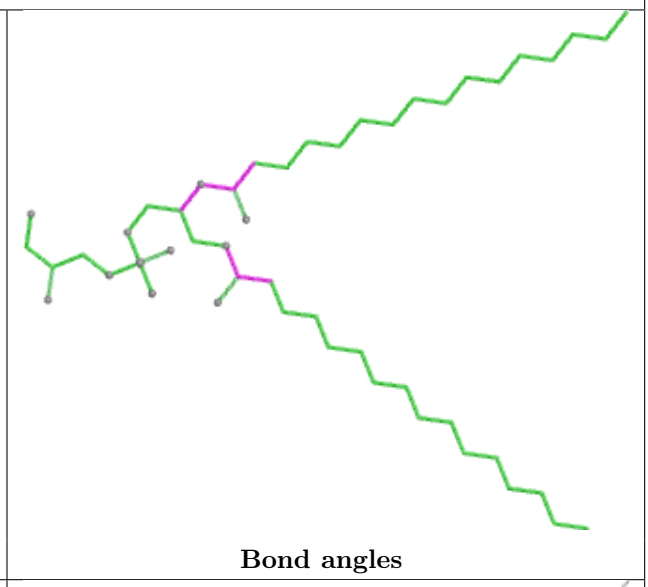


Bond lengths



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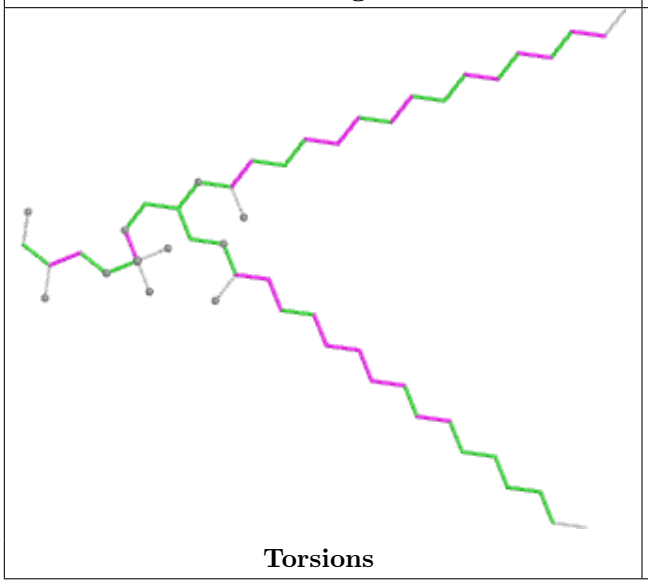

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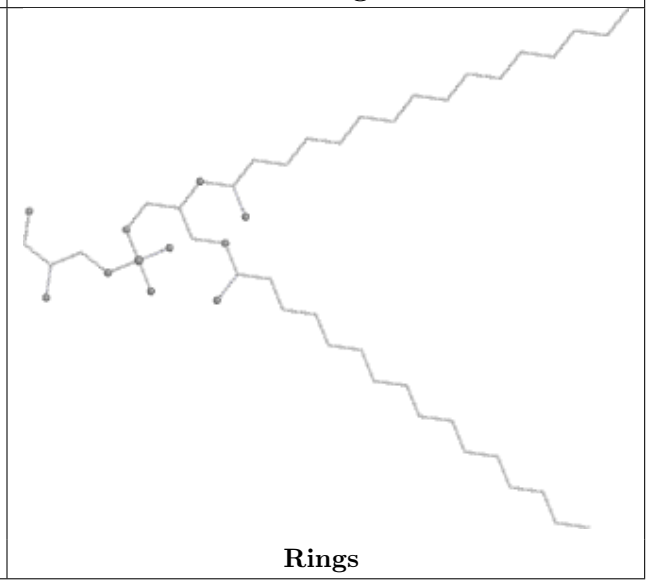
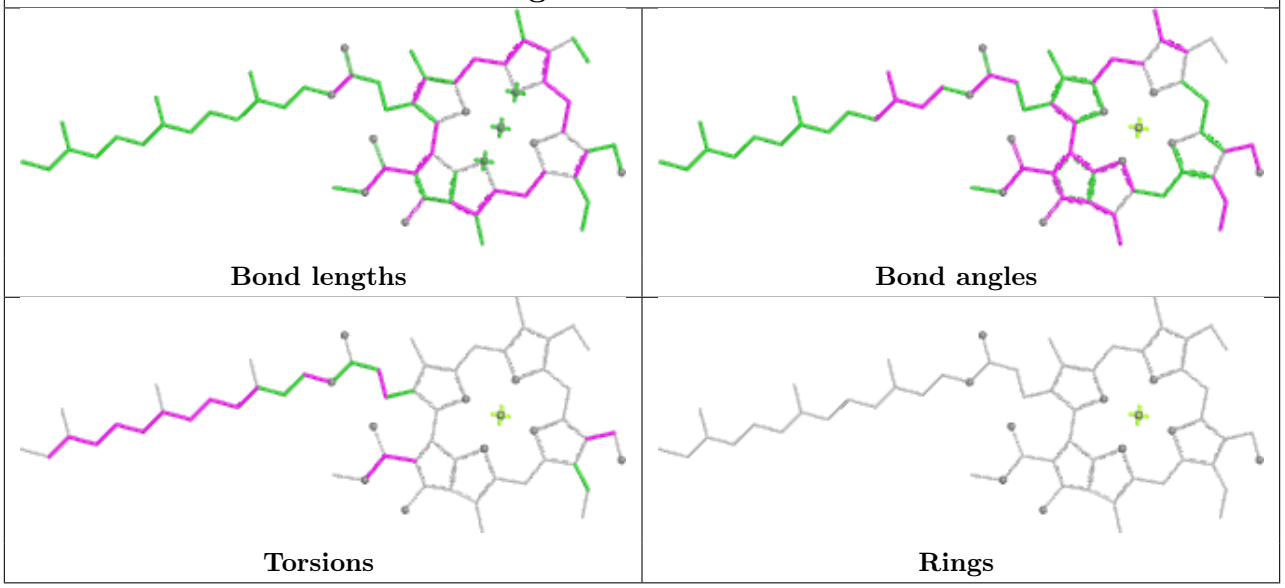


Rings

Ligand CHL 1 312



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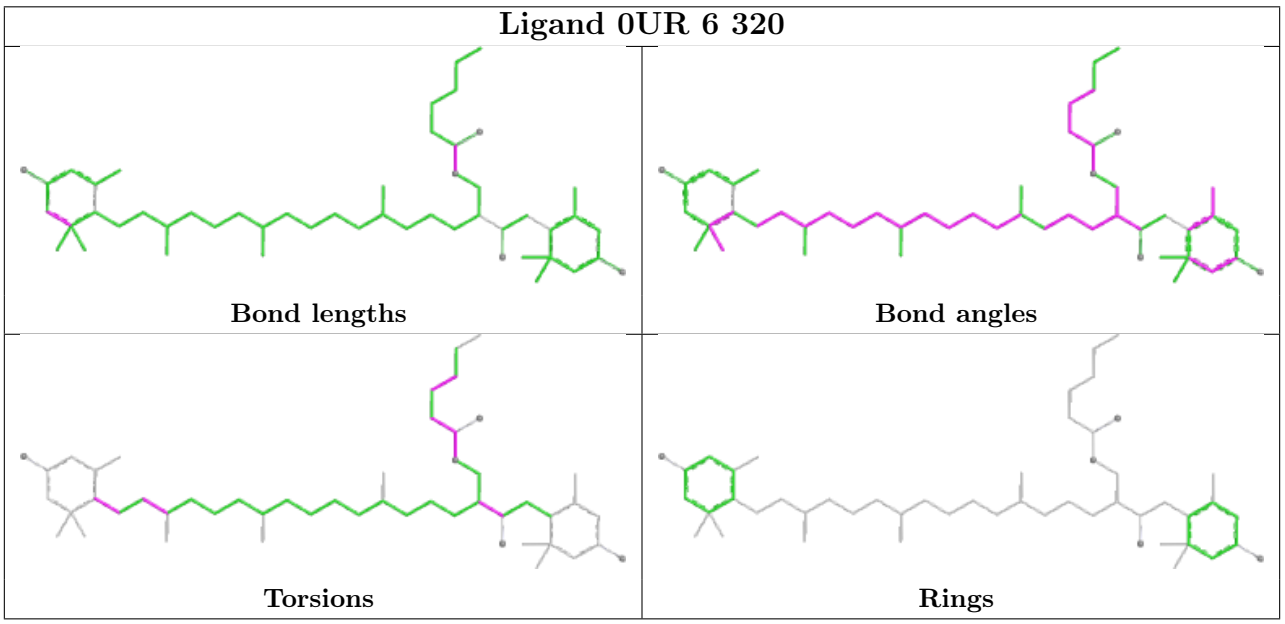

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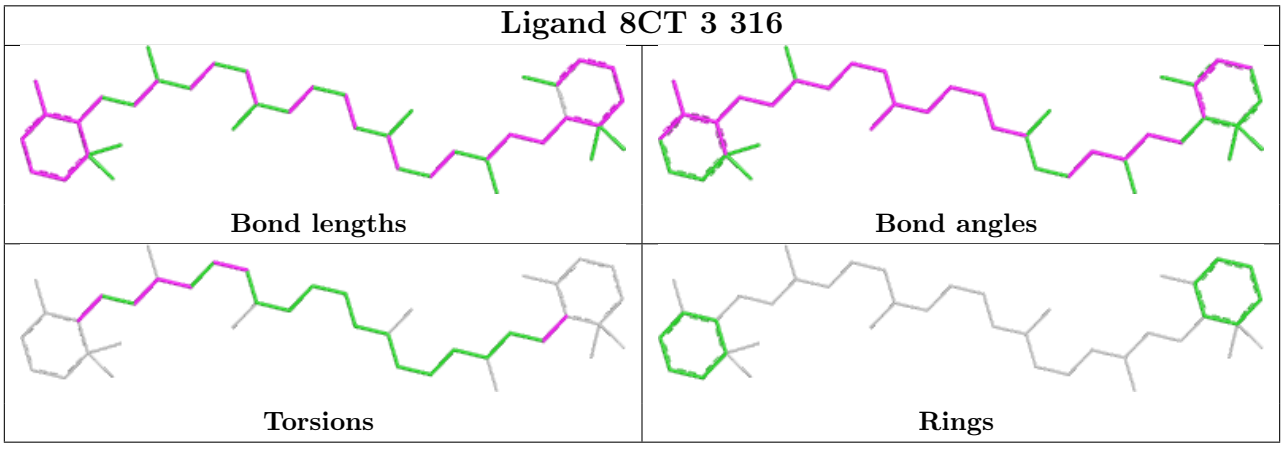

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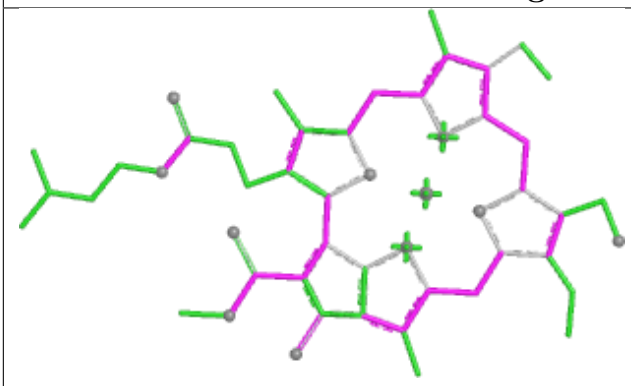

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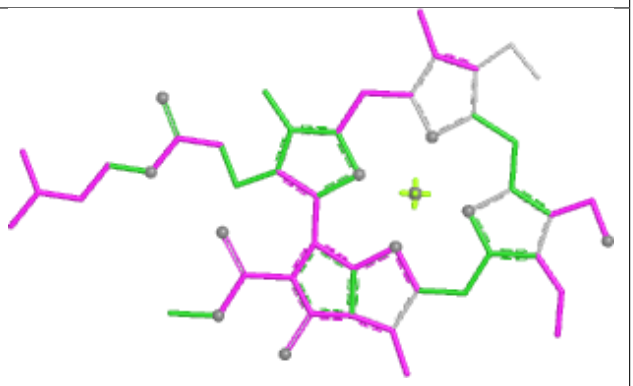
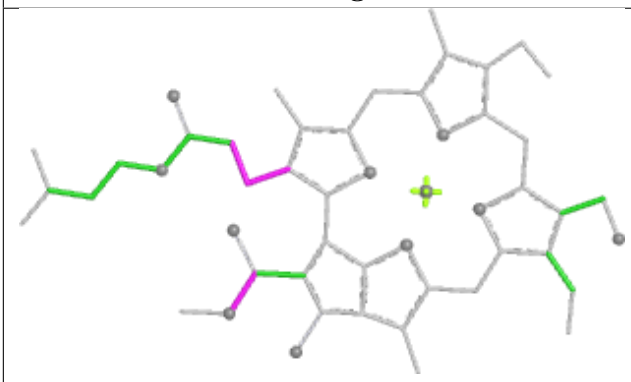
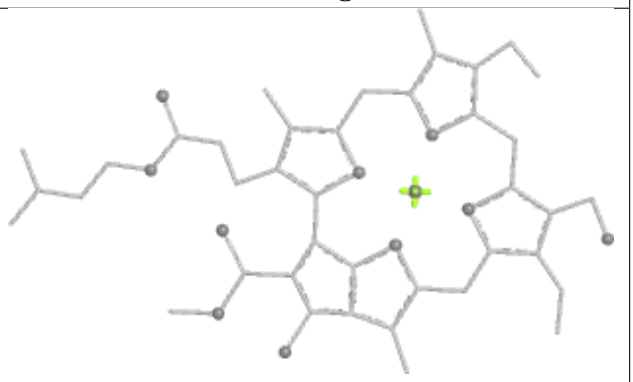


Bond angles

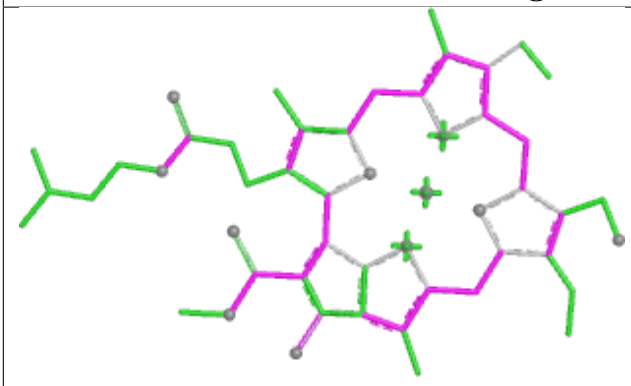


Torsions



Rings

Ligand CHL 2 306



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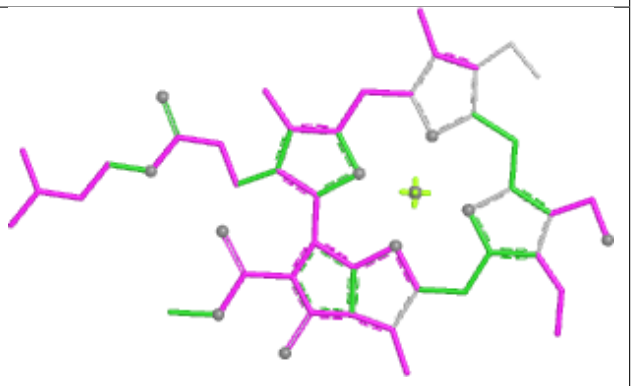

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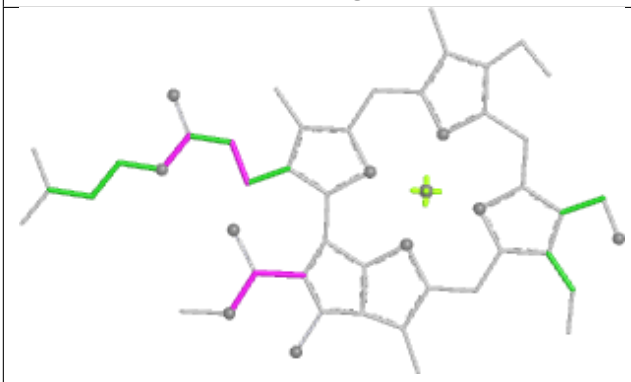

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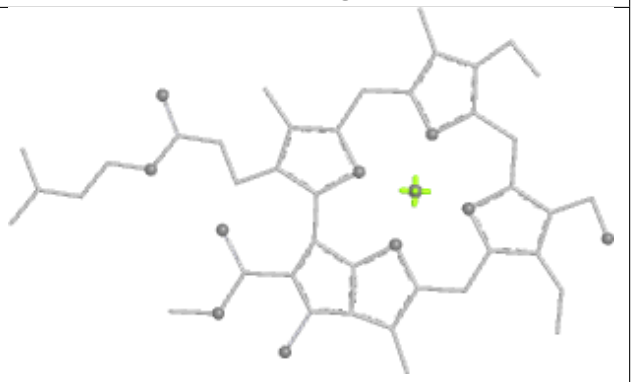

Rings

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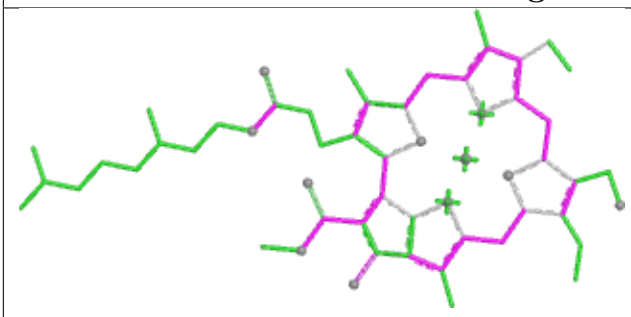
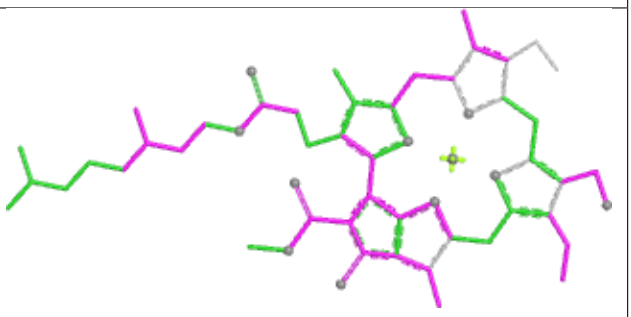
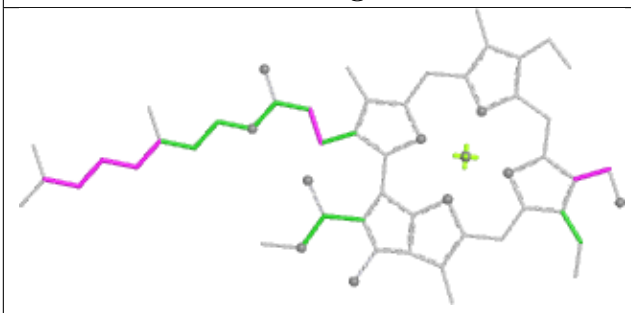
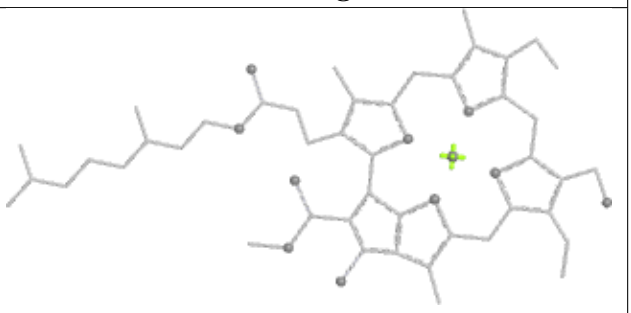
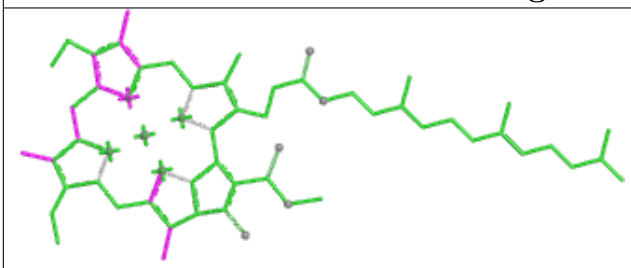
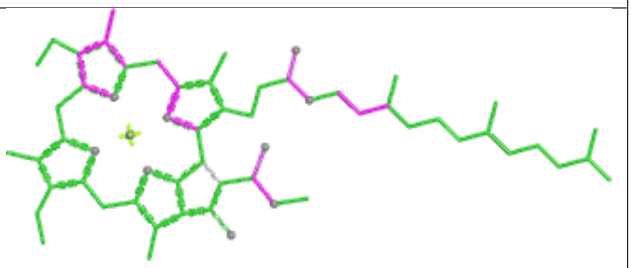
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 308	
	
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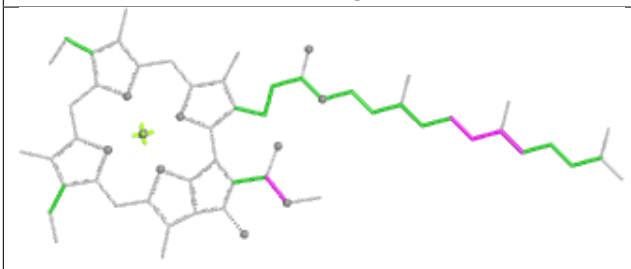
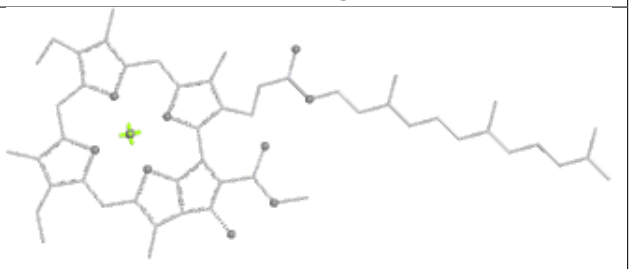
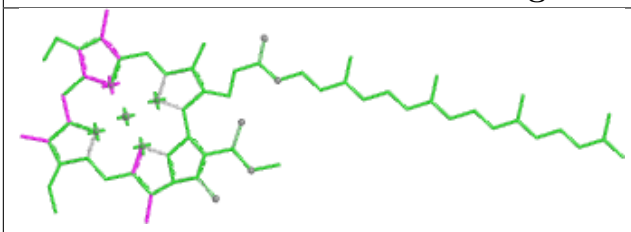
	
Torsions	Rings

Ligand CLA 7 308



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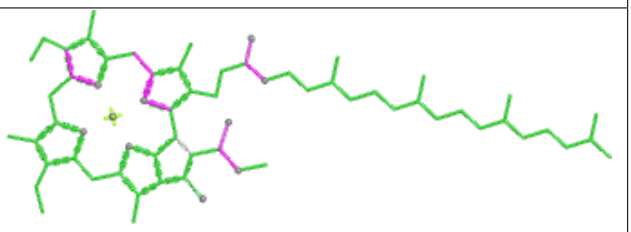

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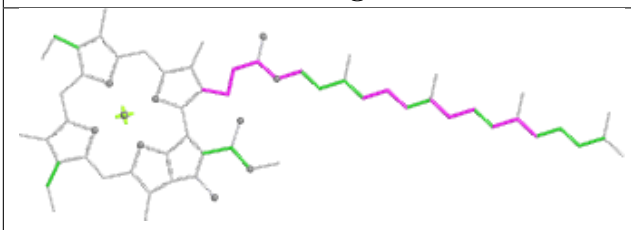
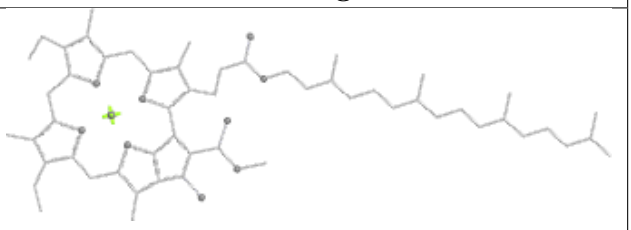
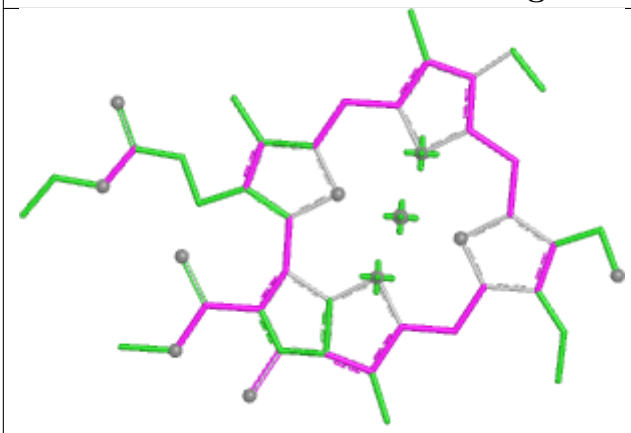


Torsions



Rings

Ligand CHL 2 305



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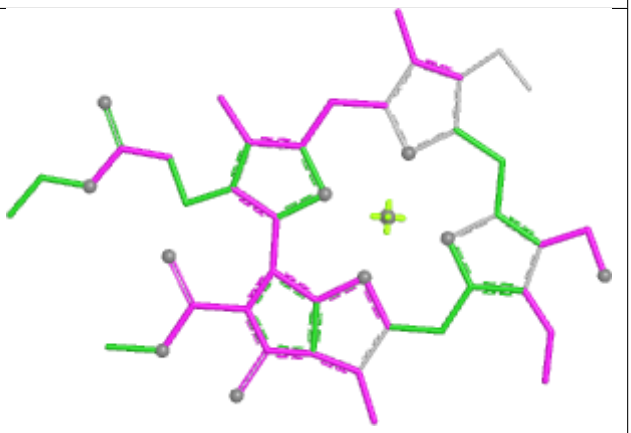

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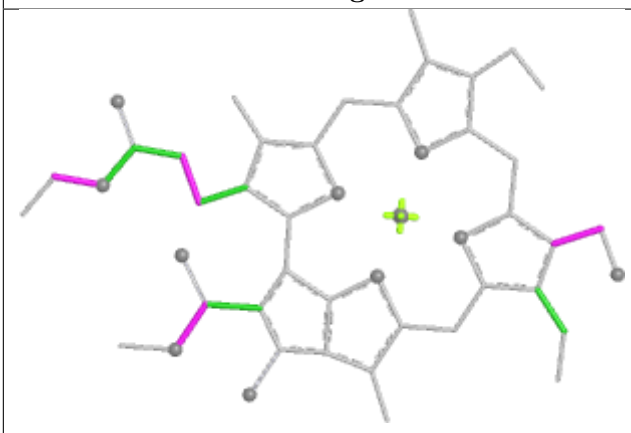

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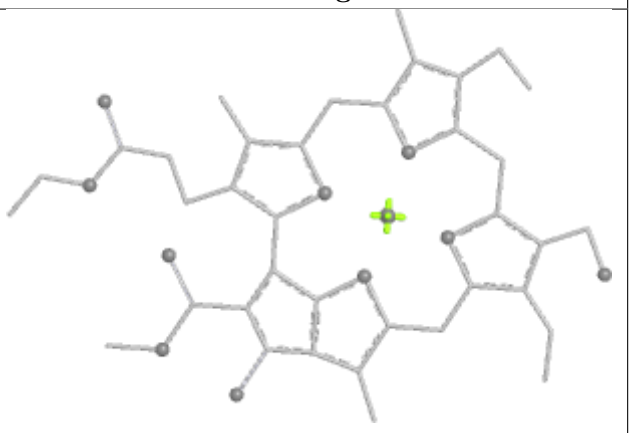

Rings

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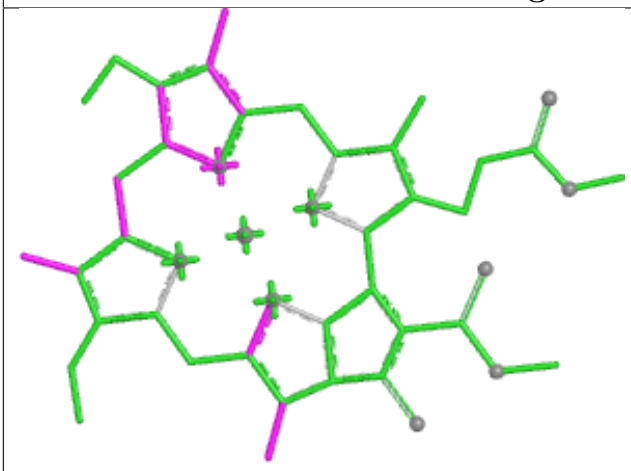

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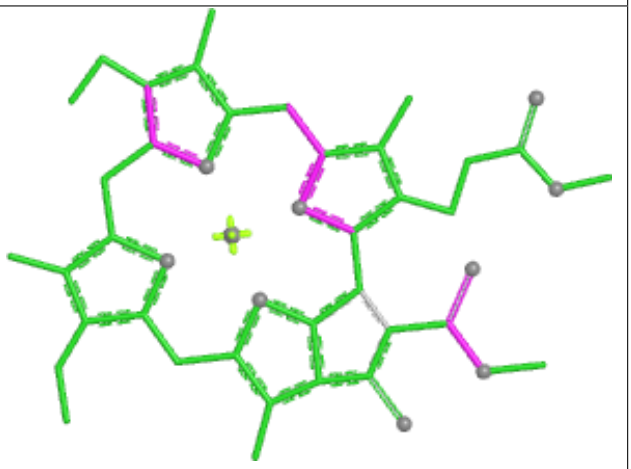
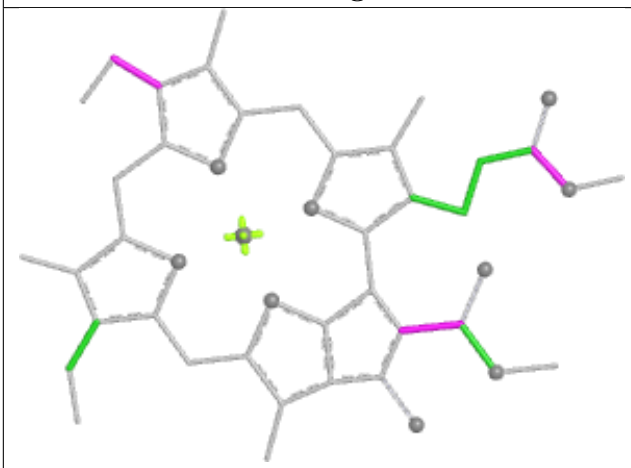


Bond angles



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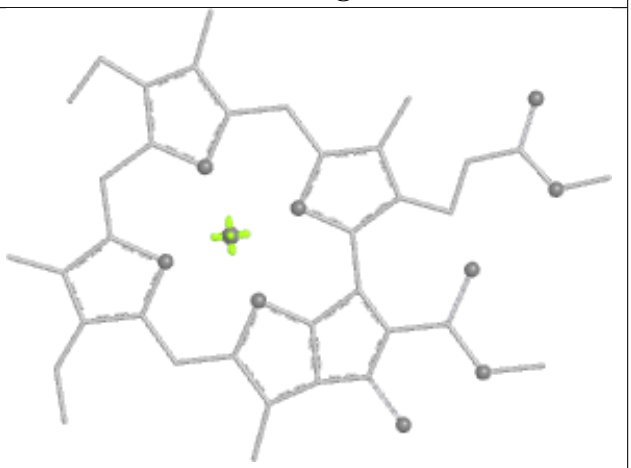
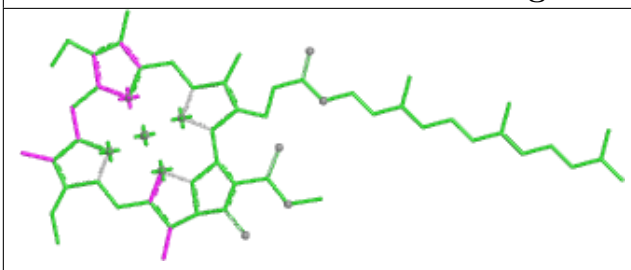


Rings

Ligand CLA 0 308



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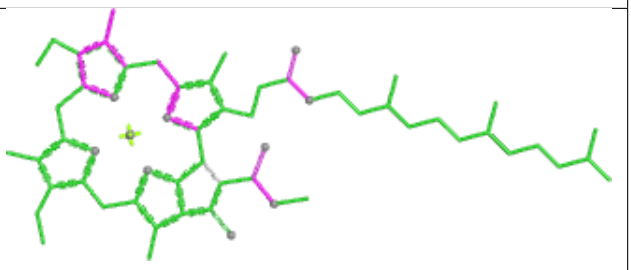
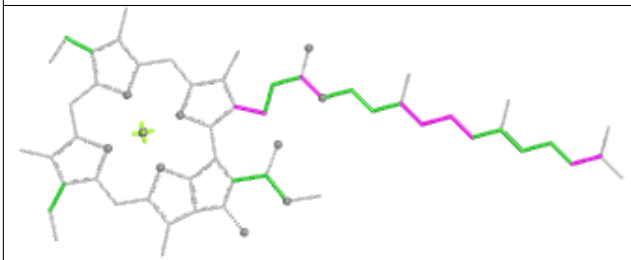


Bond angles



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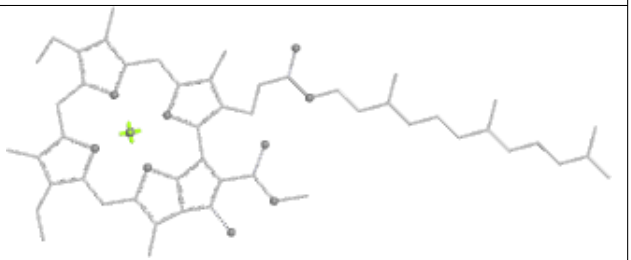
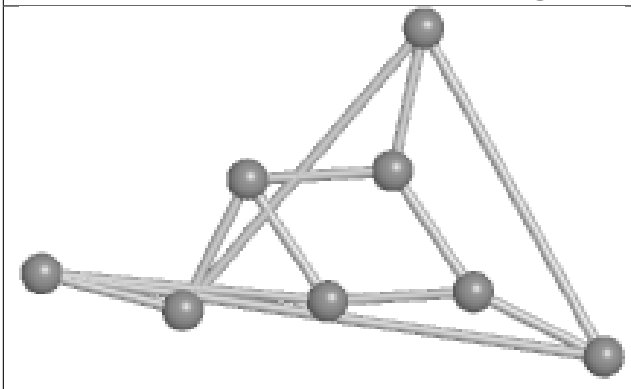
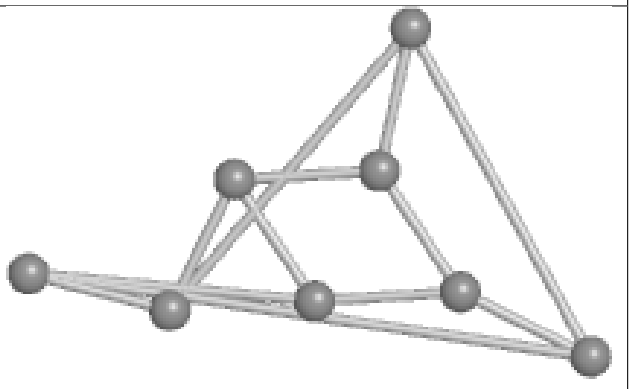


Rings

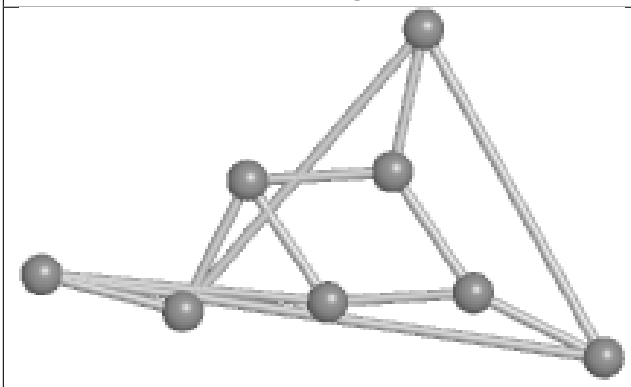
Ligand SF4 C 101



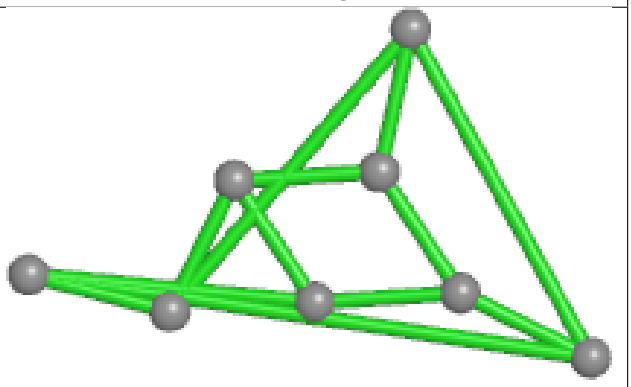
Bond lengths



Bond angles

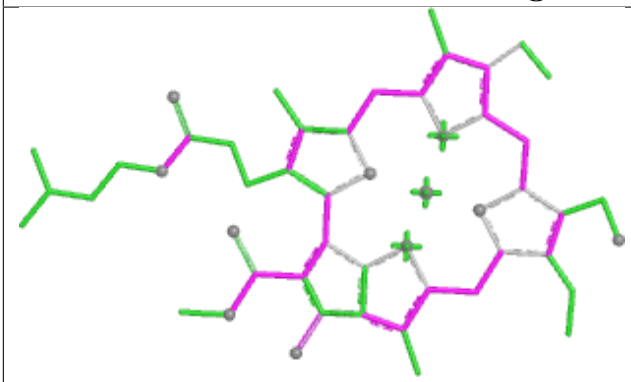


Torsions



Rings

Ligand CHL 4 313



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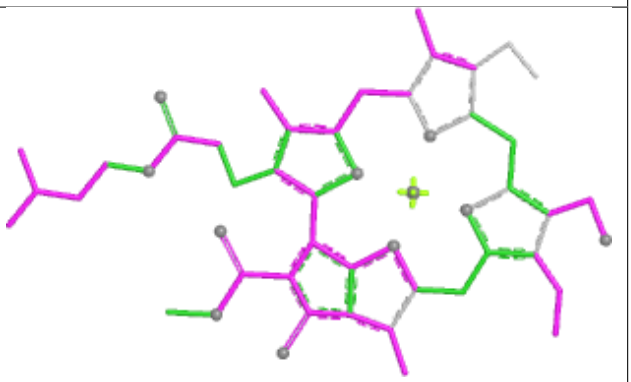

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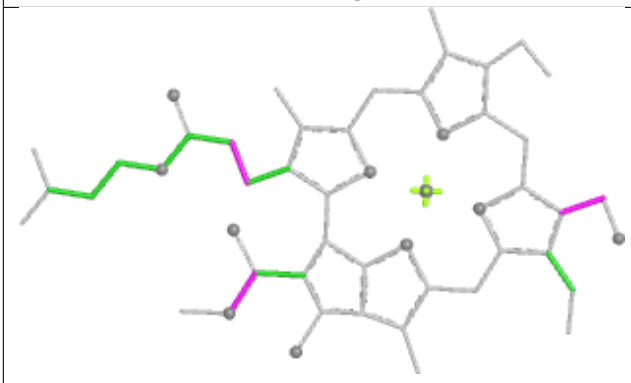

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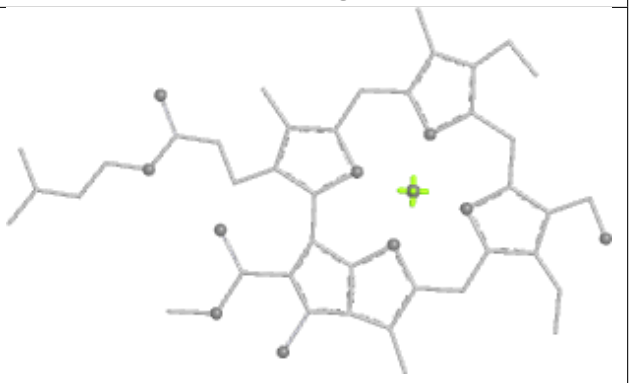
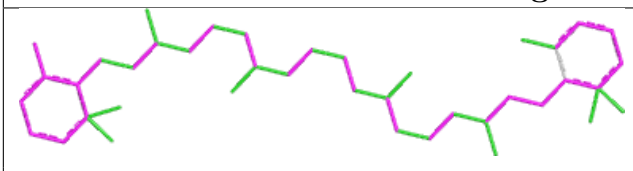


Rings

Ligand 8CT 7 318



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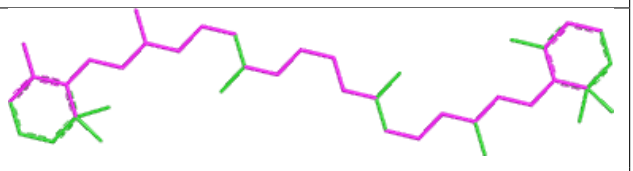
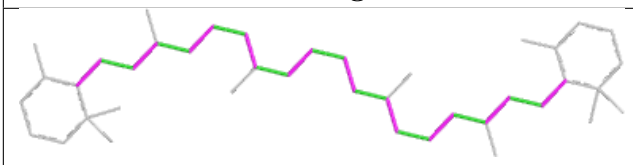


Bond angles



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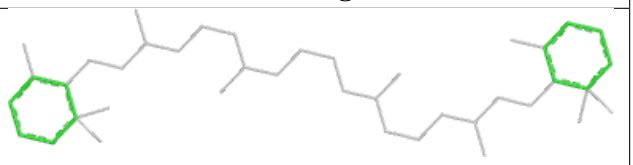
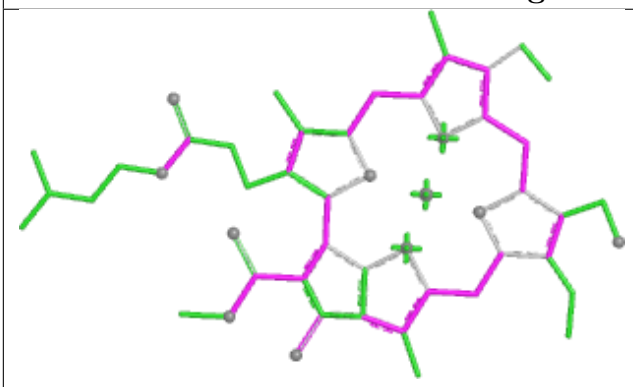


Rings

Ligand CHL 6 307



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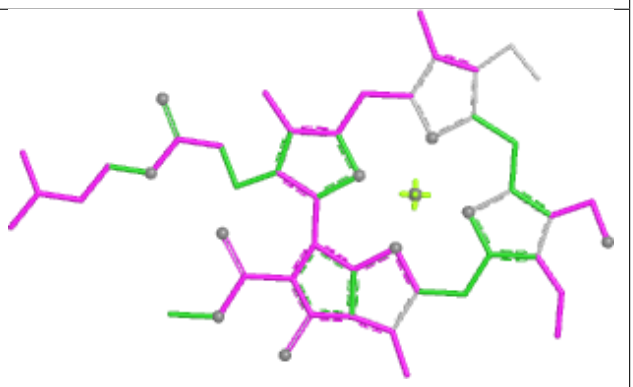
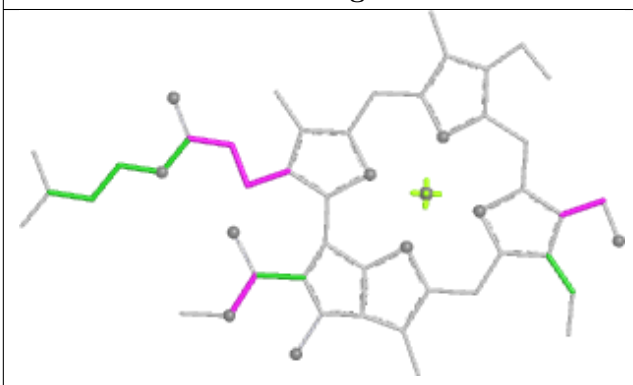


Bond angles



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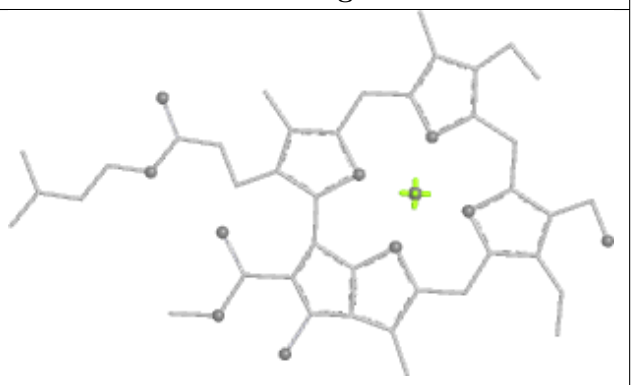
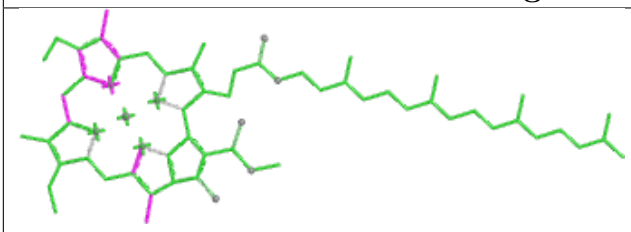
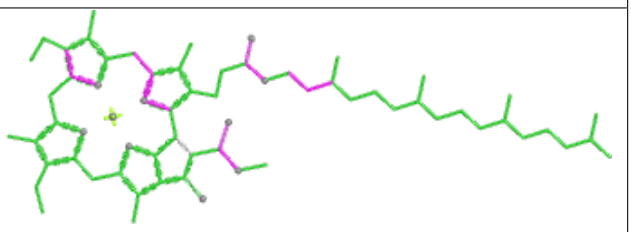
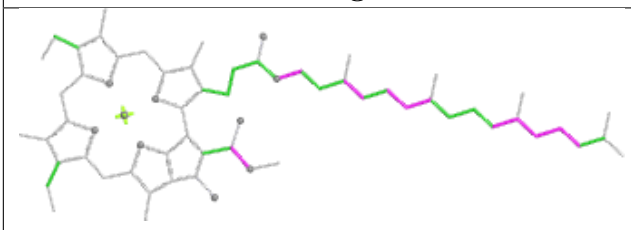
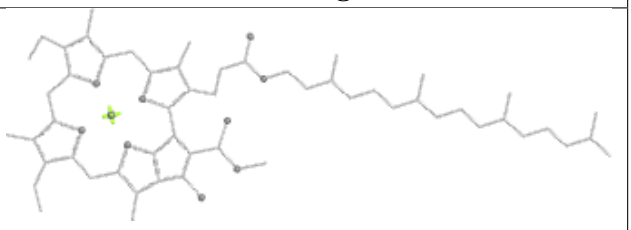


Rings

Ligand CLA A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

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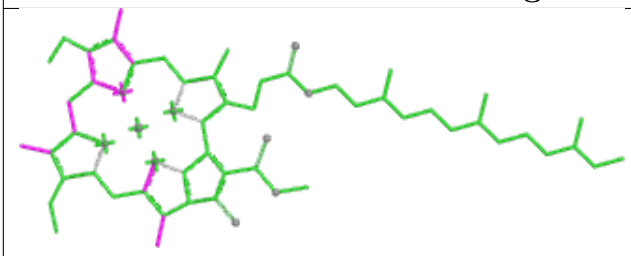
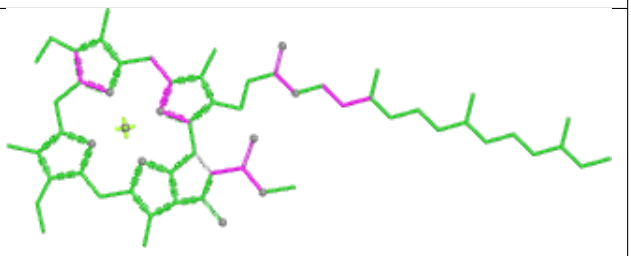
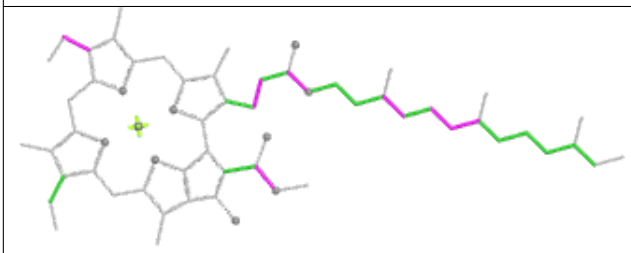
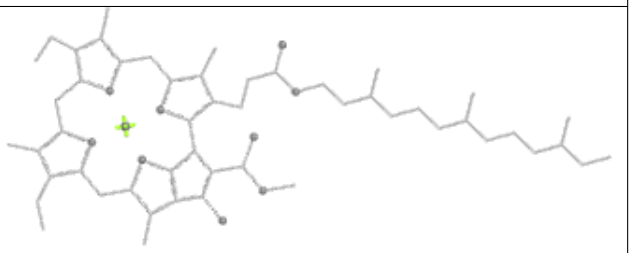
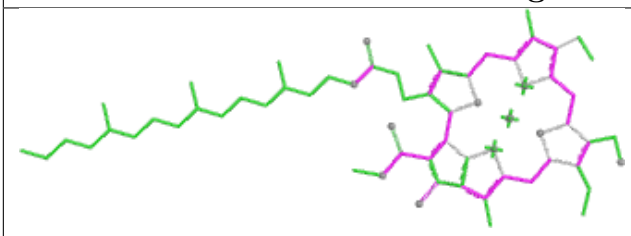
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 0 302



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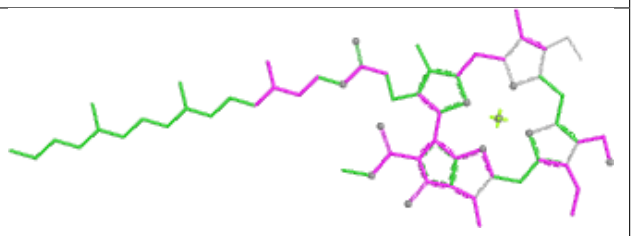
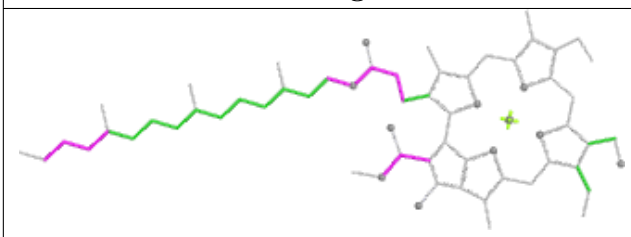
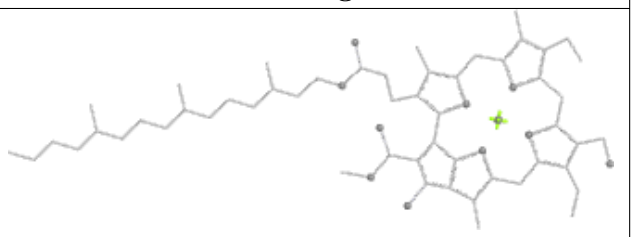


Bond angles

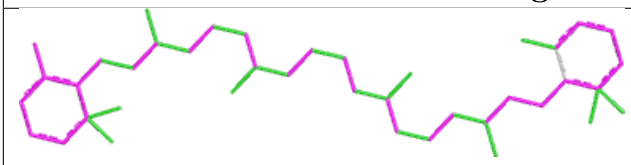


Torsions



Rings

Ligand 8CT 9 313



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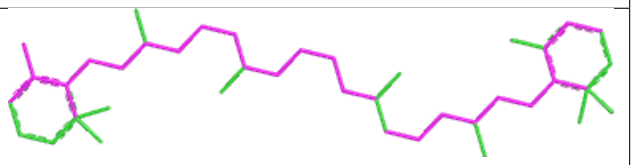

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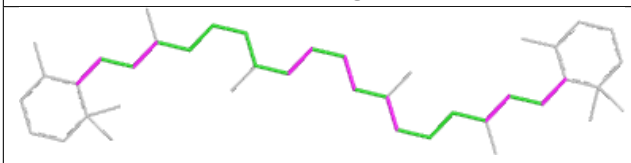

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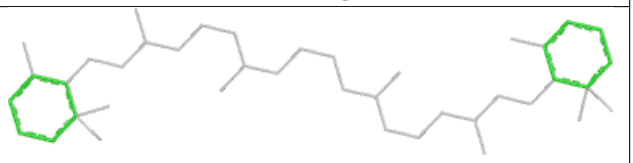
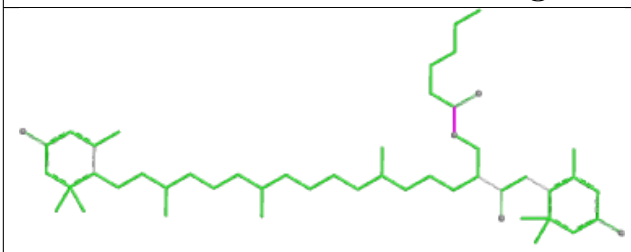


Rings

Ligand 0UR 3 318



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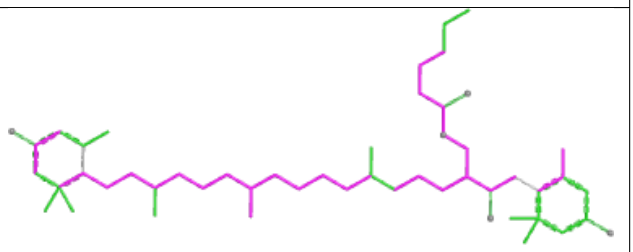
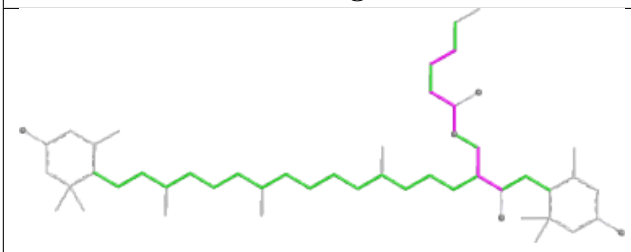


Bond angles



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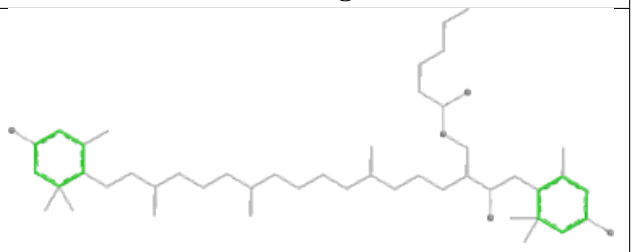
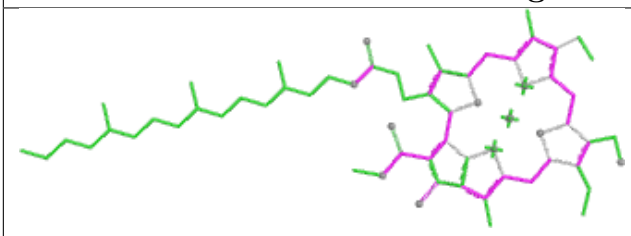


Rings

Ligand CHL 5 301



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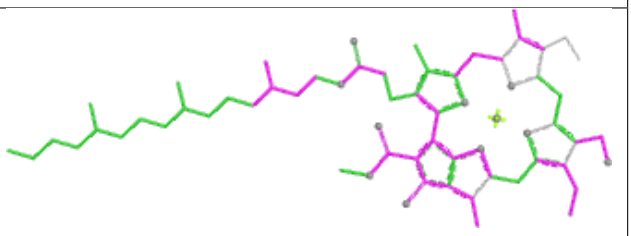

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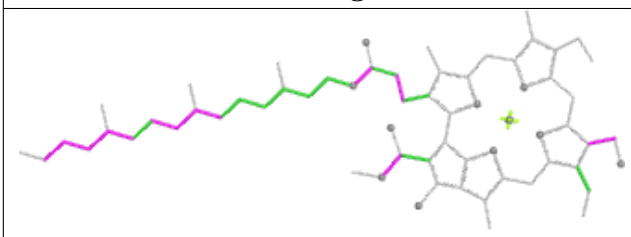

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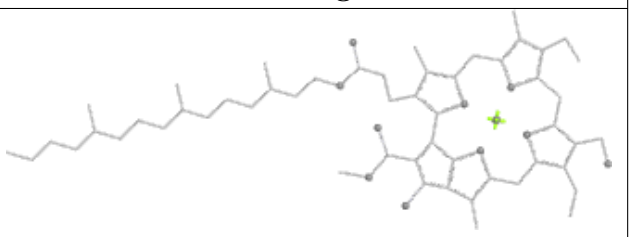
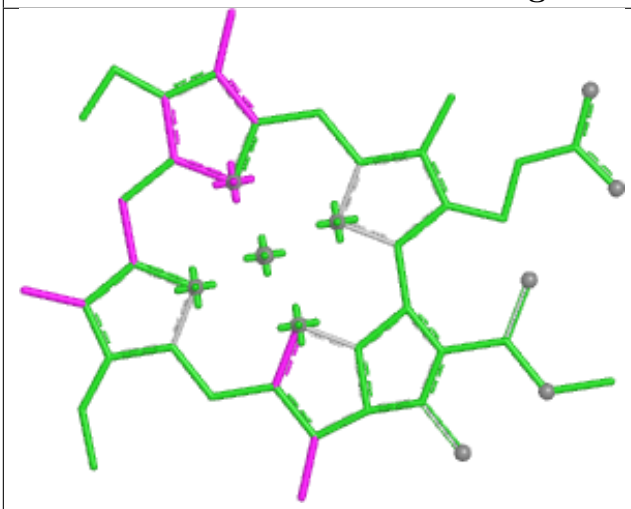


Rings

Ligand CLA 2 313



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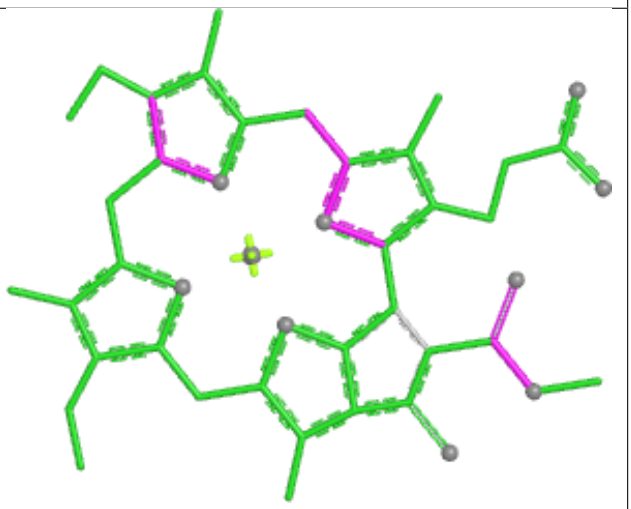
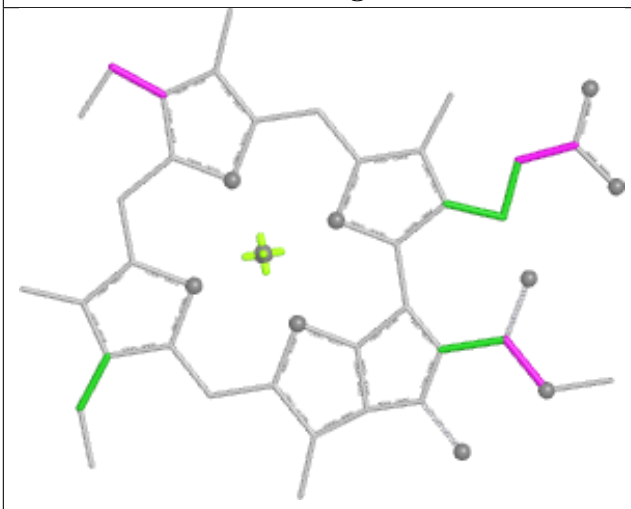


Bond angles



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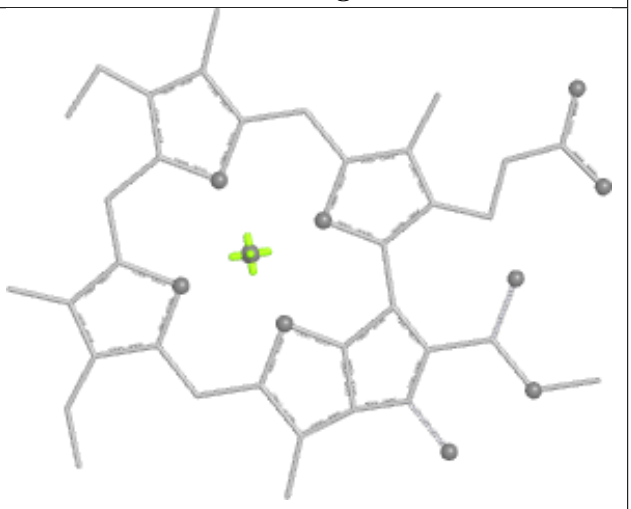
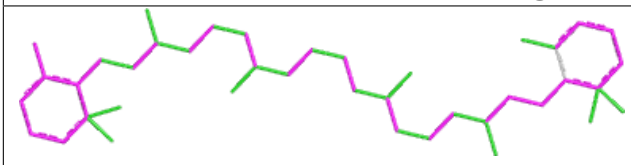
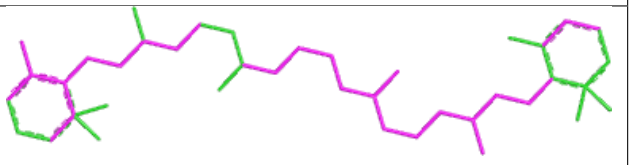
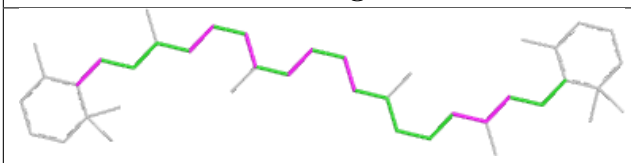
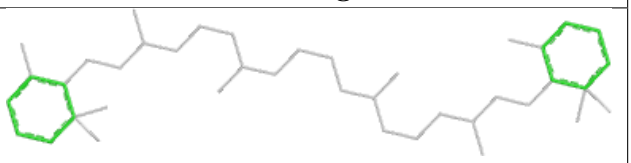
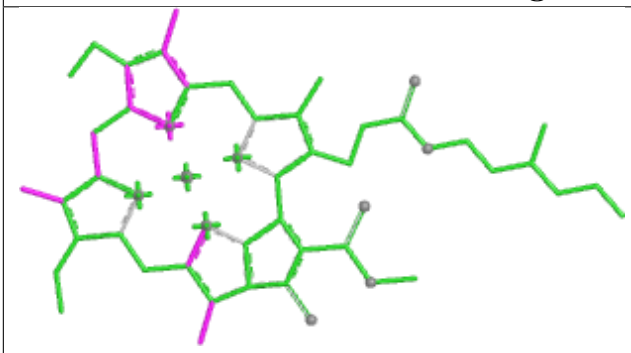
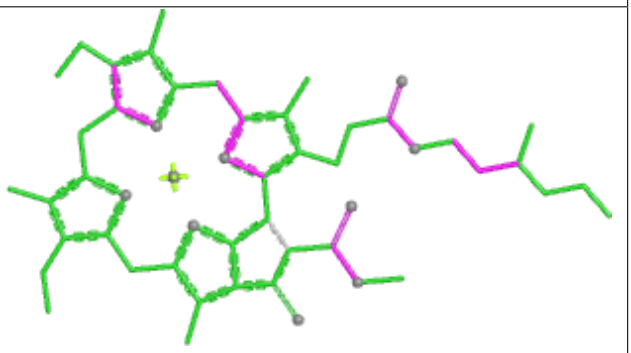
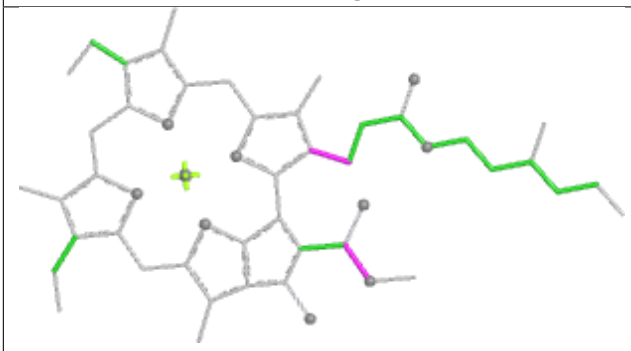
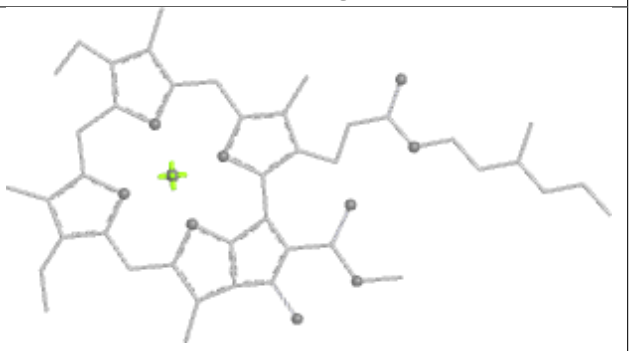
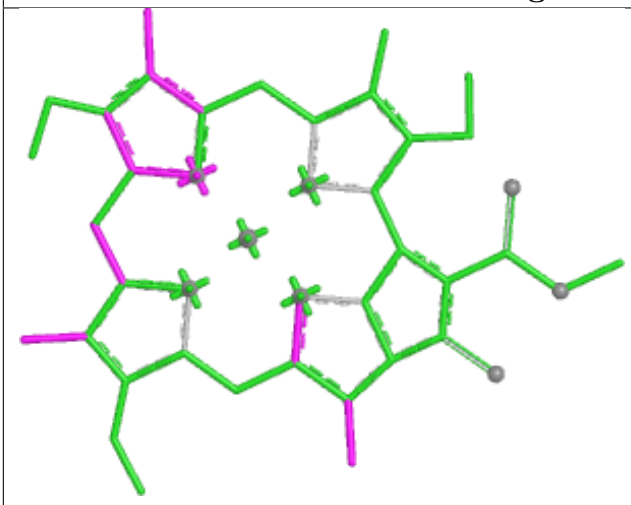


Rings

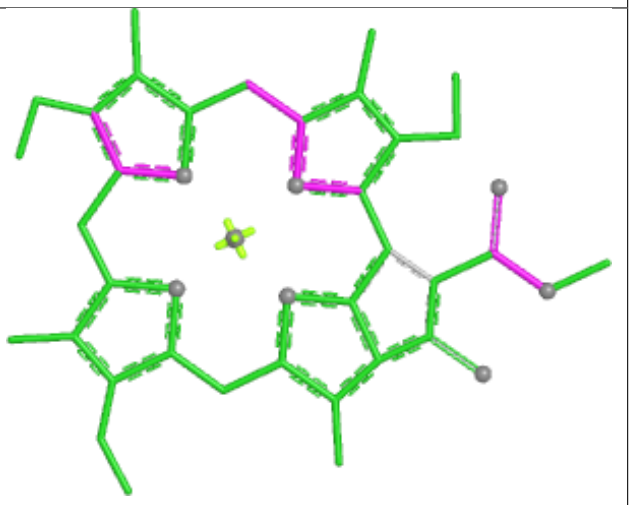
Ligand 8CT 6 324	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

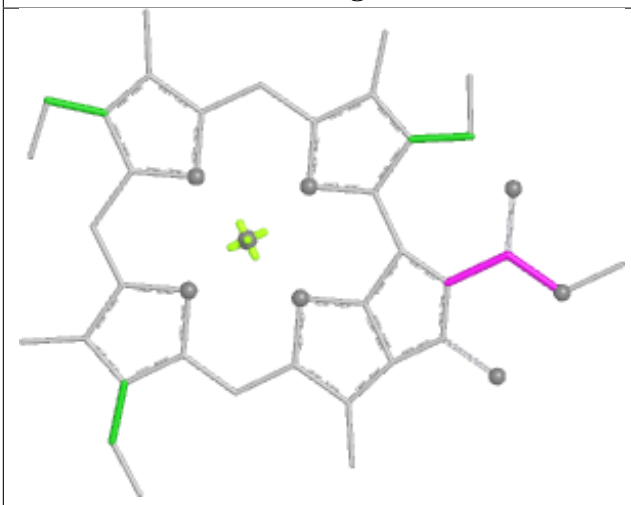
Ligand CLA J 103



Bond lengths



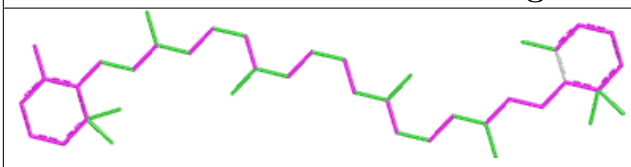
Bond angles



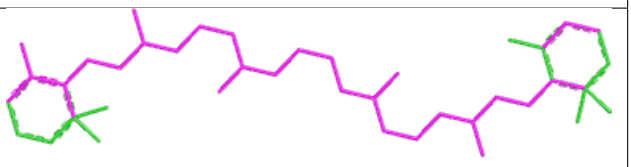
Torsions

Rings

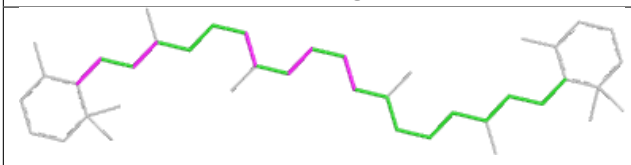
Ligand 8CT O 202



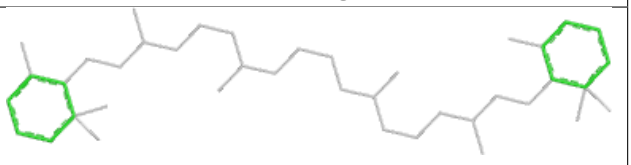
Bond lengths



Bond angles

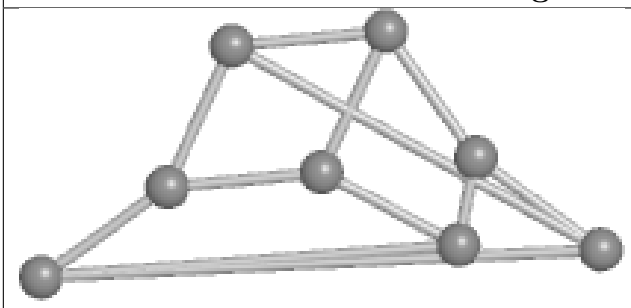


Torsions



Rings

Ligand SF4 B 803



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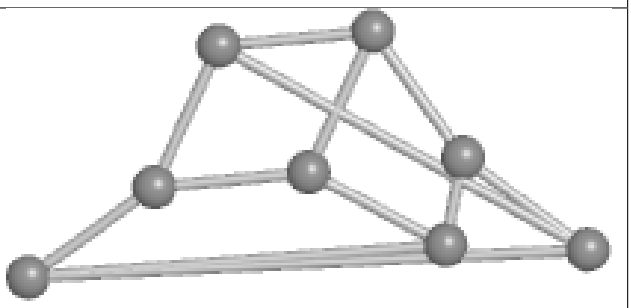
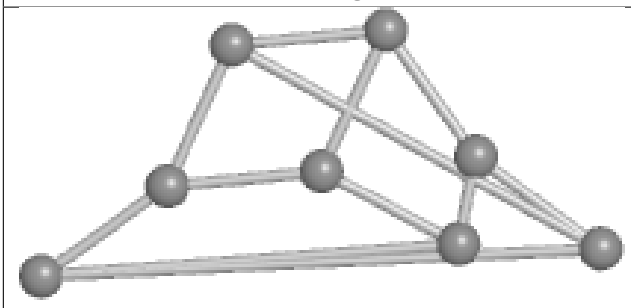


Bond angles



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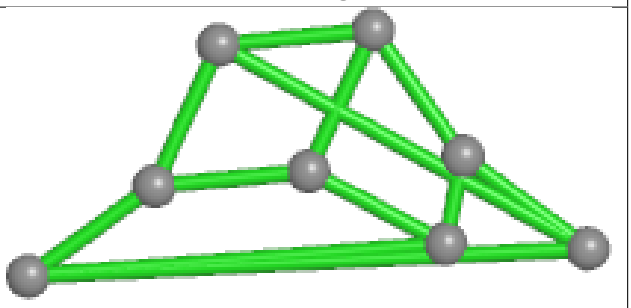
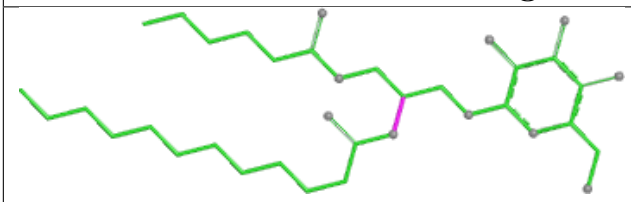


Rings

Ligand LMG A 854



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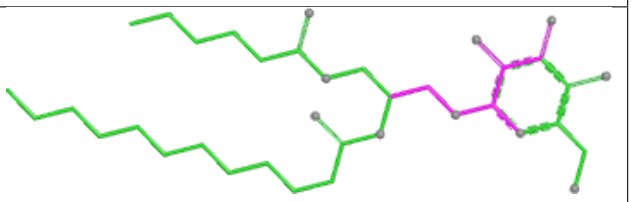
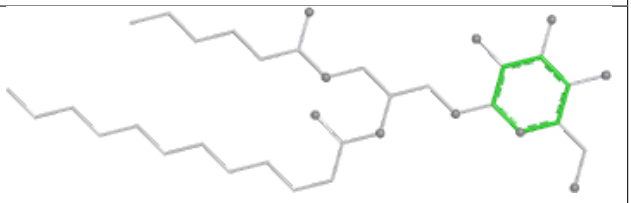


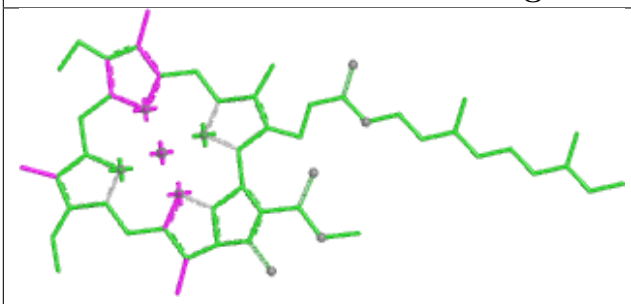
Bond angles

Torsions



Rings

Ligand CLA B 830



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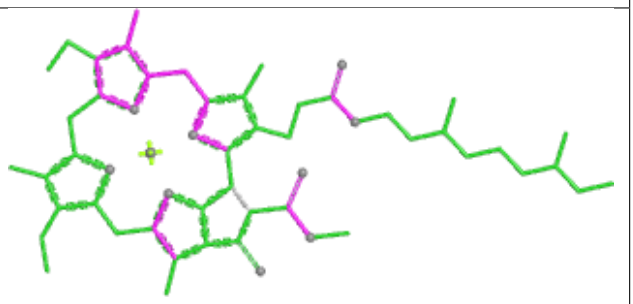
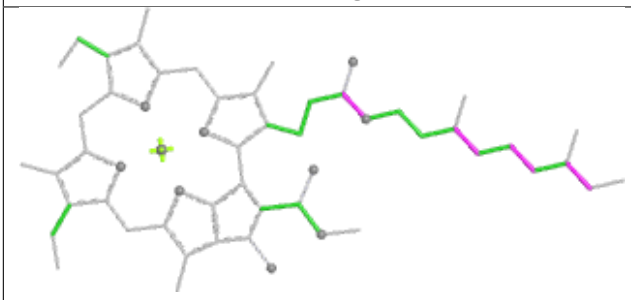
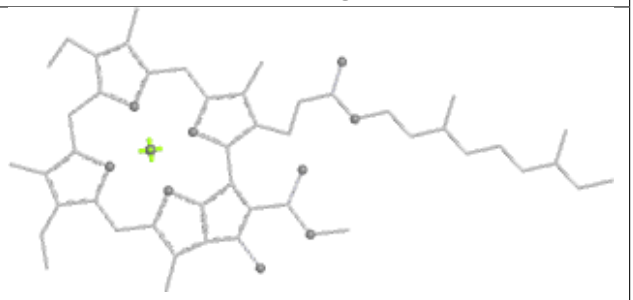


Bond angles

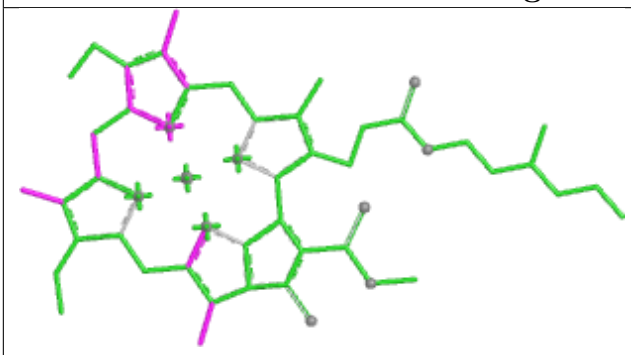


Torsions

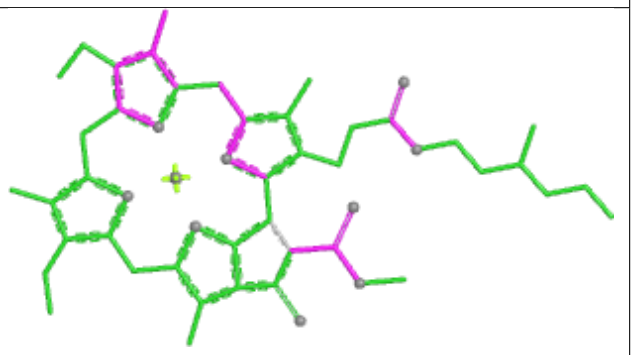


Rings

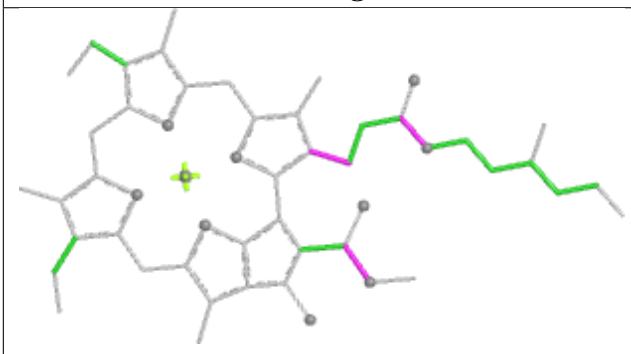
Ligand CLA O 201



Bond lengths



Bond angles



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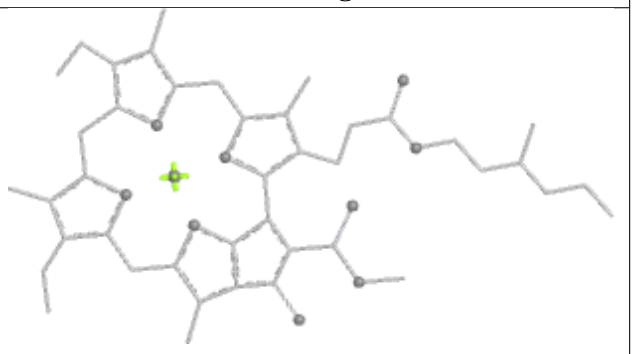
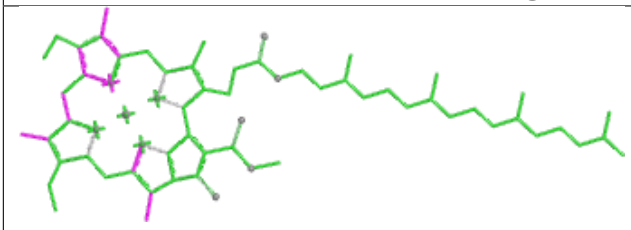


Rings

Ligand CLA A 832



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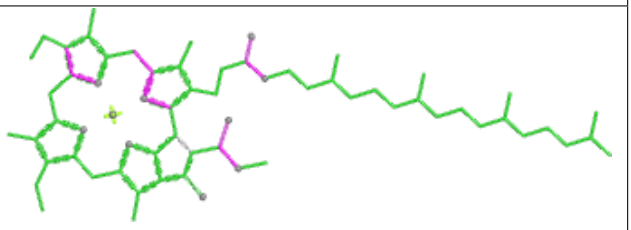
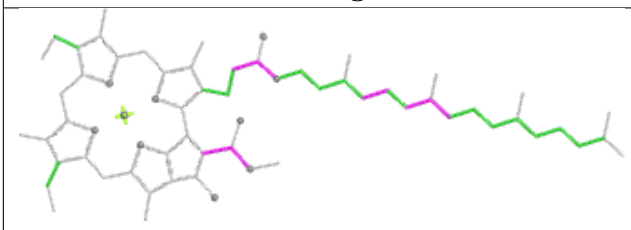


Bond angles



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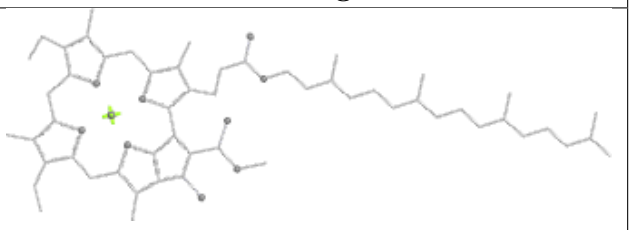
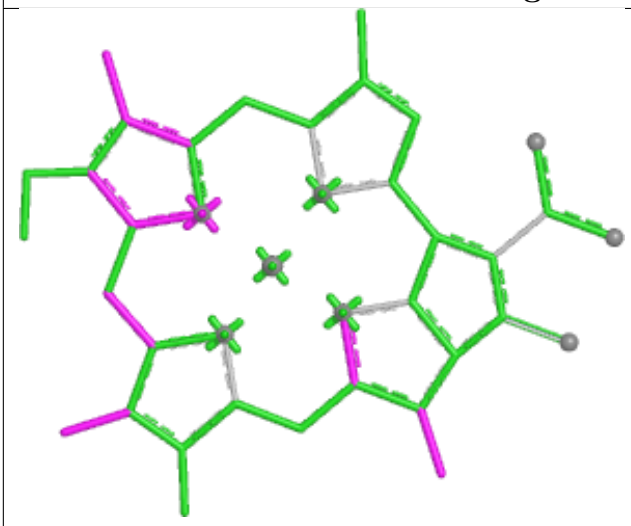


Rings

Ligand CLA O 205



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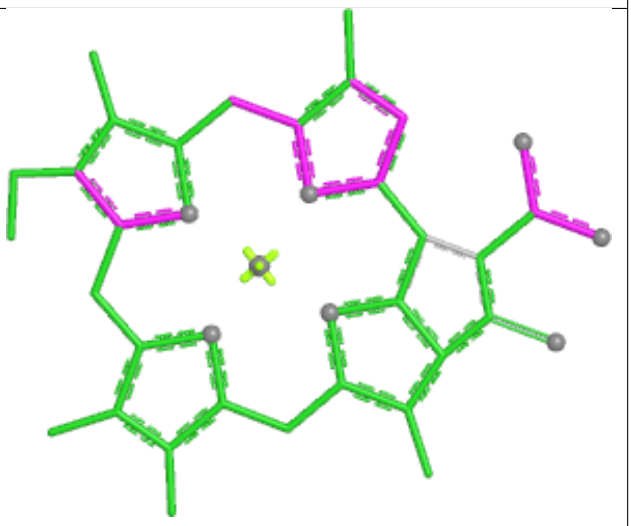
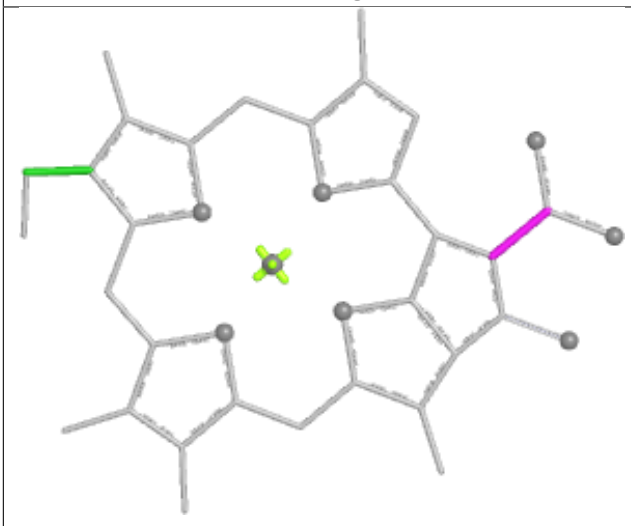


Bond angles



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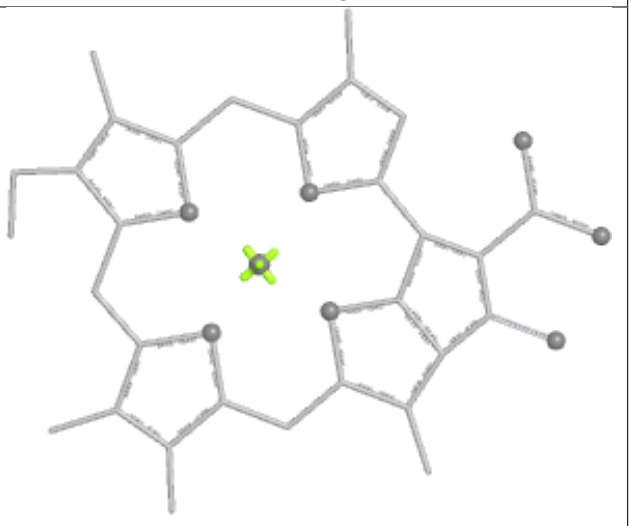
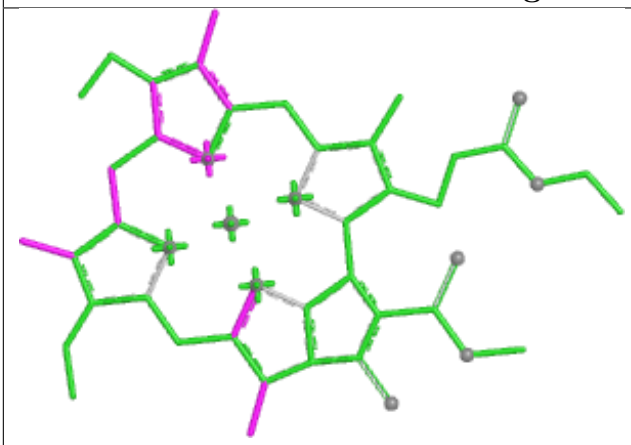


Rings

Ligand CLA H 203



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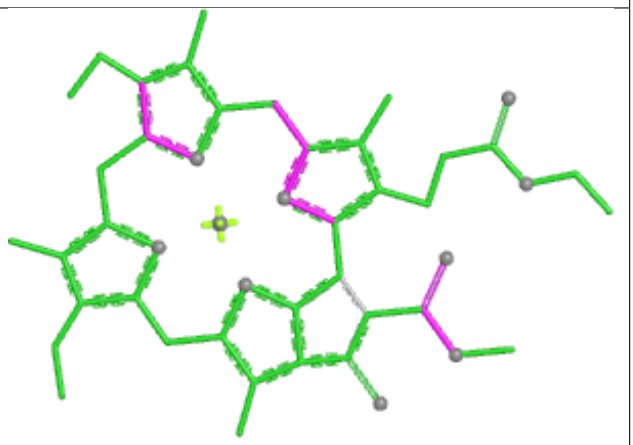
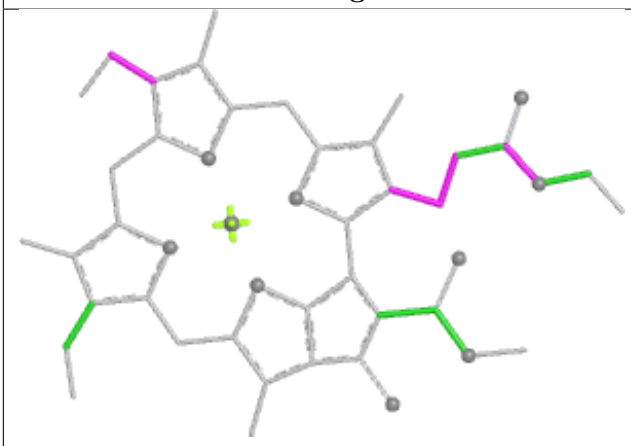


Bond angles



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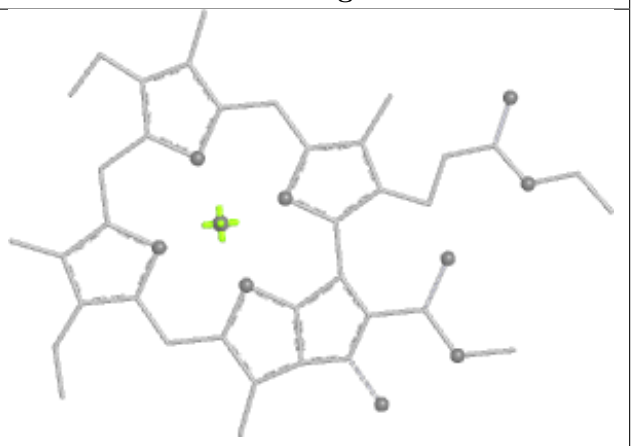
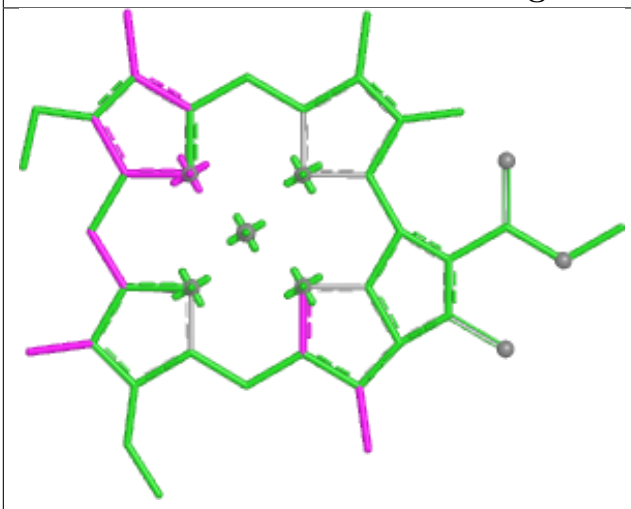


Rings

Ligand CLA 9 309



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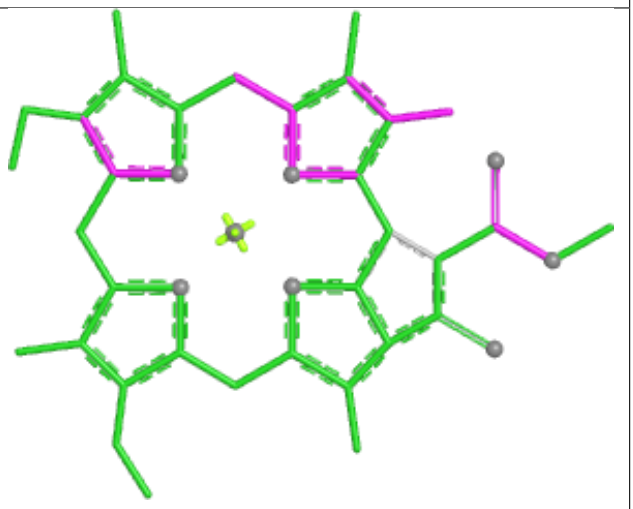
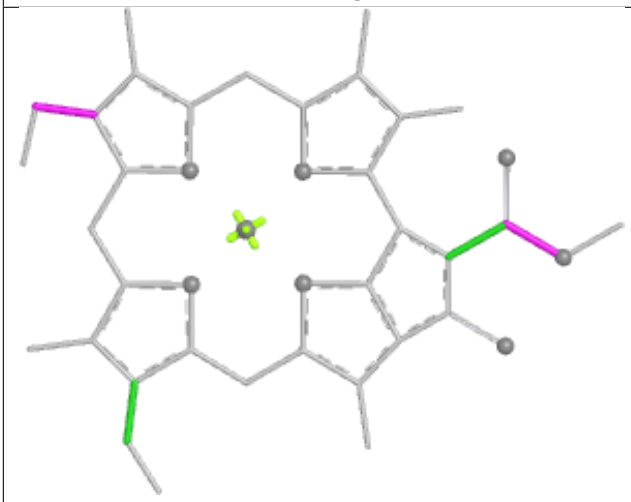
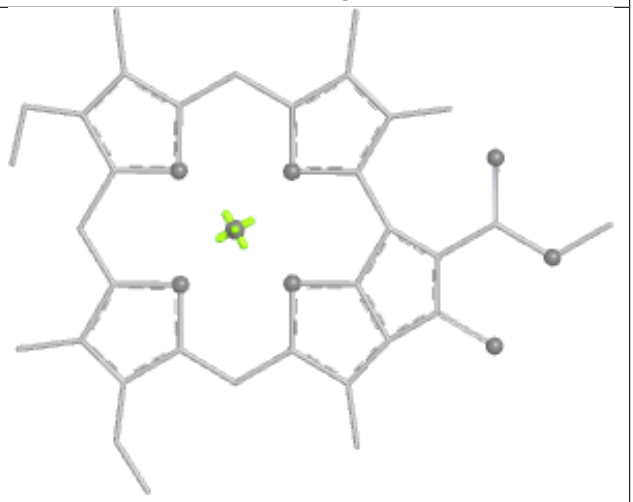


Bond angles

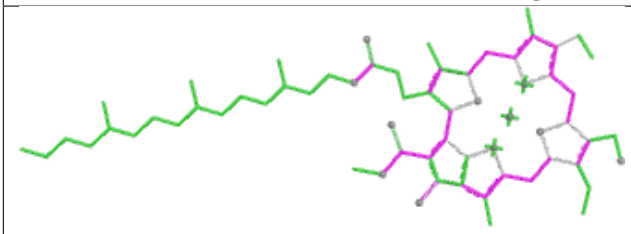


Torsions



Rings

Ligand CHL 8 303



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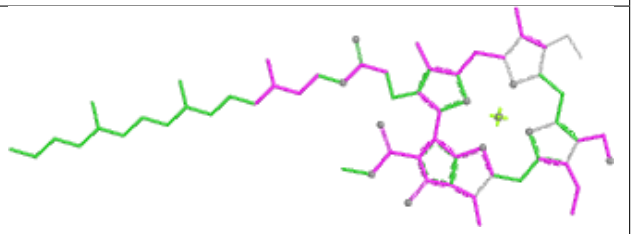
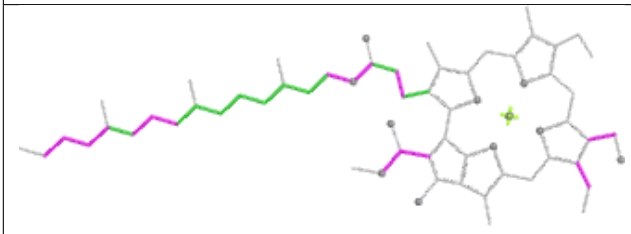


Bond angles



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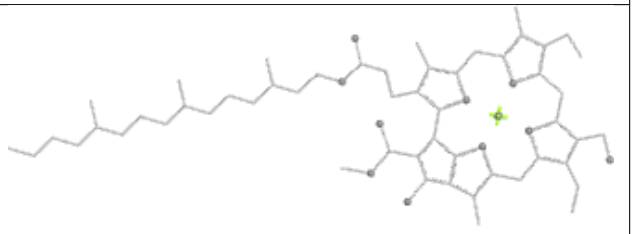
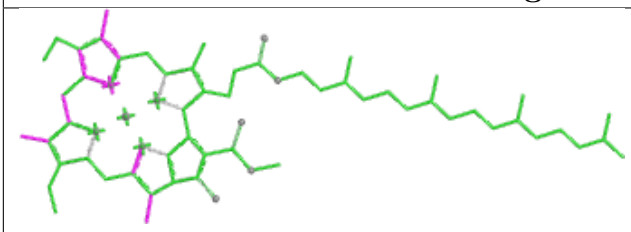


Rings

Ligand CLA B 802



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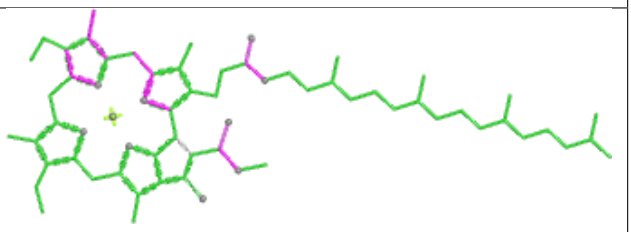
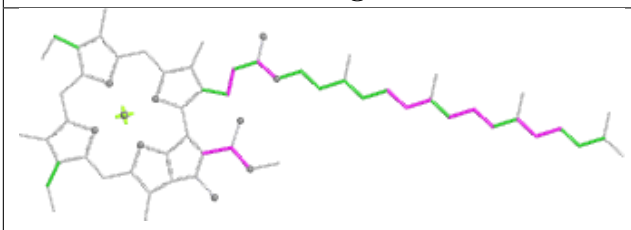


Bond angles



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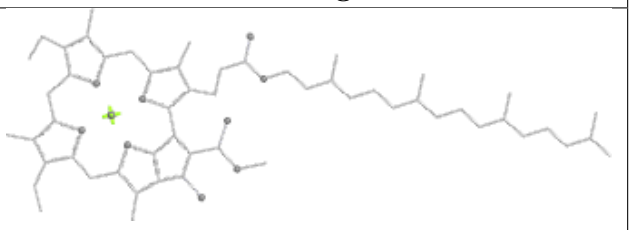
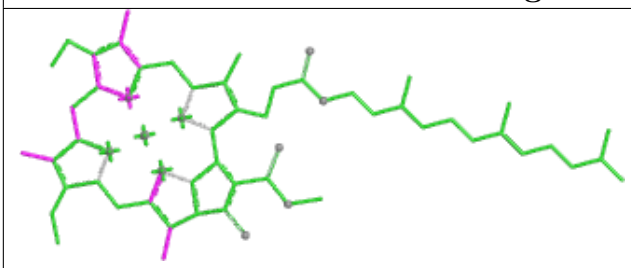


Rings

Ligand CLA B 816



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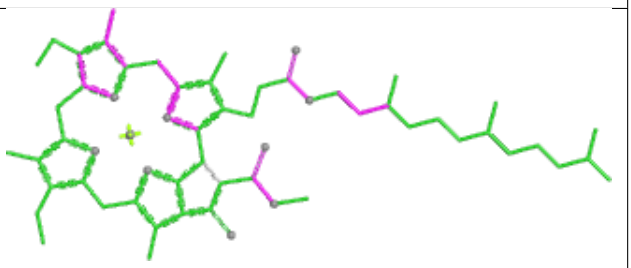
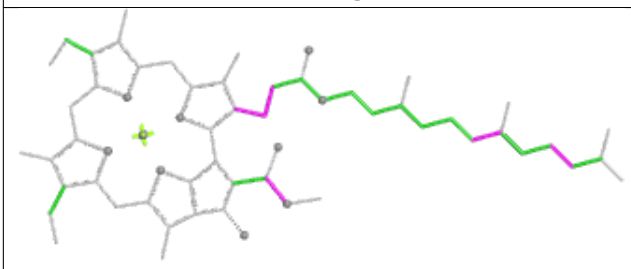
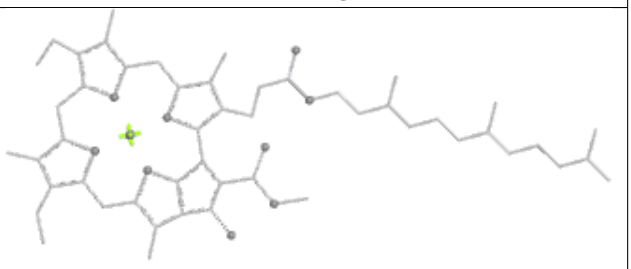


Bond angles

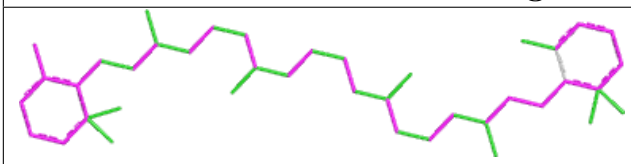


Torsions



Rings

Ligand 8CT O 208



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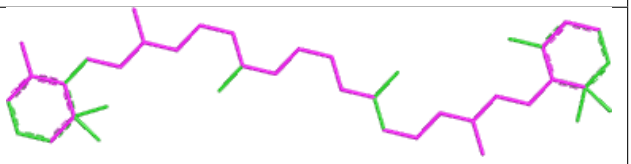
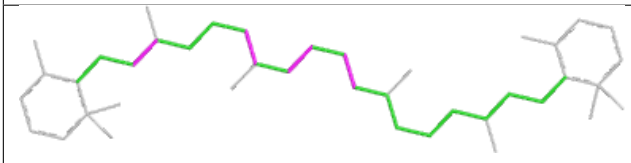
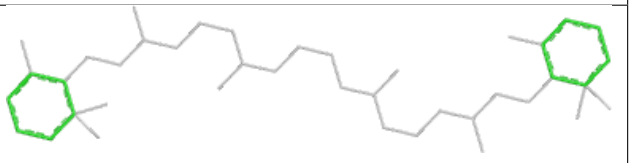


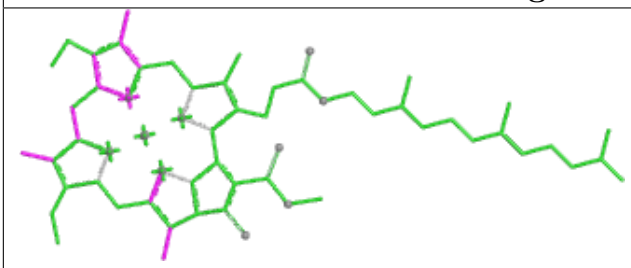
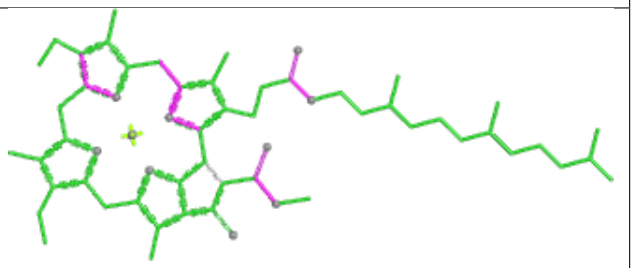
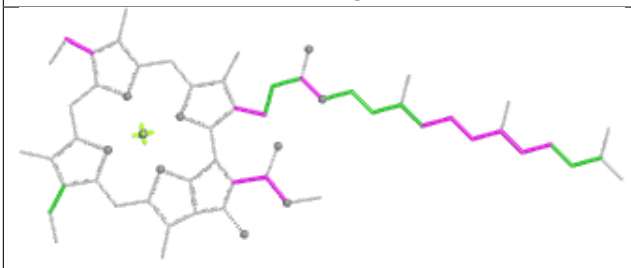
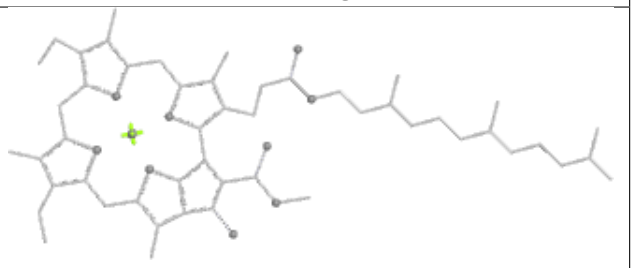
Bond angles

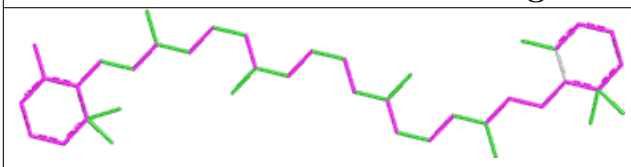
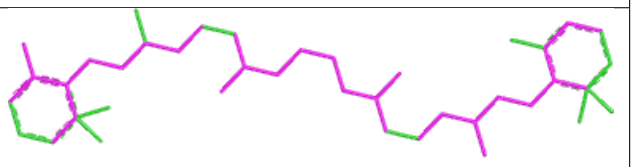
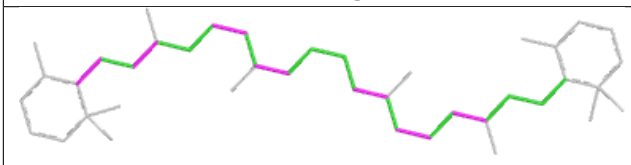
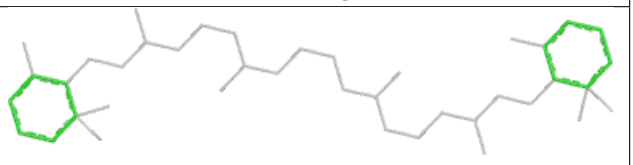


Torsions



Rings

Ligand CLA 2 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

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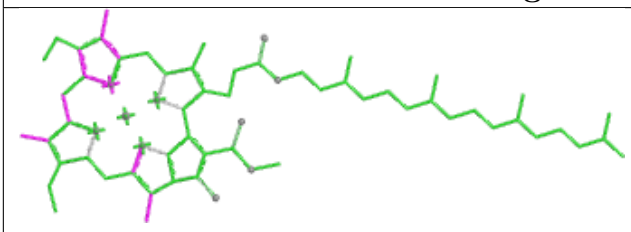
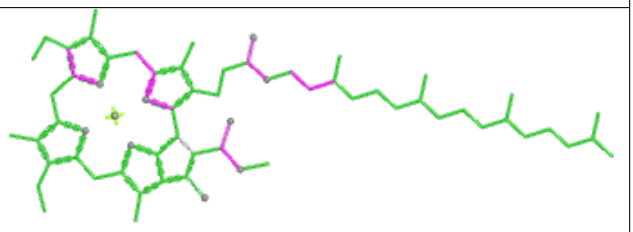
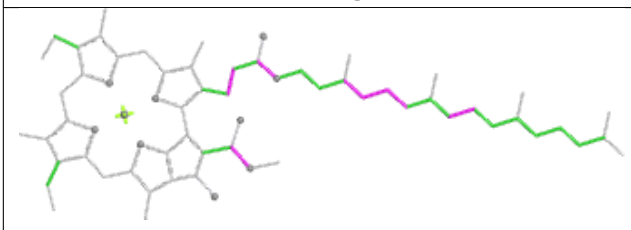
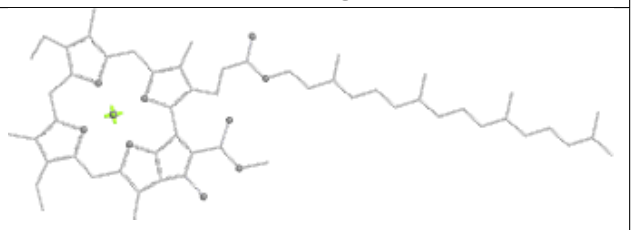
 Bond lengths	 Bond angles
 Torsions	 Rings

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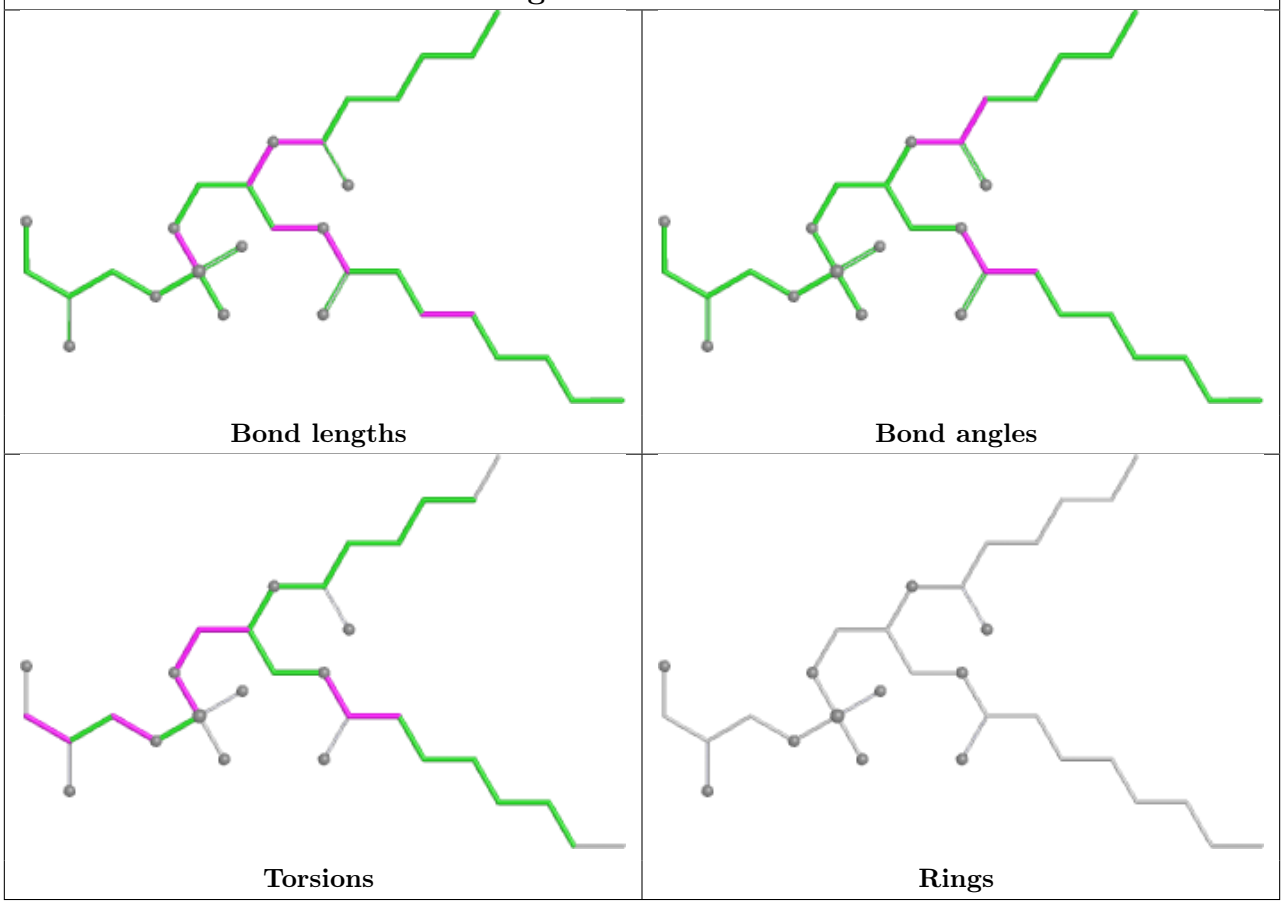
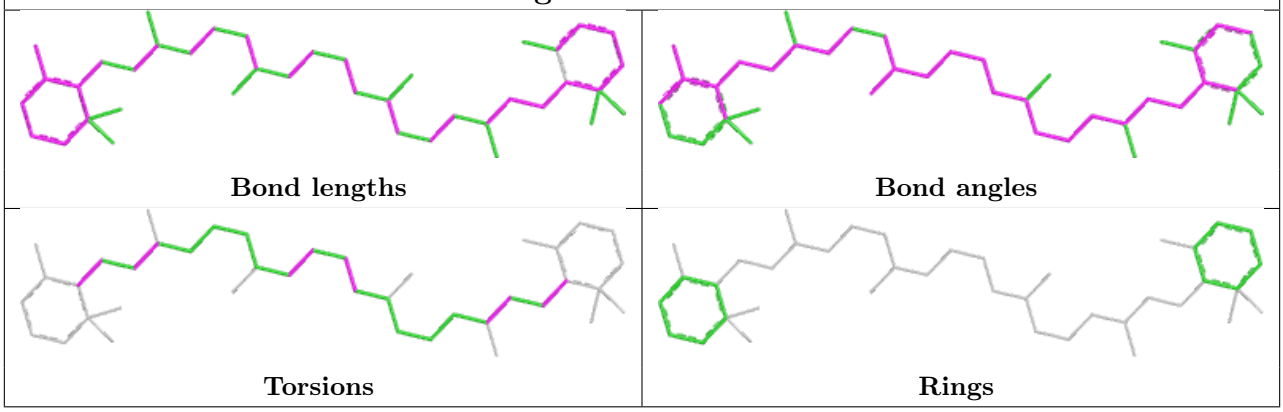


Ligand 8CT I 101



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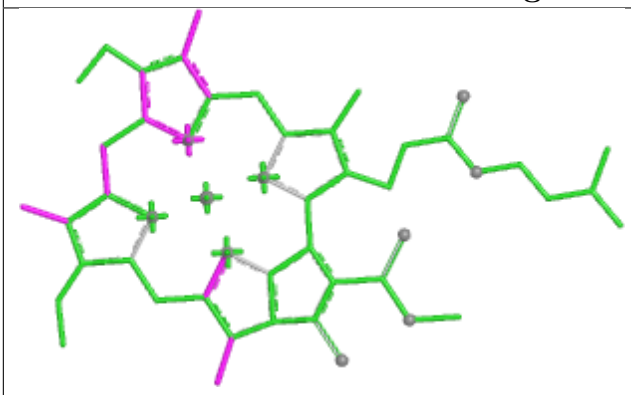

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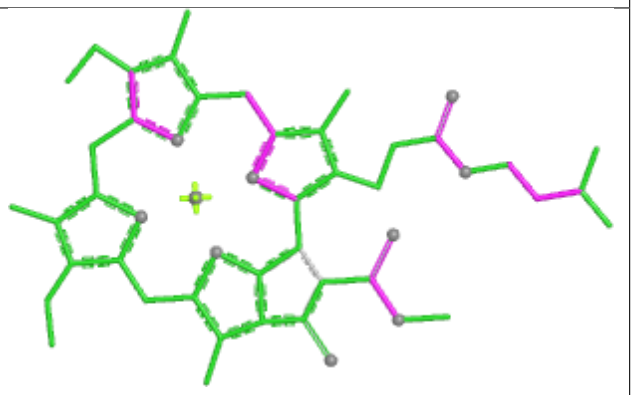
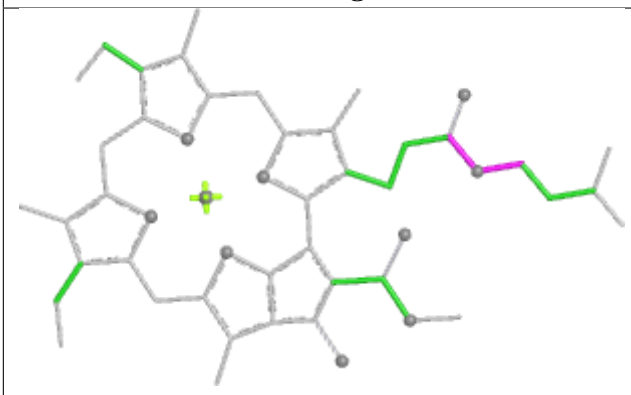


Bond angles



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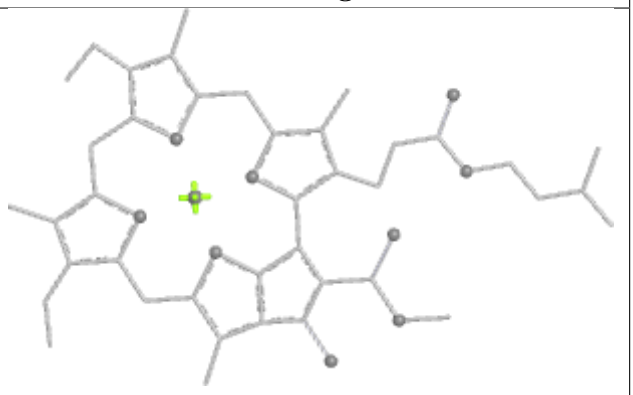
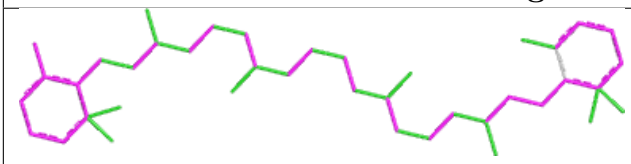


Rings

Ligand 8CT B 850



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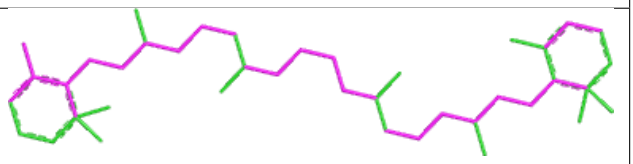

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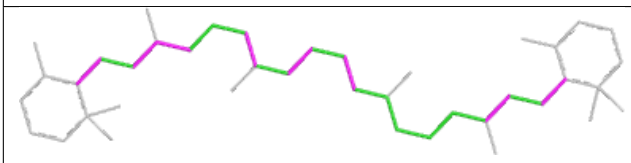

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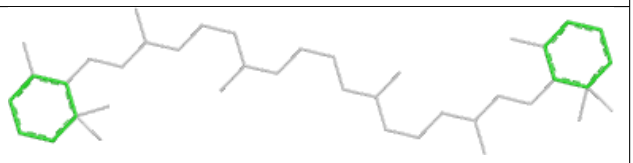
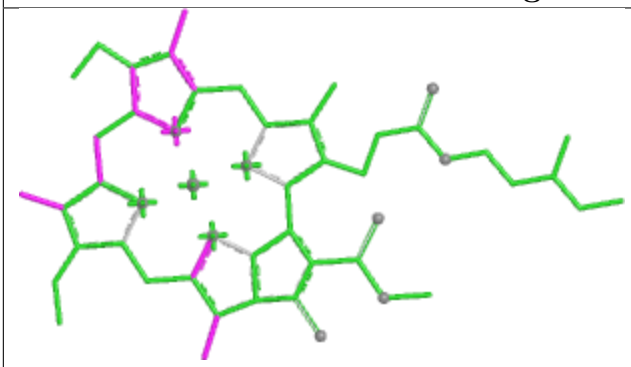


Rings

Ligand CLA H 205



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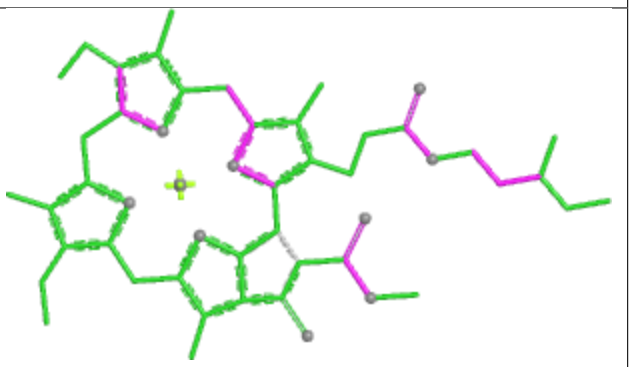

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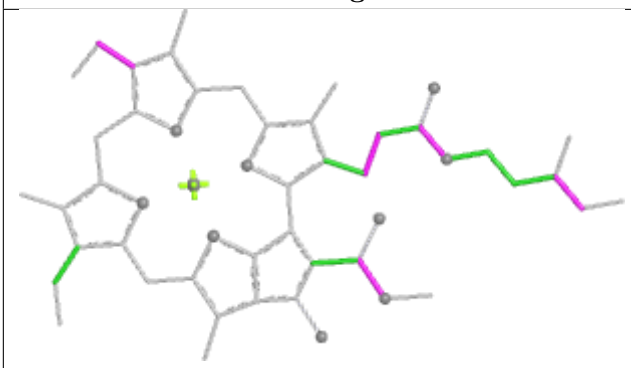

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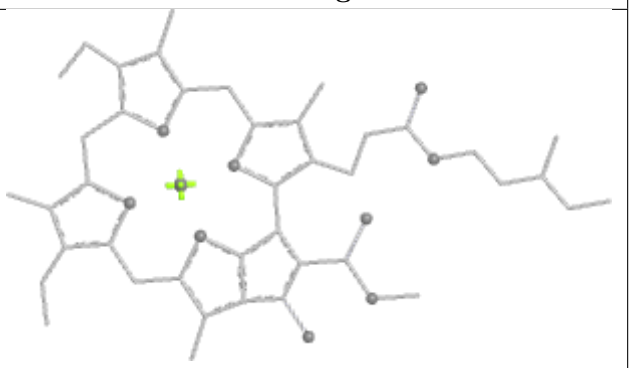
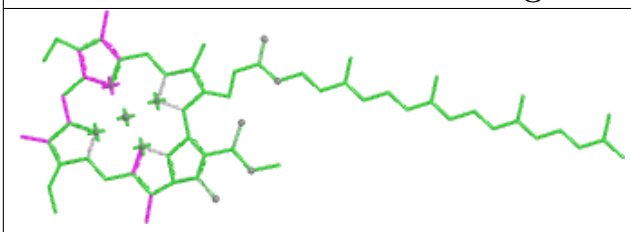


Rings

Ligand CLA B 825



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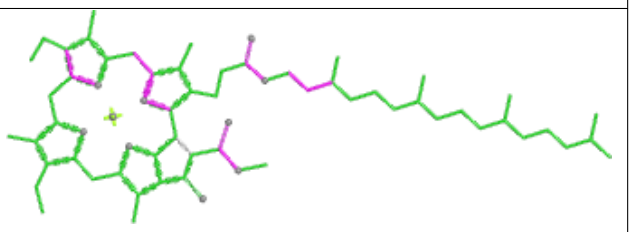

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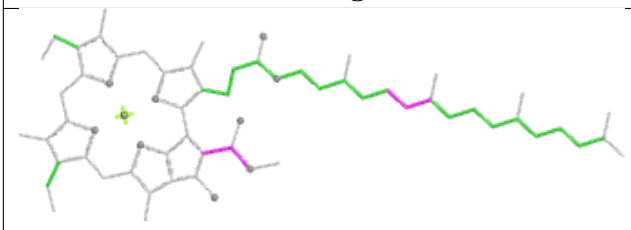

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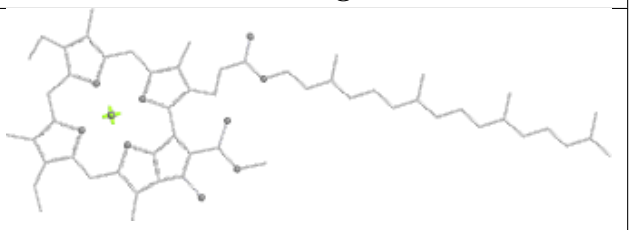
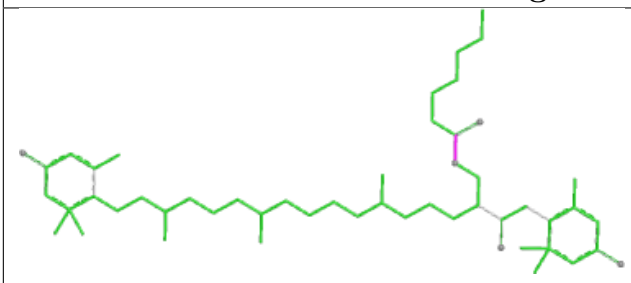


Rings

Ligand 0UR 9 314



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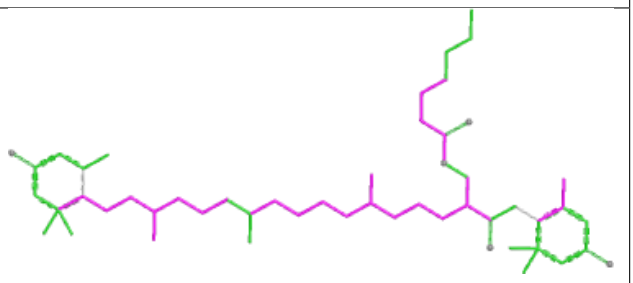

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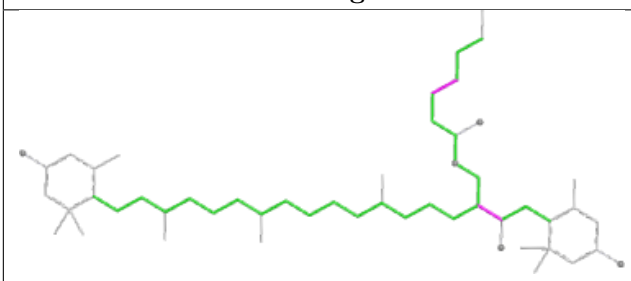

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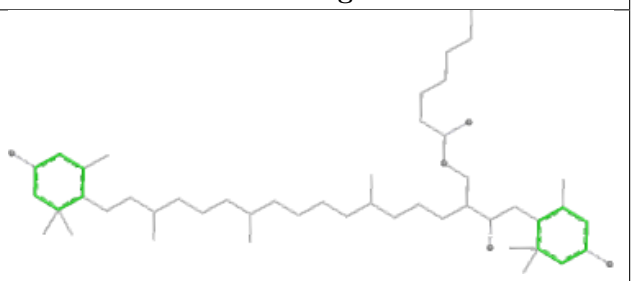
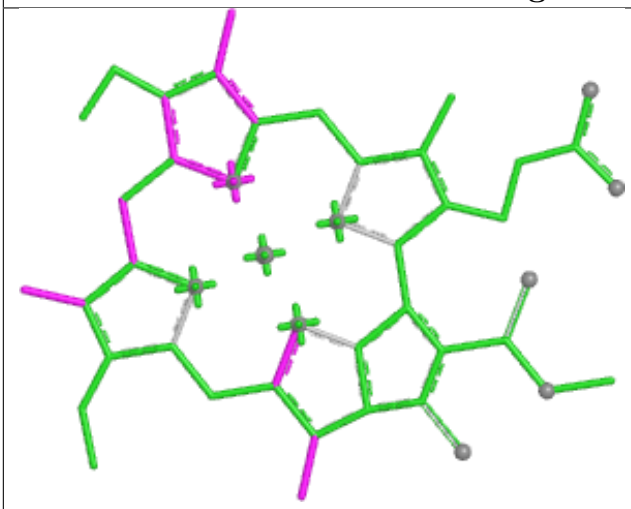


Rings

Ligand CLA 1 307



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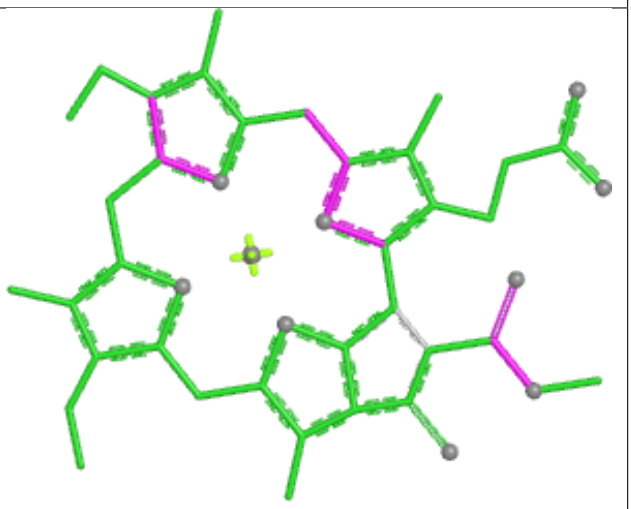

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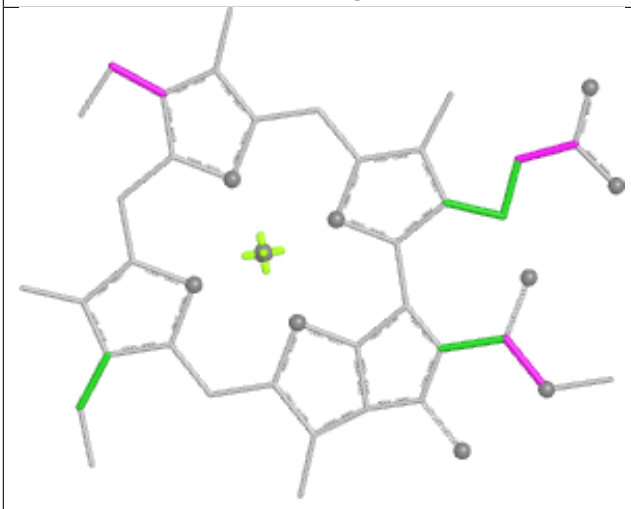
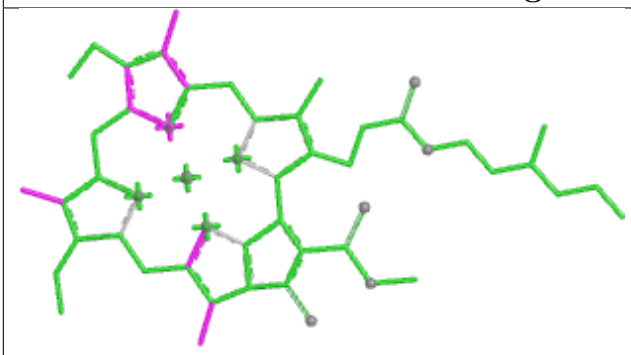


Torsions

Rings

Ligand CLA B 812



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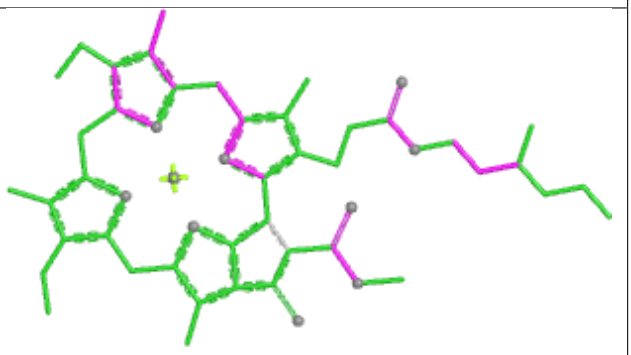

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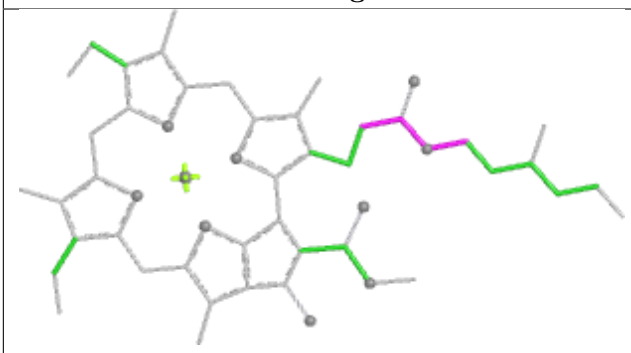

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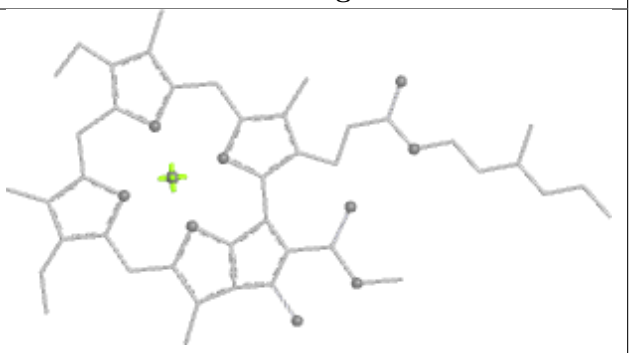
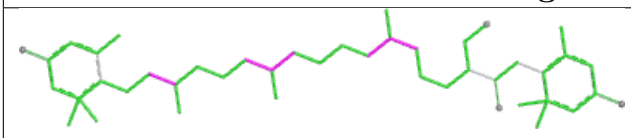


Rings

Ligand 0IE 3 319



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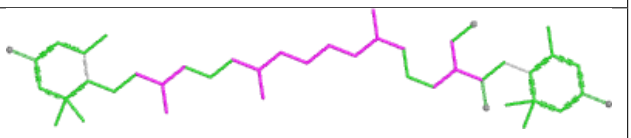
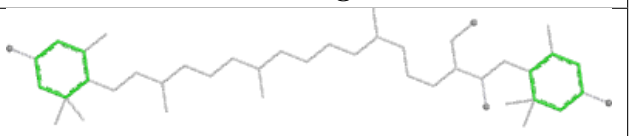


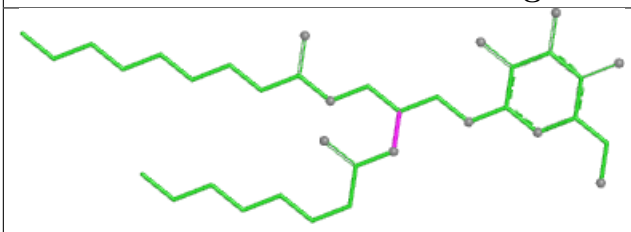
Bond angles

Torsions



Rings

Ligand LMG 2 318



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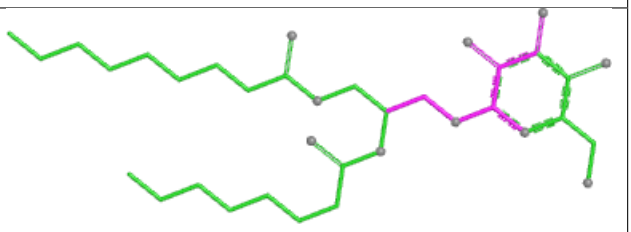

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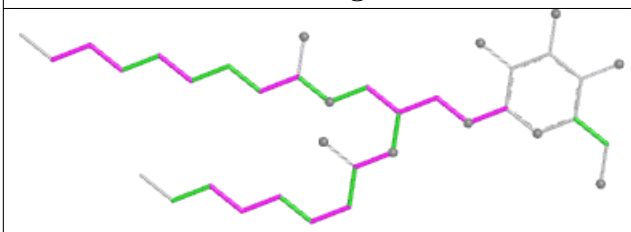

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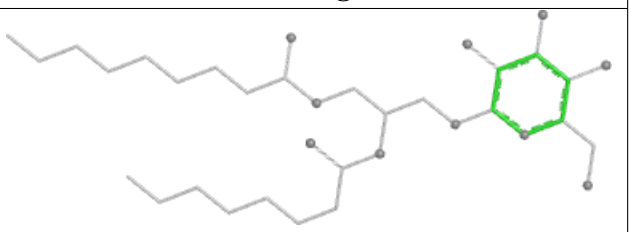
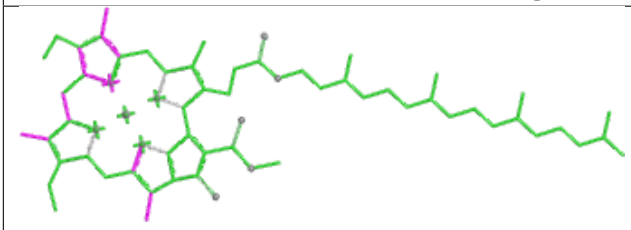


Rings

Ligand CLA 3 308



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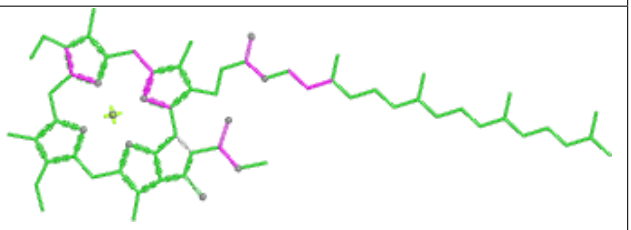
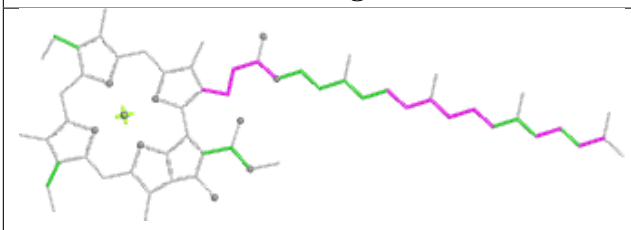


Bond angles



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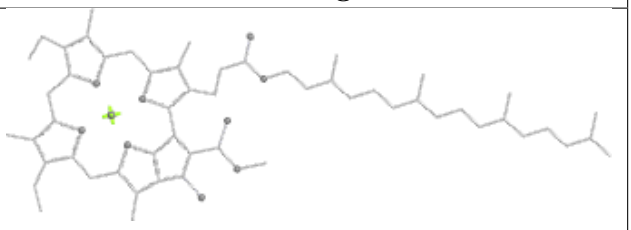
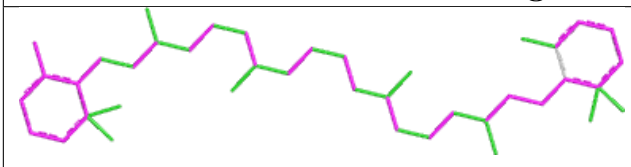


Rings

Ligand 8CT B 847



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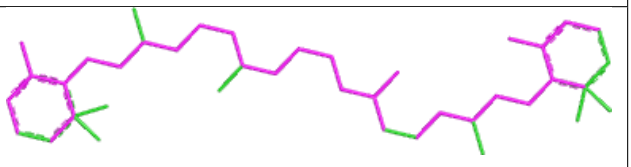
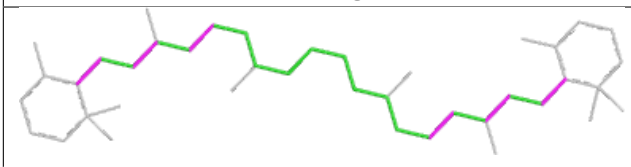


Bond angles



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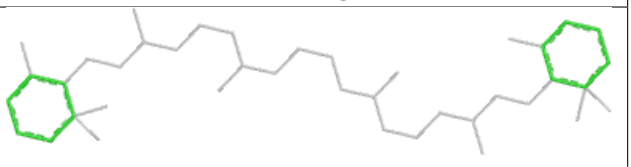
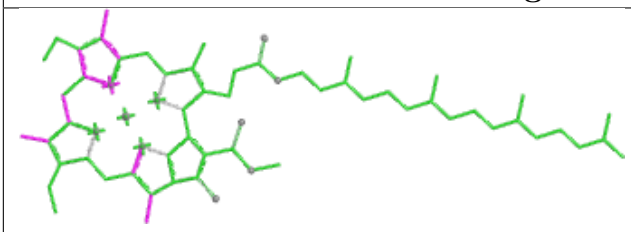
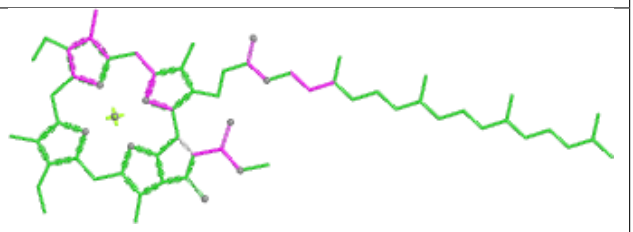


Rings

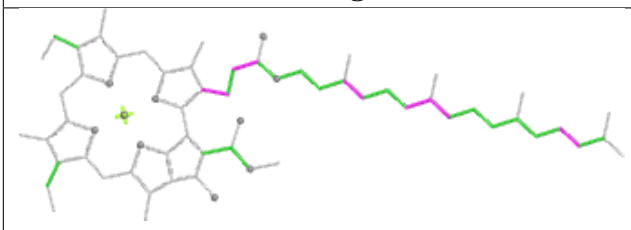
Ligand CLA B 808



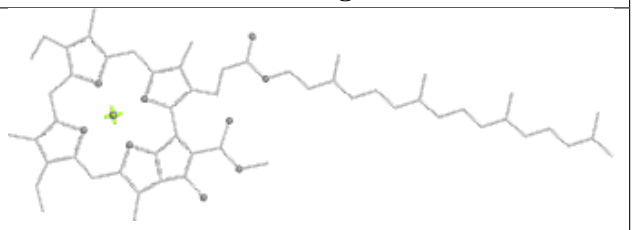
Bond lengths



Bond angles

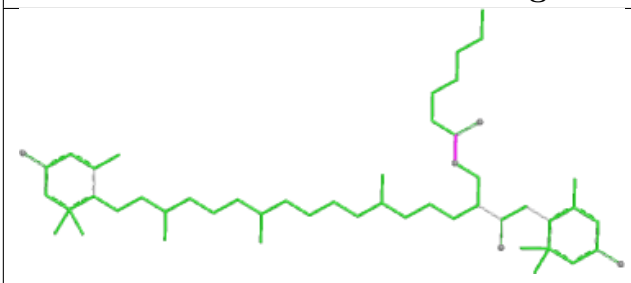


Torsions



Rings

Ligand 0UR 5 315



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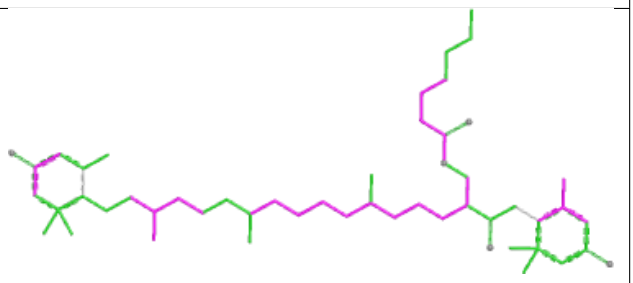

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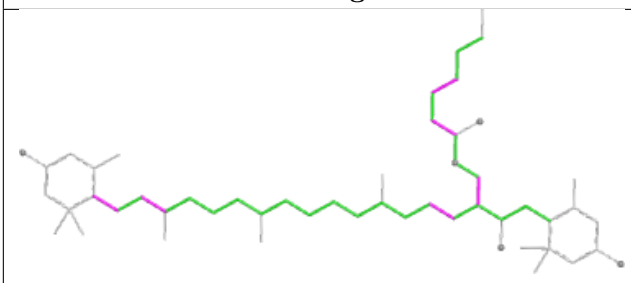

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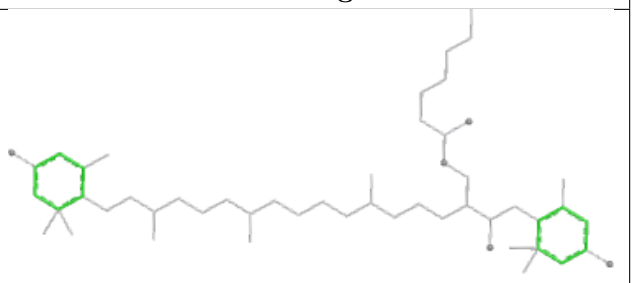
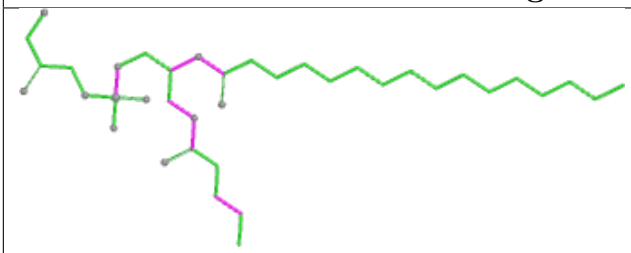


Rings

Ligand LHG 7 323



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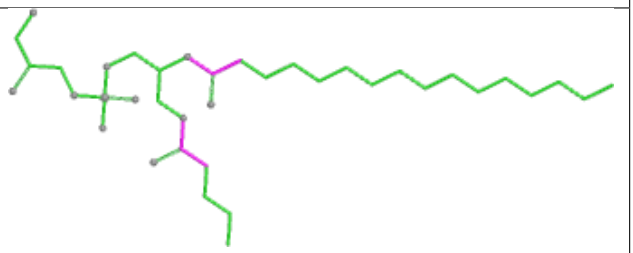

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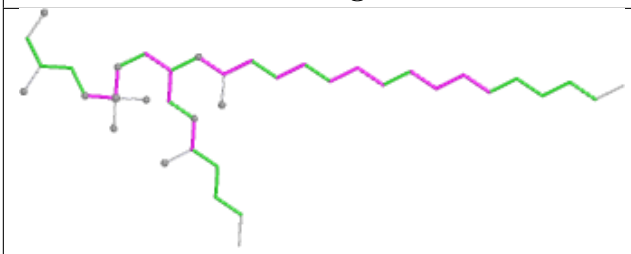

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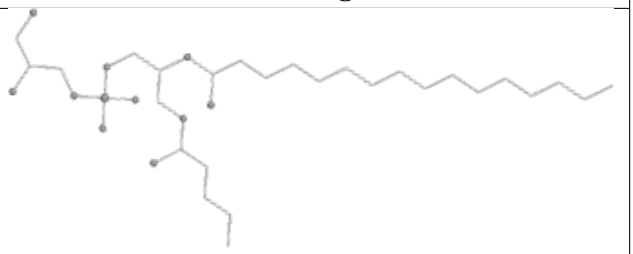
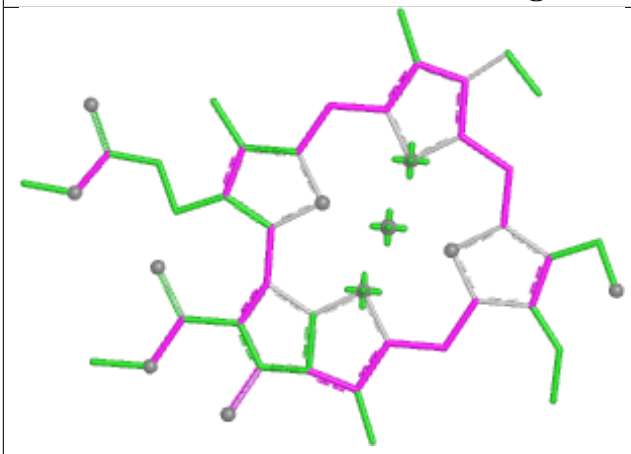


Rings

Ligand CHL 9 312



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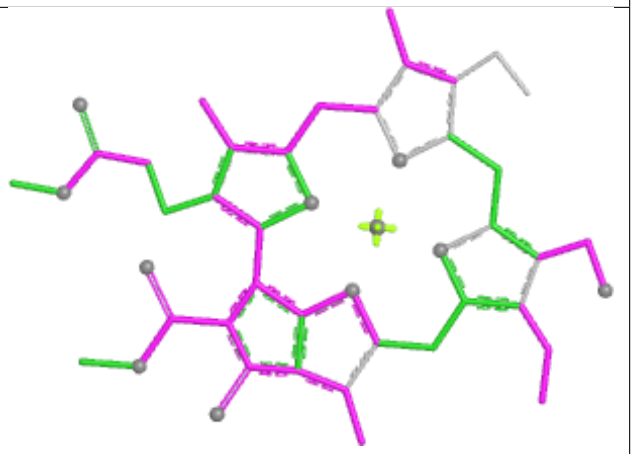

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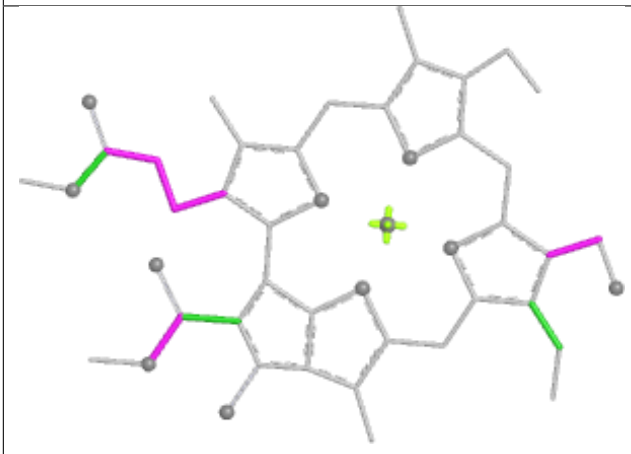
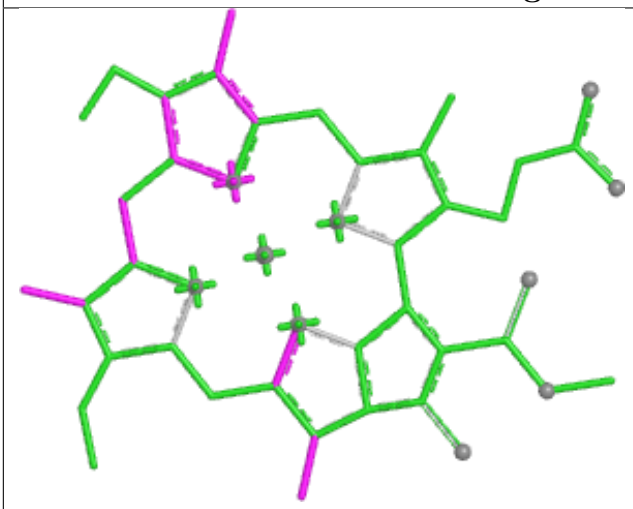


Torsions

Rings

Ligand CLA A 815



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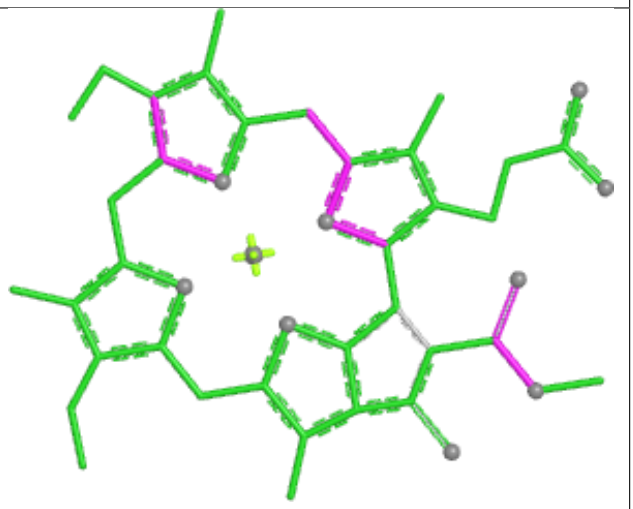

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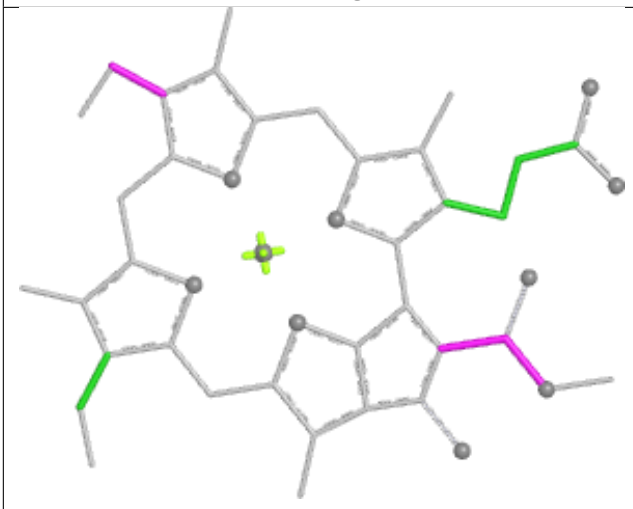
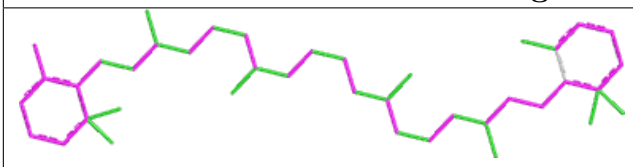


Torsions

Rings

Ligand 8CT 1 314



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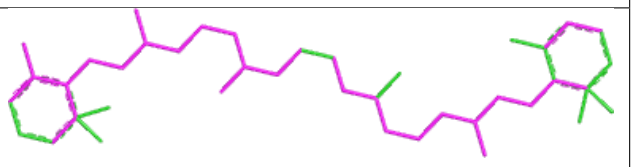

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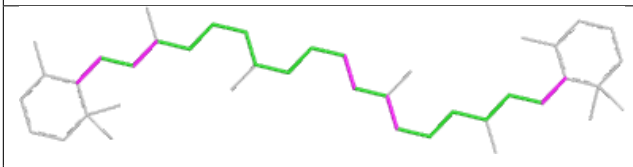

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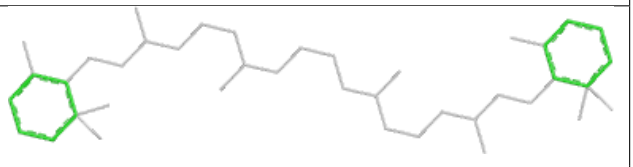
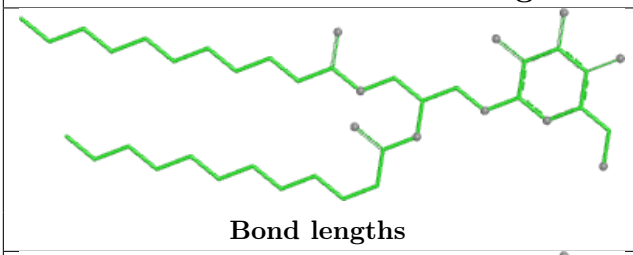


Rings

Ligand LMG M 101



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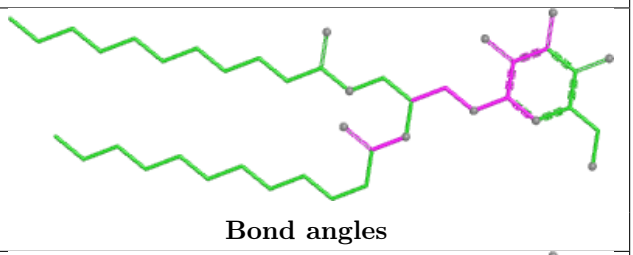

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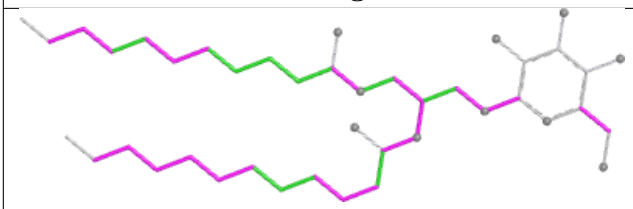

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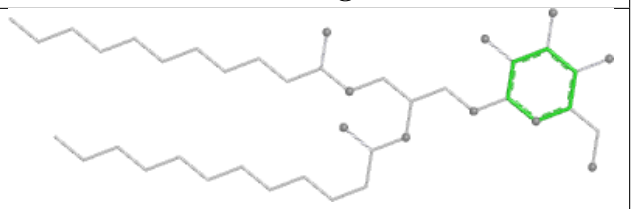
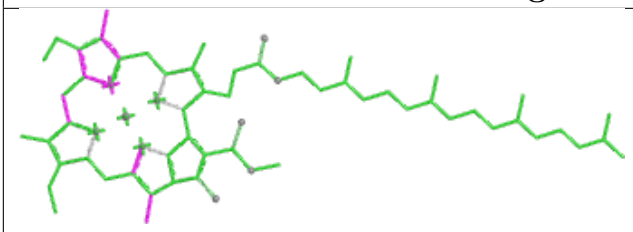


Rings

Ligand CLA 8 305



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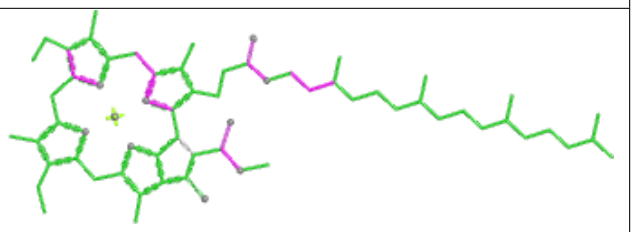

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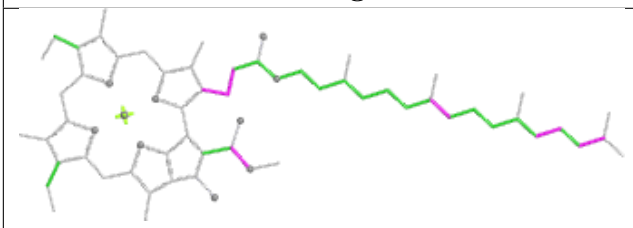

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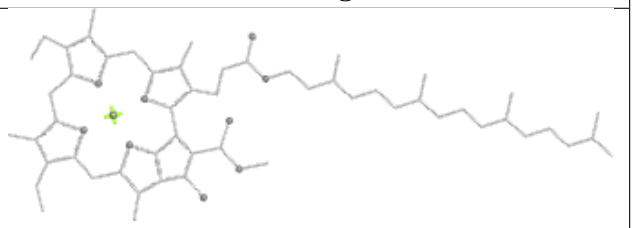
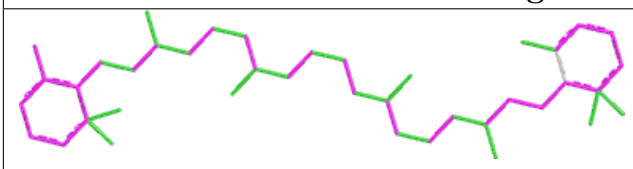


Rings

Ligand 8CT A 846



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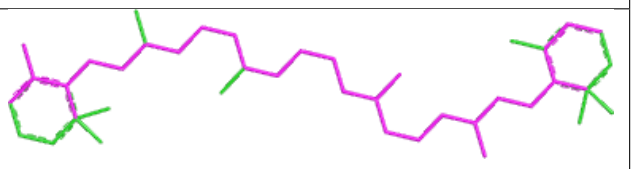
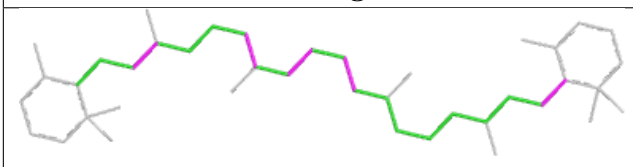


Bond angles



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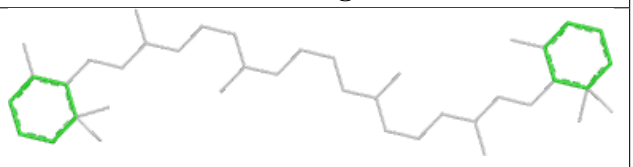
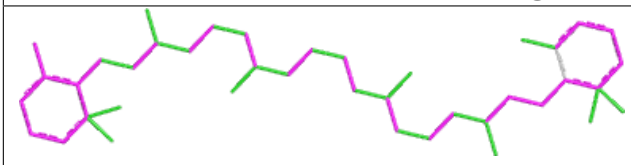
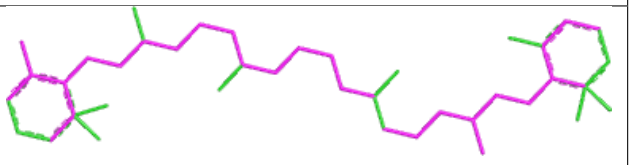
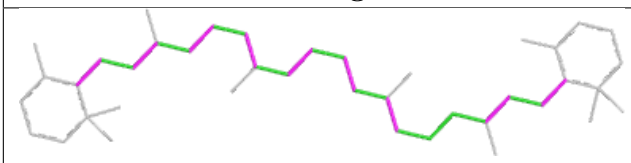
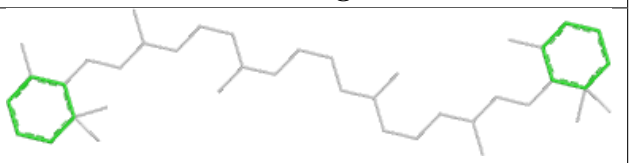
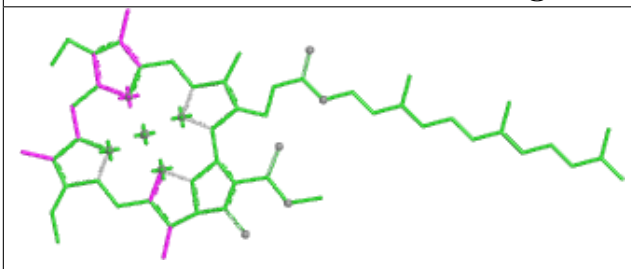
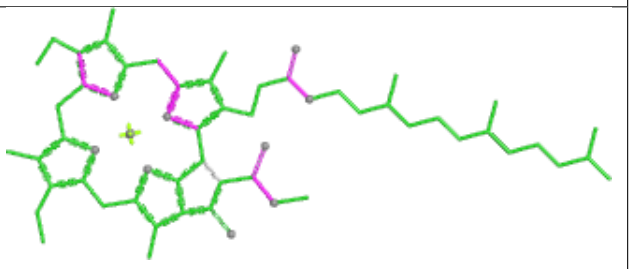
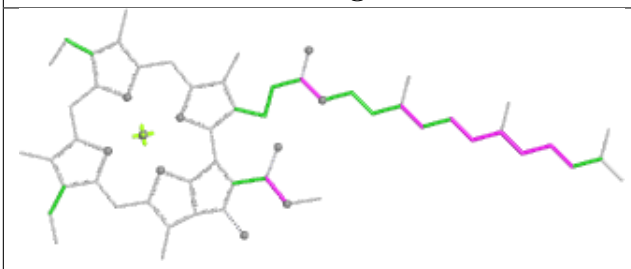
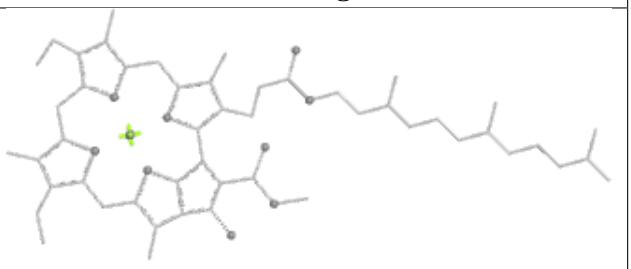
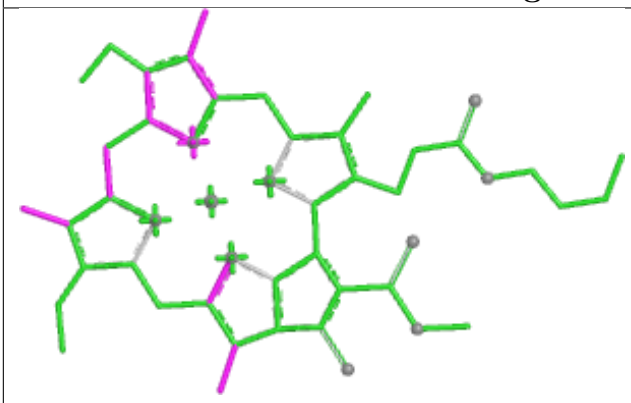


Rings

Ligand 8CT F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 821



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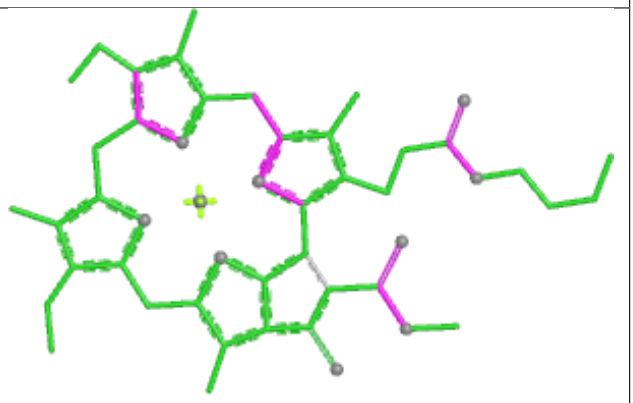
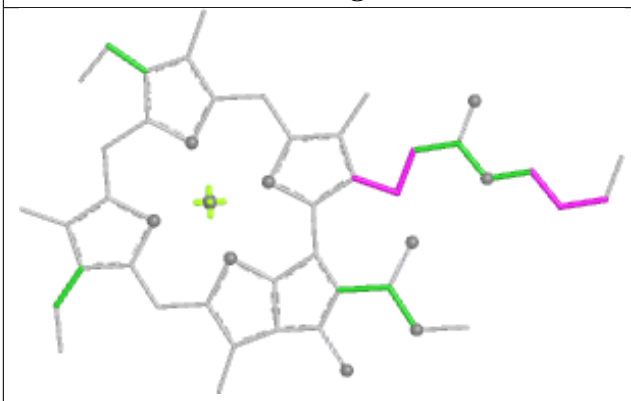


Bond angles



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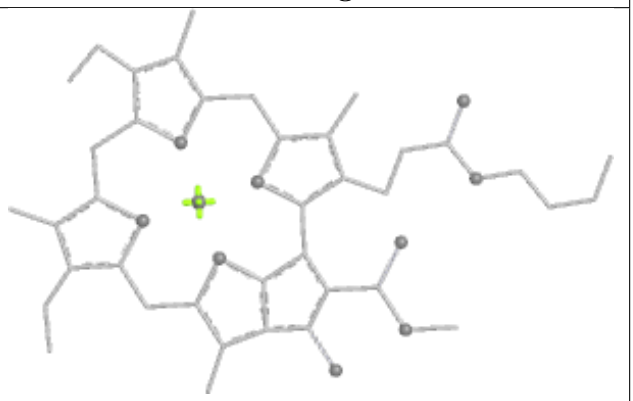
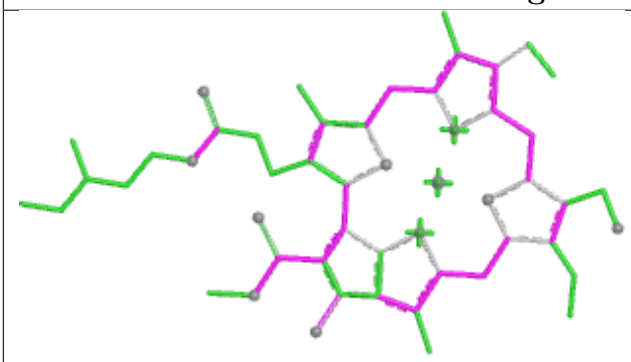


Rings

Ligand CHL 6 313



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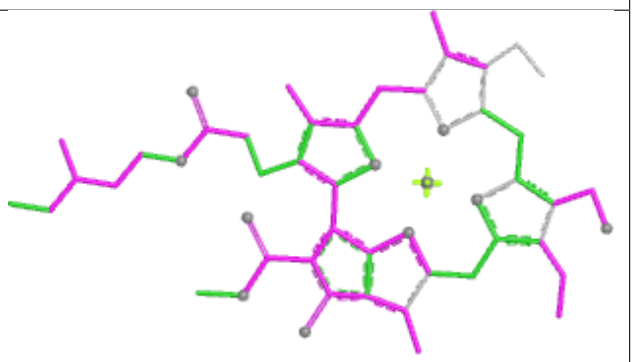
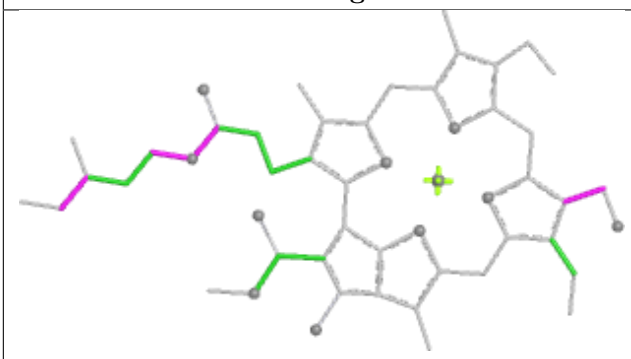


Bond angles



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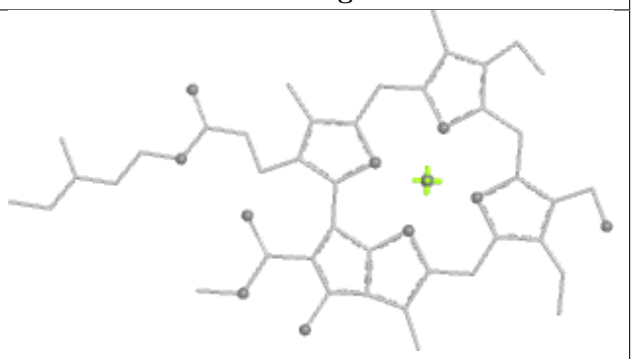
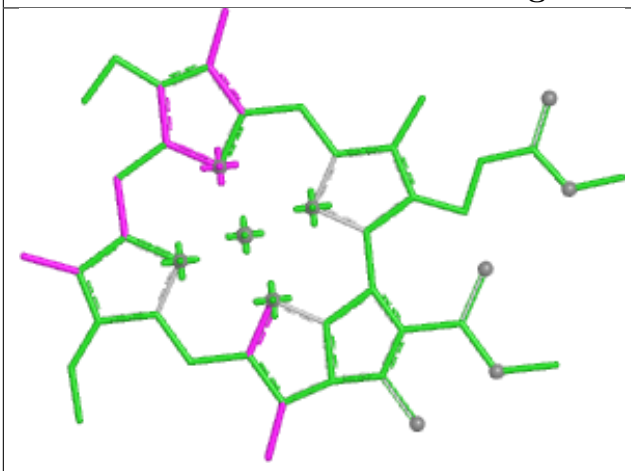


Rings

Ligand CLA 6 317



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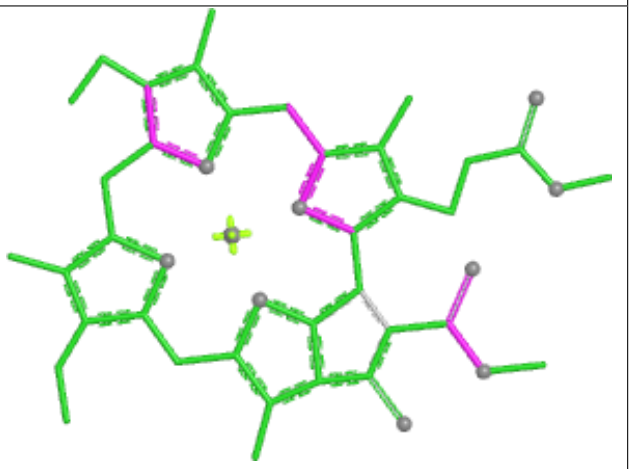
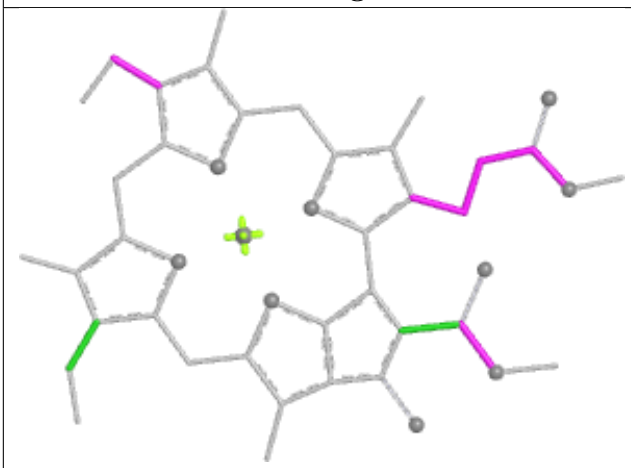


Bond angles



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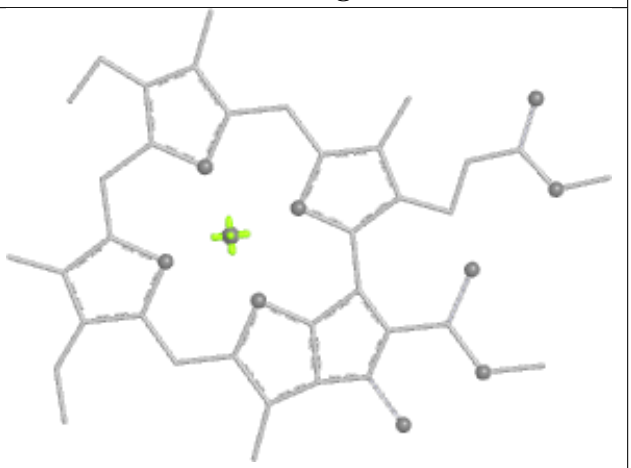
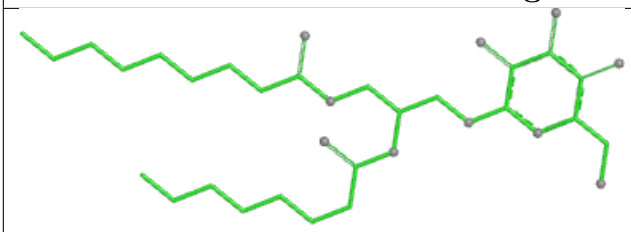
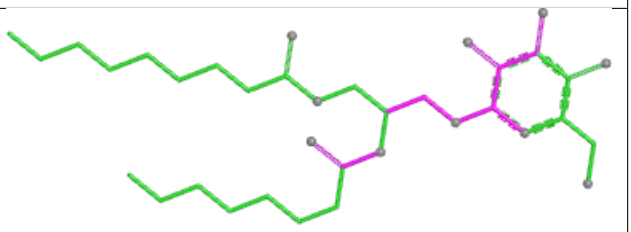


Rings

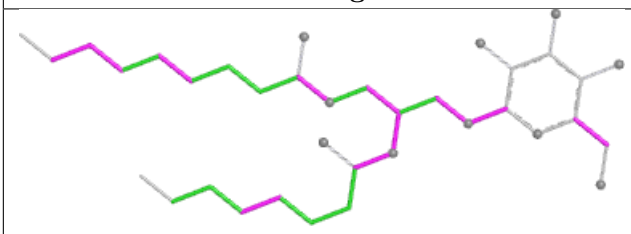
Ligand LMG 3 321



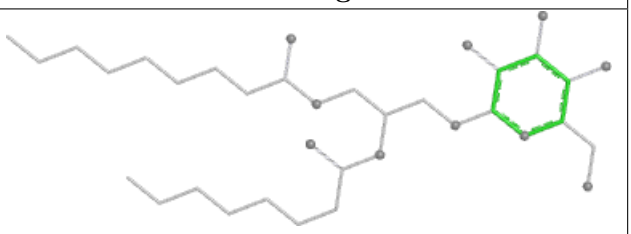
Bond lengths



Bond angles

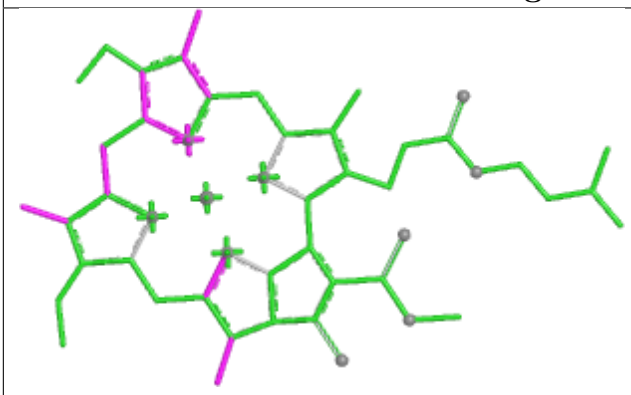


Torsions



Rings

Ligand CLA B 831



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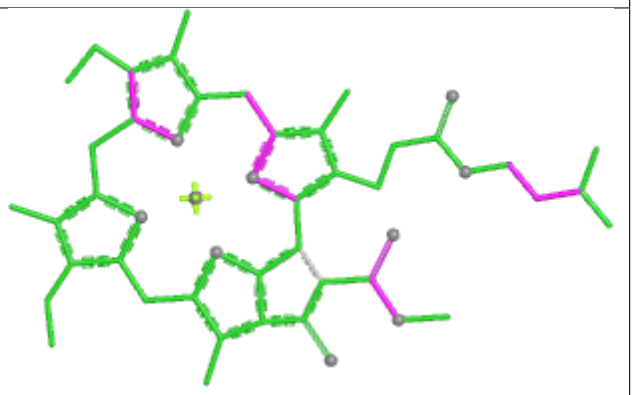
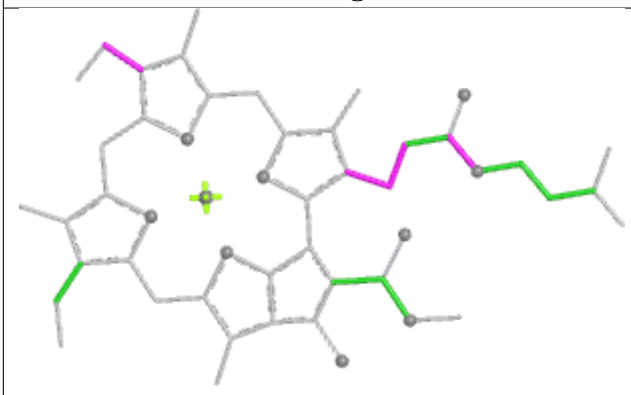
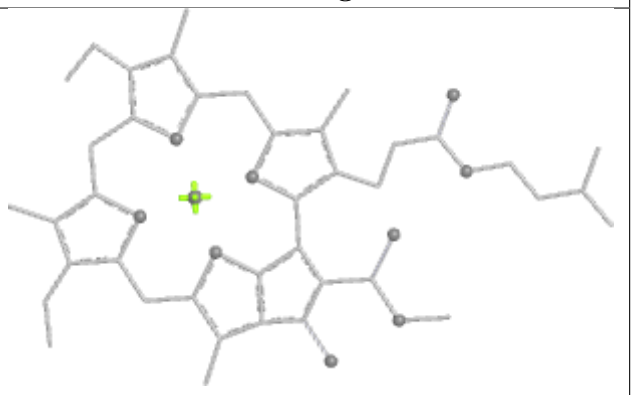


Bond angles

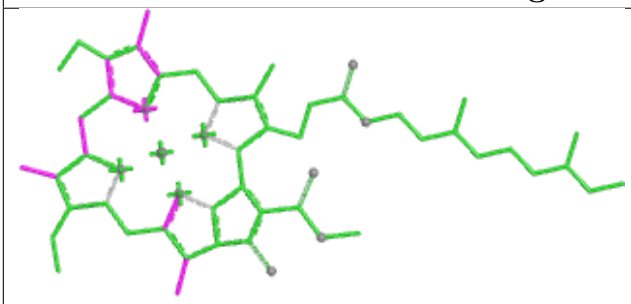


Torsions



Rings

Ligand CLA 2 302



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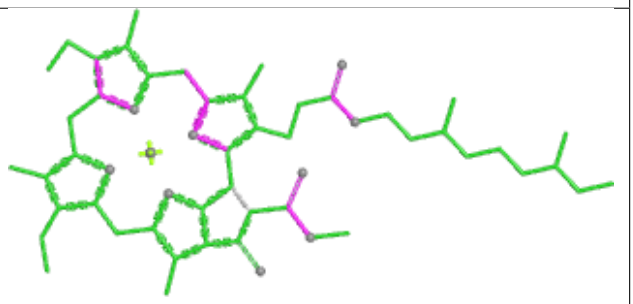
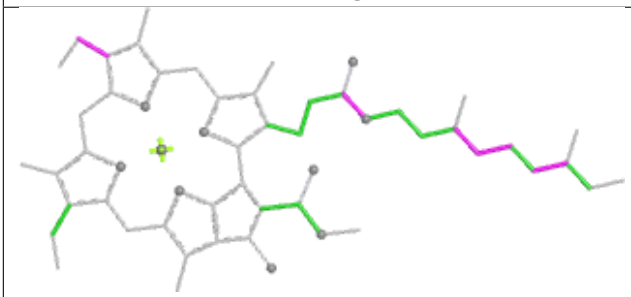


Bond angles



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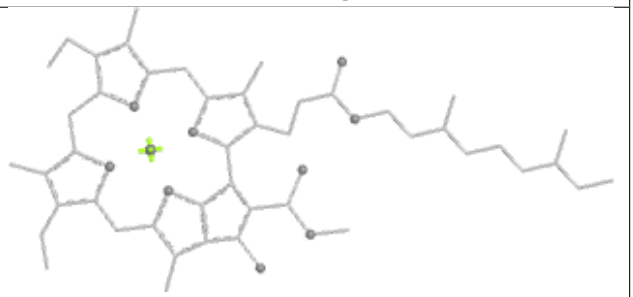
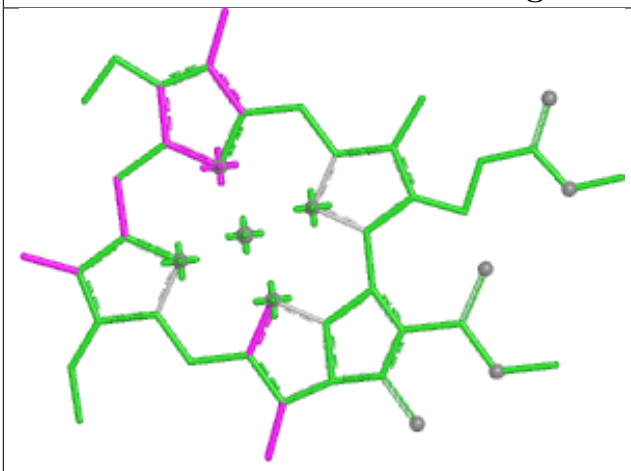


Rings

Ligand CLA L 203



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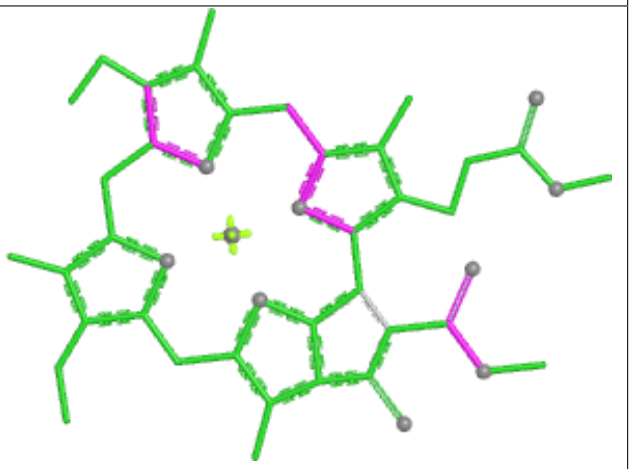

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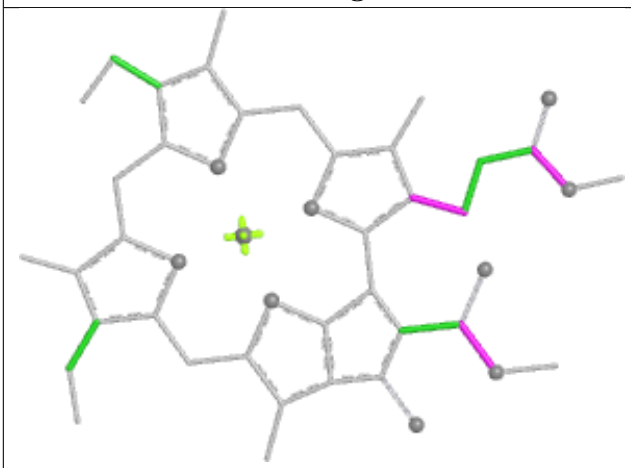

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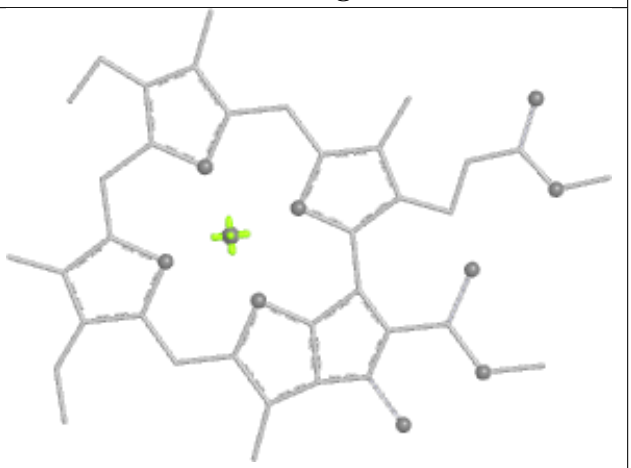
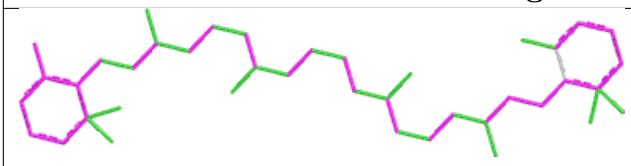


Rings

Ligand 8CT G 104



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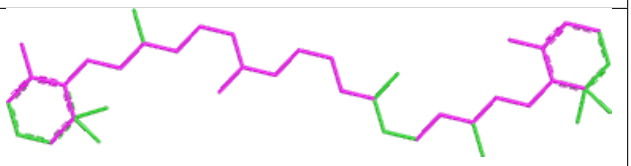
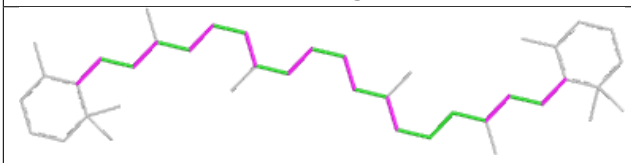


Bond angles



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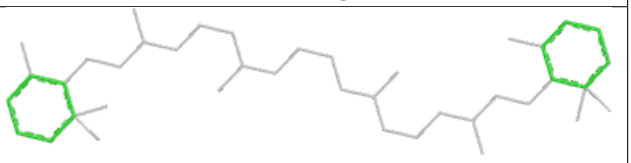
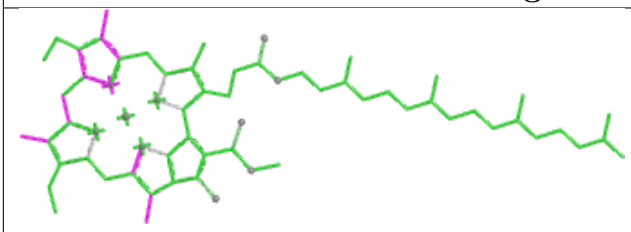


Rings

Ligand CLA A 831



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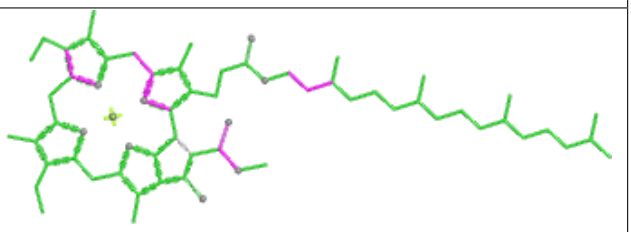
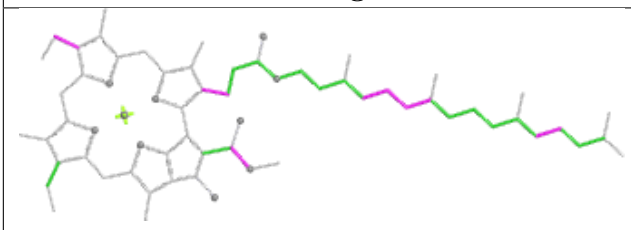


Bond angles



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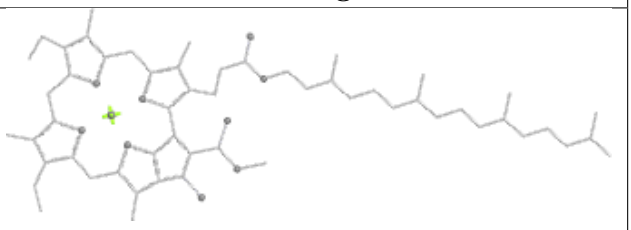
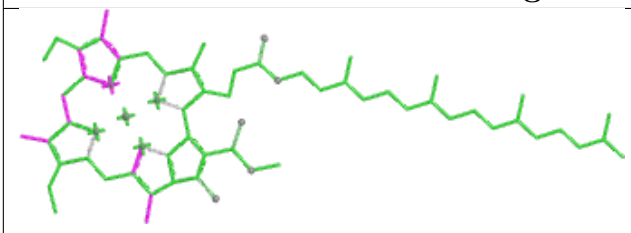


Rings

Ligand CLA A 807



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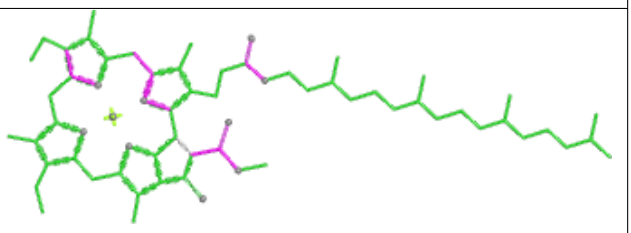

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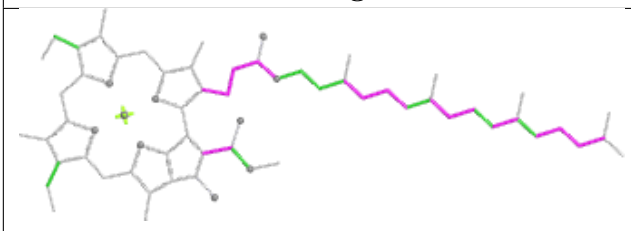

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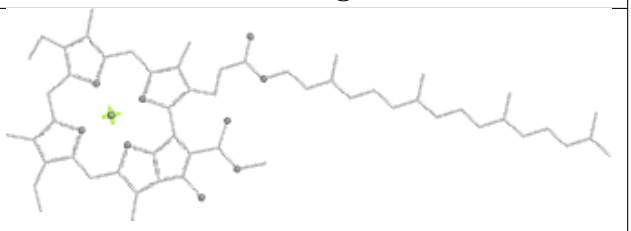
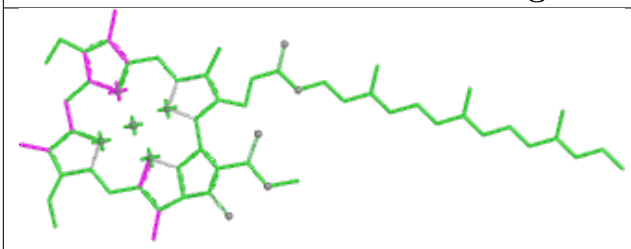


Rings

Ligand CLA 0 303



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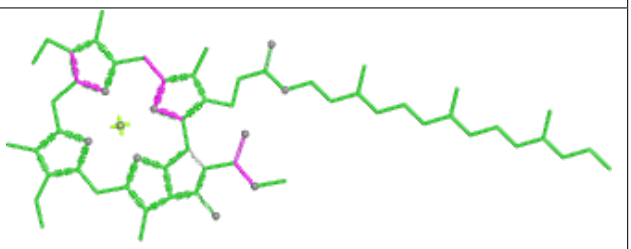

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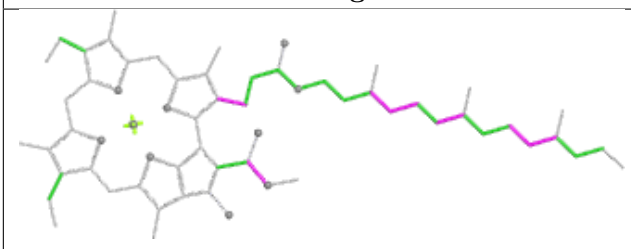

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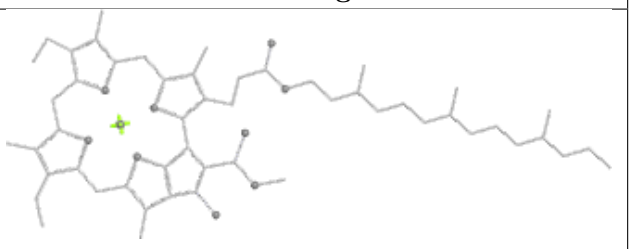
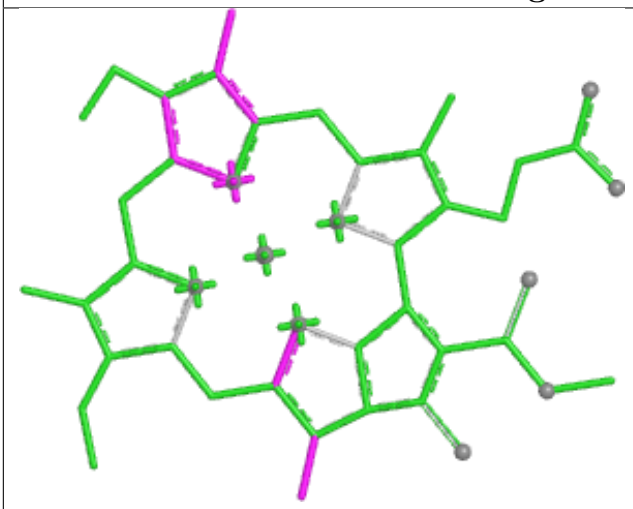


Rings

Ligand CLA 7 316



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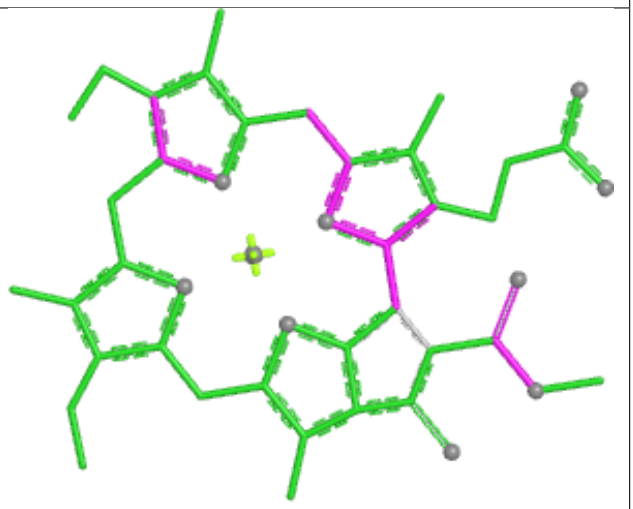

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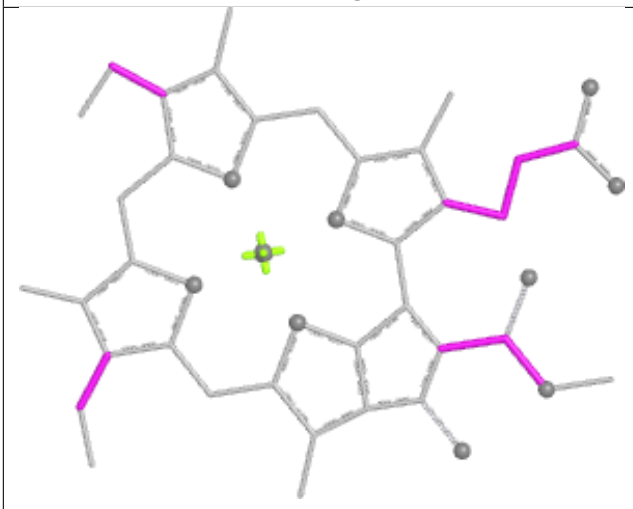
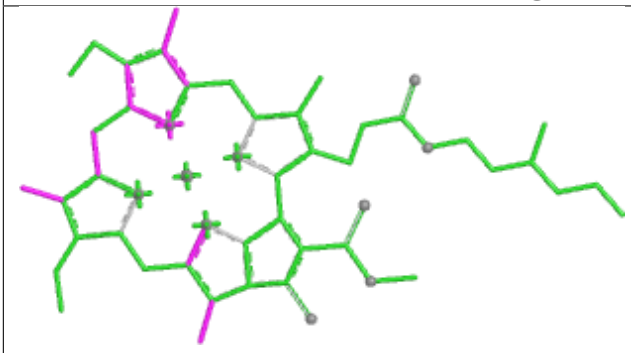


Torsions

Rings

Ligand CLA 1 310



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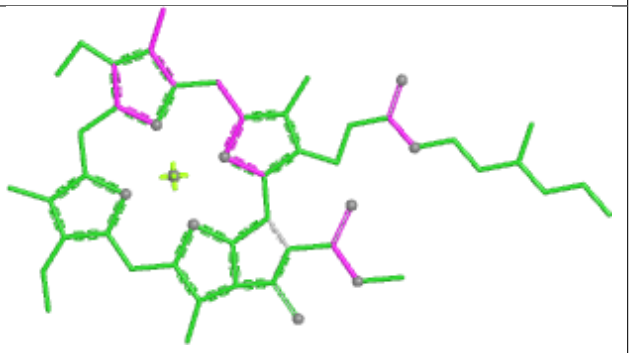

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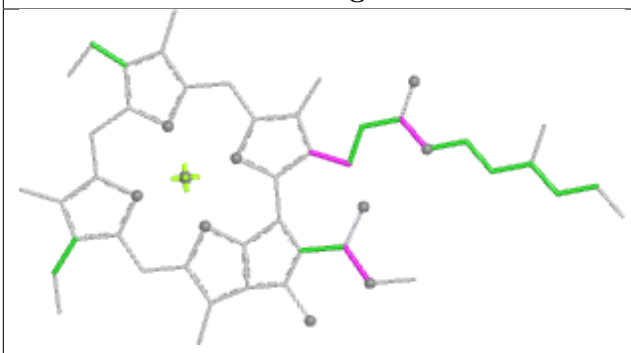

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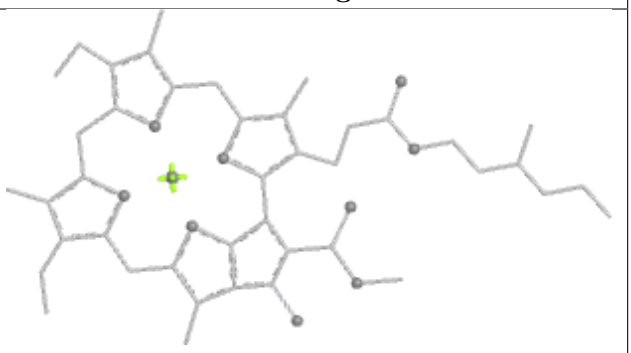
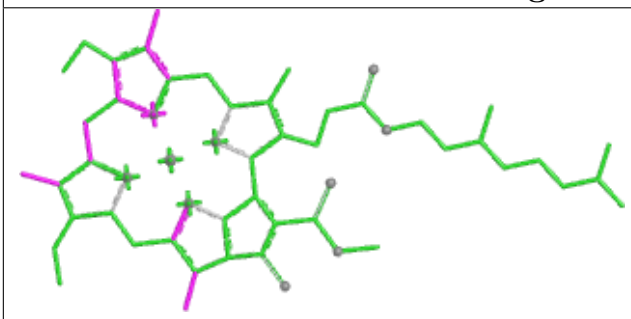


Rings

Ligand CLA 3 303



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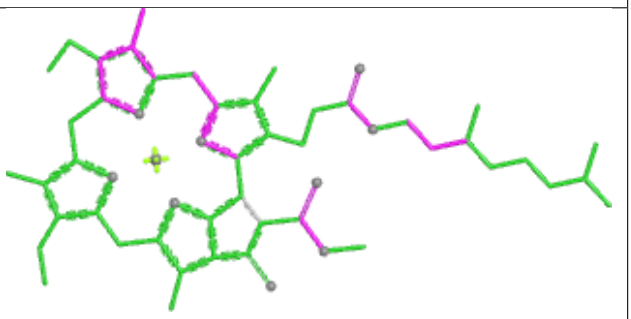

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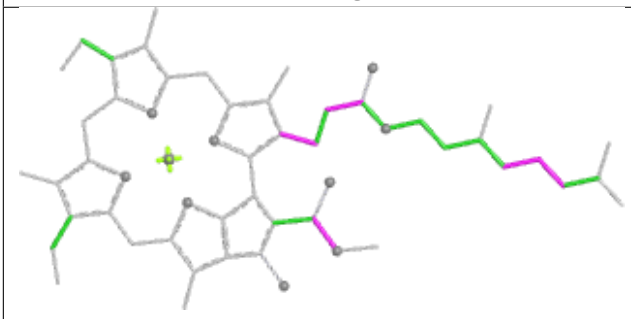

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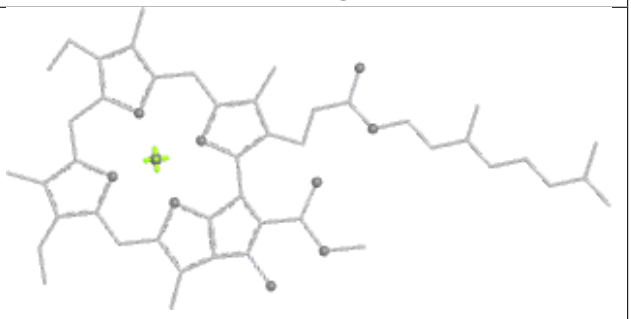
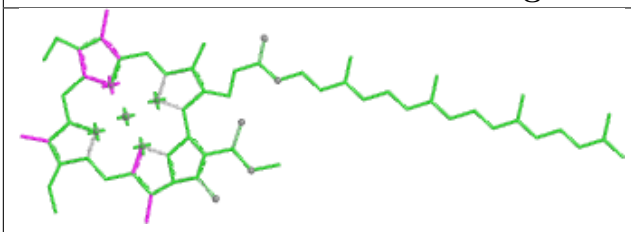


Rings

Ligand CLA A 810



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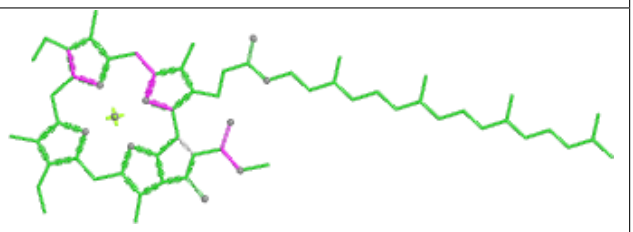

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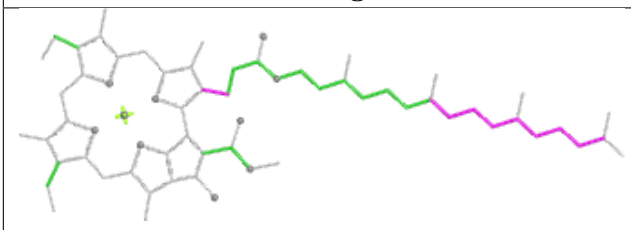

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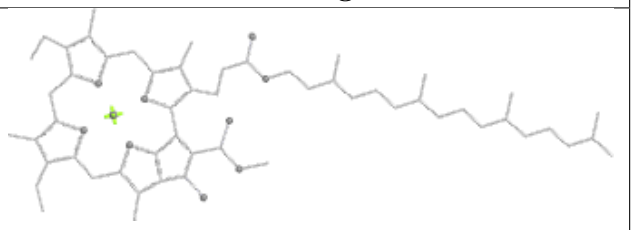
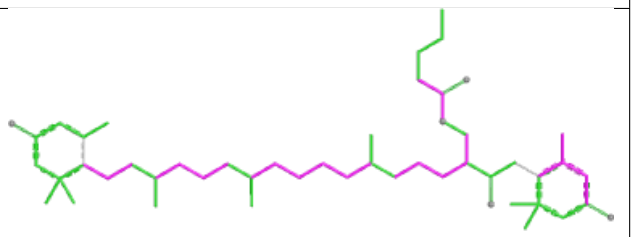


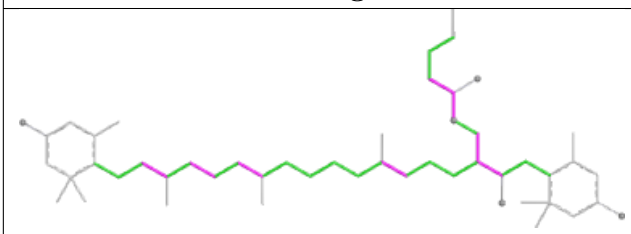
Rings

Ligand 0UR 4 318

Bond lengths



Bond angles



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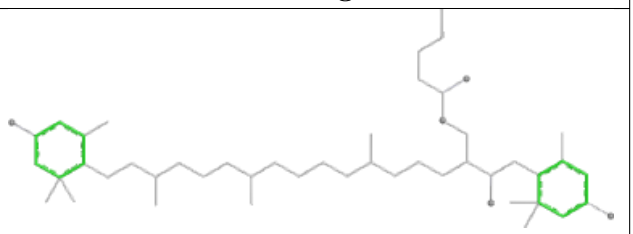
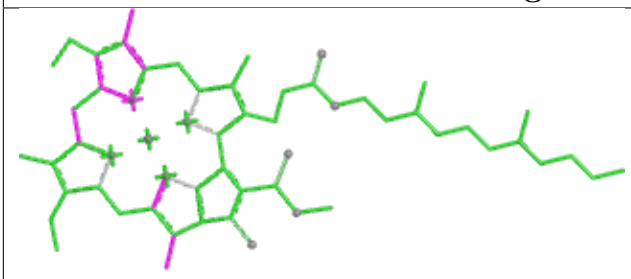
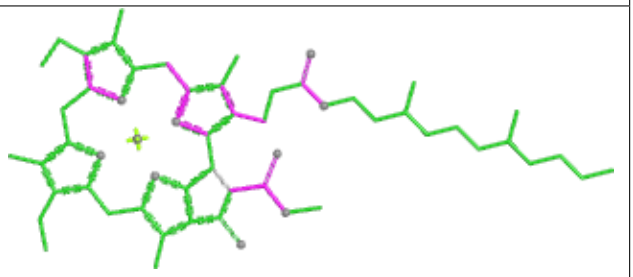
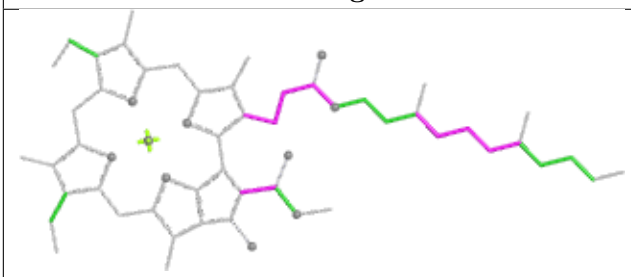
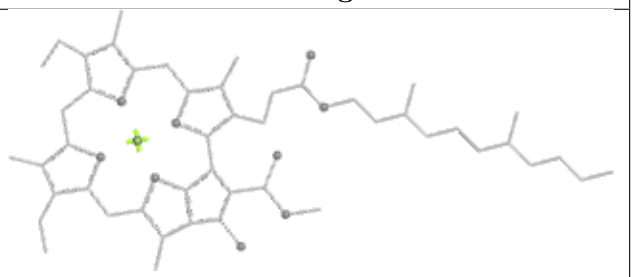
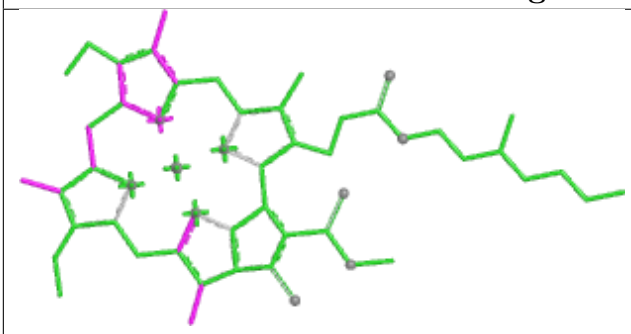
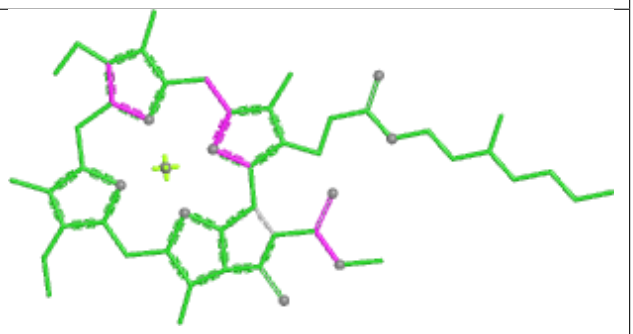
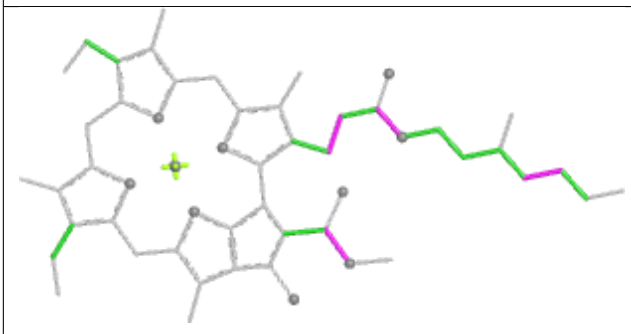
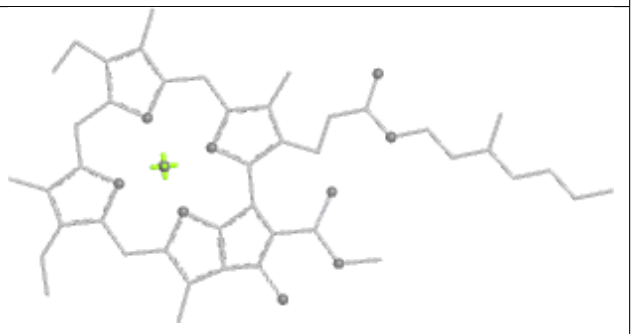
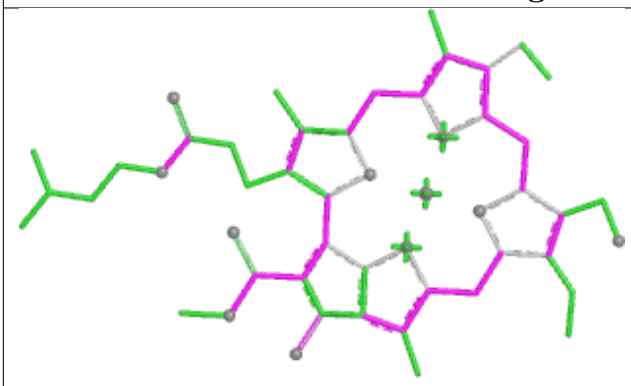


Rings

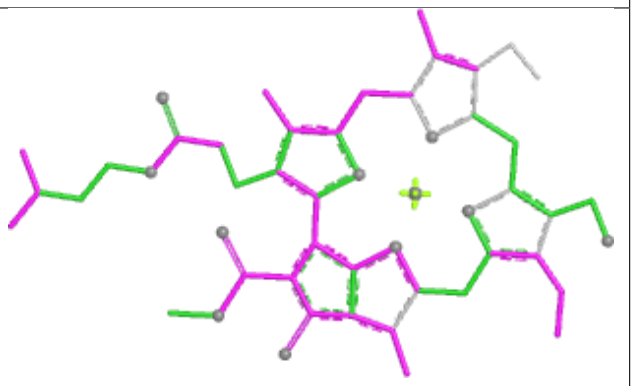
Ligand CLA B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

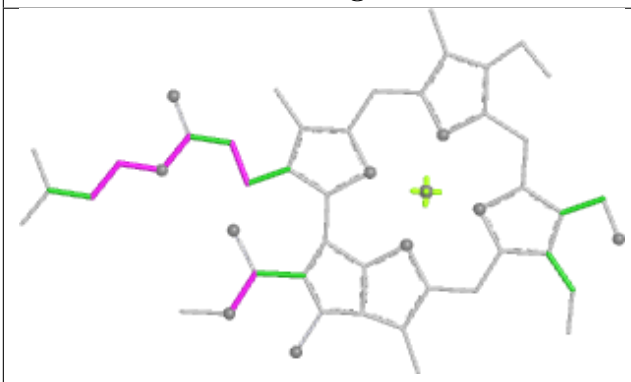
Ligand CHL 1 304



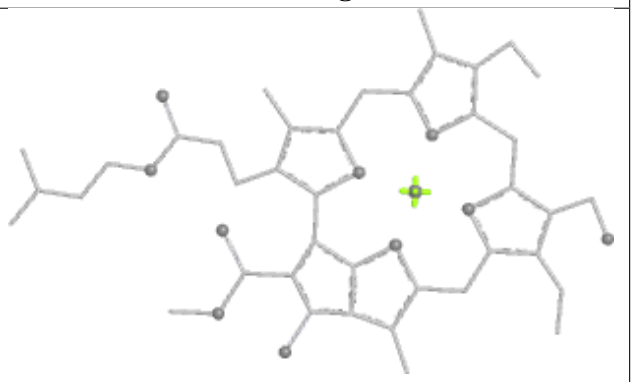
Bond lengths



Bond angles

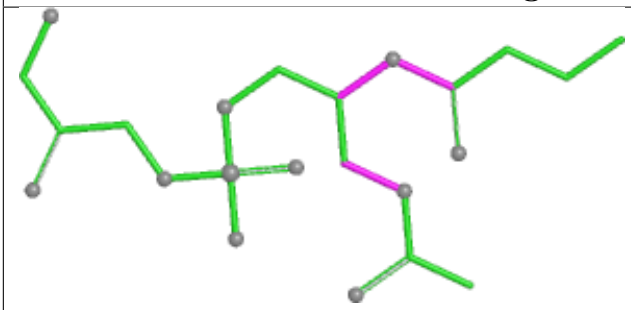


Torsions



Rings

Ligand LHG B 851



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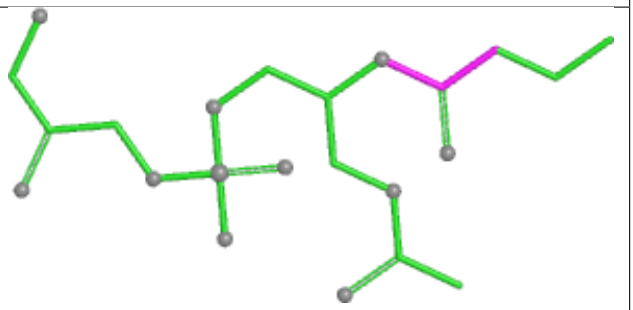

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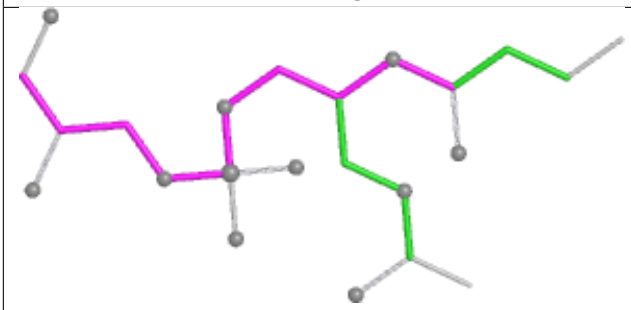

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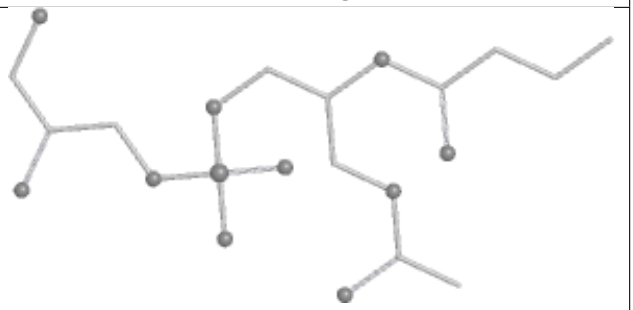
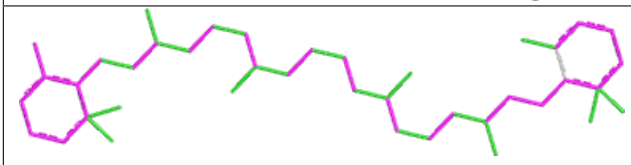


Rings

Ligand 8CT A 844



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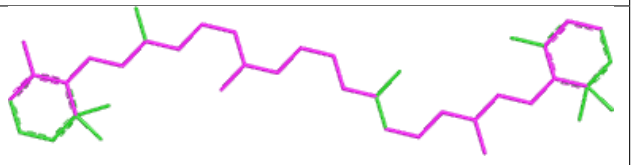

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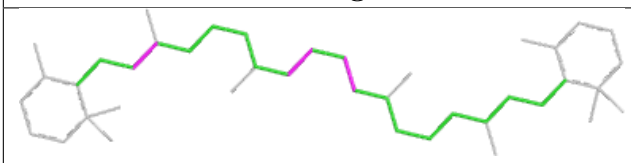

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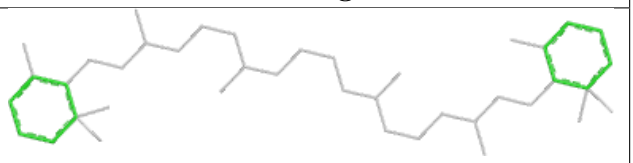
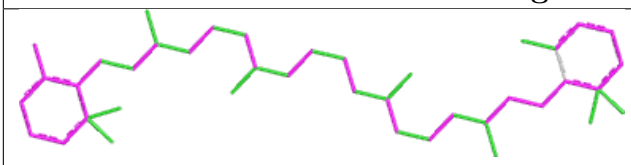


Rings

Ligand 8CT 7 319



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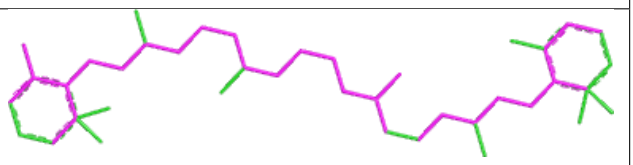

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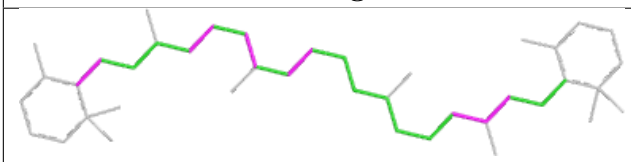

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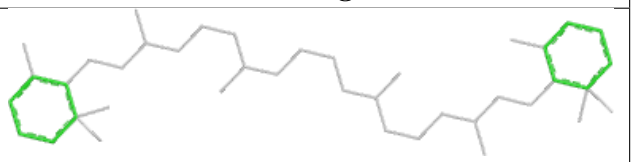
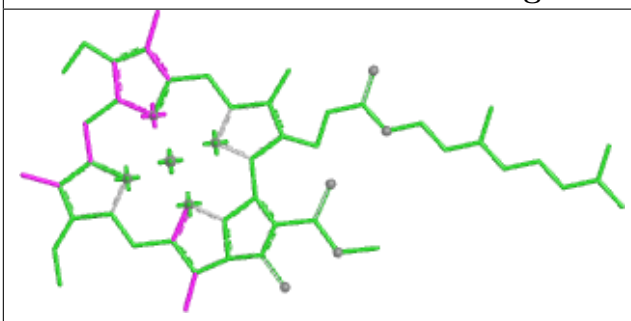


Rings

Ligand CLA A 823



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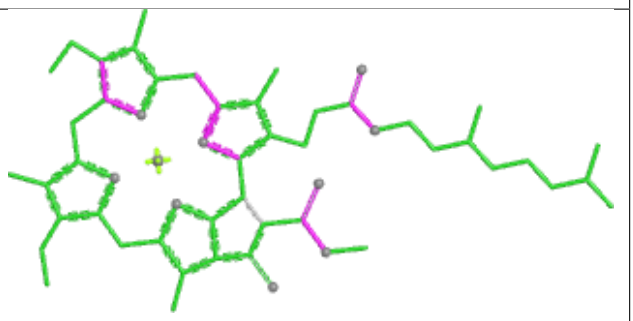
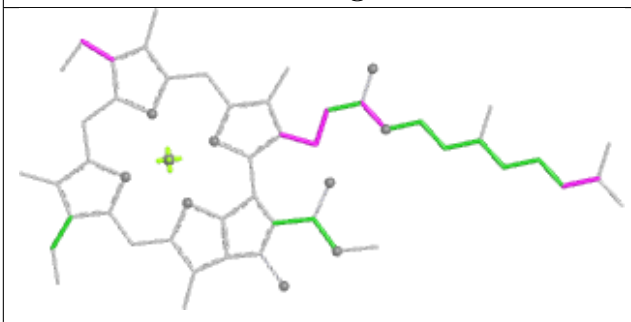


Bond angles



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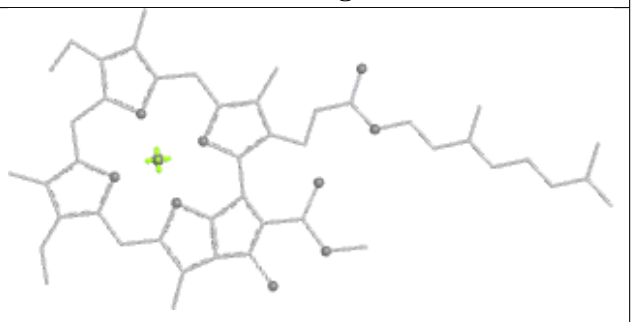
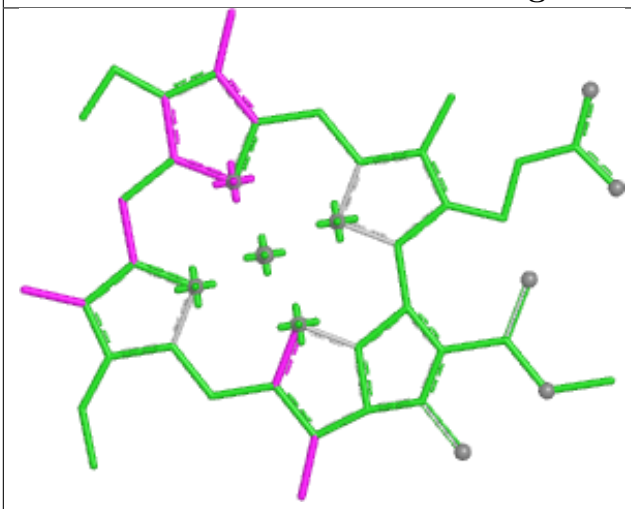


Rings

Ligand CLA 8 315



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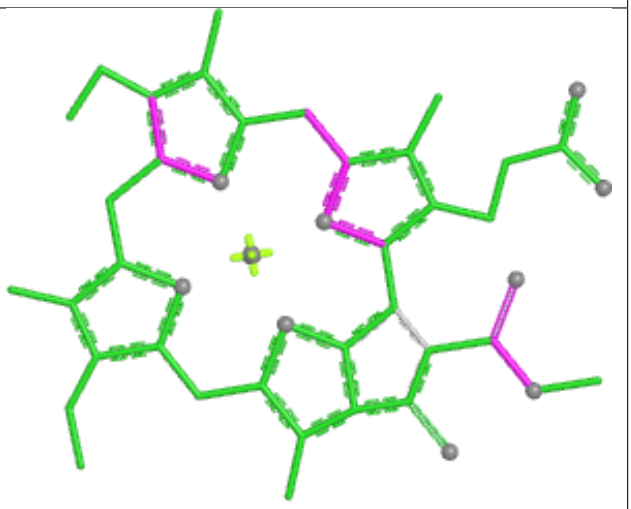

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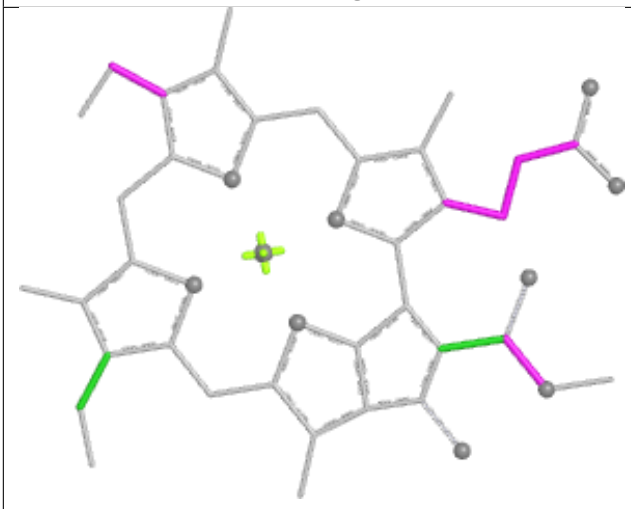
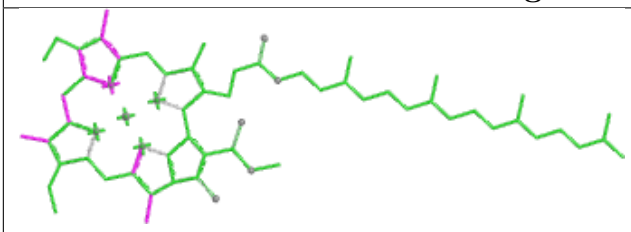


Torsions

Rings

Ligand CLA B 805



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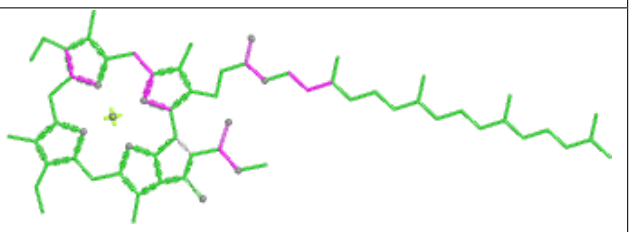
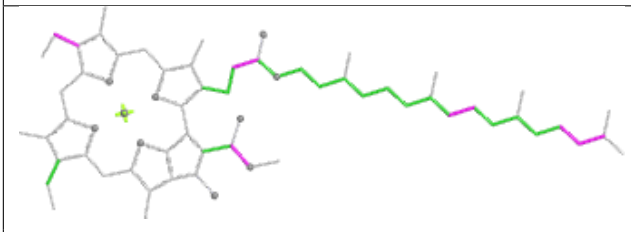
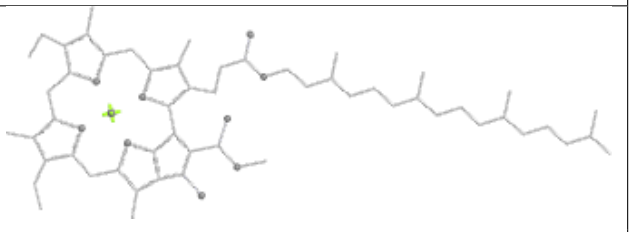


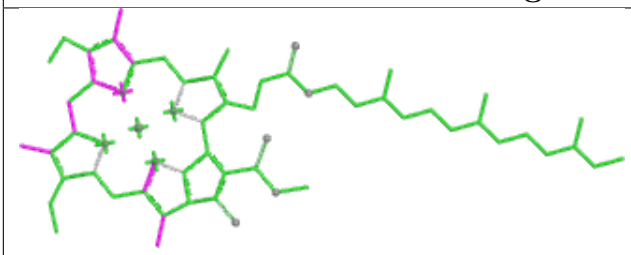
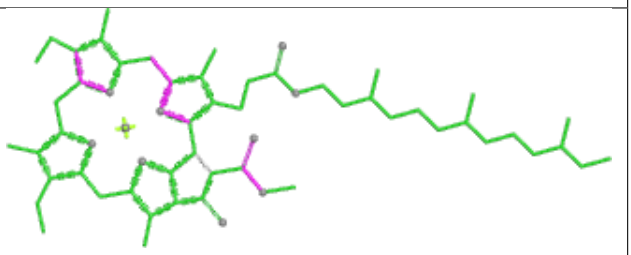
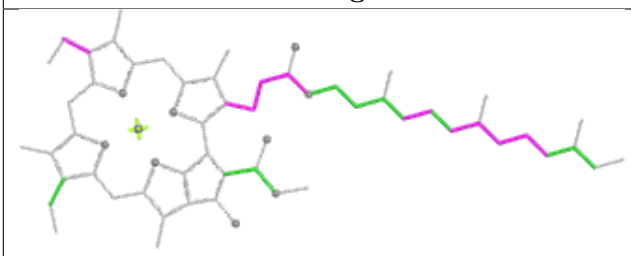
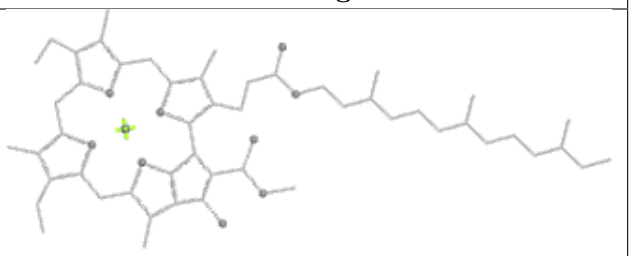
Bond angles

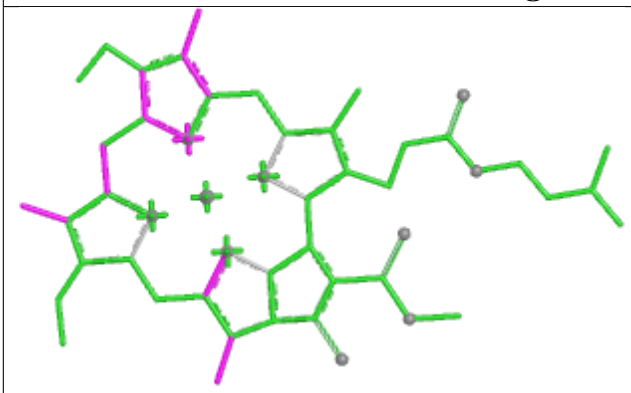
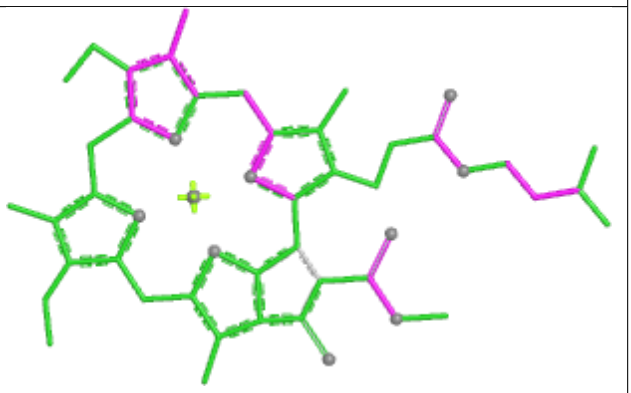
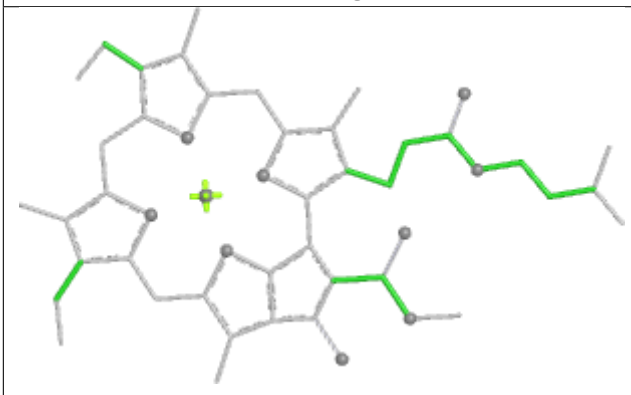
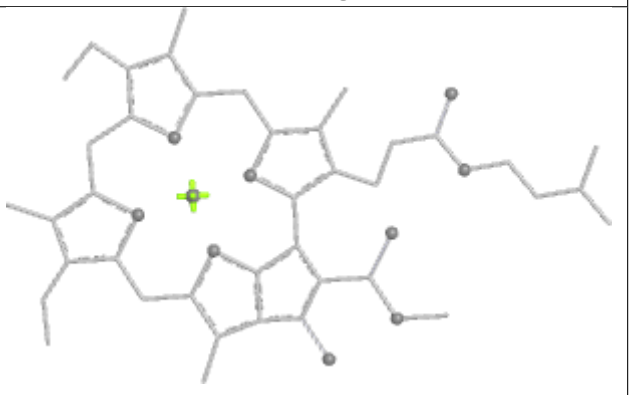


Torsions

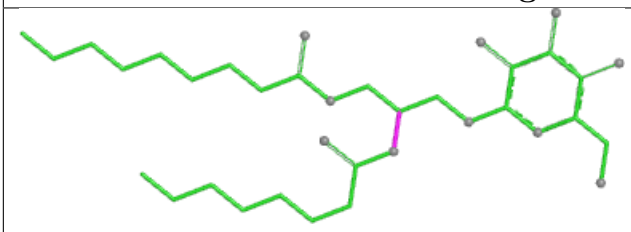


Rings

Ligand CLA B 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 851



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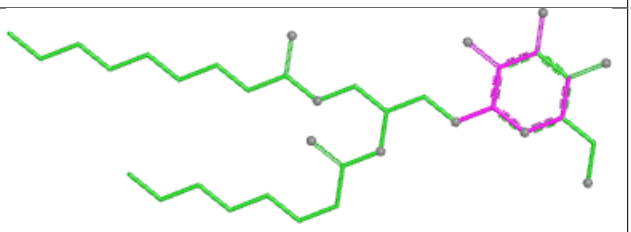
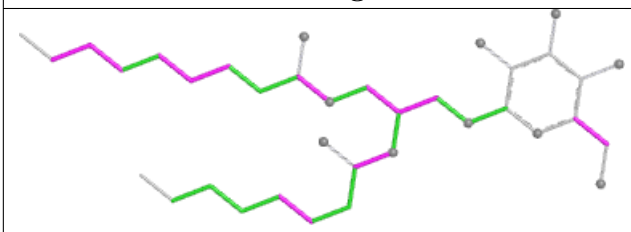
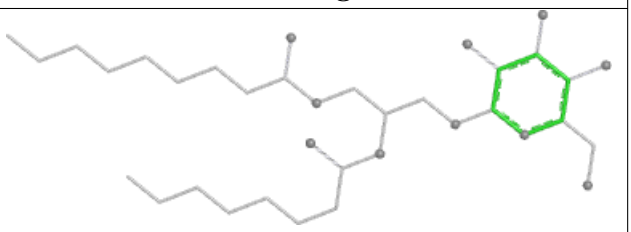


Bond angles

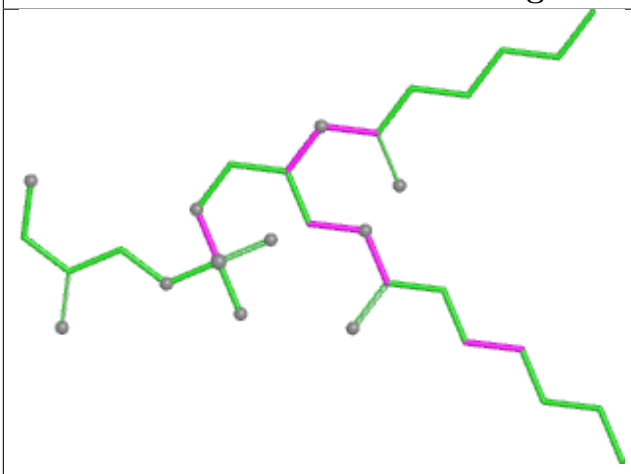


Torsions



Rings

Ligand LHG 7 322



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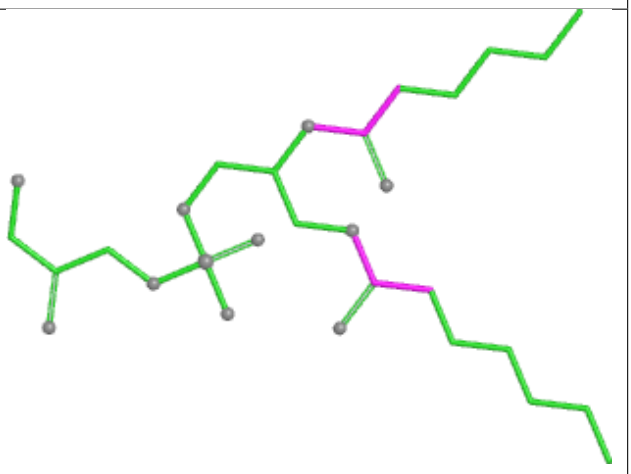
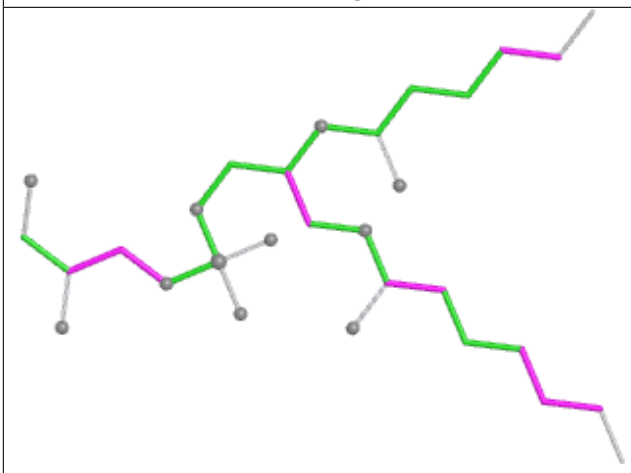


Bond angles



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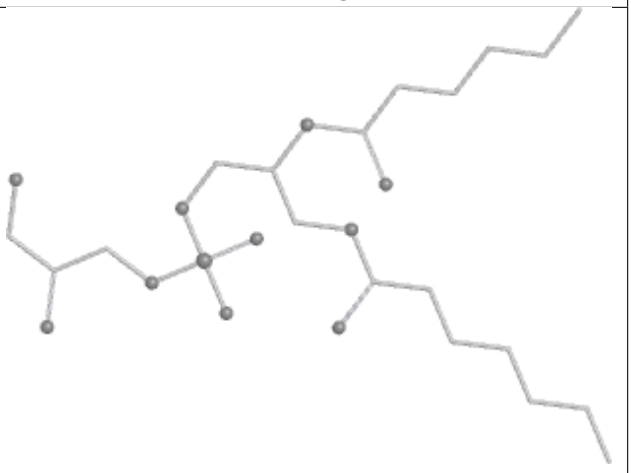
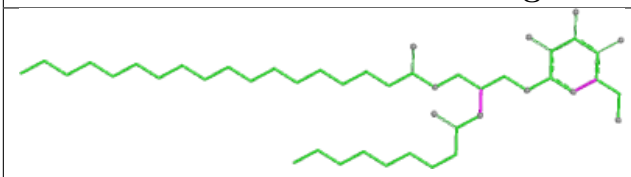


Rings

Ligand LMG J 105



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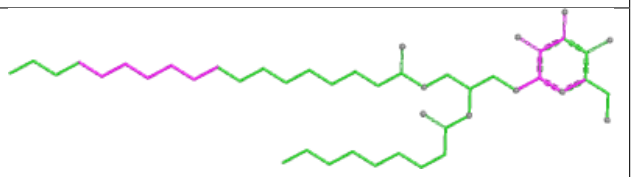
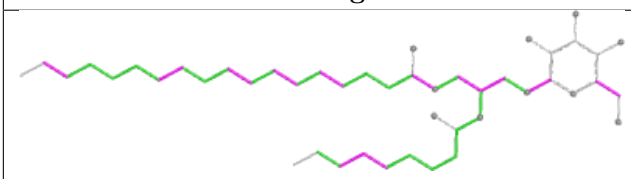
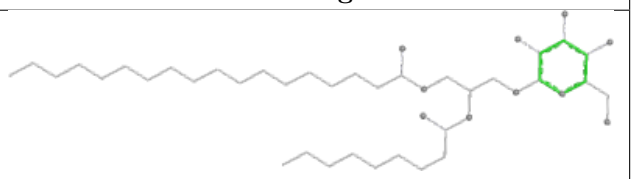


Bond angles

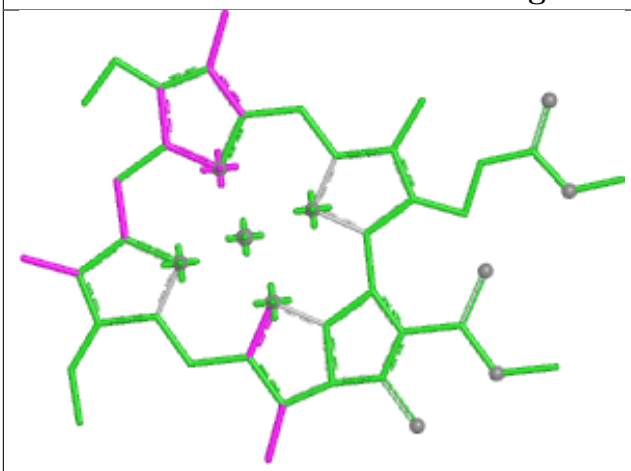


Torsions



Rings

Ligand CLA 8 312



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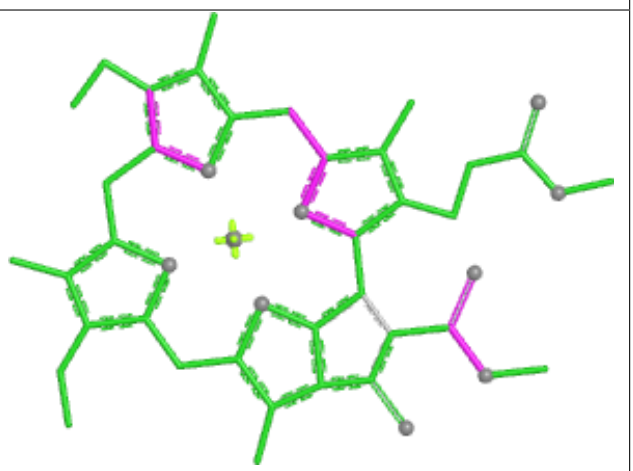
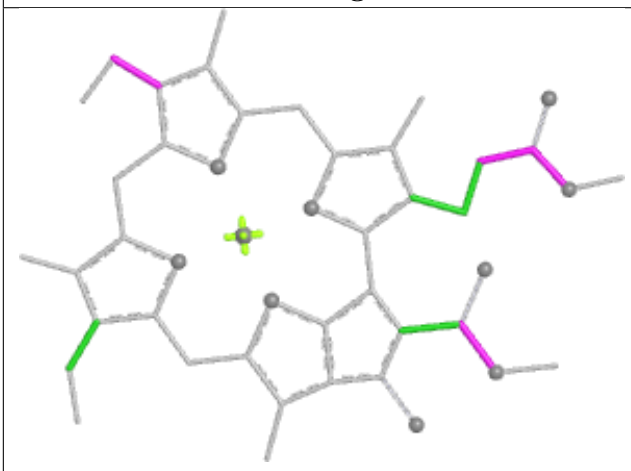
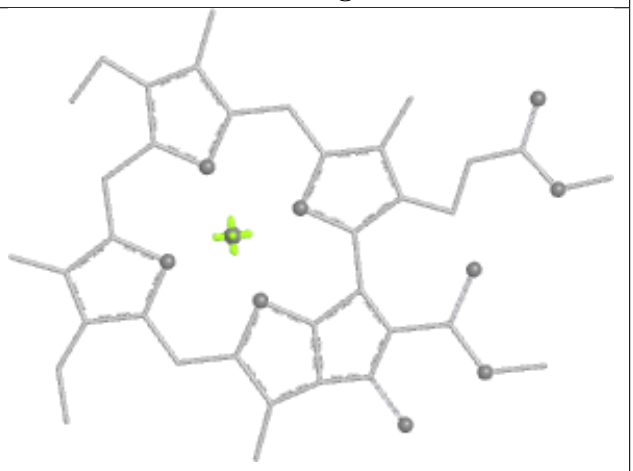


Bond angles

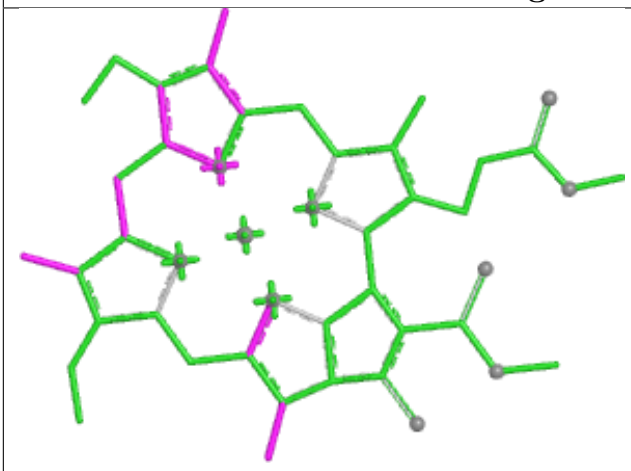


Torsions



Rings

Ligand CLA 5 313



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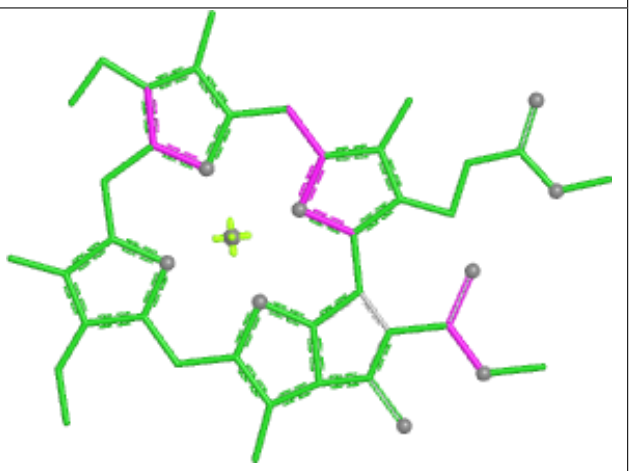
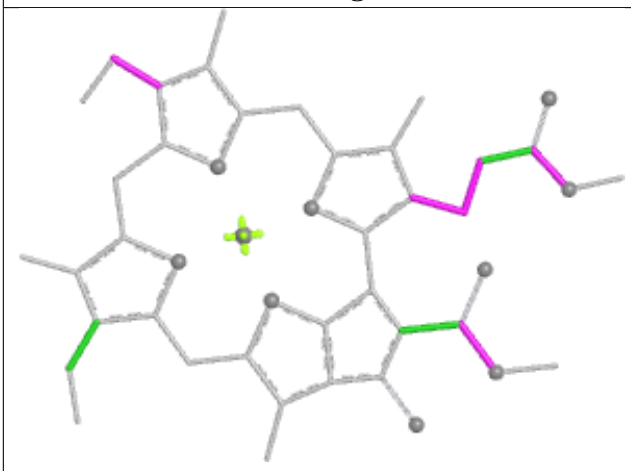
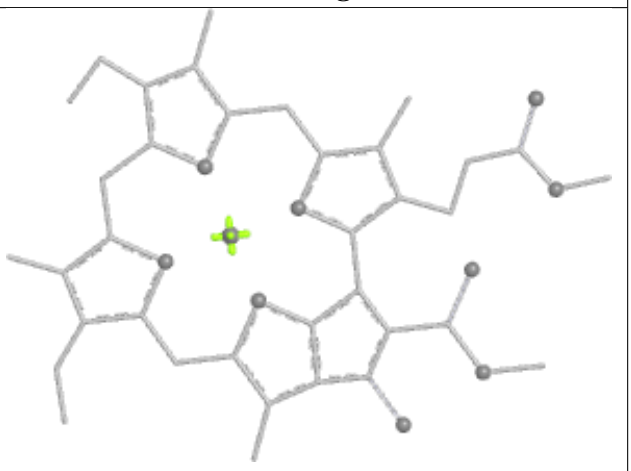


Bond angles

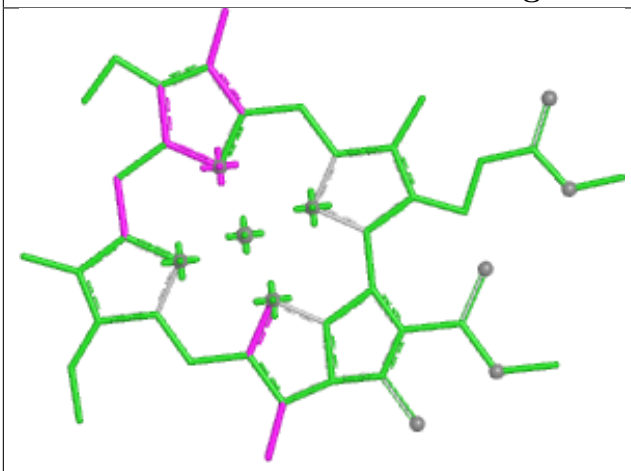


Torsions



Rings

Ligand CLA G 103



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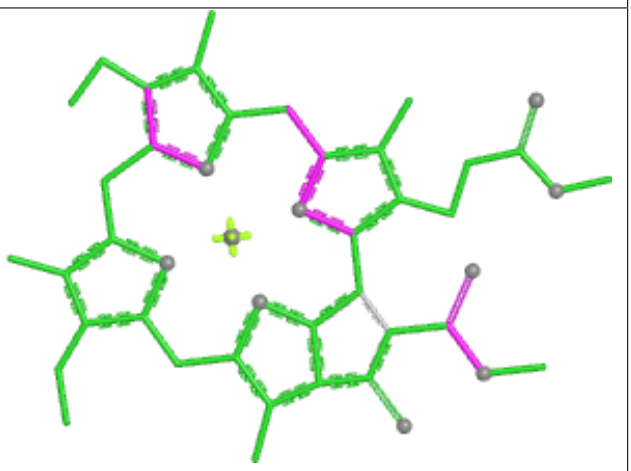
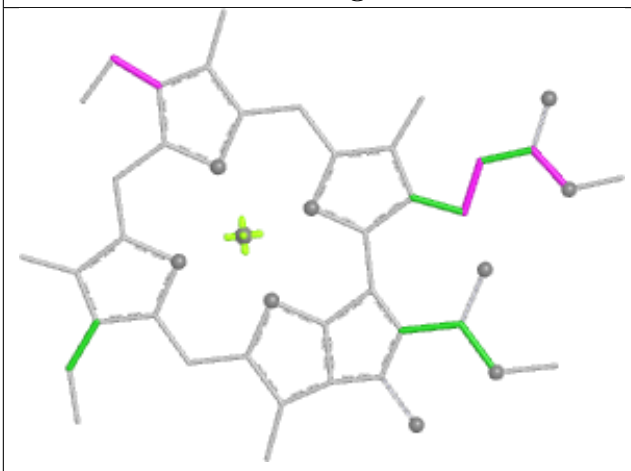
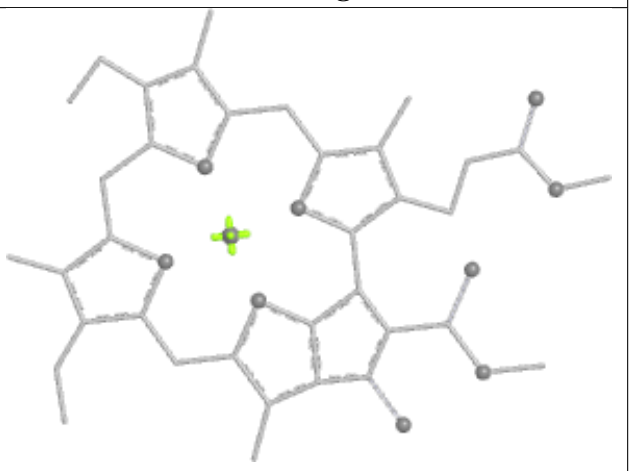


Bond angles

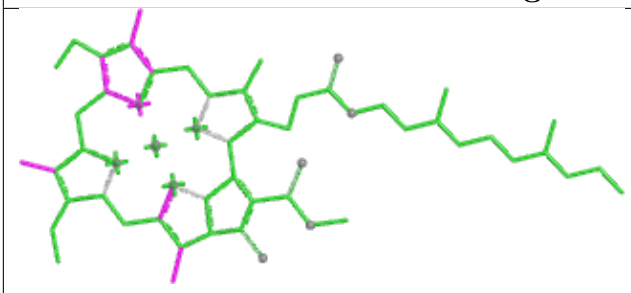


Torsions



Rings

Ligand CLA A 813



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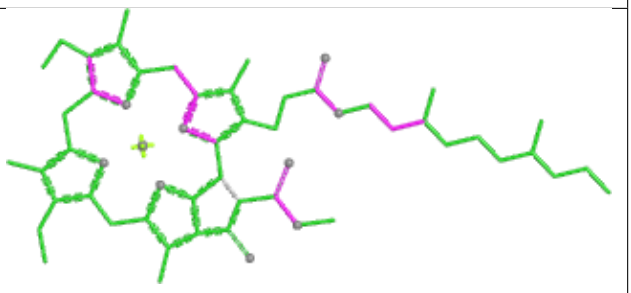
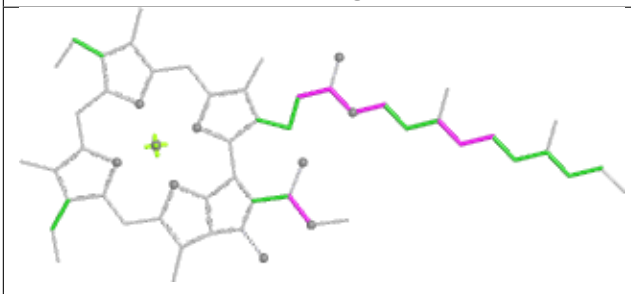


Bond angles



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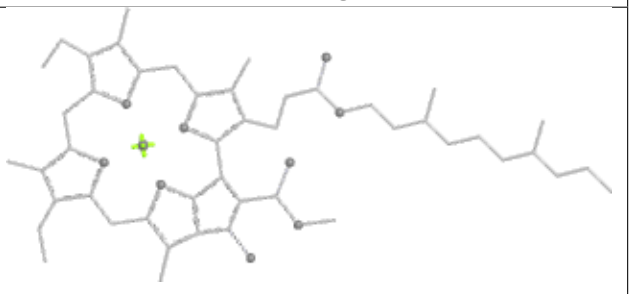
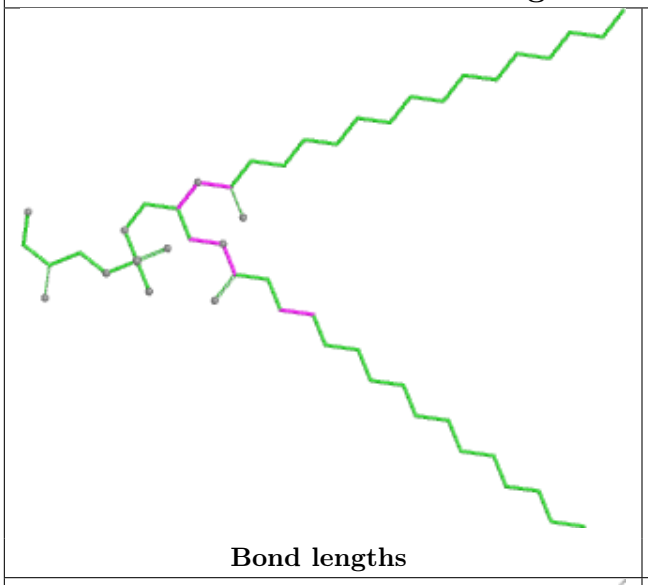


Rings

Ligand LHG 1 317



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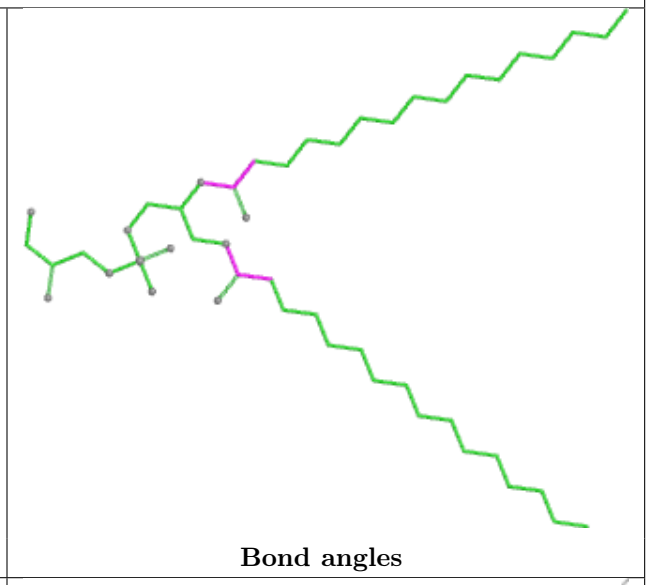
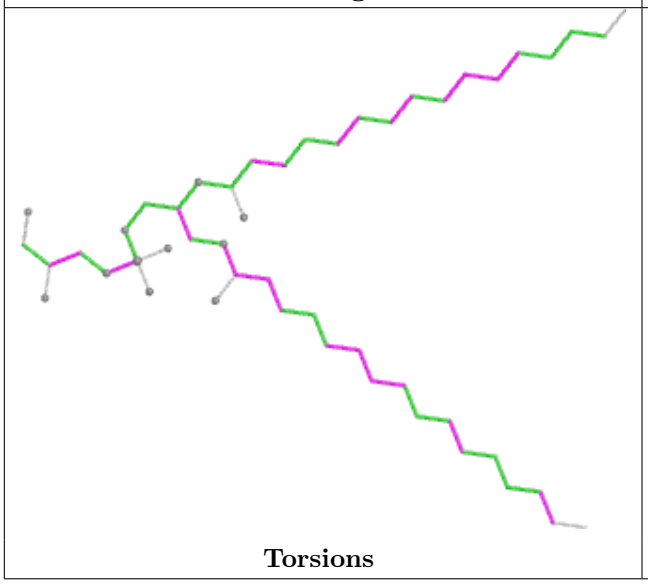


Bond angles



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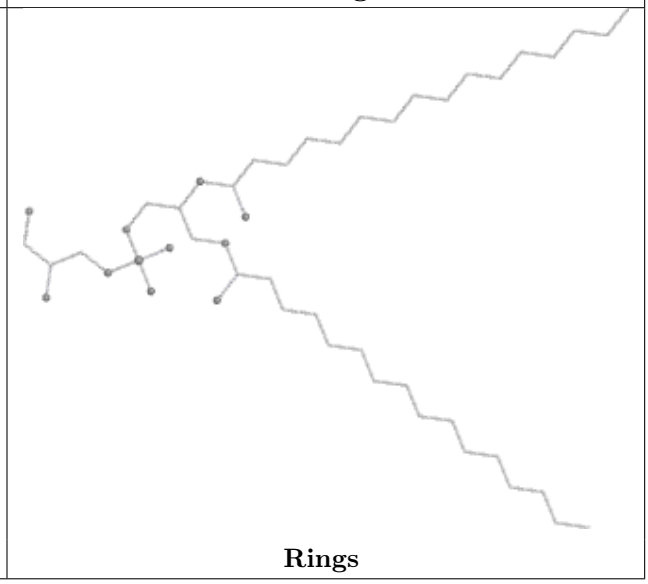
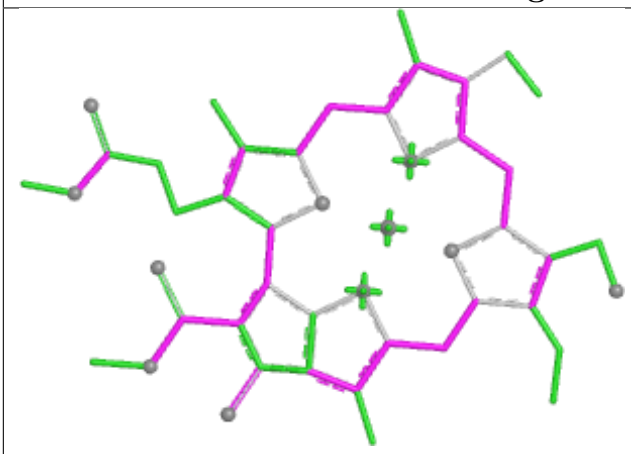


Rings

Ligand CHL 7 313



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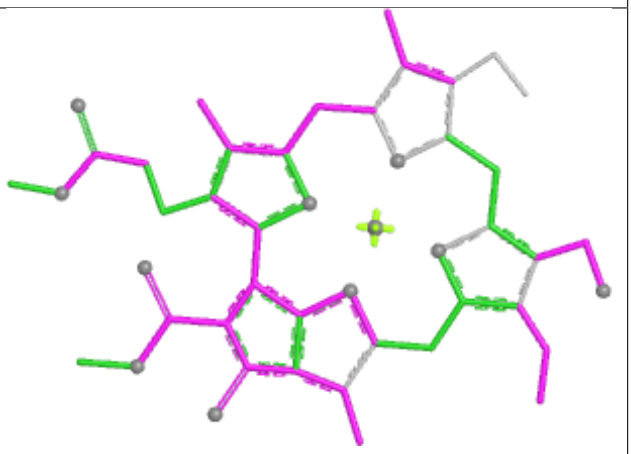
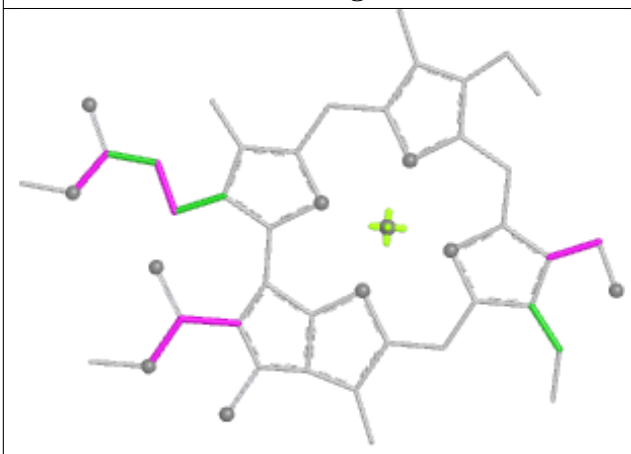


Bond angles



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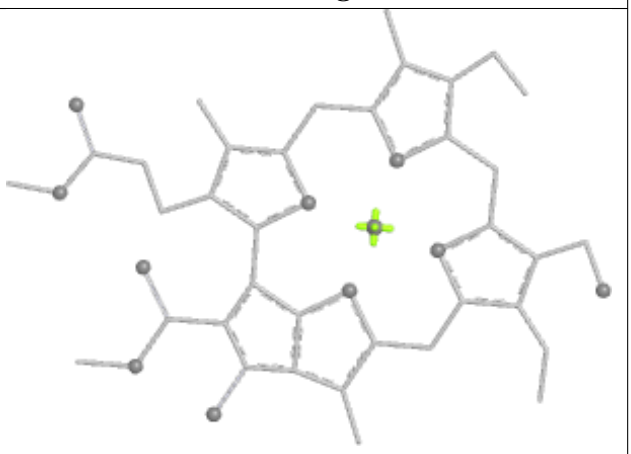
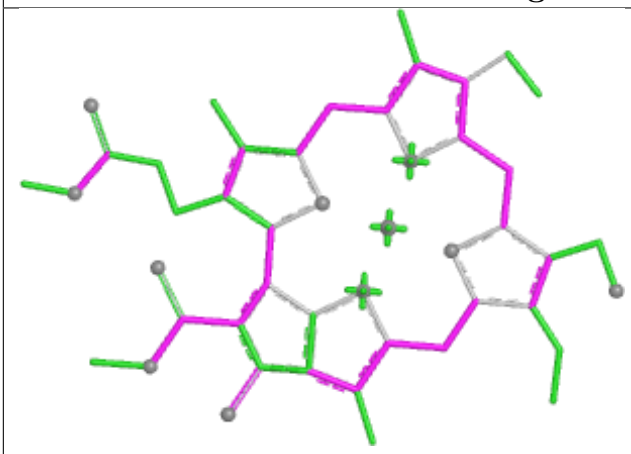


Rings

Ligand CHL 9 301



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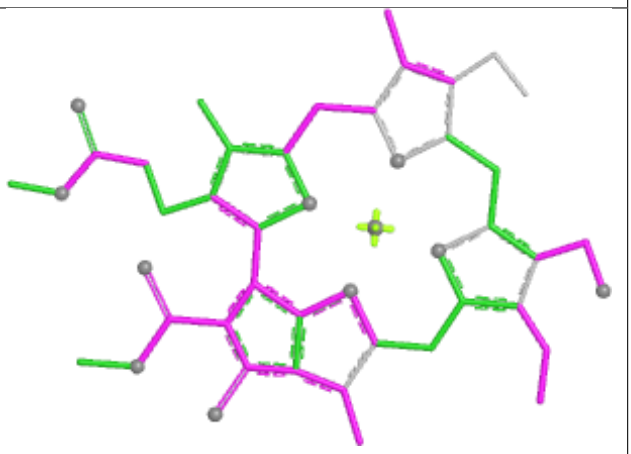
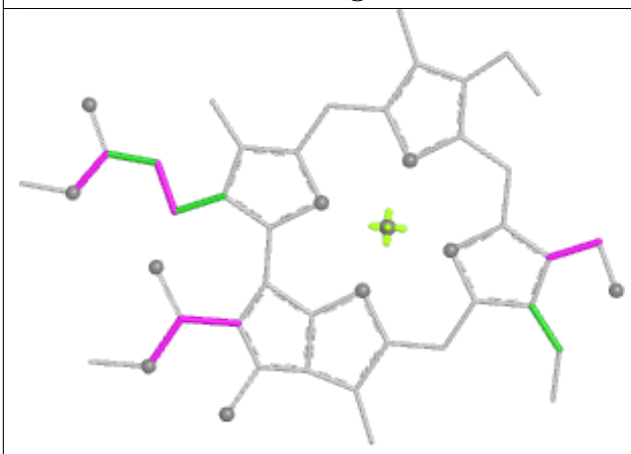


Bond angles



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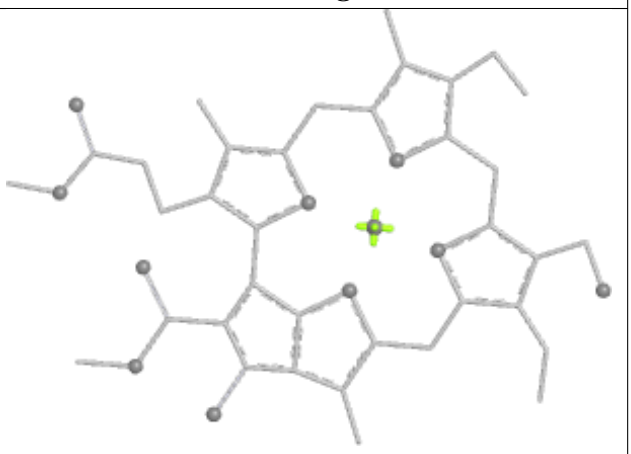
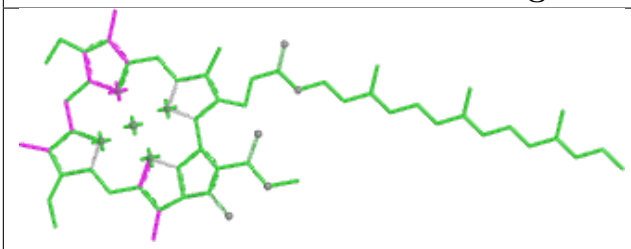


Rings

Ligand CLA 3 310



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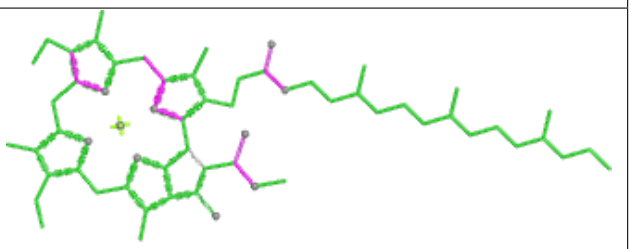

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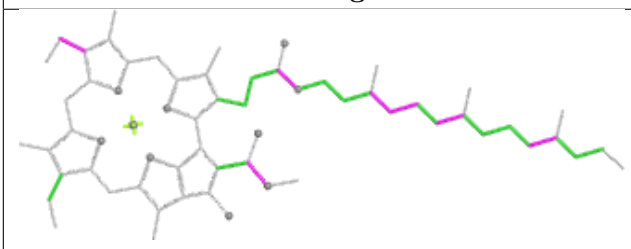

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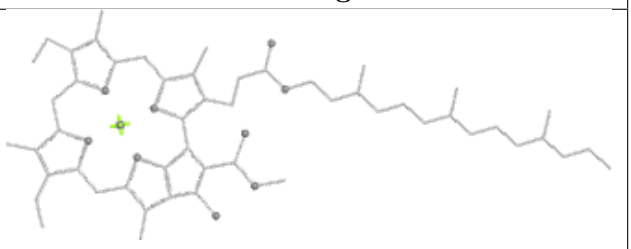
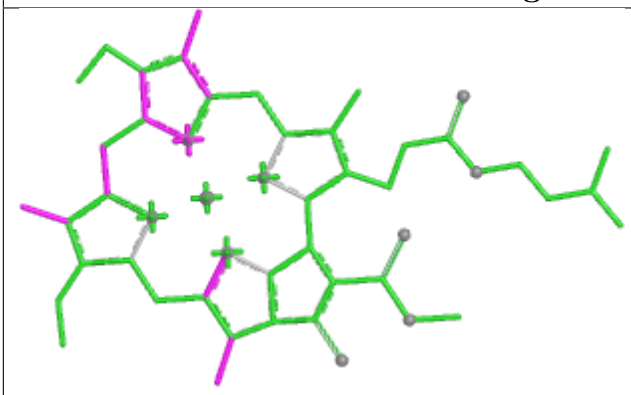


Rings

Ligand CLA K 104



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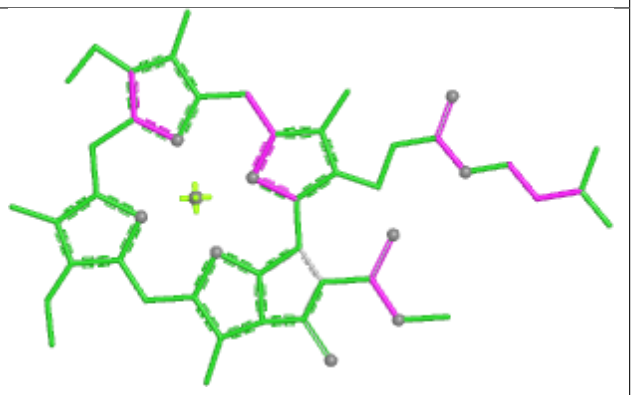

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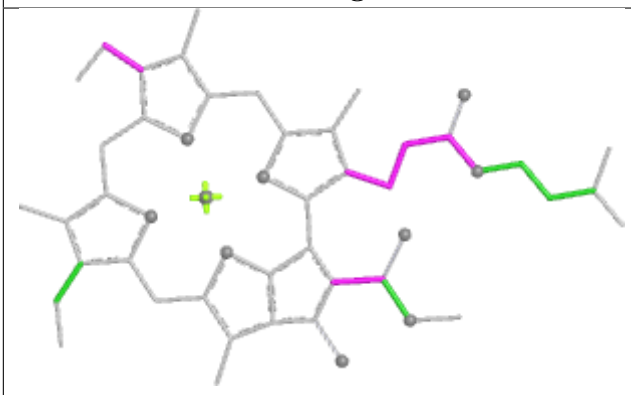

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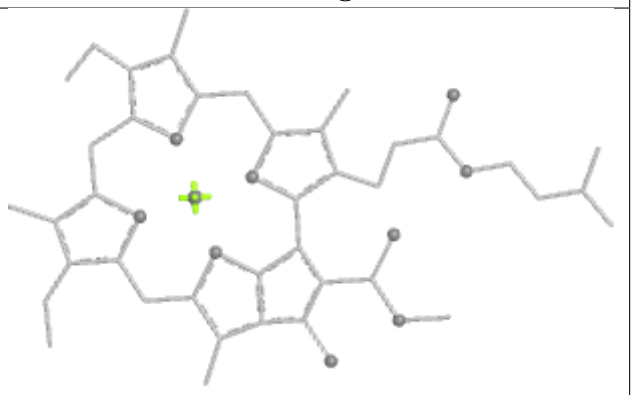
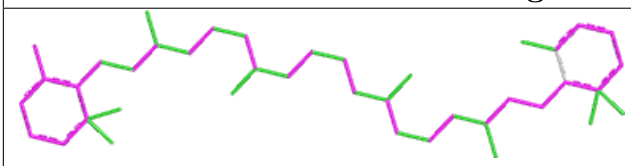


Rings

Ligand 8CT A 849



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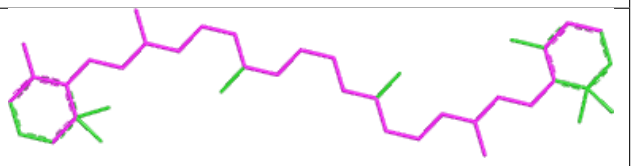
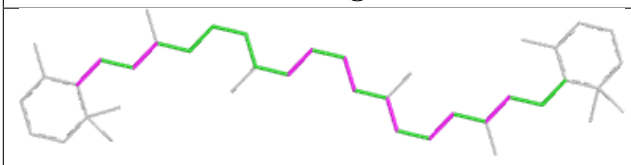


Bond angles



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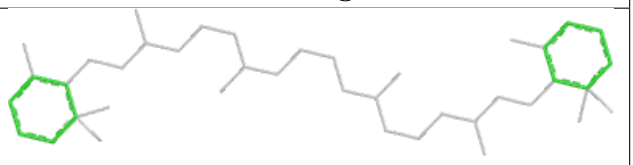
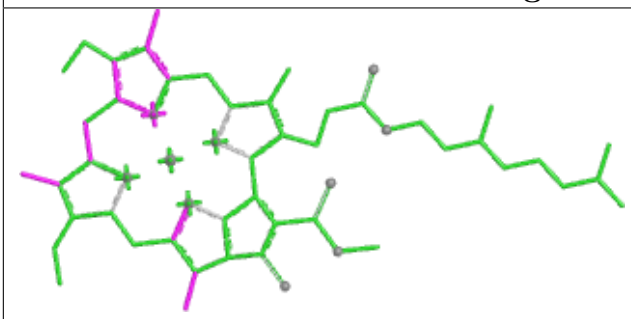


Rings

Ligand CLA A 803



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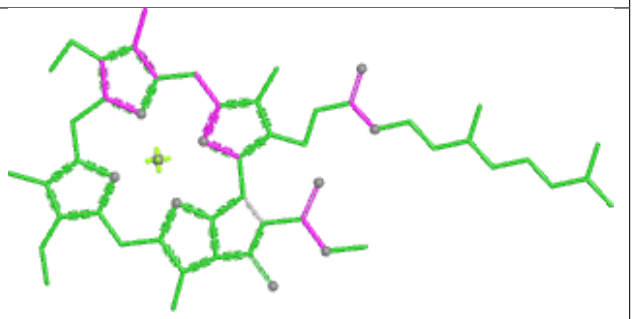
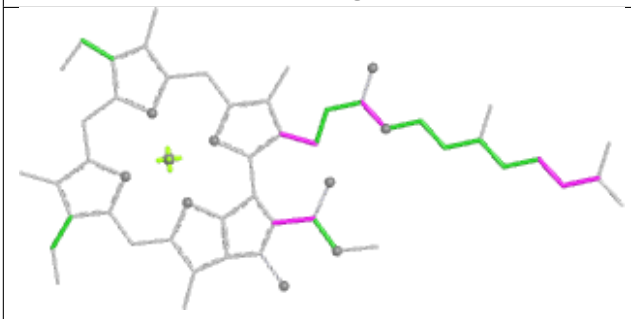


Bond angles



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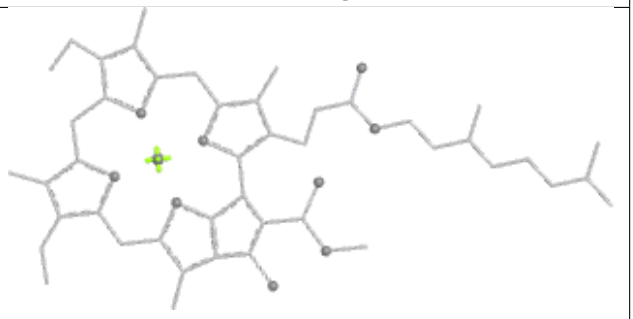
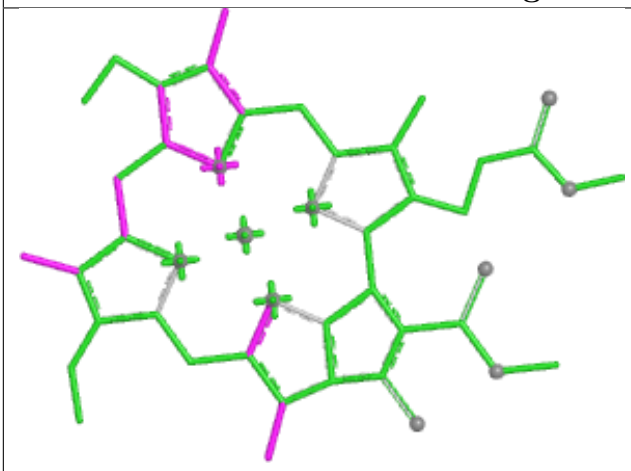


Rings

Ligand CLA K 103



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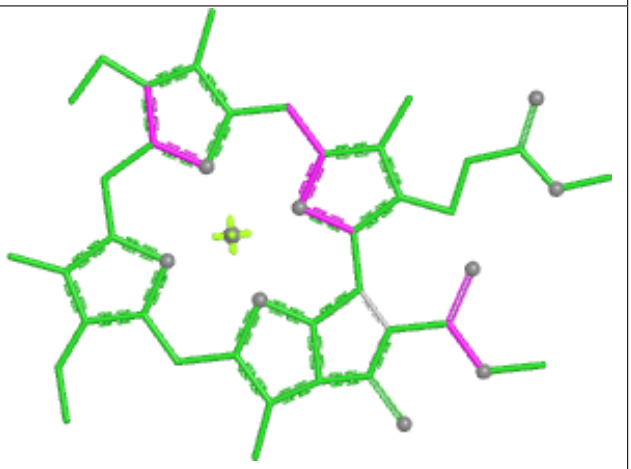

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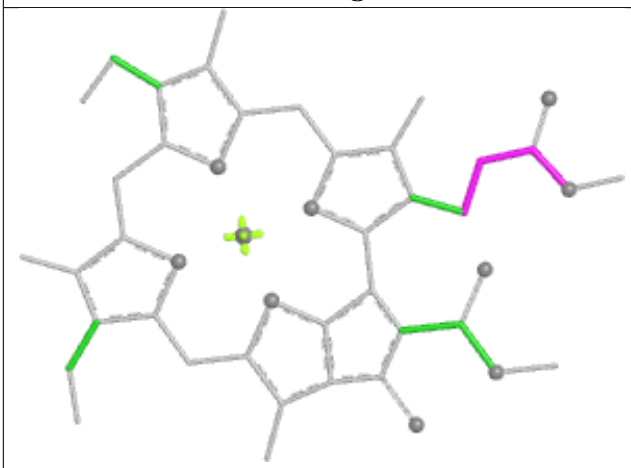

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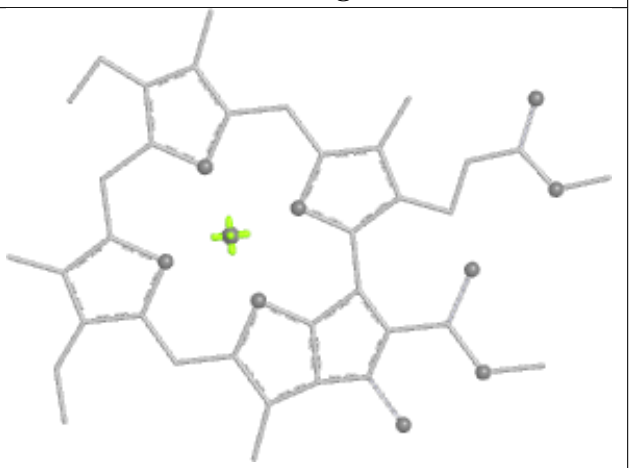
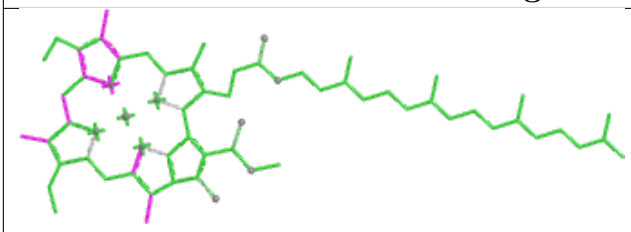


Rings

Ligand CLA A 839



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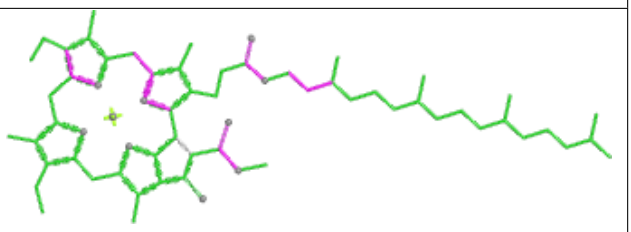

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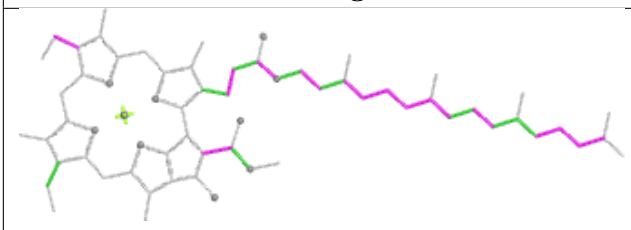

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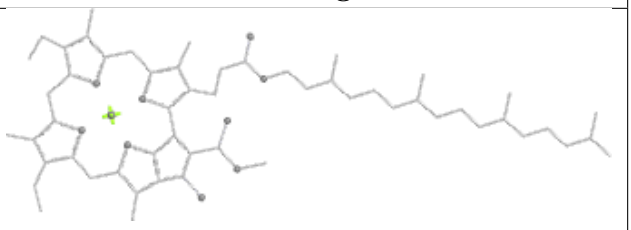
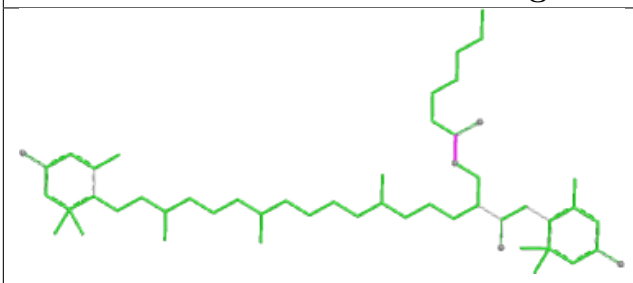


Rings

Ligand 0UR 8 319



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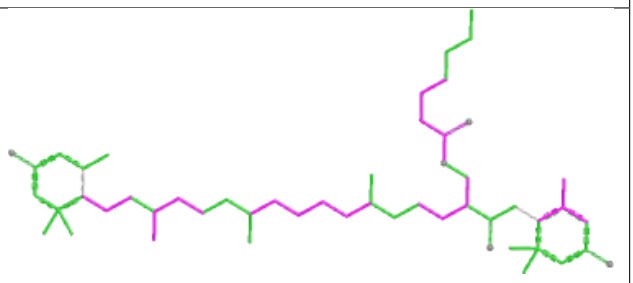
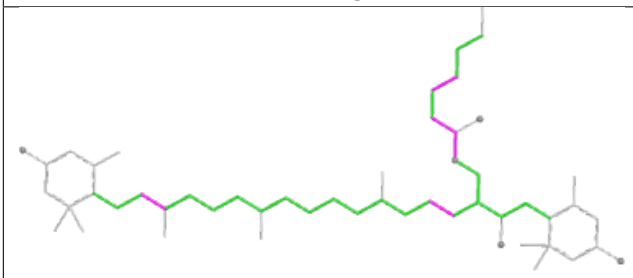


Bond angles



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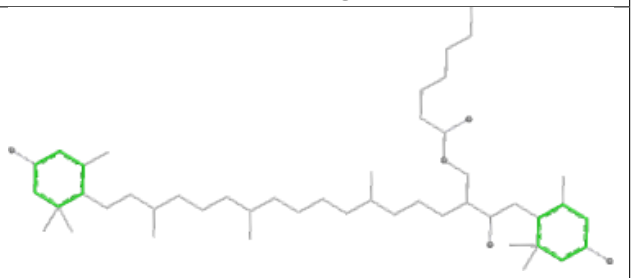
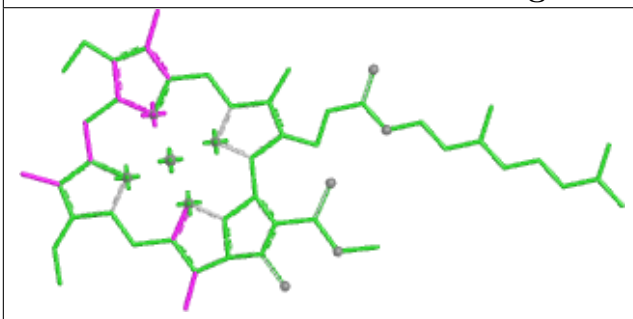


Rings

Ligand CLA 7 312



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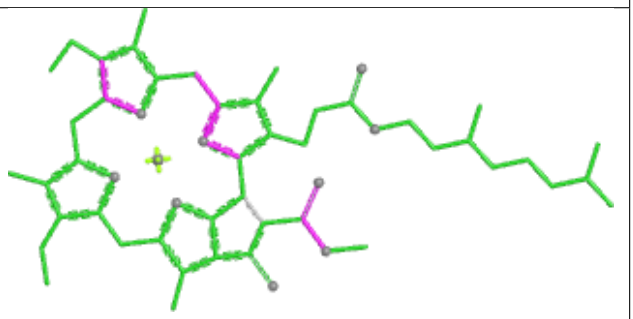
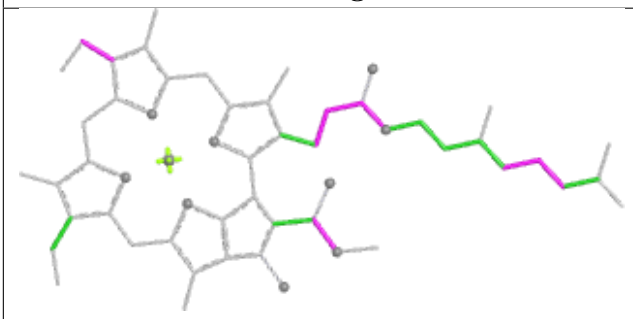


Bond angles



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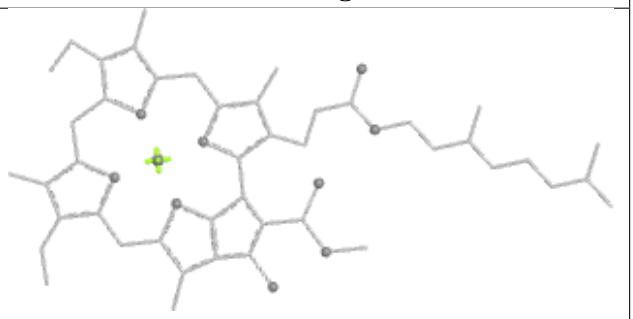
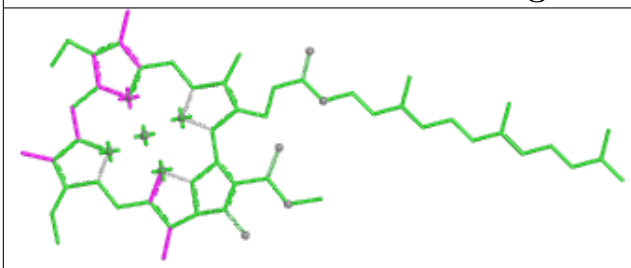


Rings

Ligand CLA 2 308



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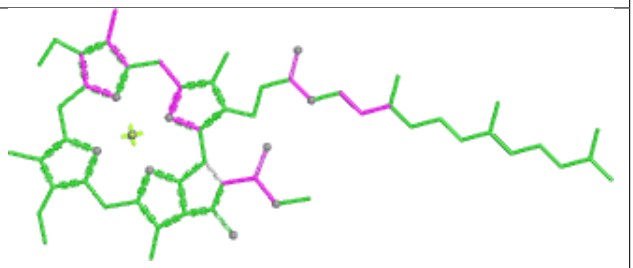
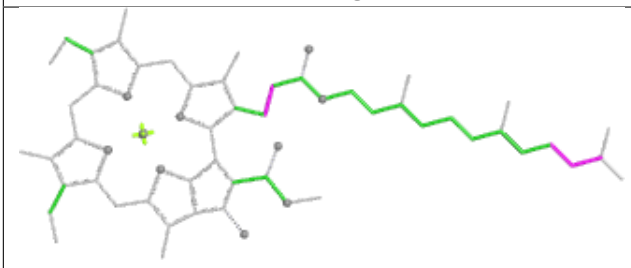


Bond angles



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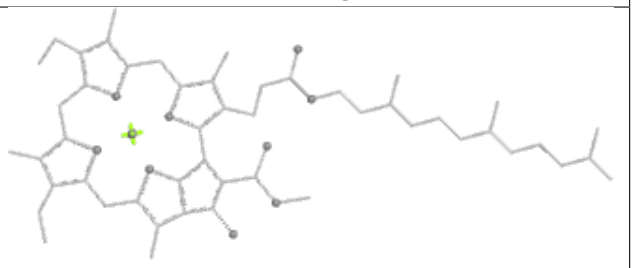
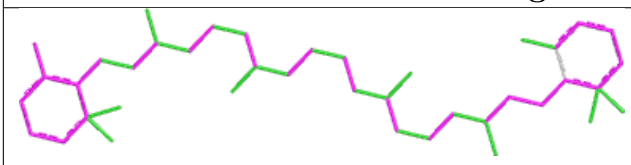


Rings

Ligand 8CT F 304



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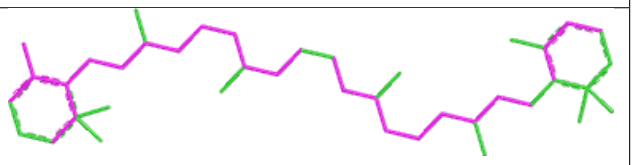

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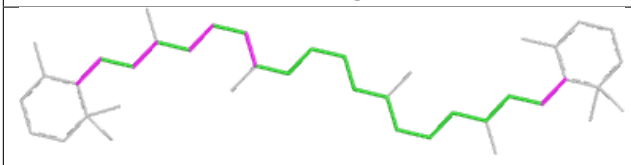
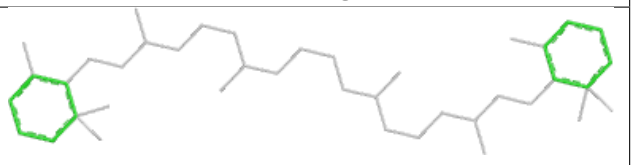
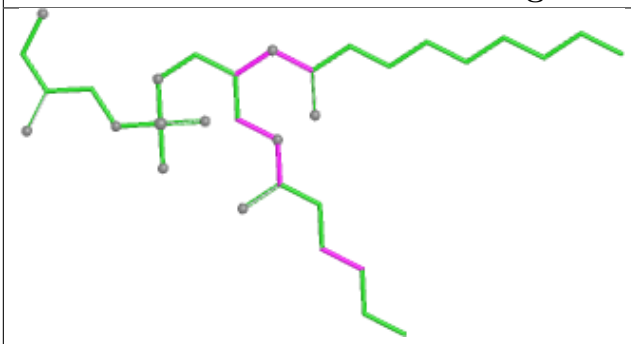


Torsions



Rings

Ligand LHG 2 317



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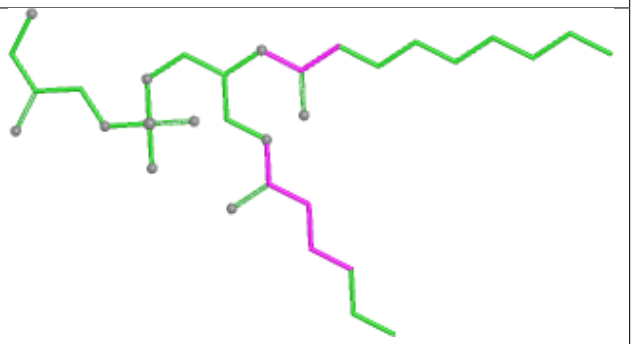

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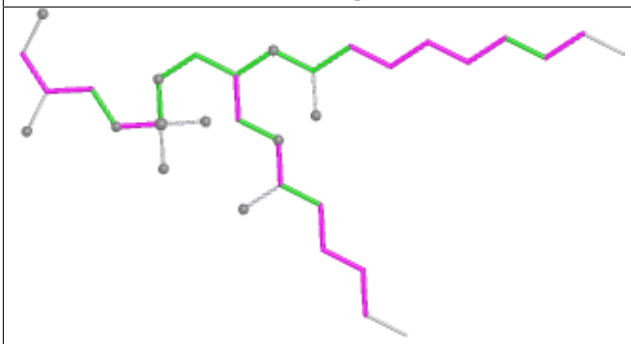

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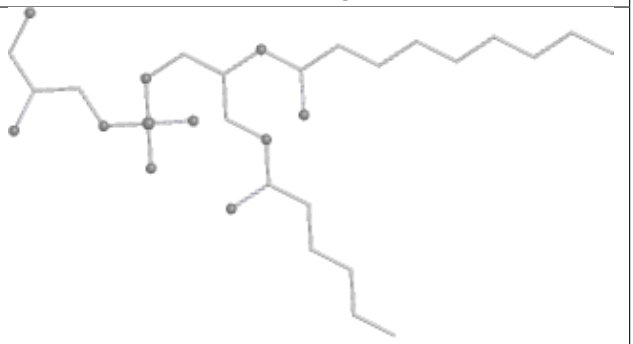
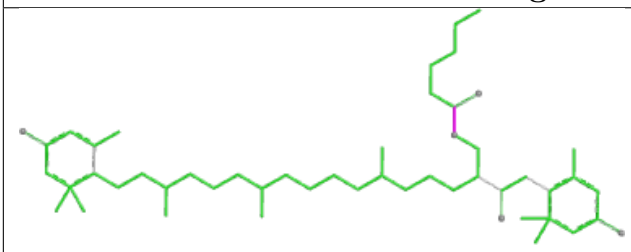


Rings

Ligand 0UR 8 318



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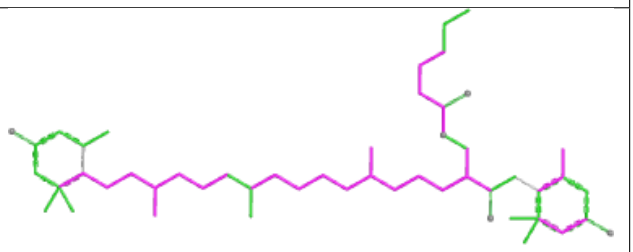

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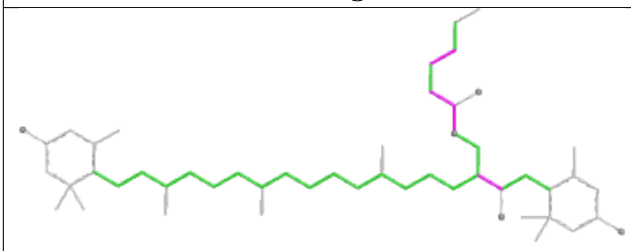

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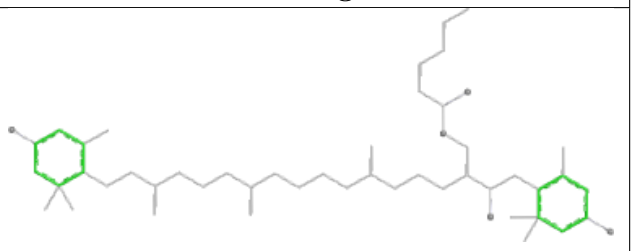
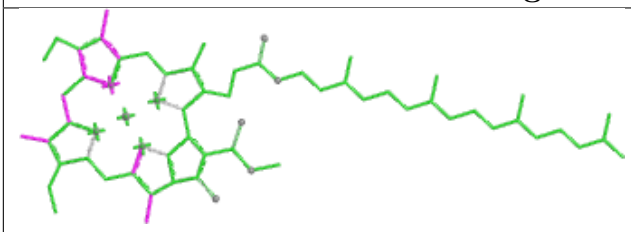


Rings

Ligand CLA A 804



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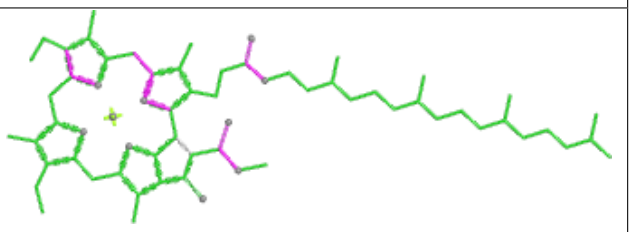

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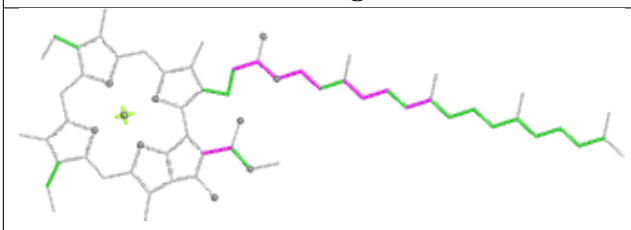

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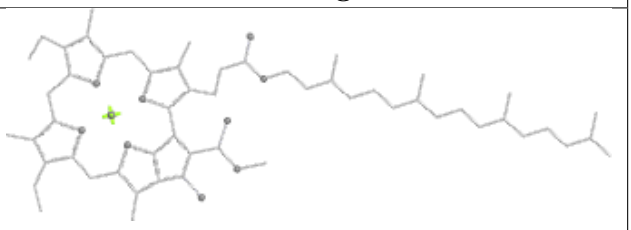
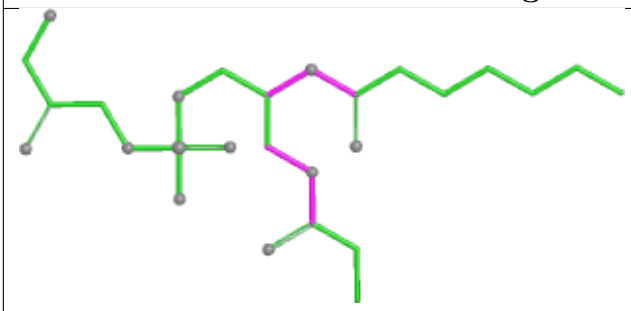


Rings

Ligand LHG A 843



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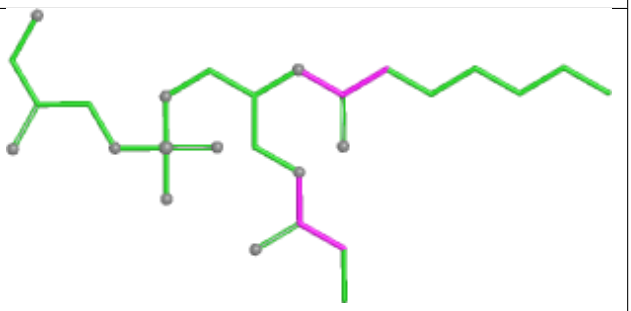

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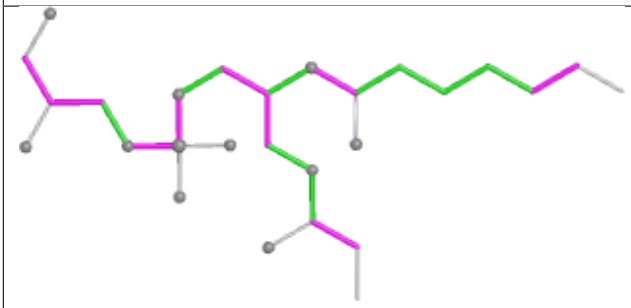

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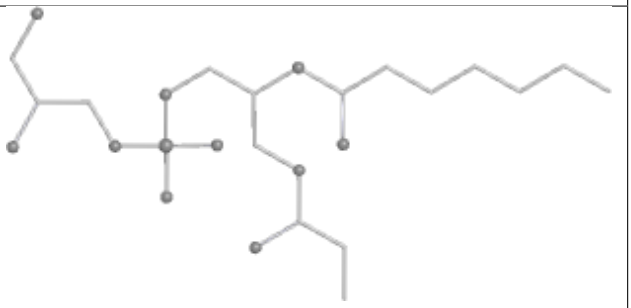
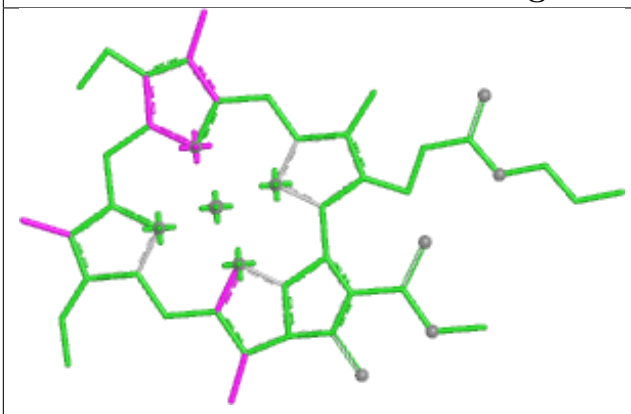


Rings

Ligand CLA 9 303



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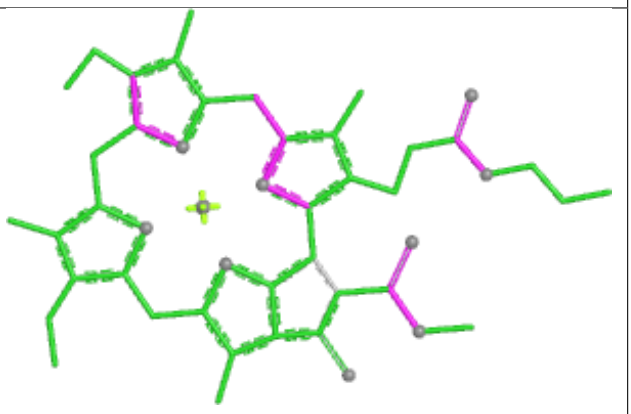

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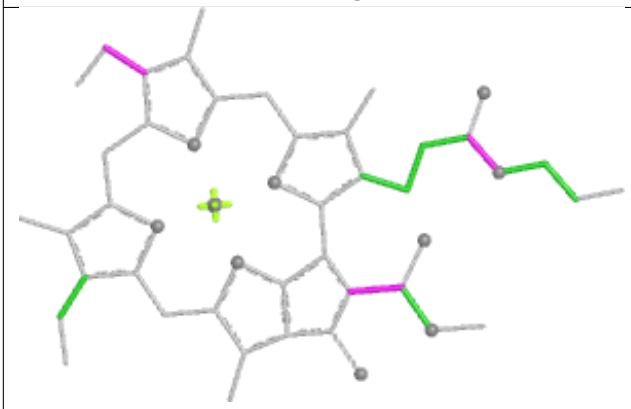

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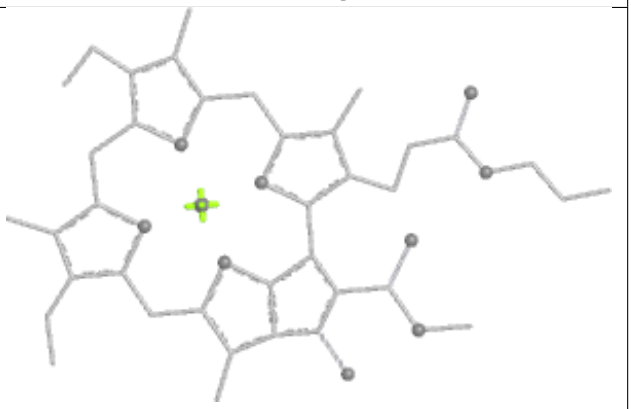
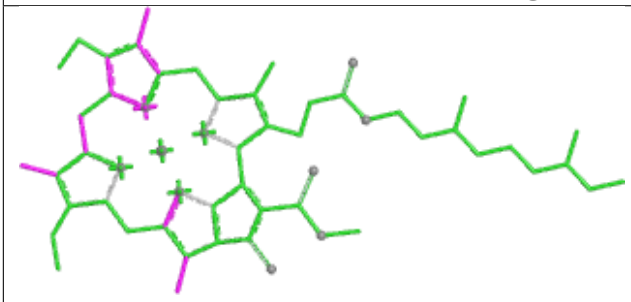


Rings

Ligand CLA B 820



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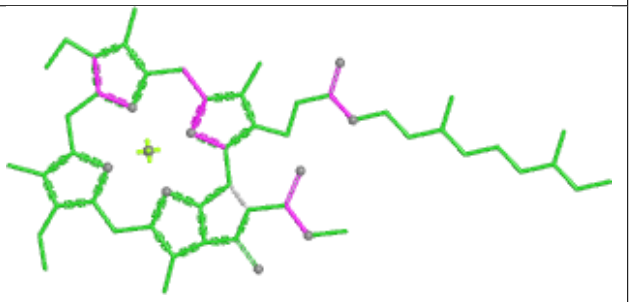

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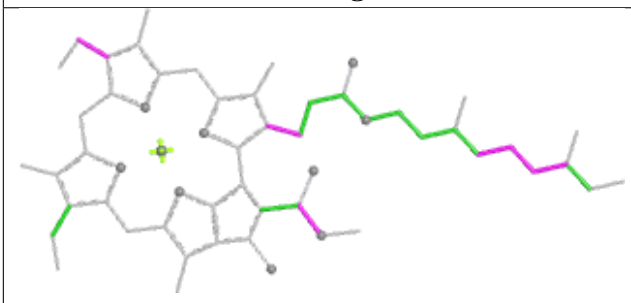

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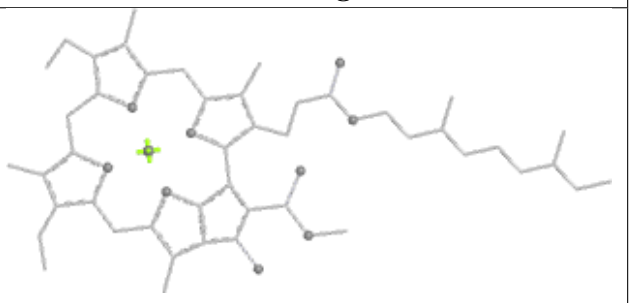
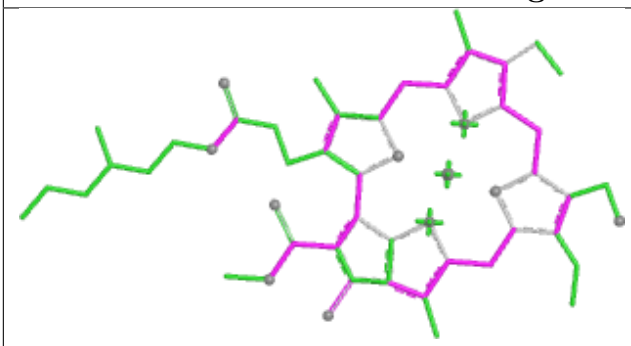


Rings

Ligand CHL 4 302



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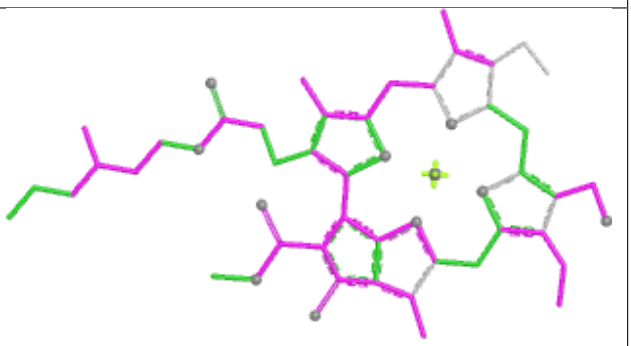

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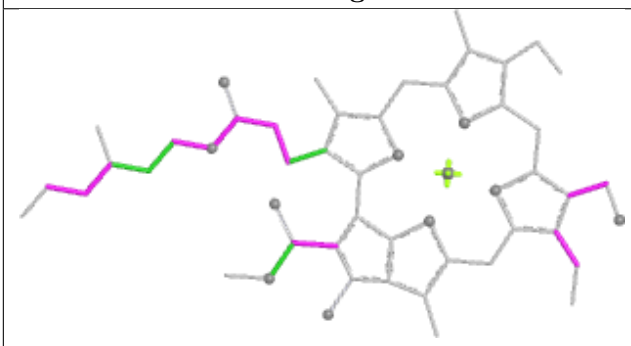

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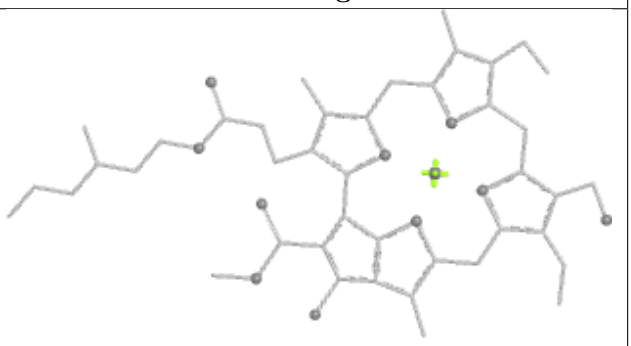
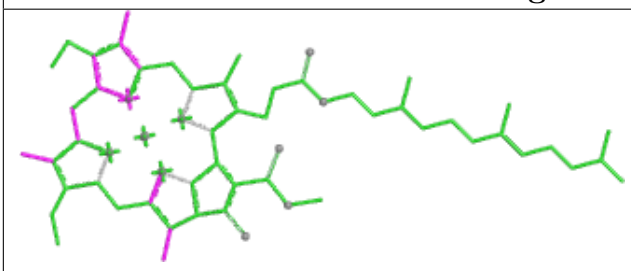


Rings

Ligand CLA 7 317



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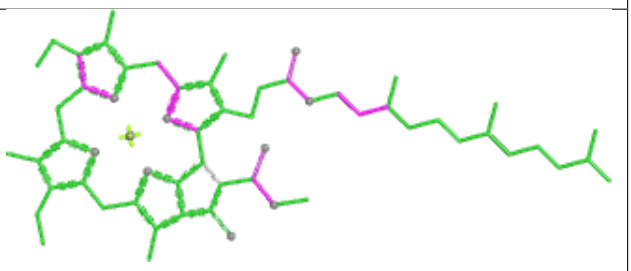
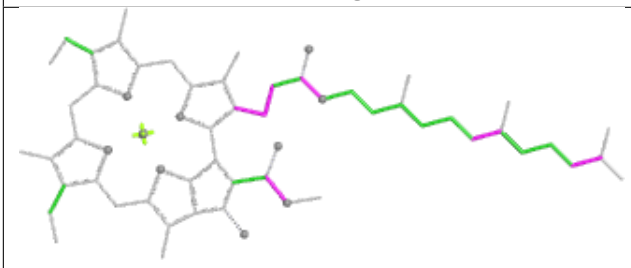


Bond angles



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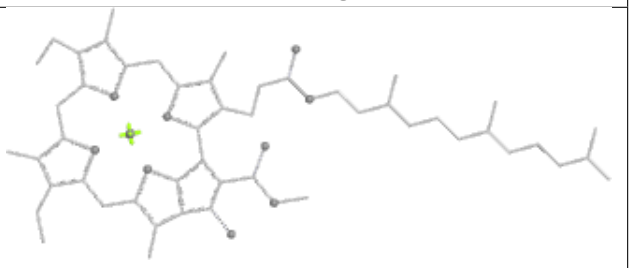
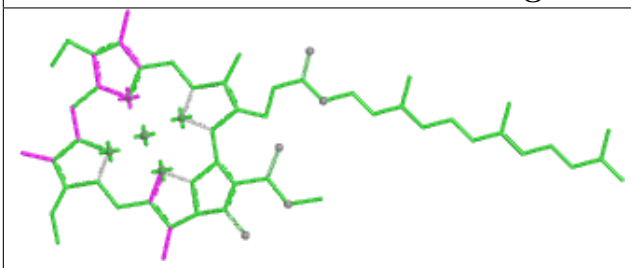


Rings

Ligand CLA B 824



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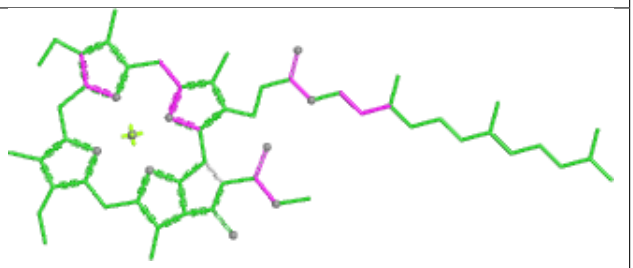

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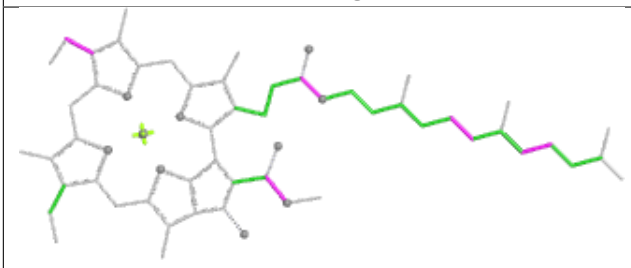

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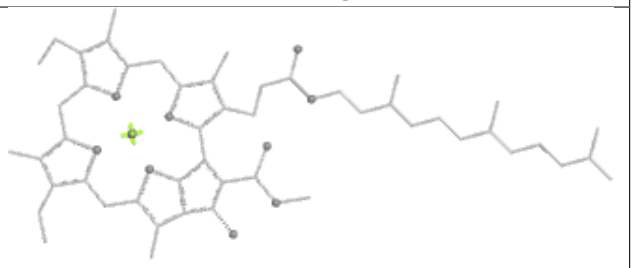
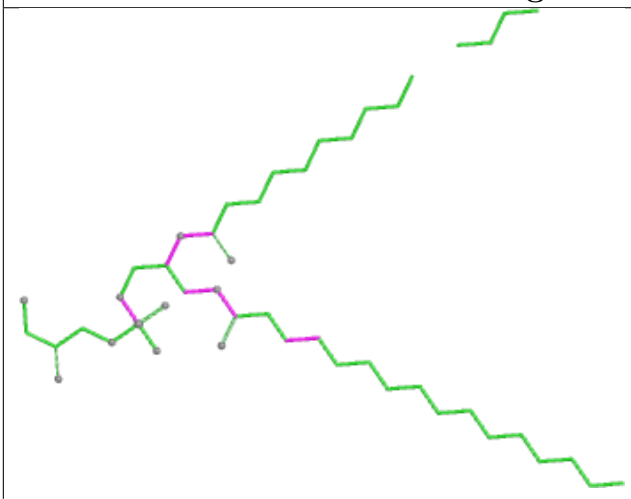


Rings

Ligand LHG 9 316



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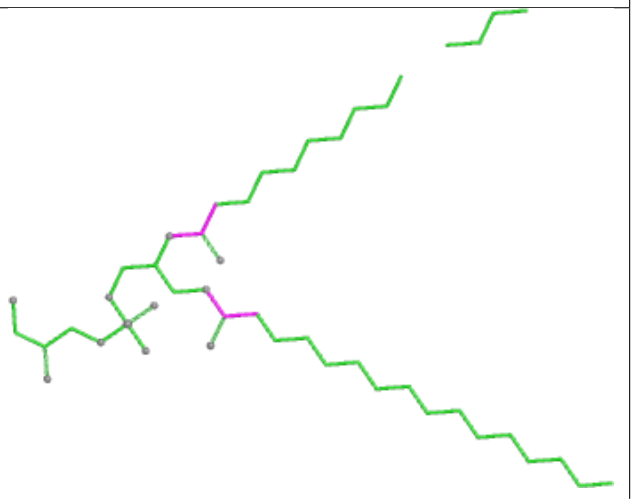
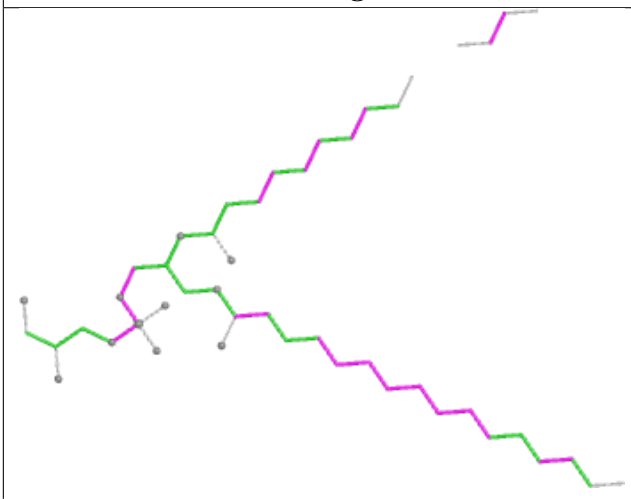


Bond angles



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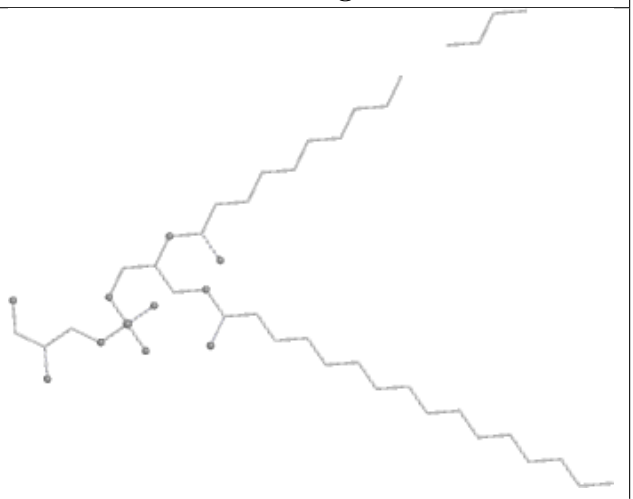
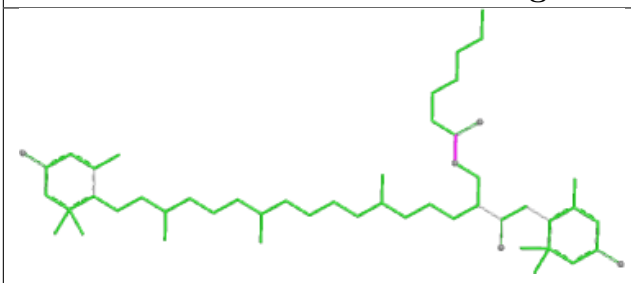
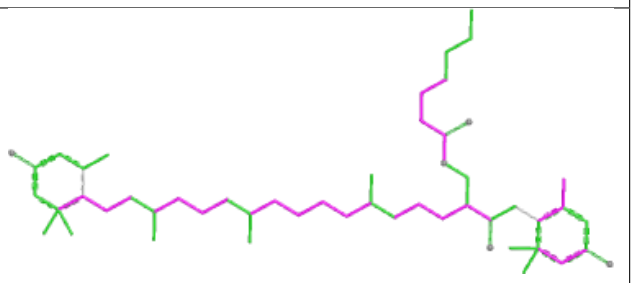
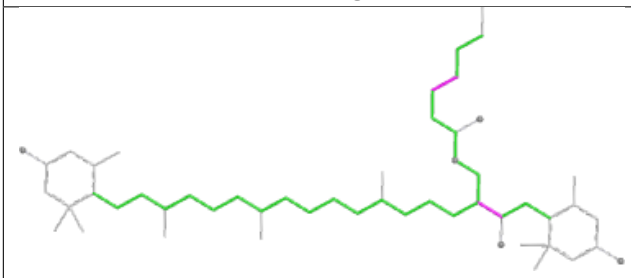
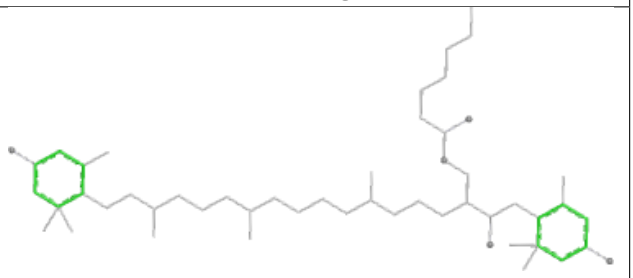
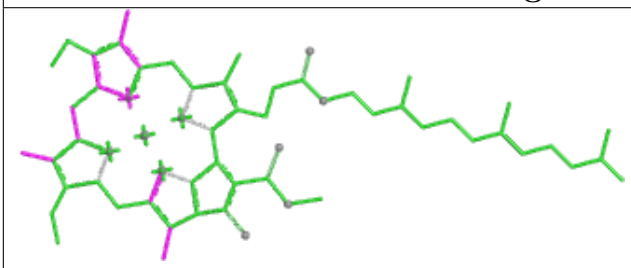
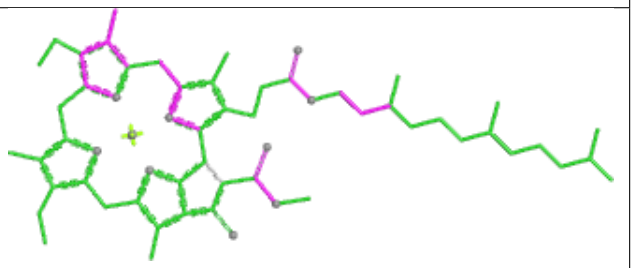
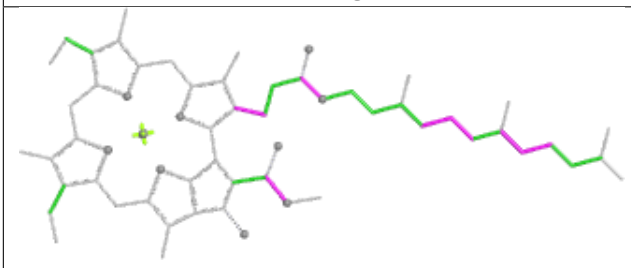
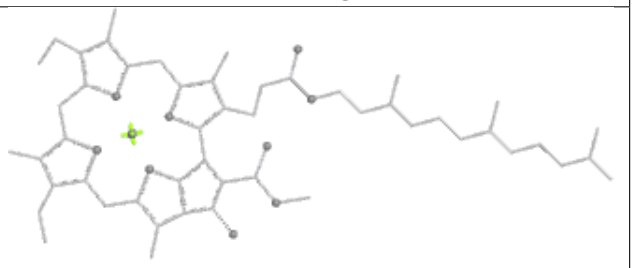
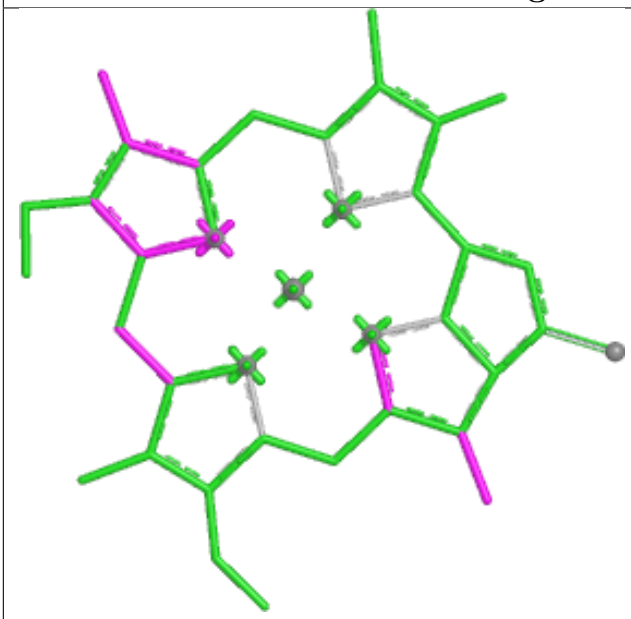


Rings

Ligand 0UR 0 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 310



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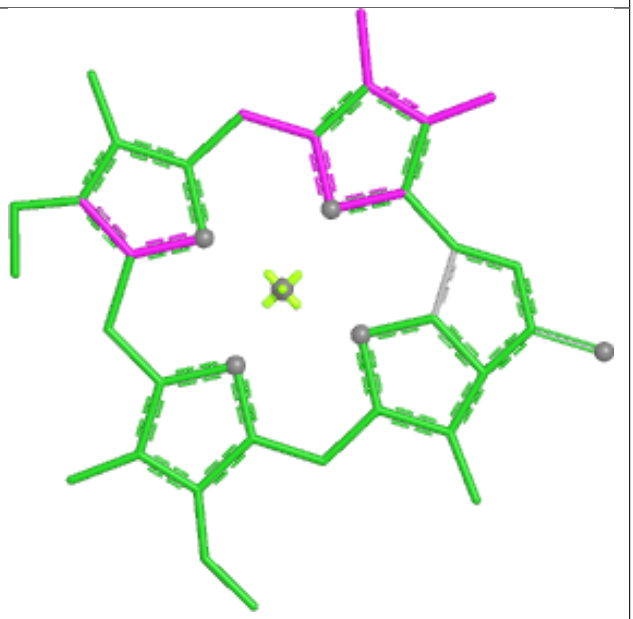
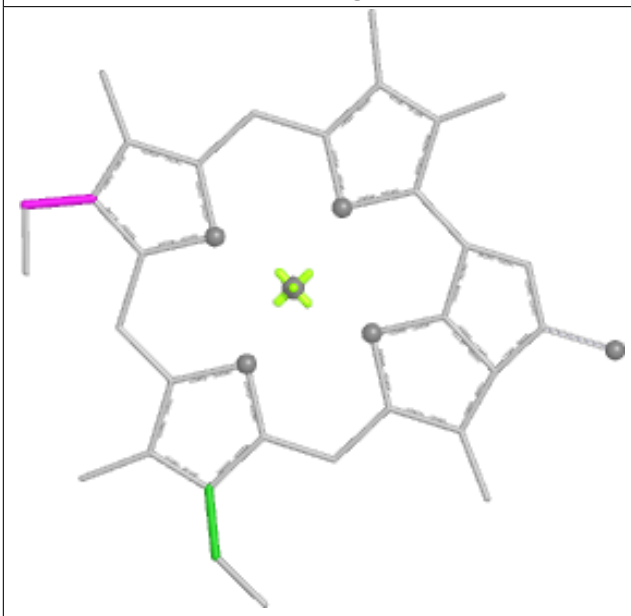
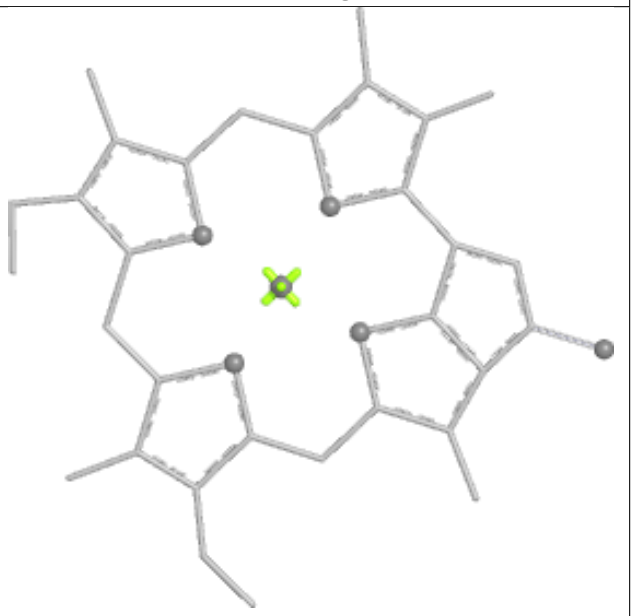


Bond angles

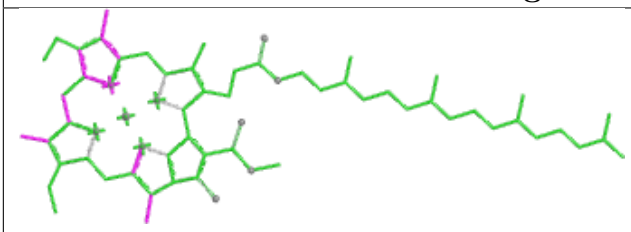


Torsions

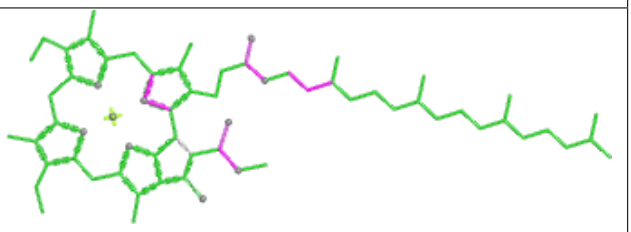


Rings

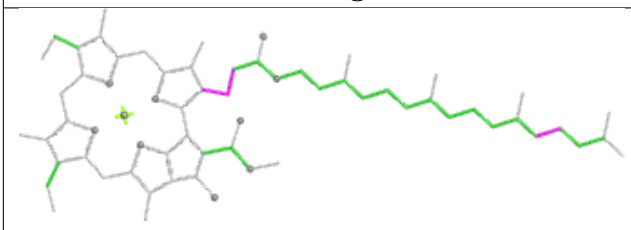
Ligand CLA A 801



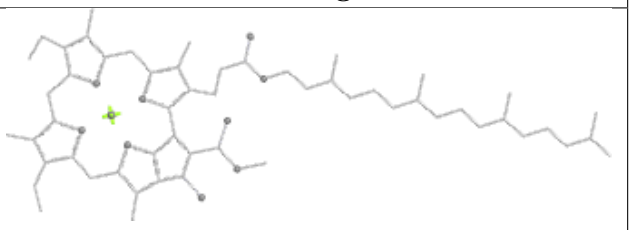
Bond lengths



Bond angles

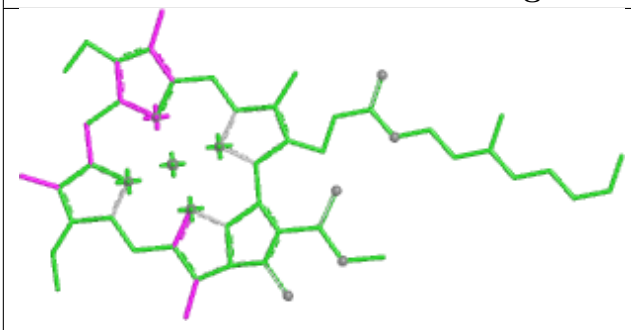


Torsions



Rings

Ligand CLA A 811



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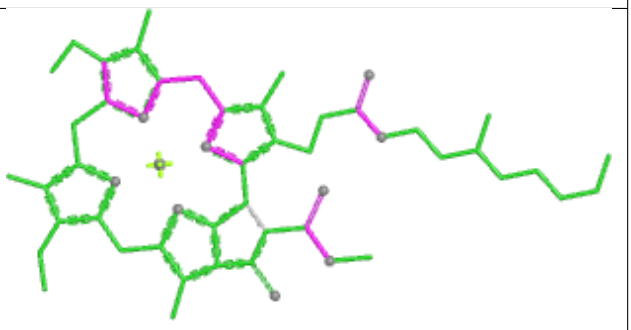

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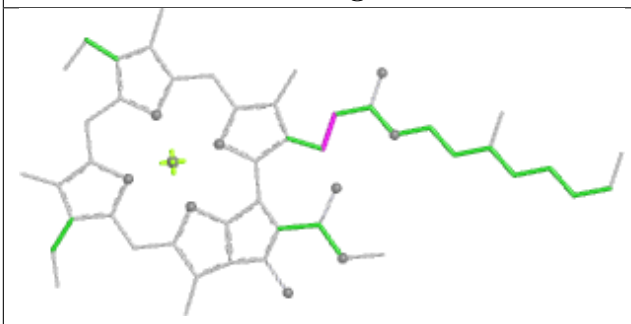

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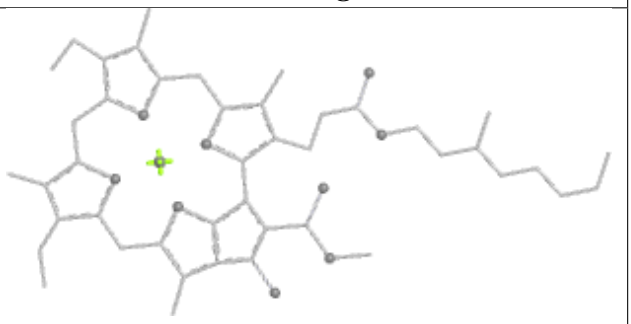
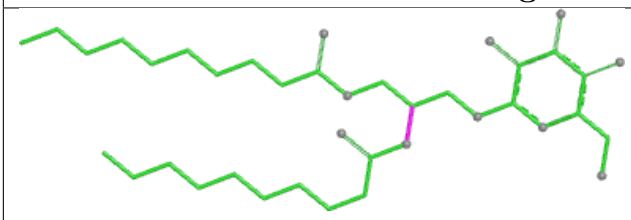


Rings

Ligand LMG O 210



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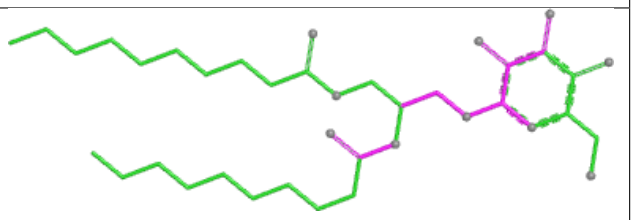
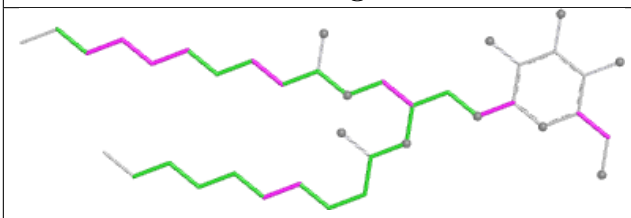


Bond angles



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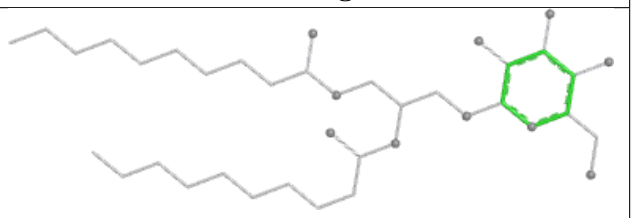
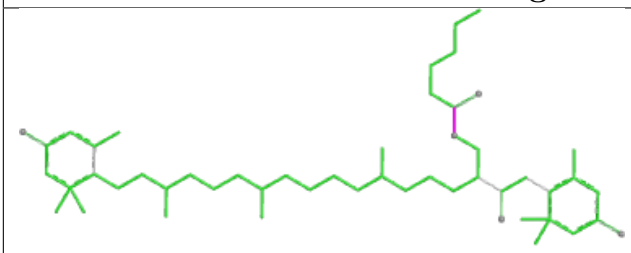


Rings

Ligand 0UR 7 320



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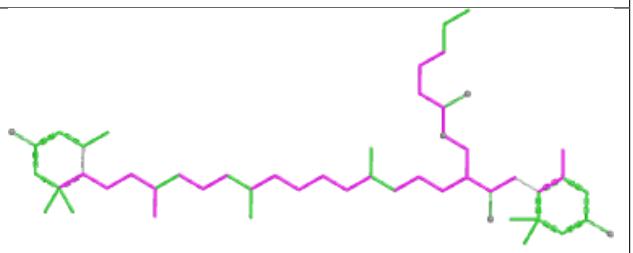

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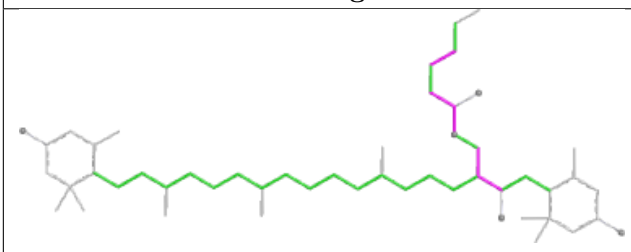

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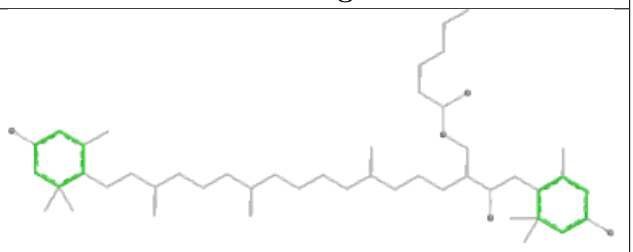
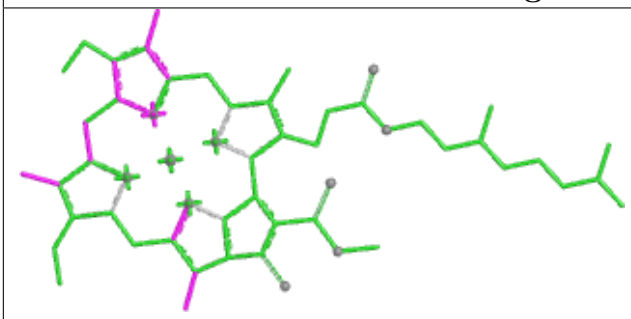
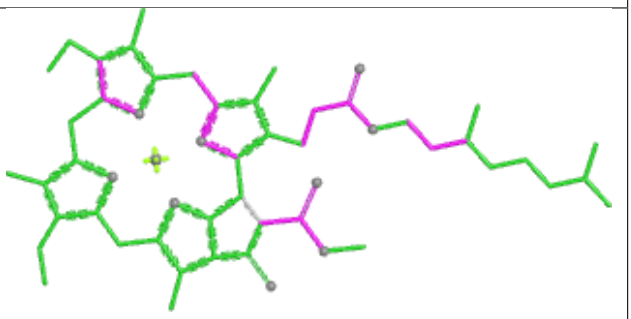
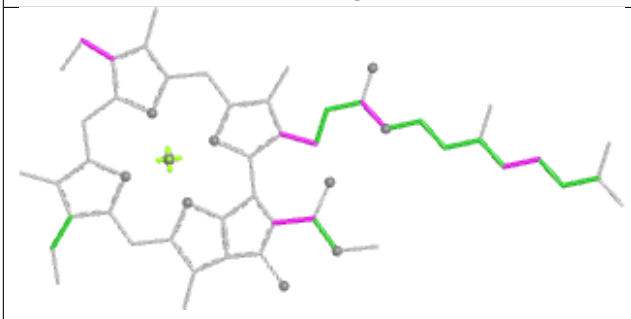
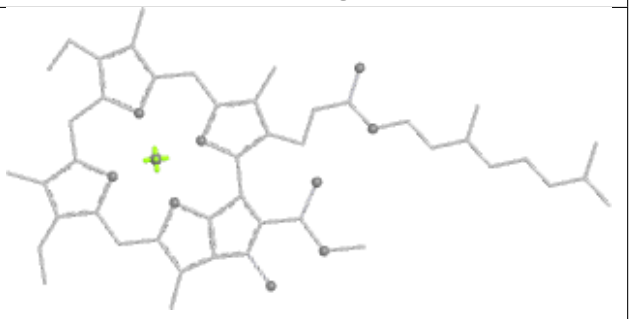


Rings

Ligand CLA B 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

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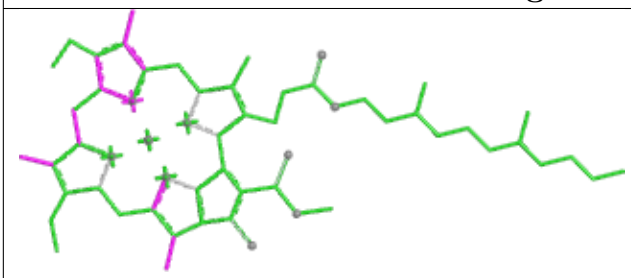
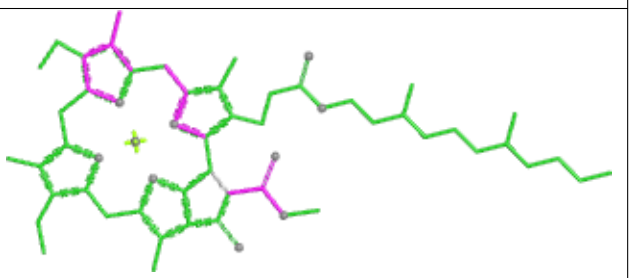
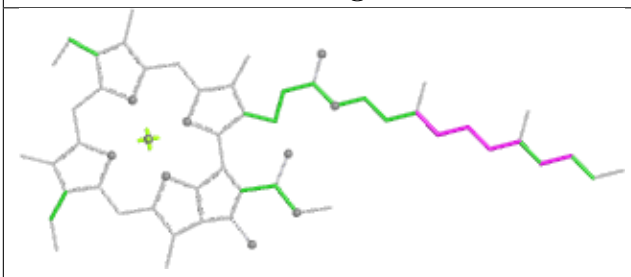
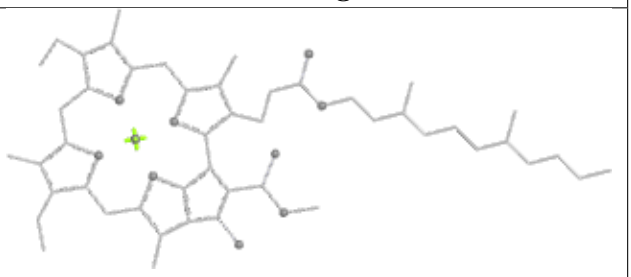
	
Bond lengths	Bond angles
	
Torsions	Rings

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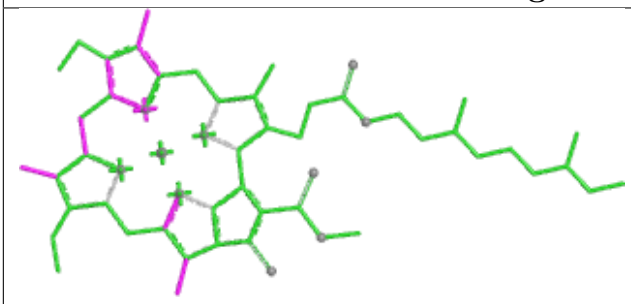	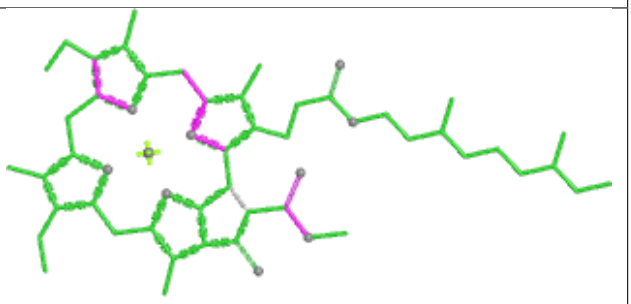
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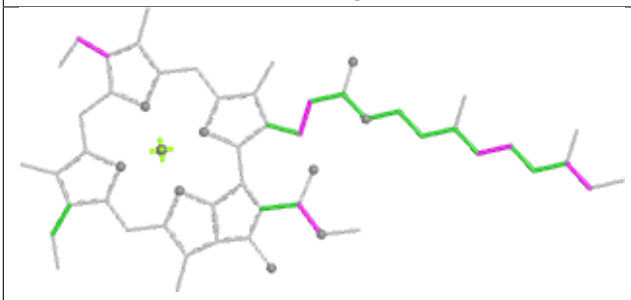
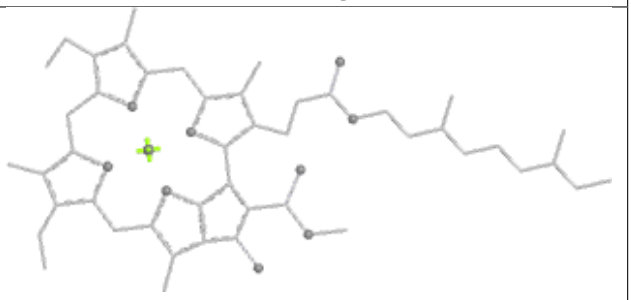
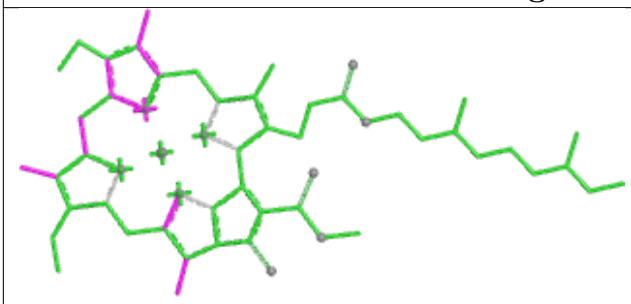
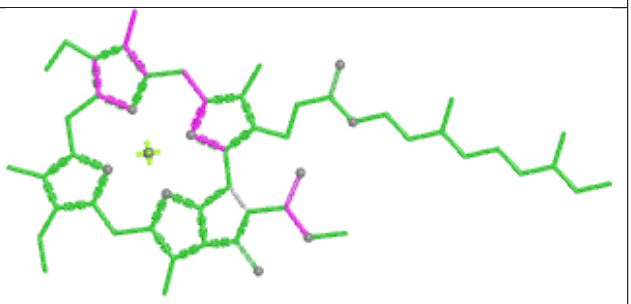
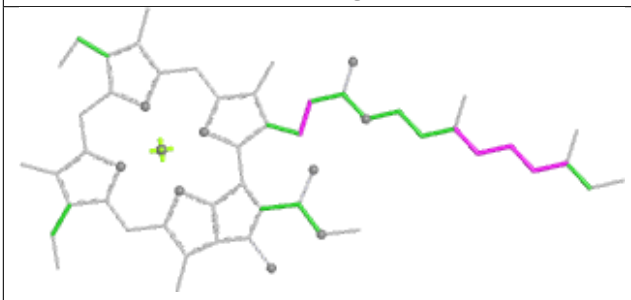
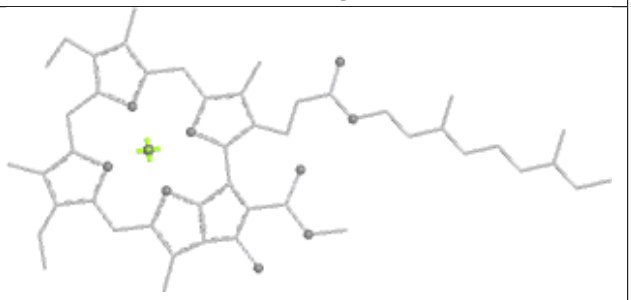
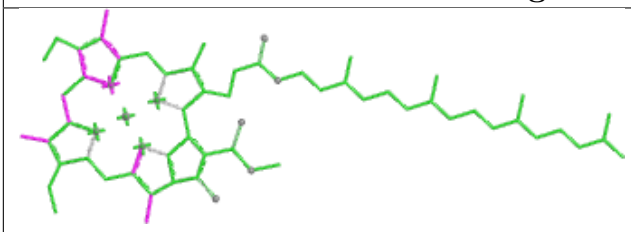
	
Torsions	Rings

Ligand CLA 9 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 307



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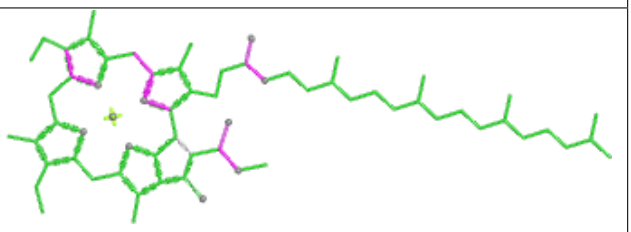
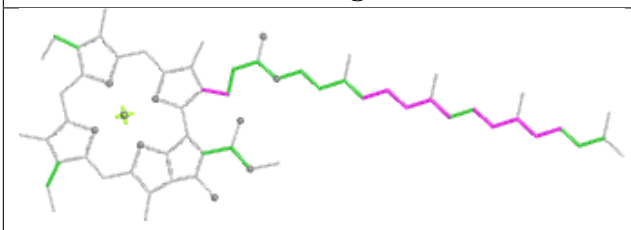


Bond angles



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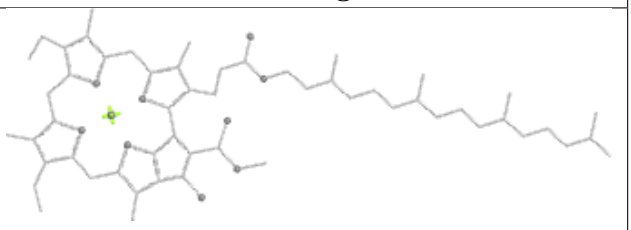
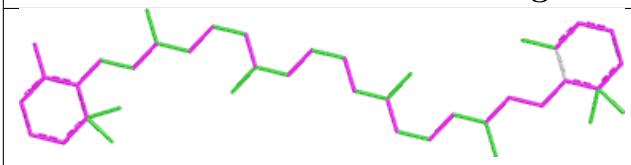


Rings

Ligand 8CT 6 319



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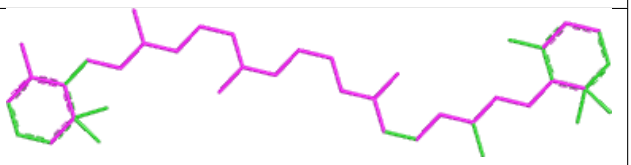
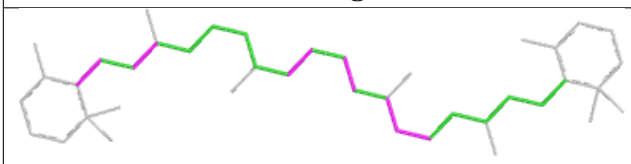


Bond angles



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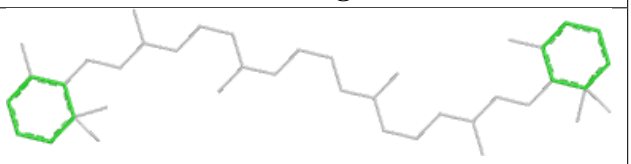
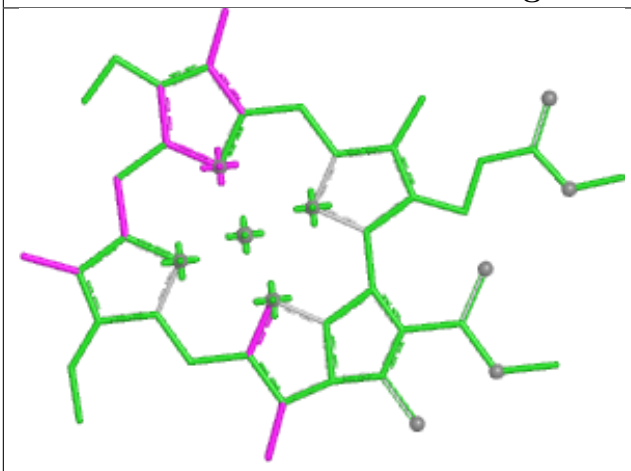


Rings

Ligand CLA H 201



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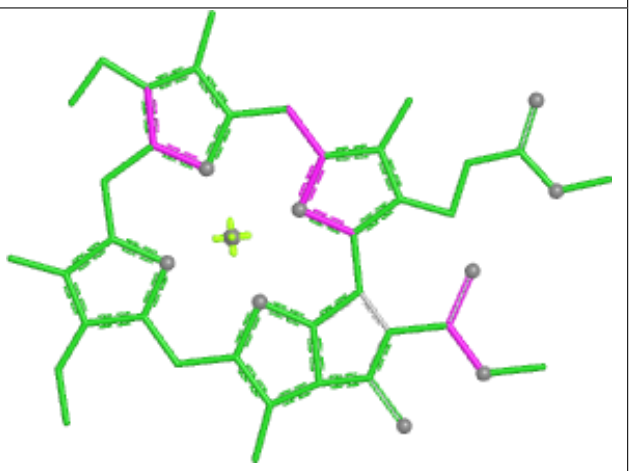

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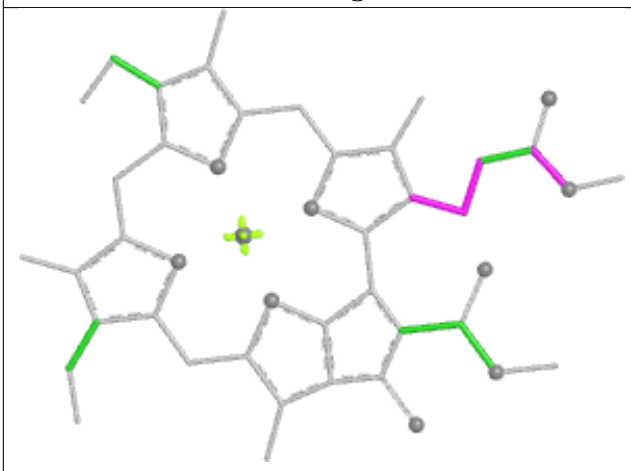

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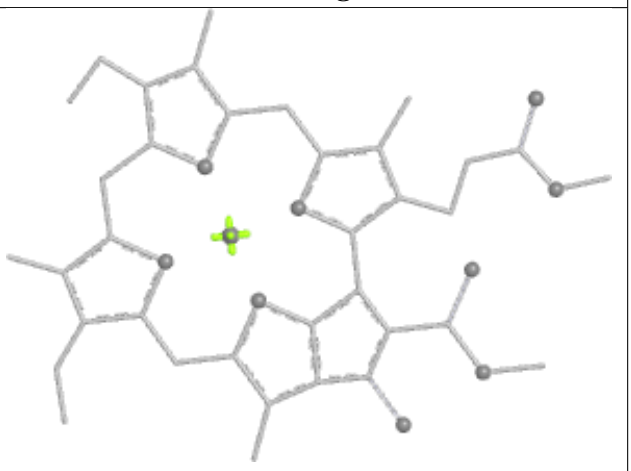
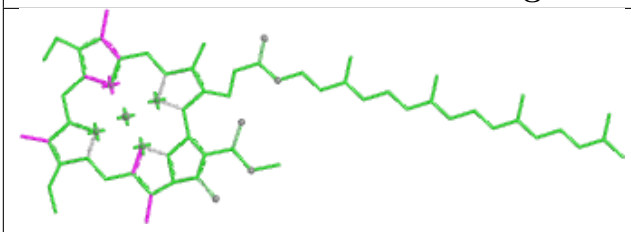


Rings

Ligand CLA A 817



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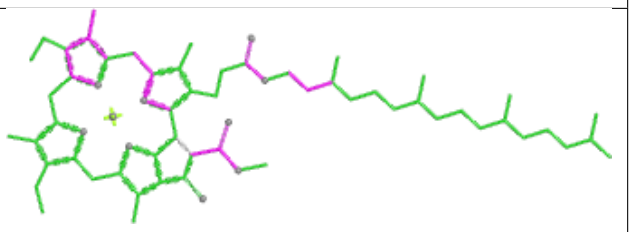
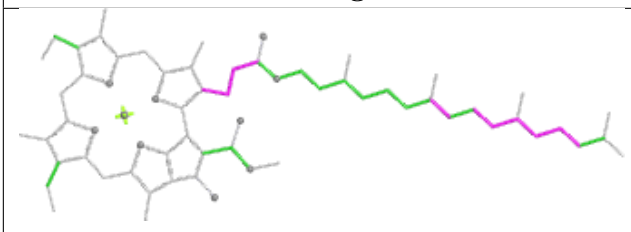
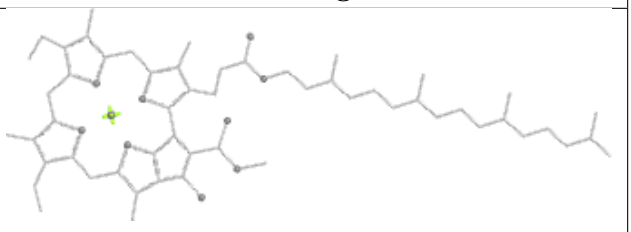


Bond angles

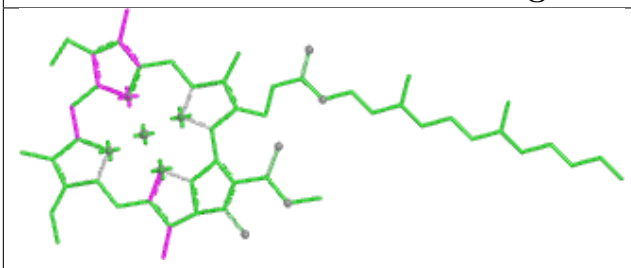


Torsions



Rings

Ligand CLA 5 302



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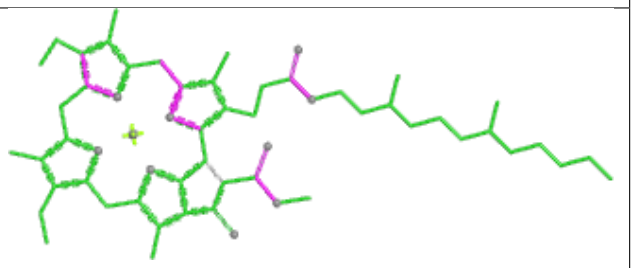
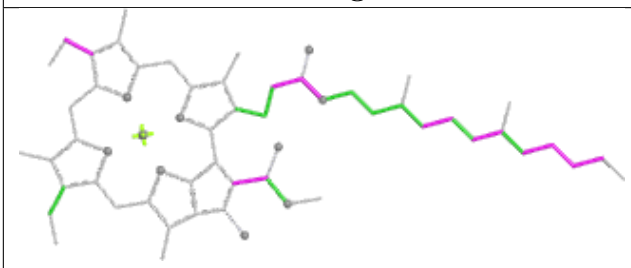


Bond angles



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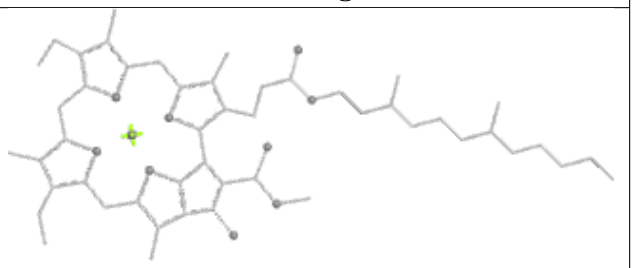
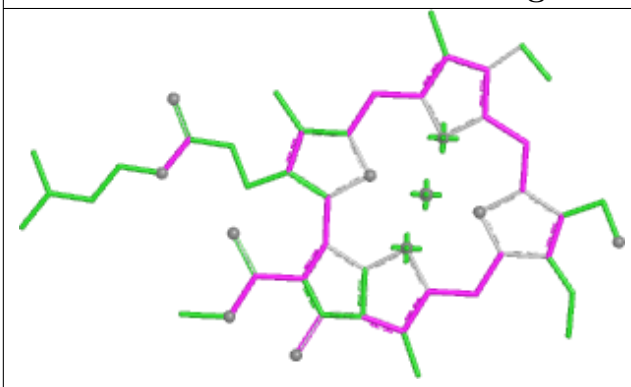


Rings

Ligand CHL 9 305



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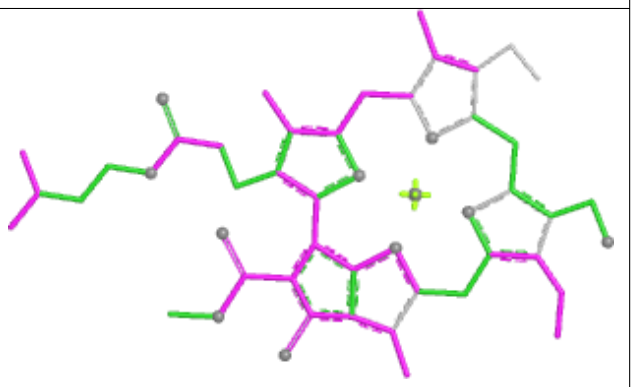
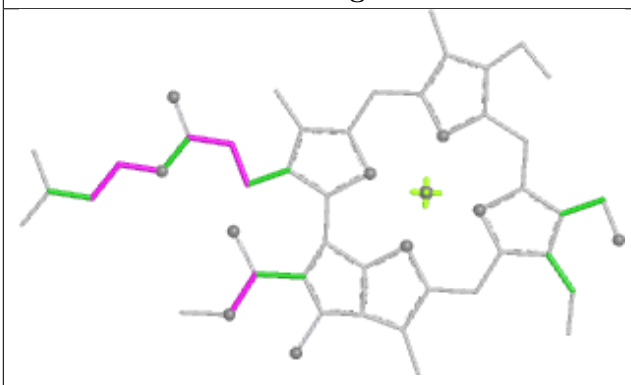
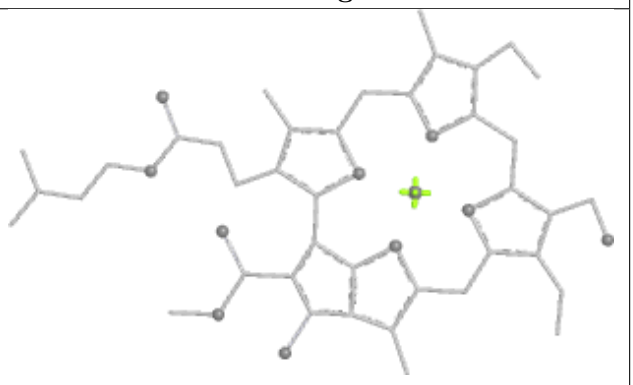


Bond angles

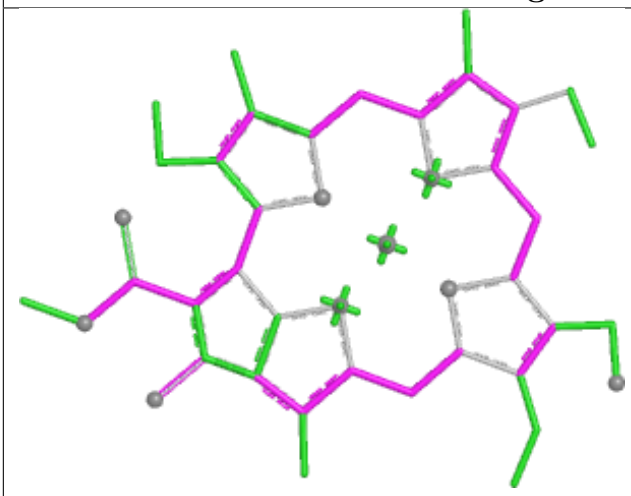


Torsions

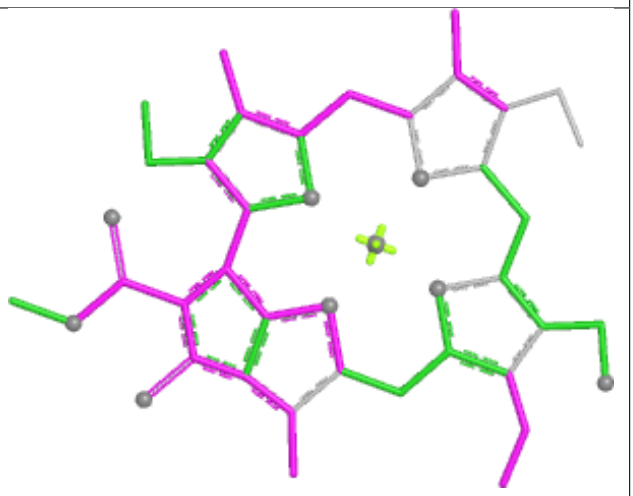


Rings

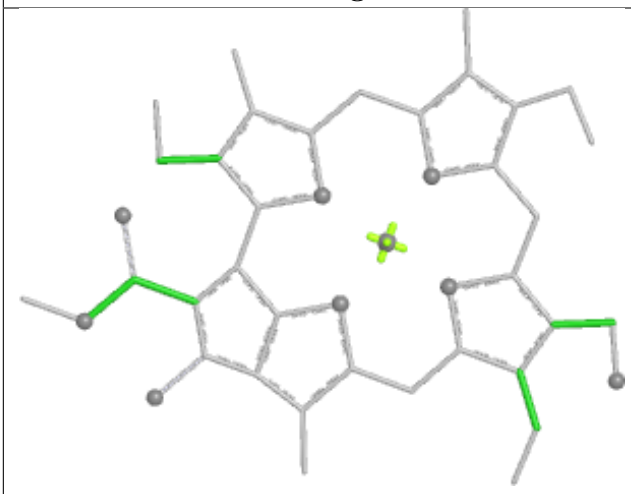
Ligand CHL 6 305



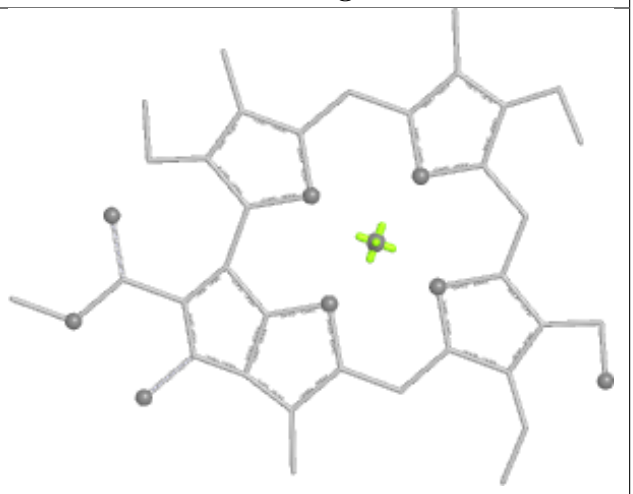
Bond lengths



Bond angles

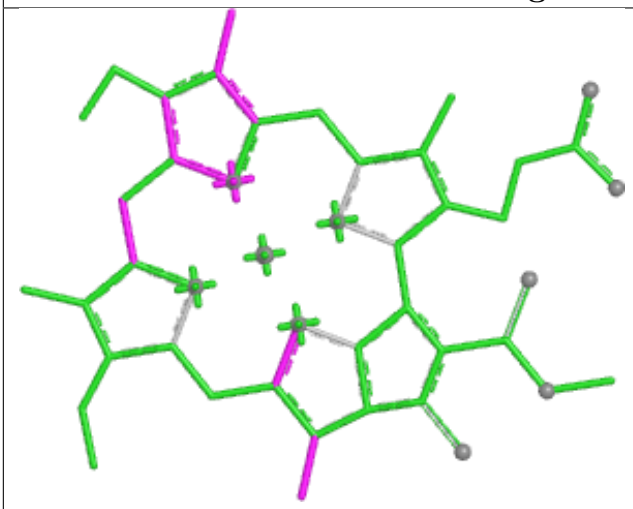


Torsions



Rings

Ligand CLA 0 313



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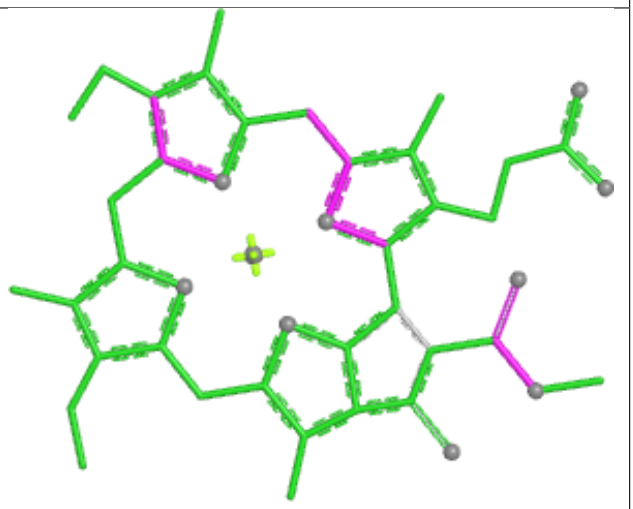

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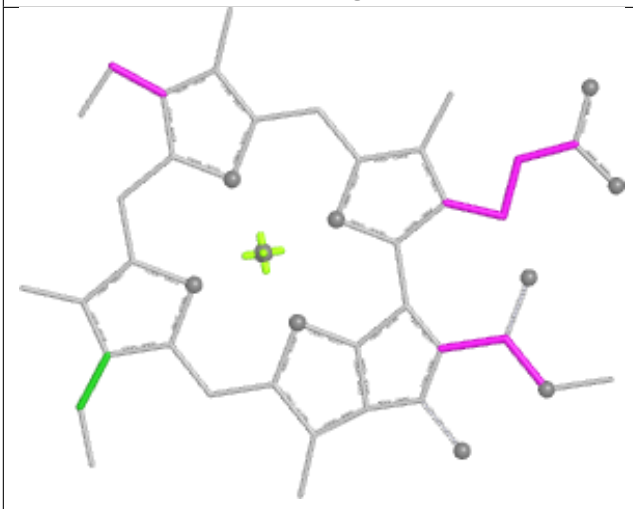
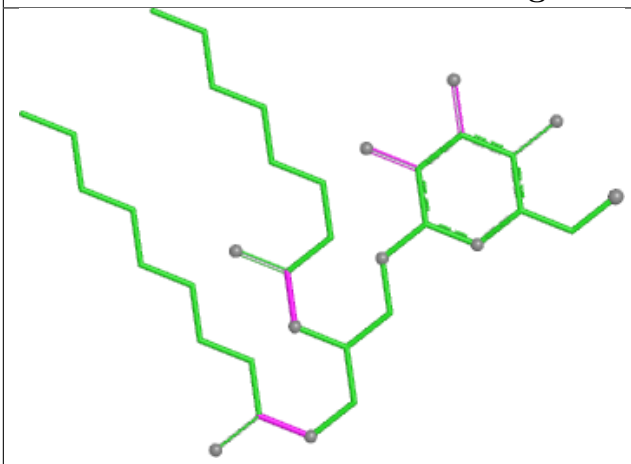


Torsions

Rings

Ligand SQD 0 318



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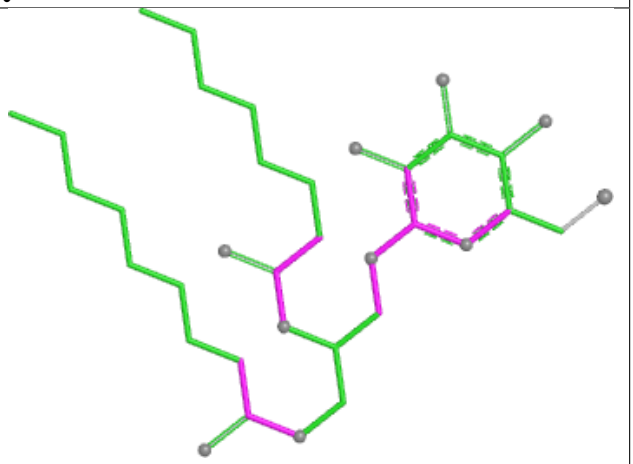
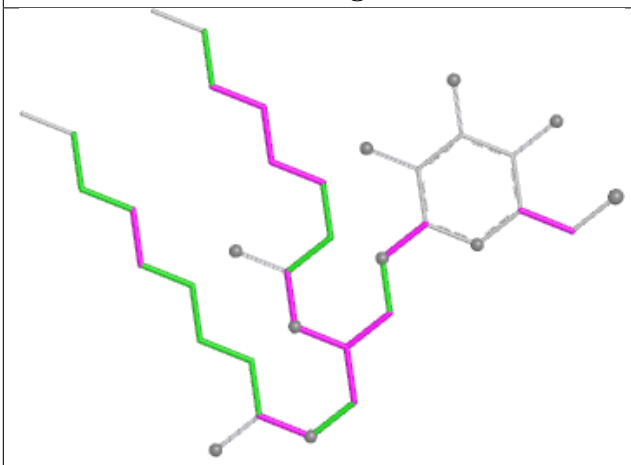


Bond angles



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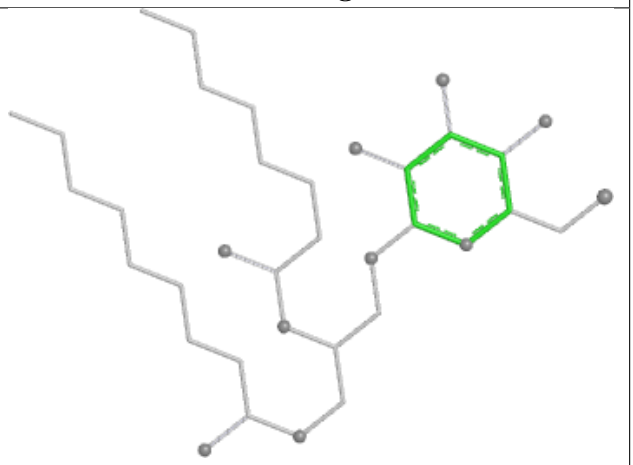
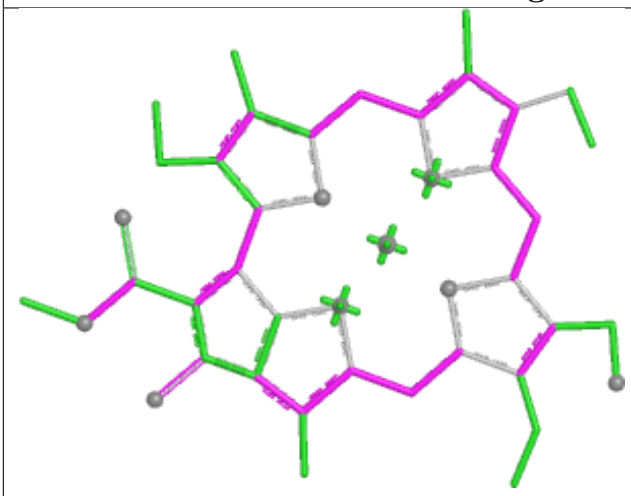


Rings

Ligand CHL 8 316



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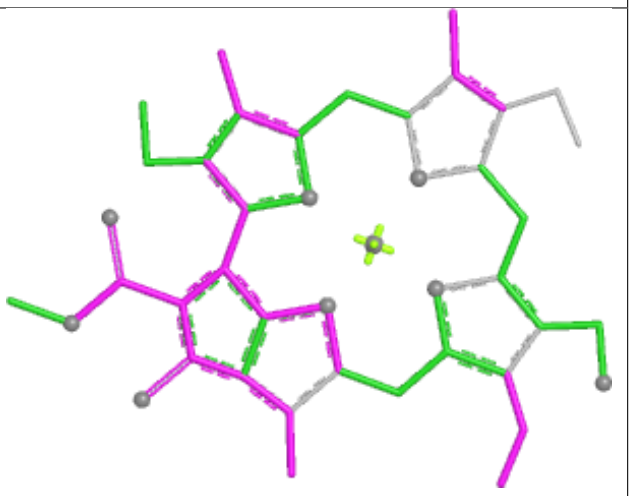

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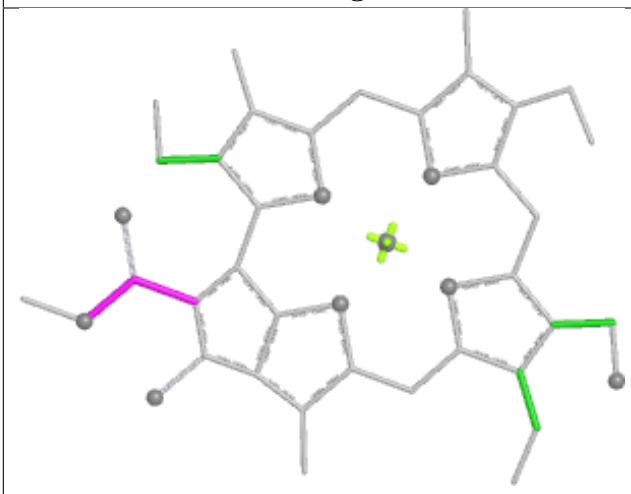

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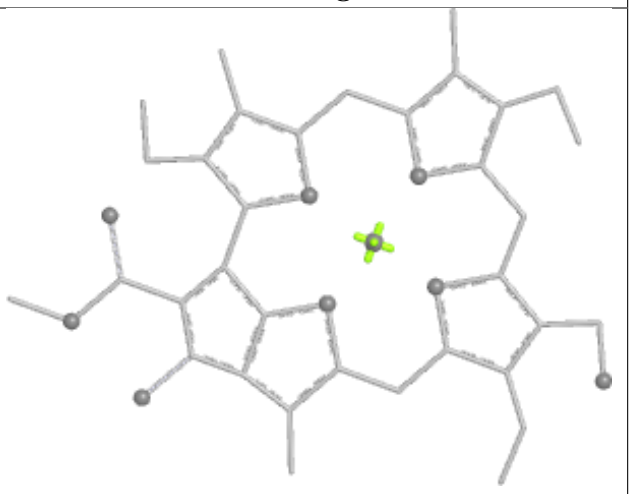
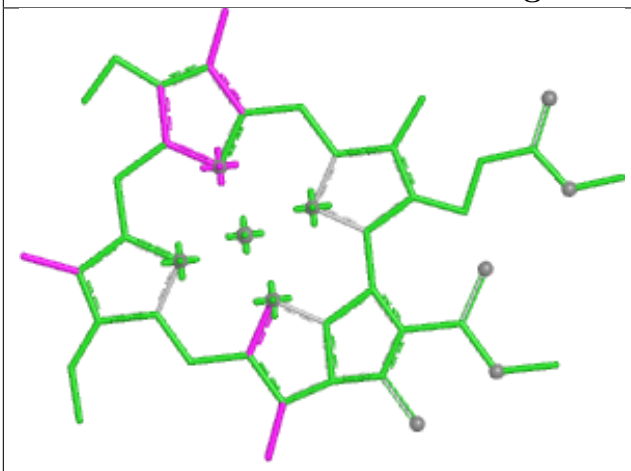


Rings

Ligand CLA A 833



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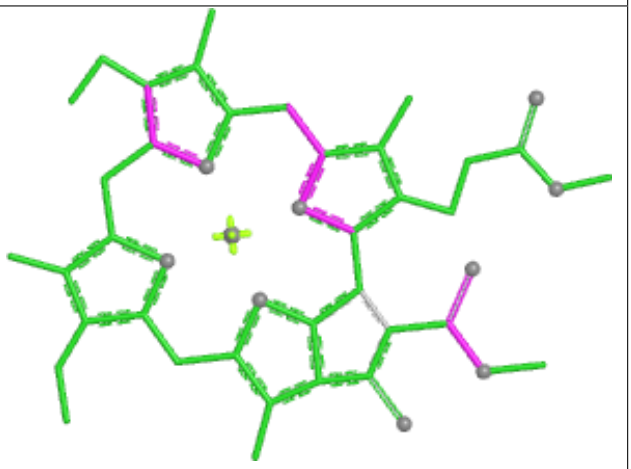

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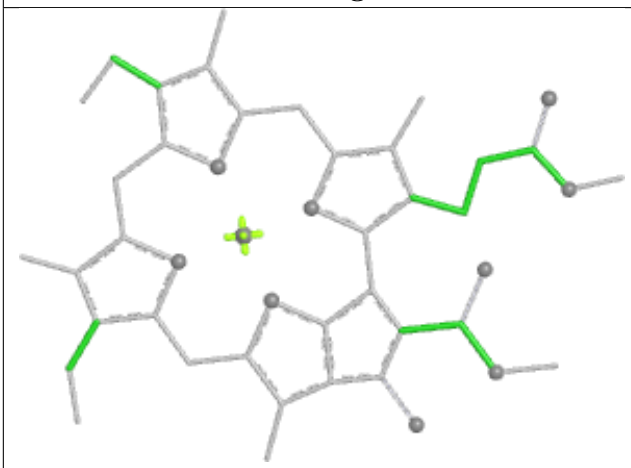

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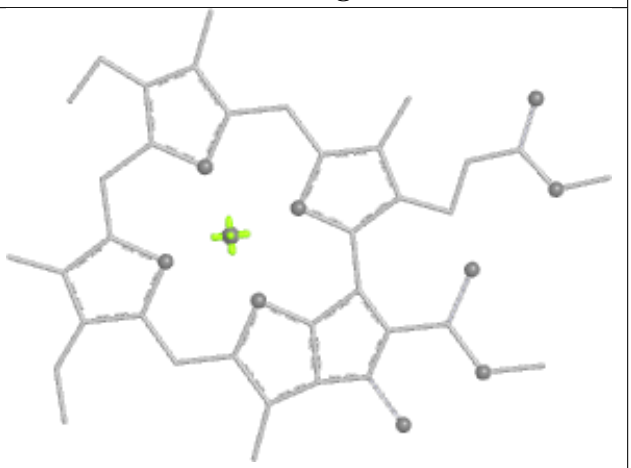
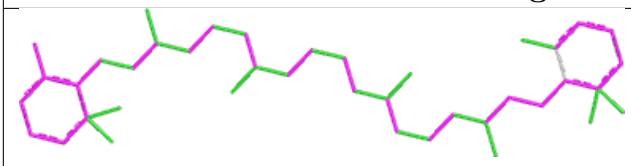


Rings

Ligand 8CT L 205



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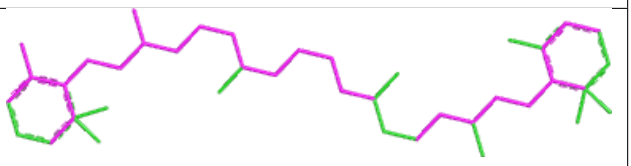
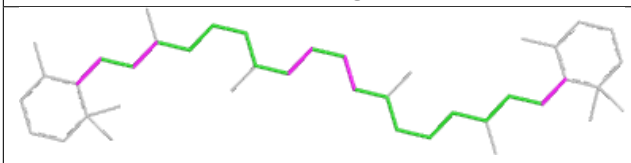


Bond angles



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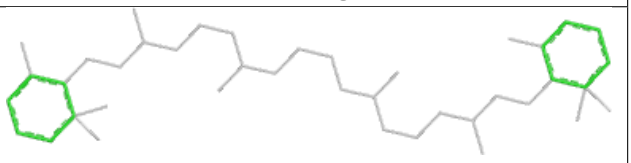
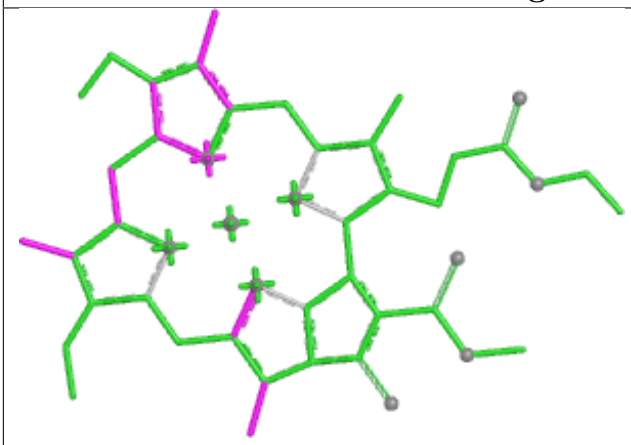


Rings

Ligand CLA 7 314



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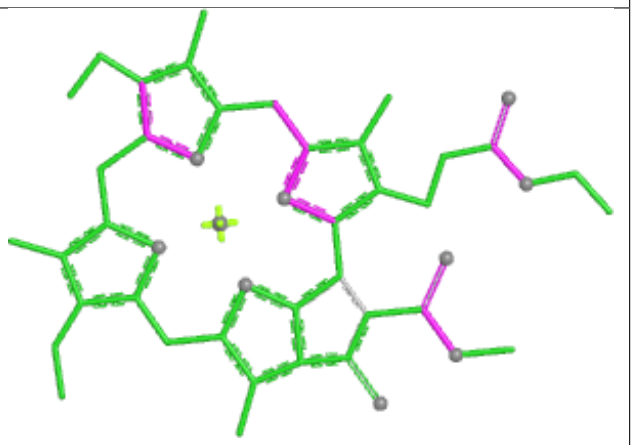
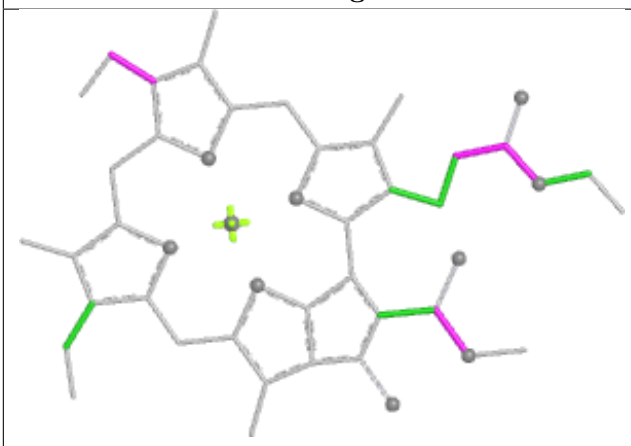


Bond angles



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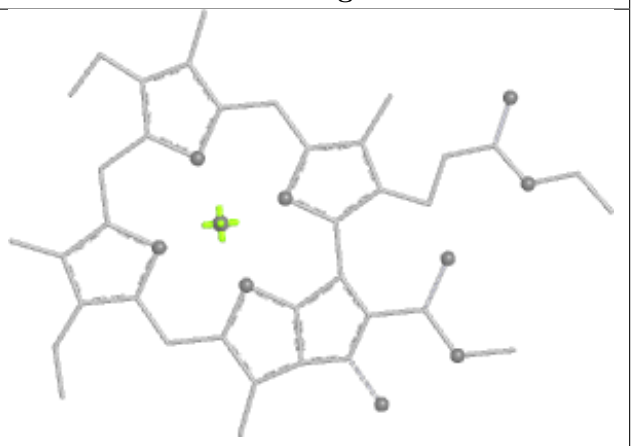
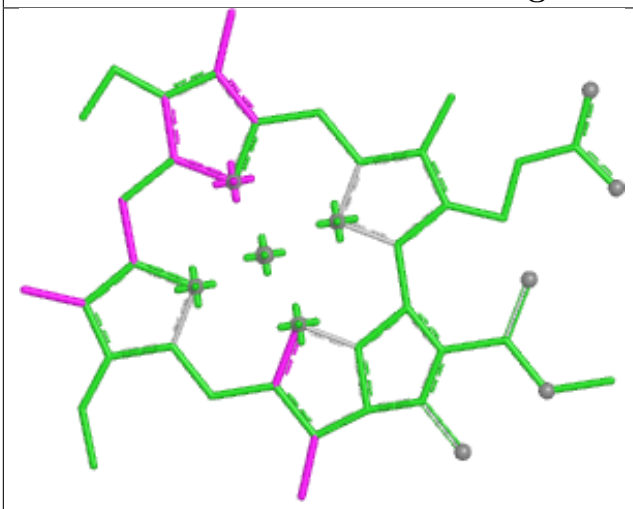


Rings

Ligand CLA 3 313



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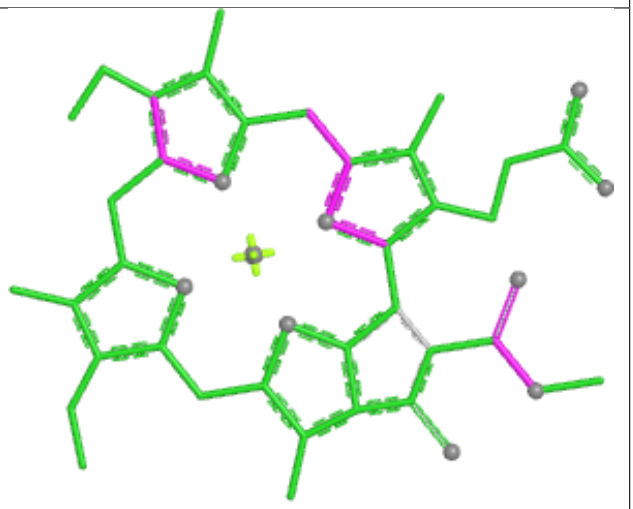

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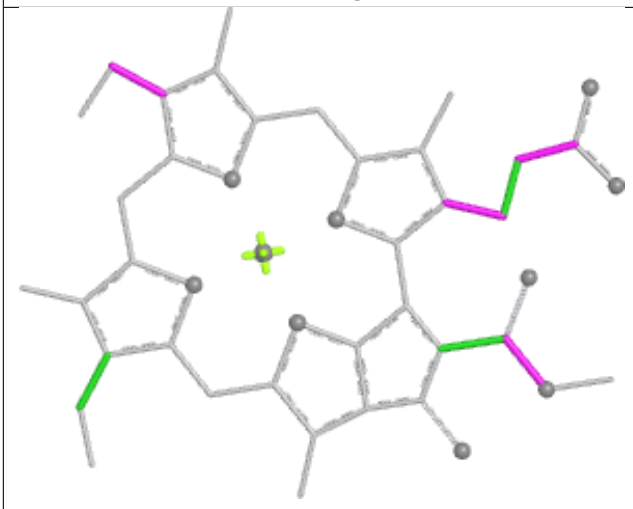
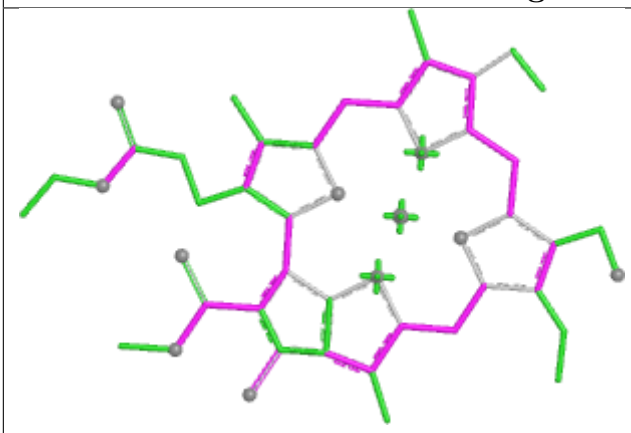


Torsions

Rings

Ligand CHL 1 305



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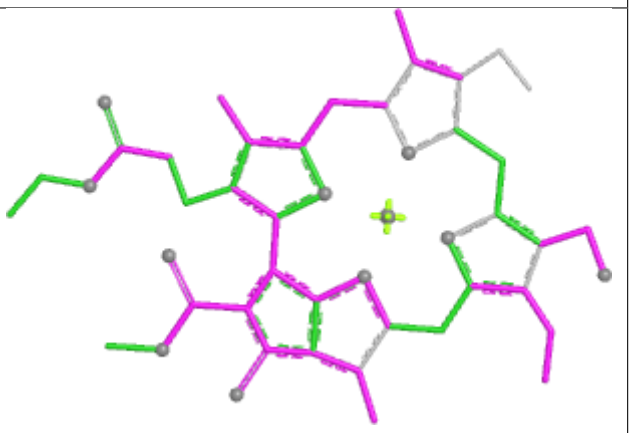
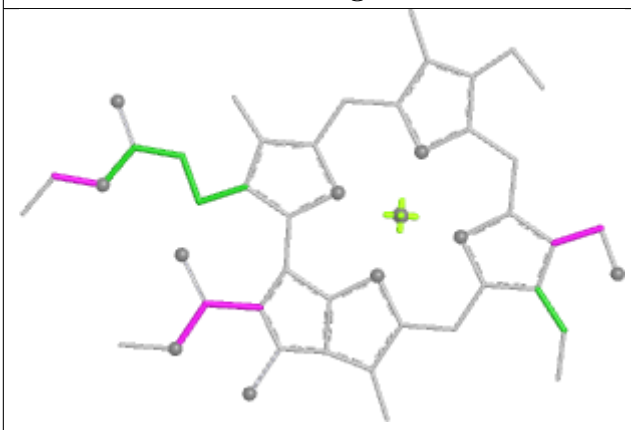


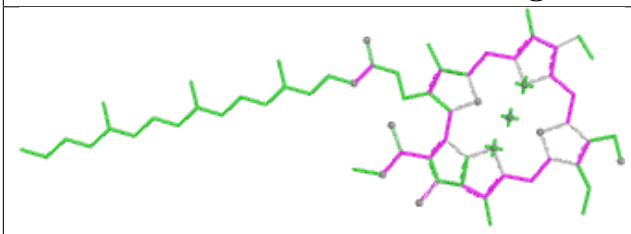
Bond angles



Torsions

Rings

Ligand CHL 2 301



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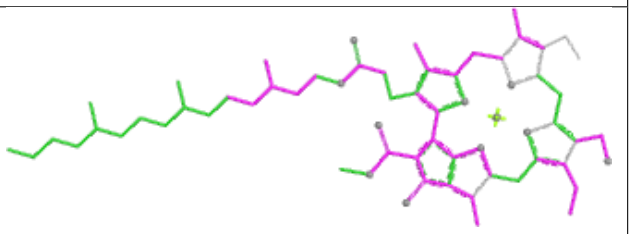
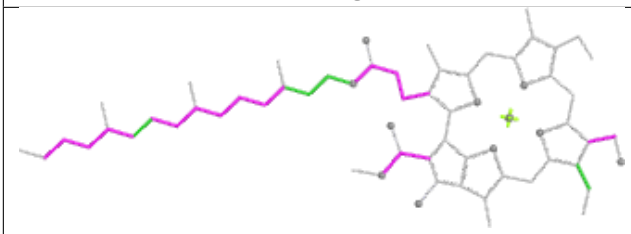
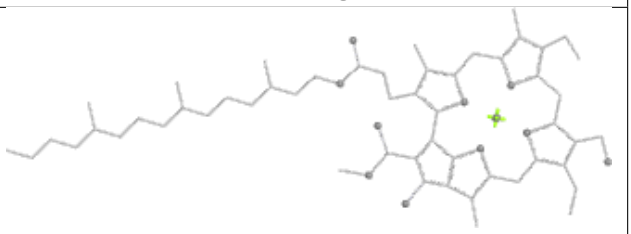


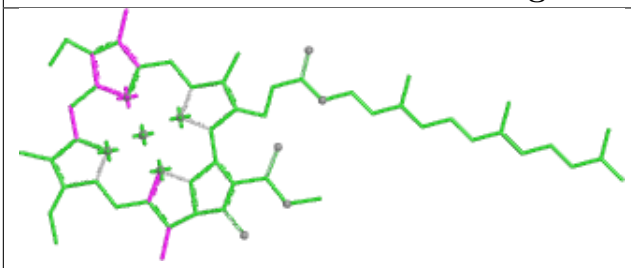
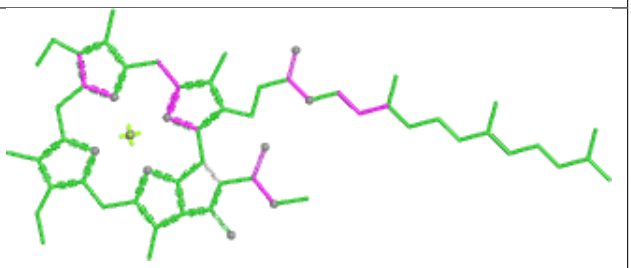
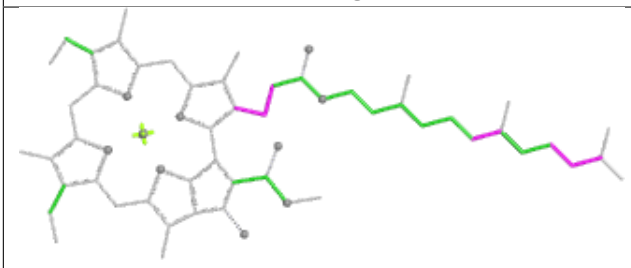
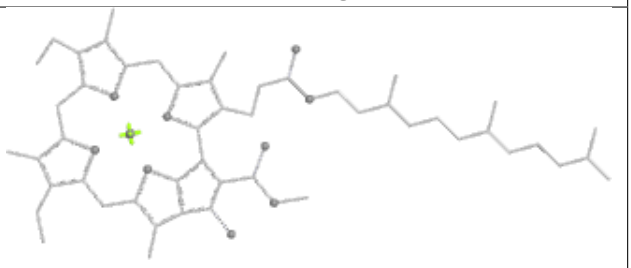
Bond angles



Torsions



Rings

Ligand CLA 4 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

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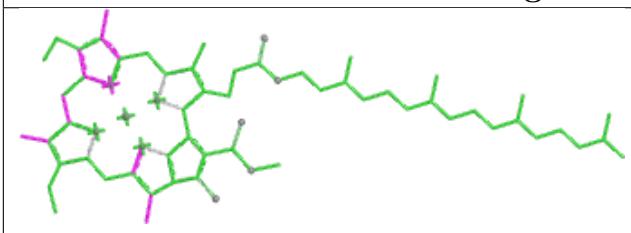
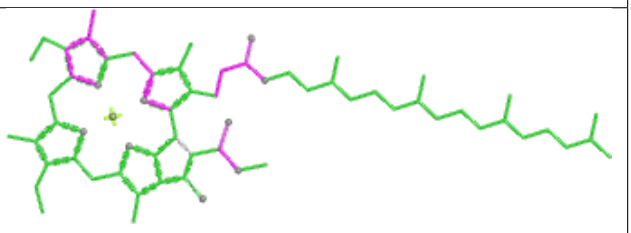
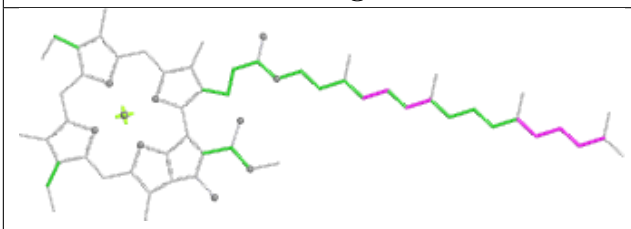
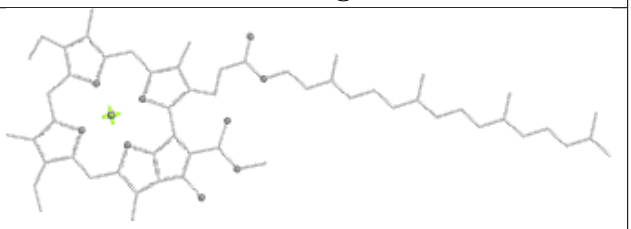
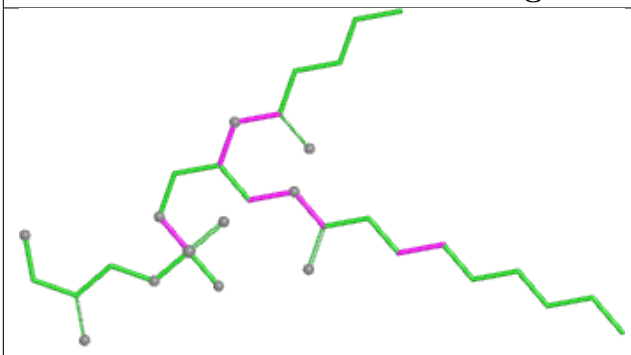
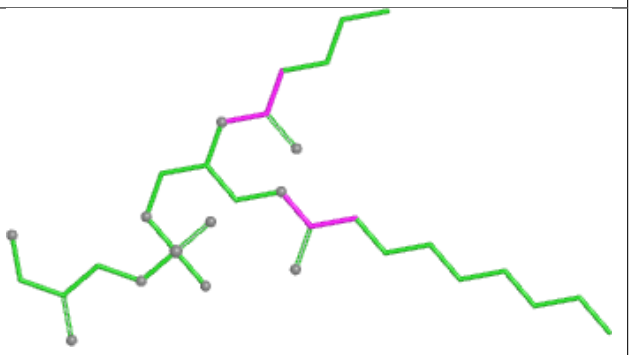
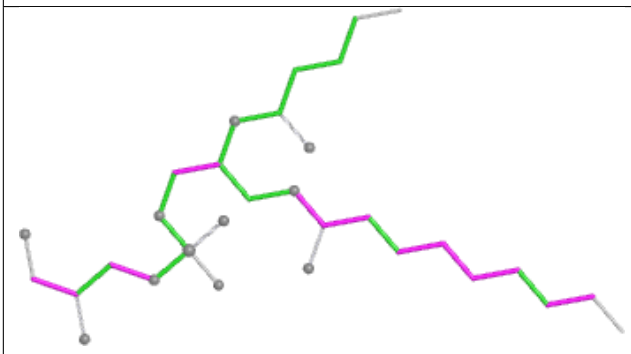
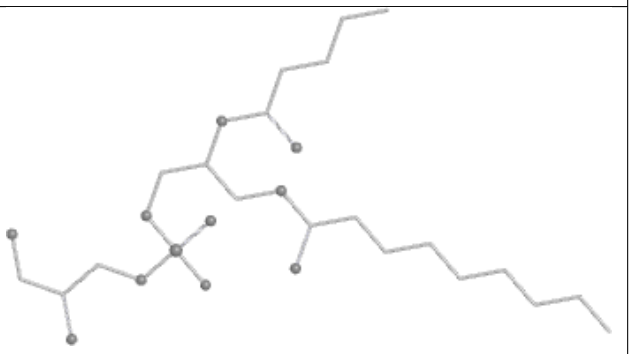
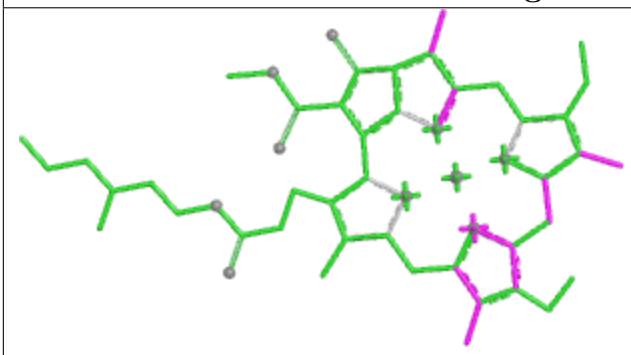
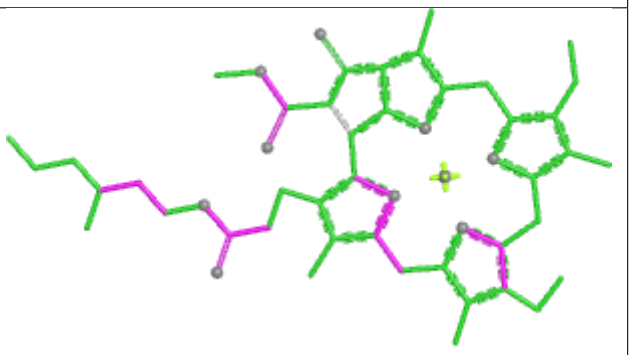
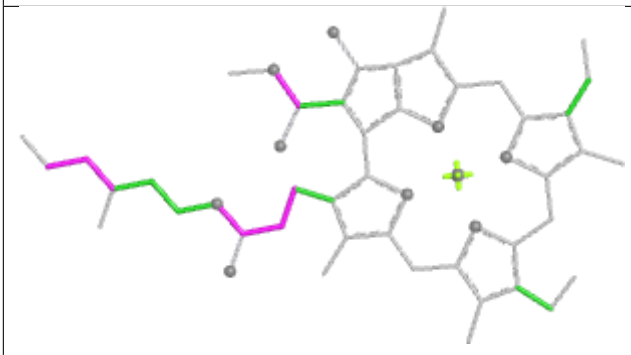
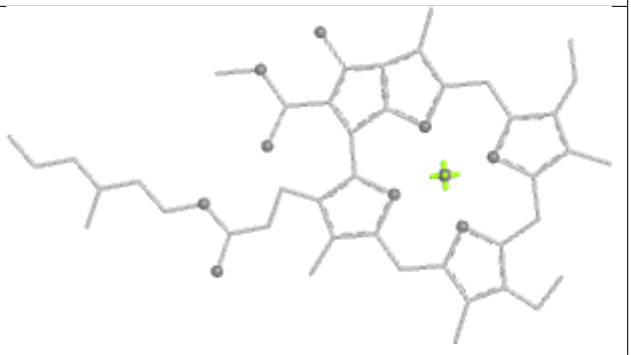
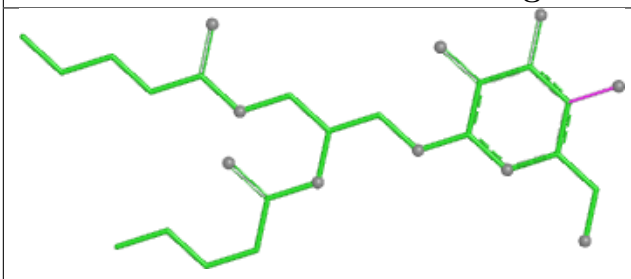
	
Bond lengths	Bond angles
	
Torsions	Rings

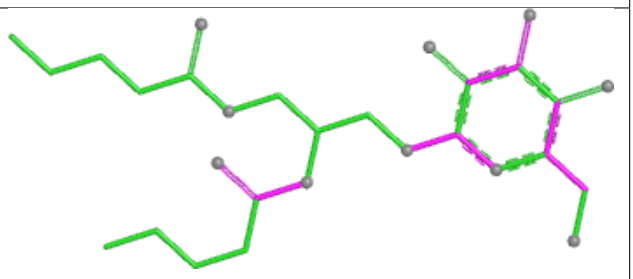
Ligand LHG L 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

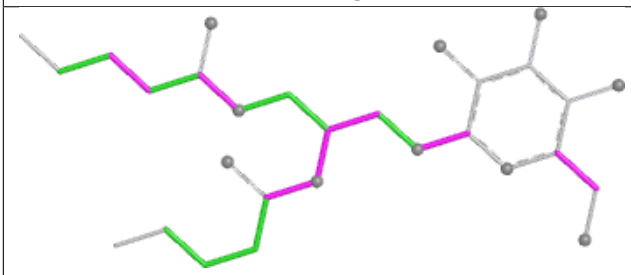
Ligand LMG J 102



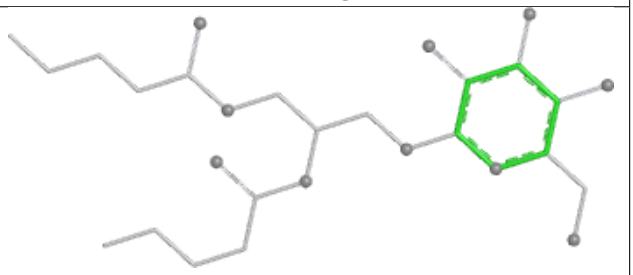
Bond lengths



Bond angles

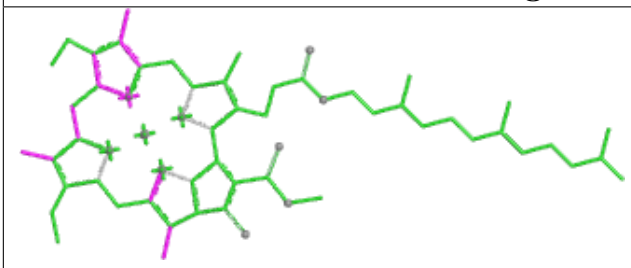


Torsions



Rings

Ligand CLA B 828



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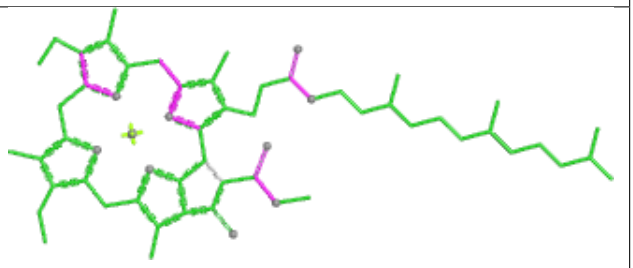
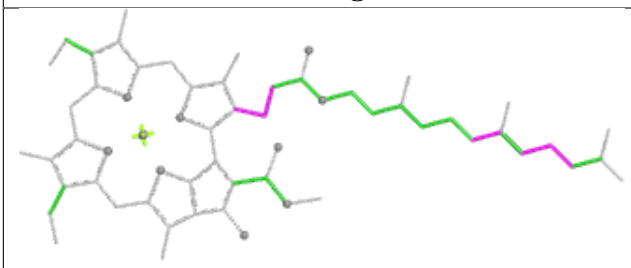
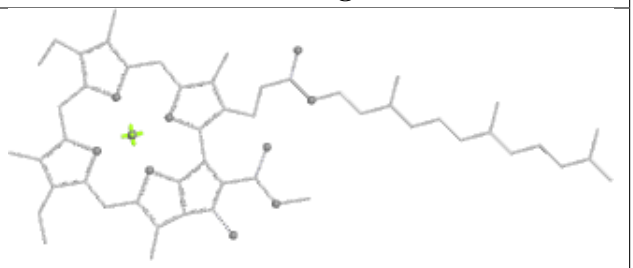


Bond angles

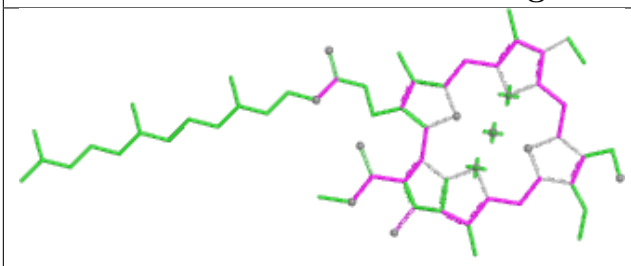


Torsions



Rings

Ligand CHL 4 301



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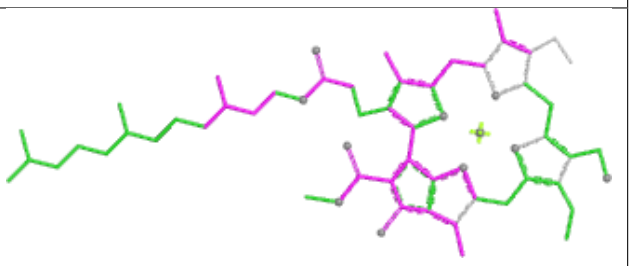

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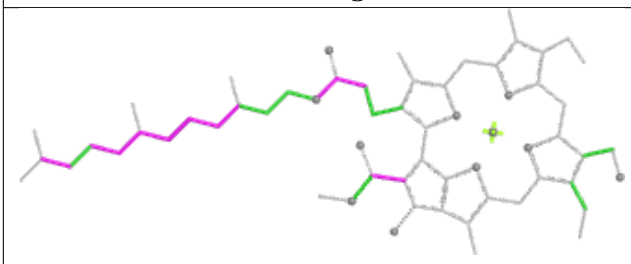
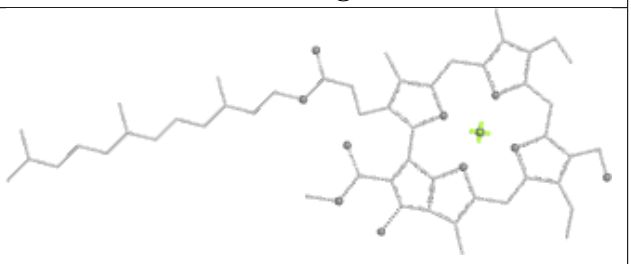
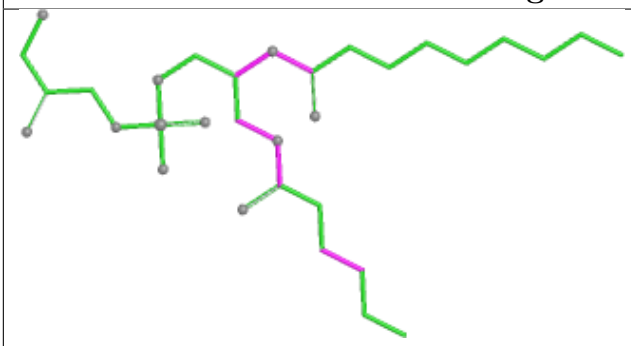


Torsions



Rings

Ligand LHG 2 319



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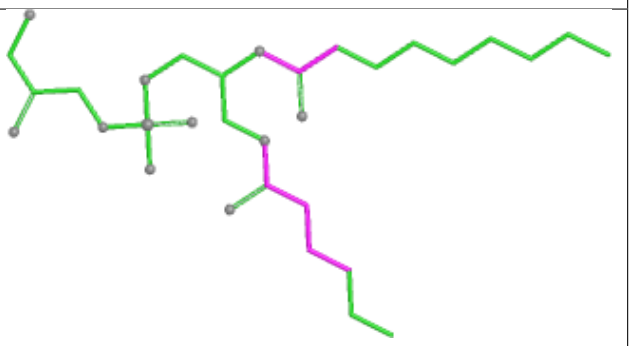

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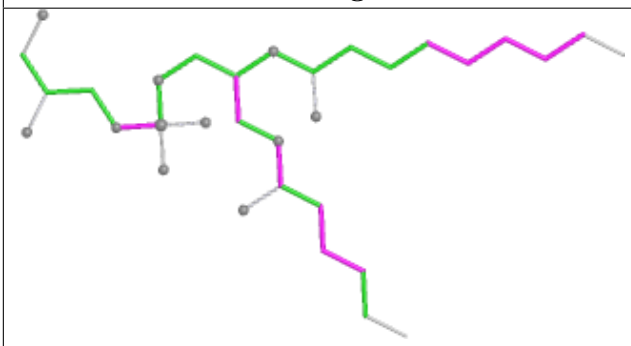

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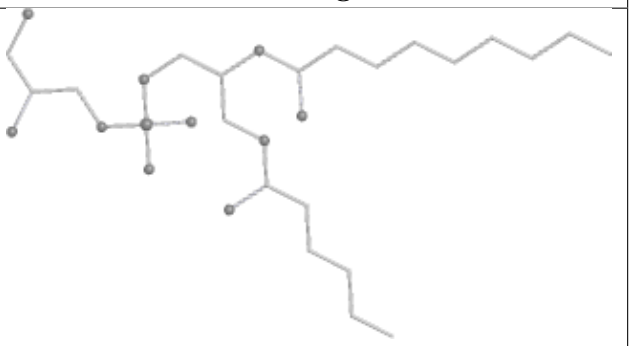
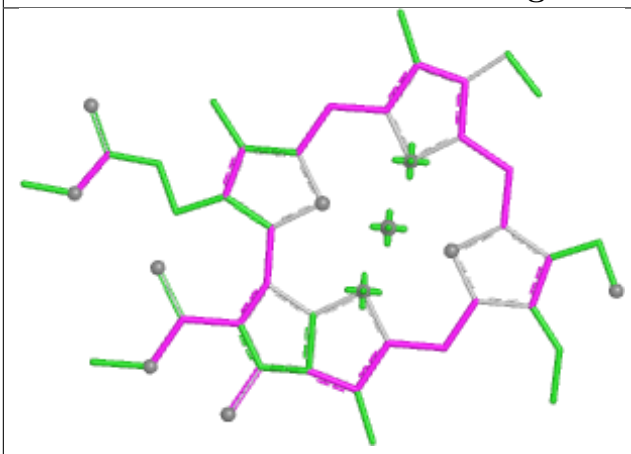


Rings

Ligand CHL 4 308



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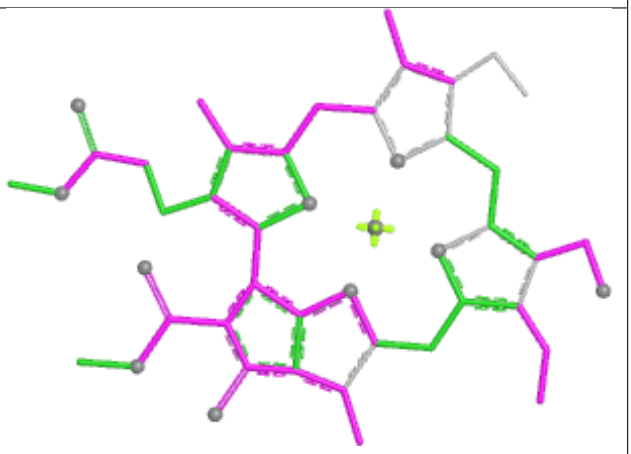

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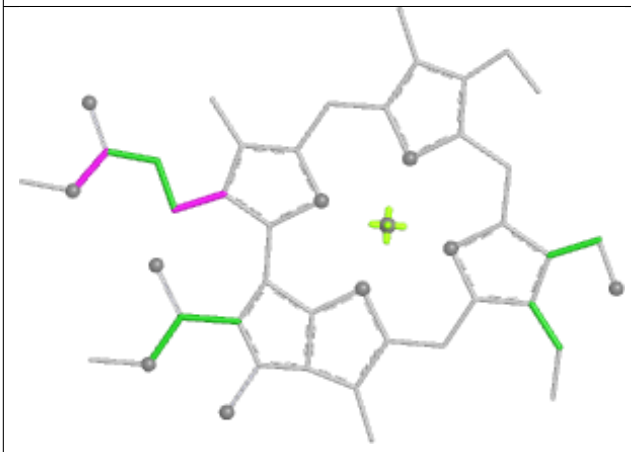
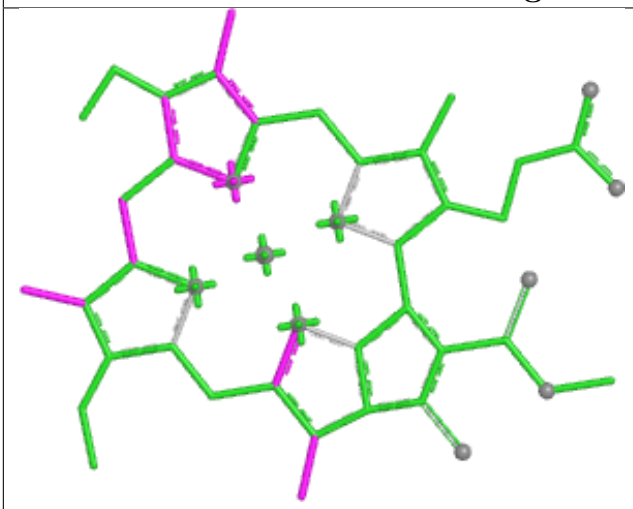


Torsions

Rings

Ligand CLA B 807



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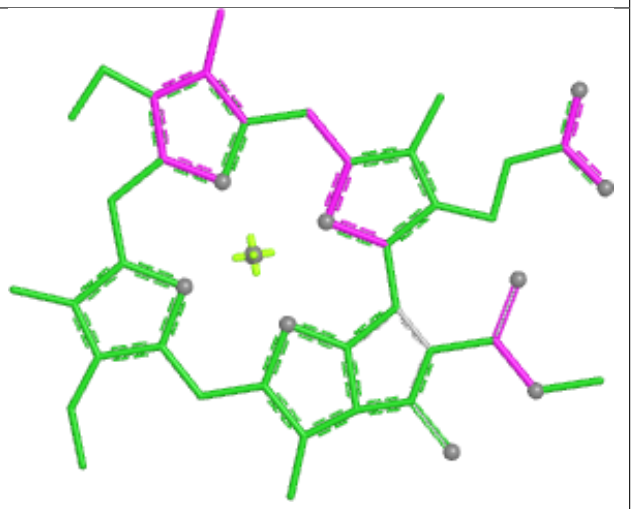

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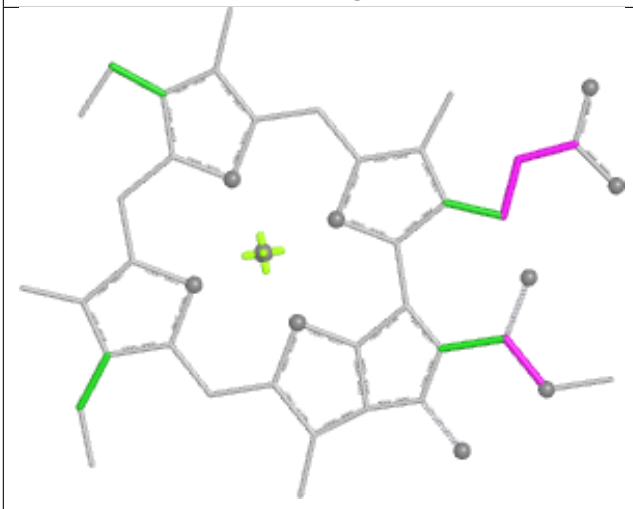
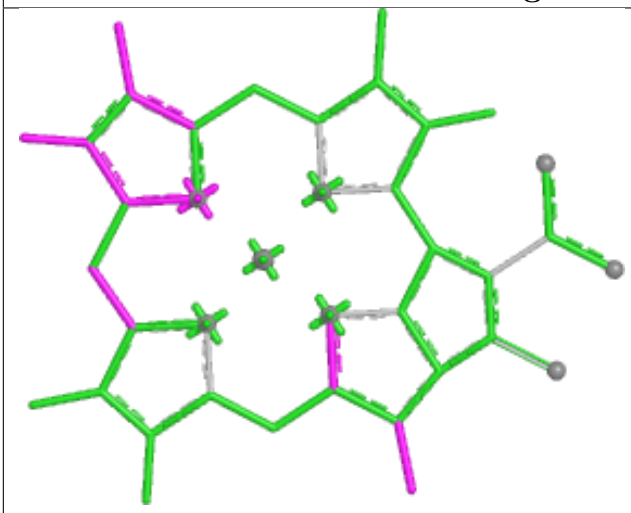


Torsions

Rings

Ligand CLA O 206



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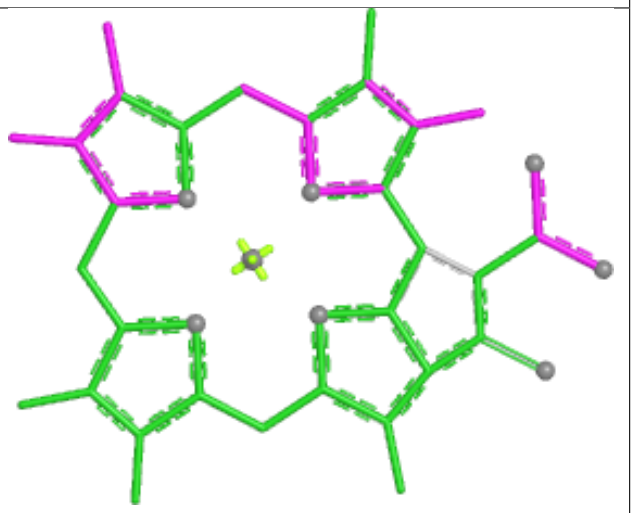

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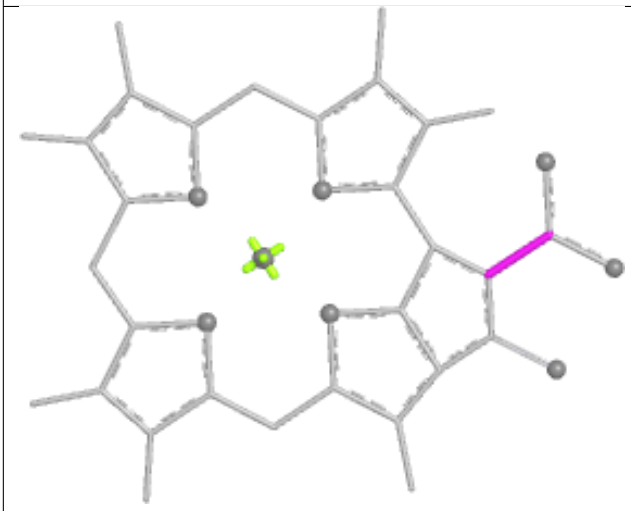

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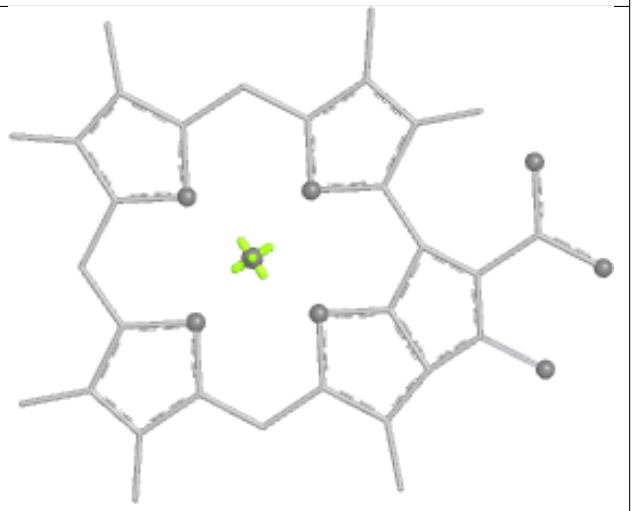
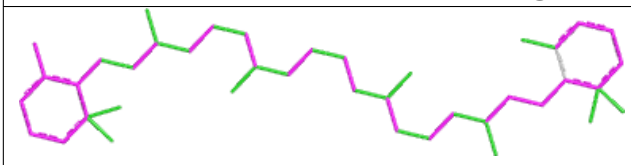


Rings

Ligand 8CT 8 317



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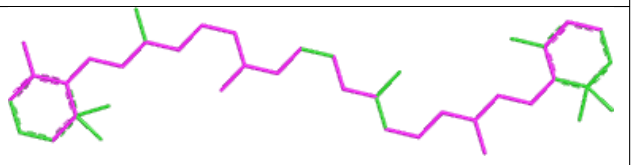

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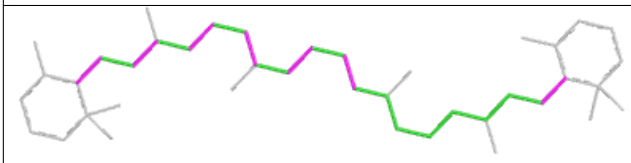

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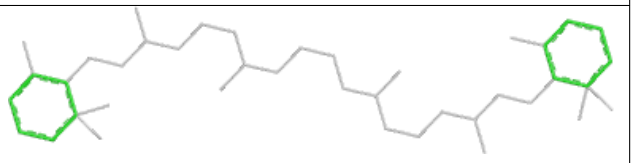
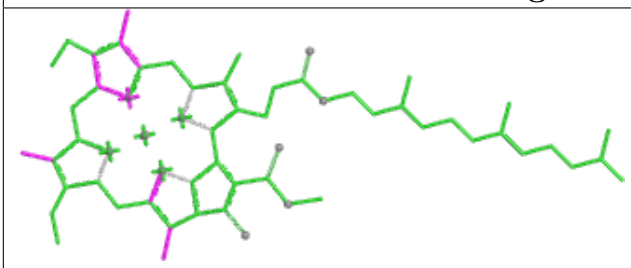


Rings

Ligand CLA 2 311



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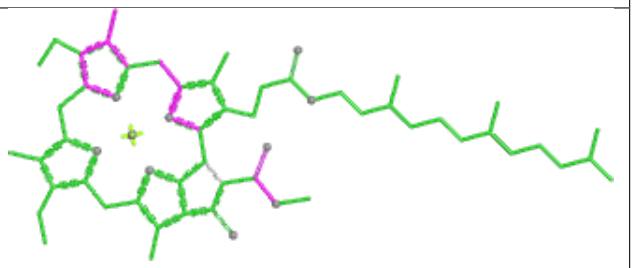
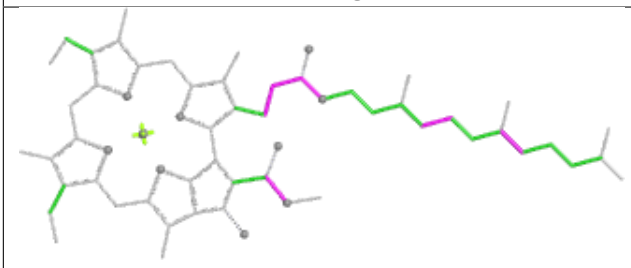


Bond angles



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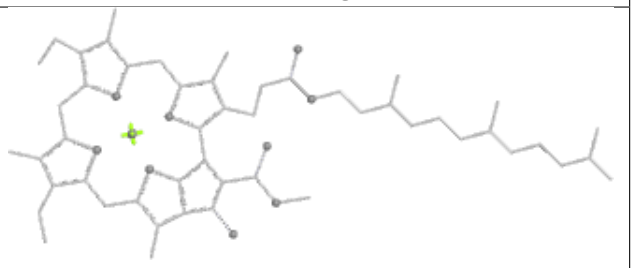
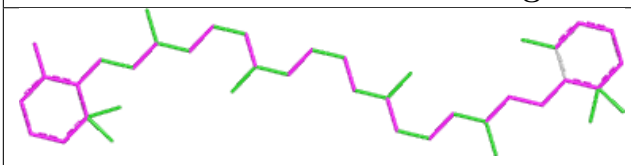


Rings

Ligand 8CT M 102



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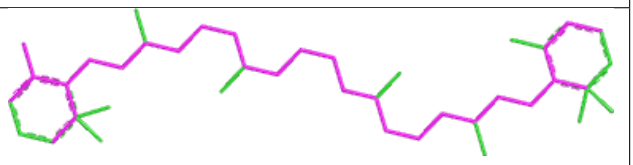
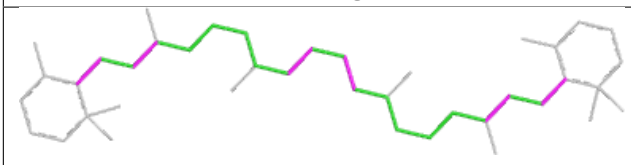


Bond angles



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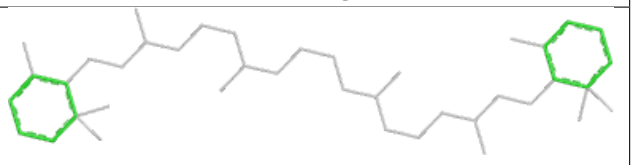
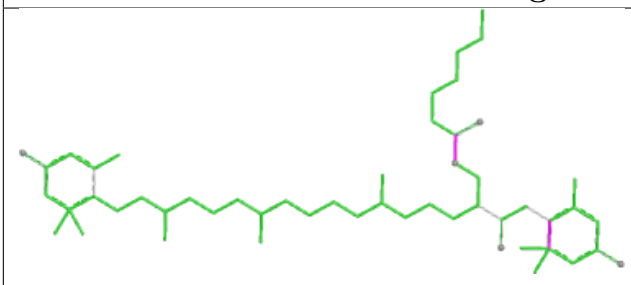


Rings

Ligand 0UR 9 315



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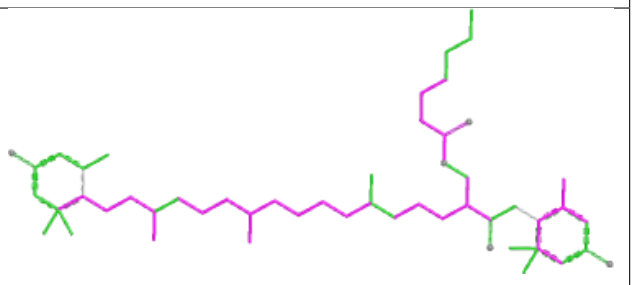

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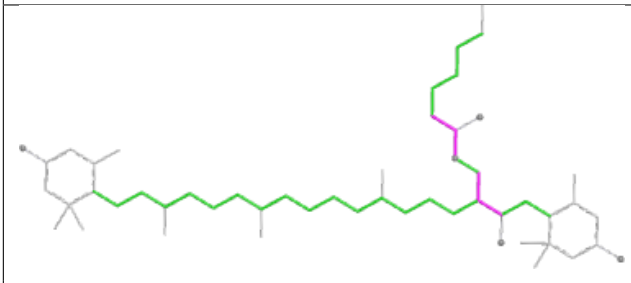

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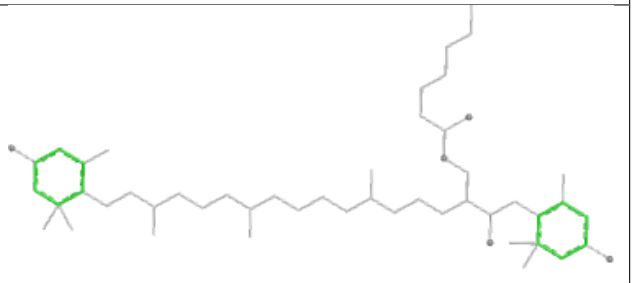
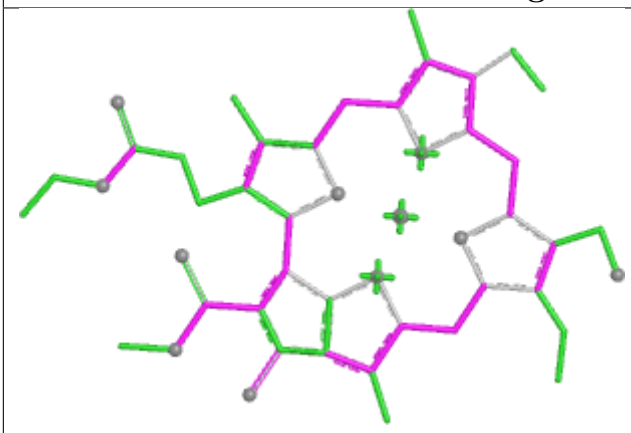


Rings

Ligand CHL 9 306



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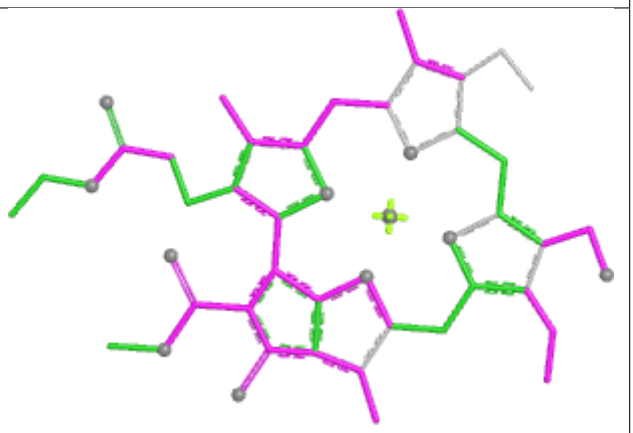

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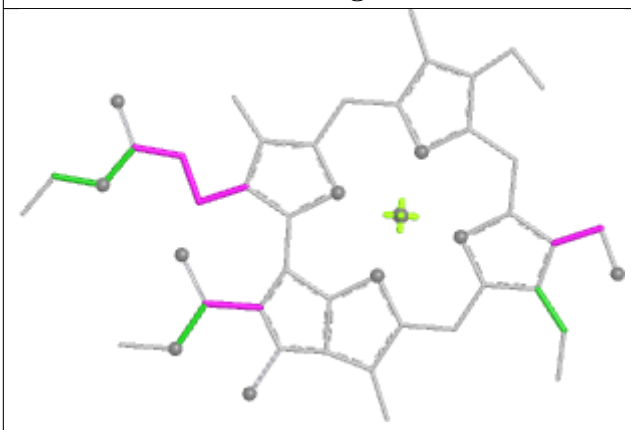

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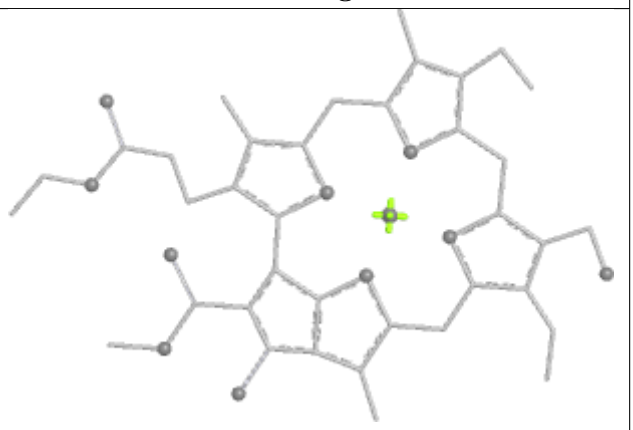
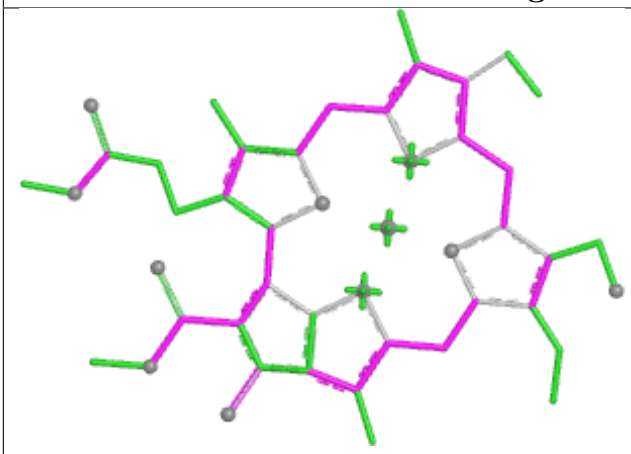


Rings

Ligand CHL 8 306



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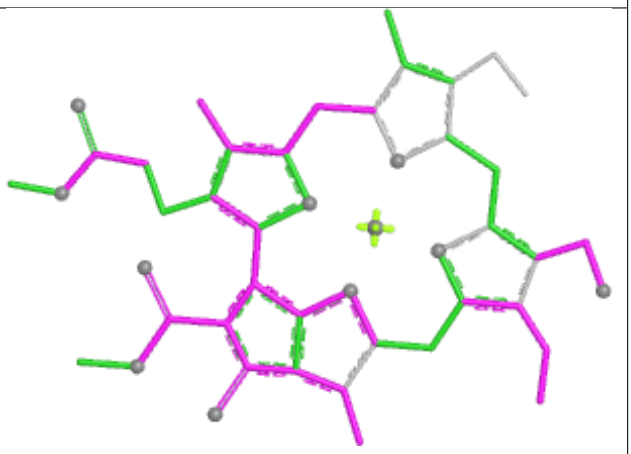

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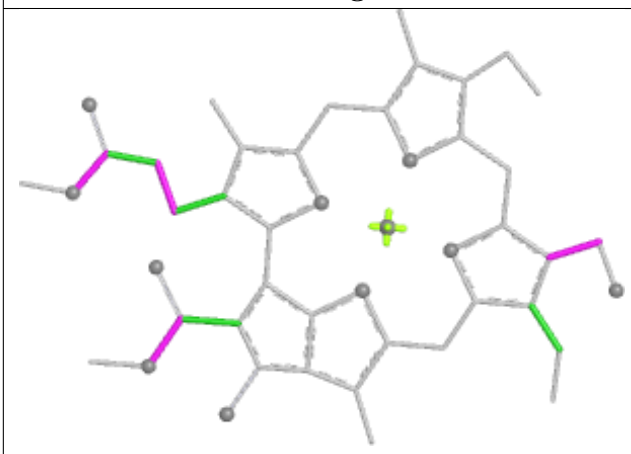

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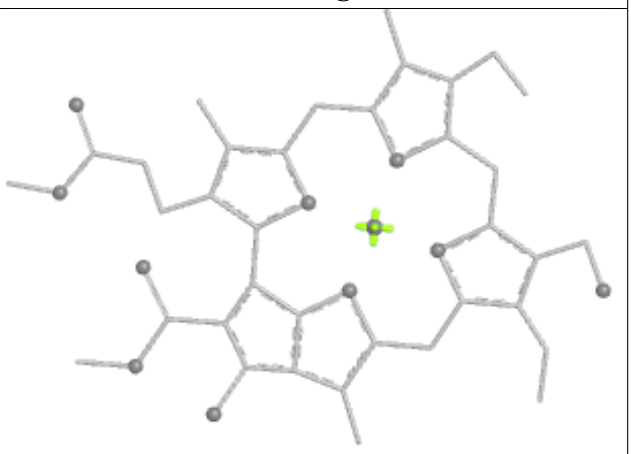
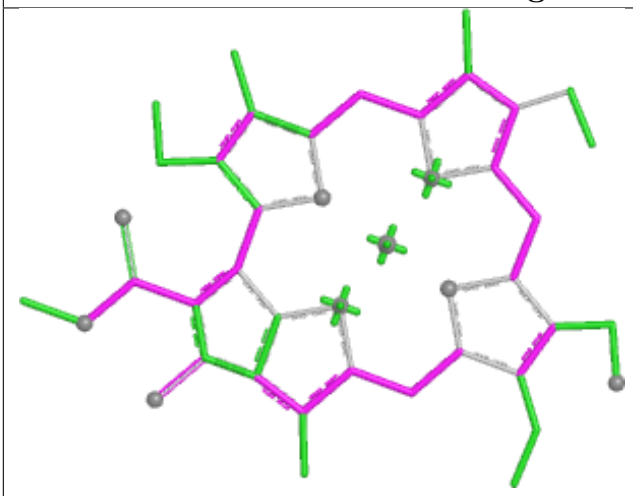


Rings

Ligand CHL 4 305



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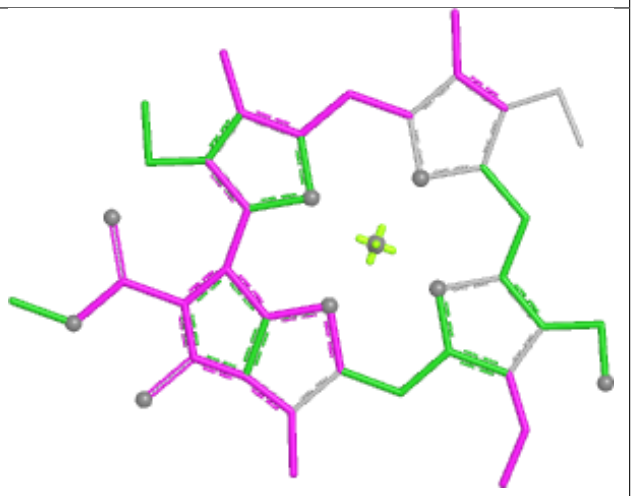
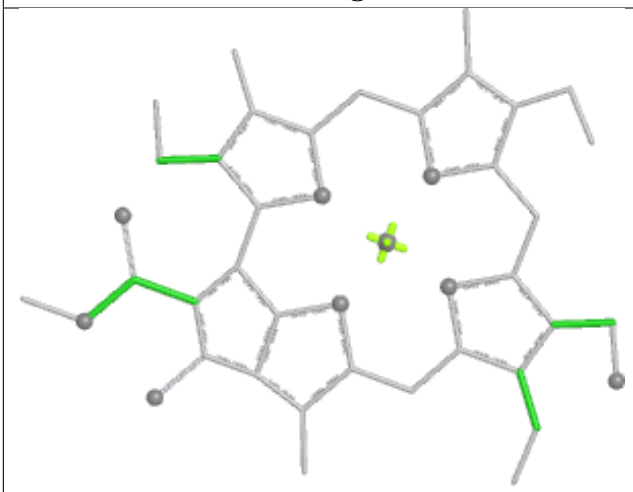


Bond angles



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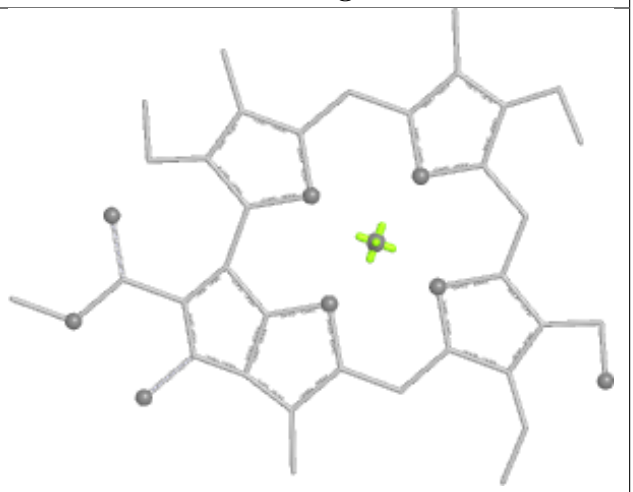
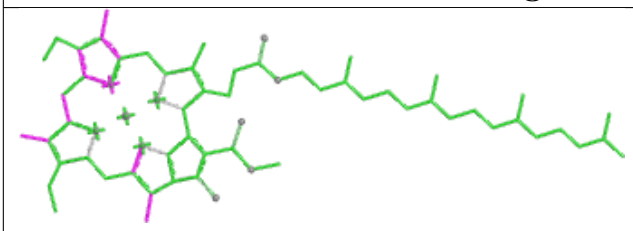


Rings

Ligand CLA A 809



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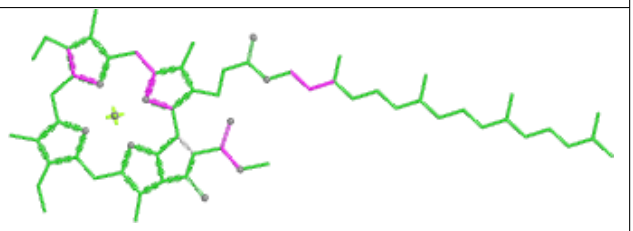
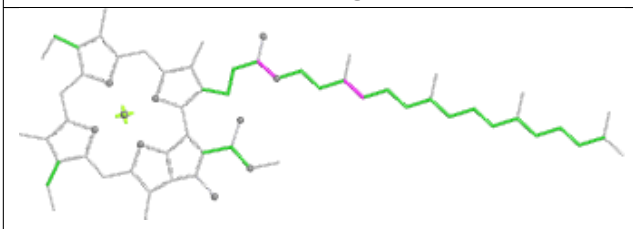
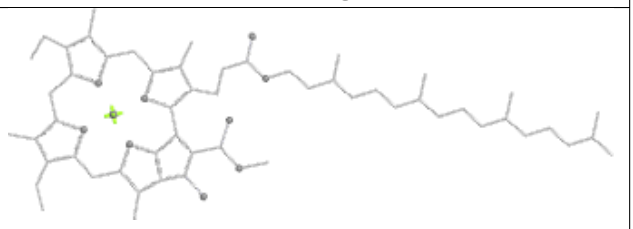


Bond angles



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.

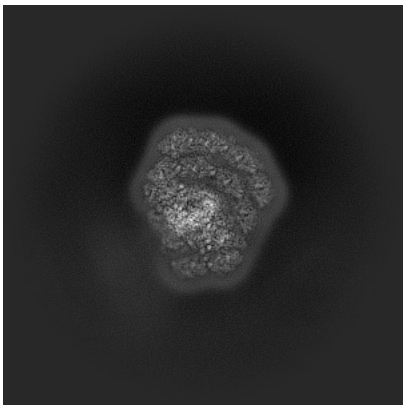
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61973. These allow visual inspection of the internal detail of the map and identification of artifacts.

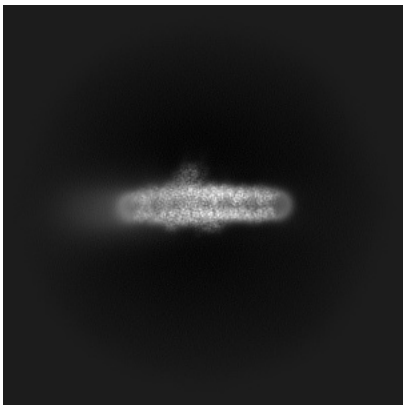
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

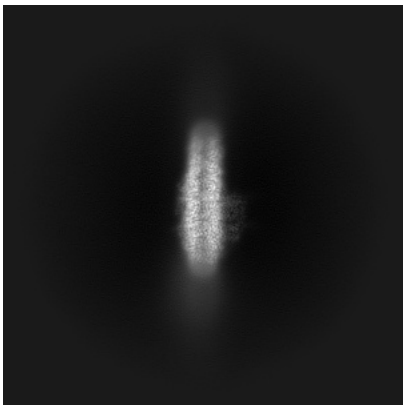
6.1.1 Primary map



X

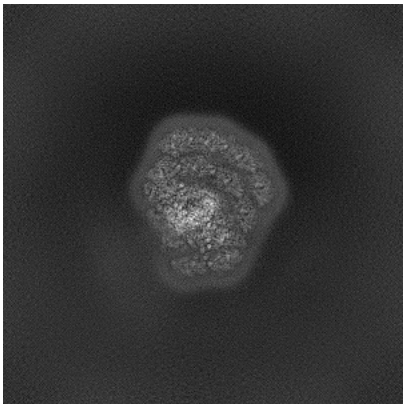


Y

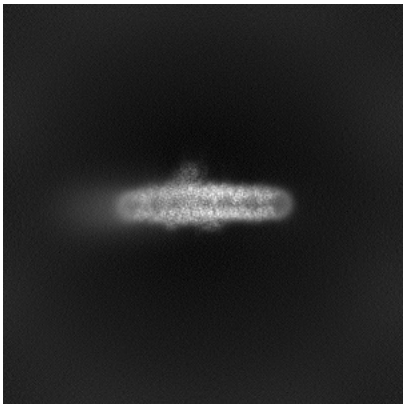


Z

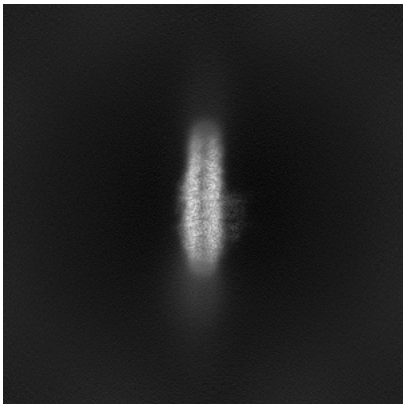
6.1.2 Raw map



X



Y

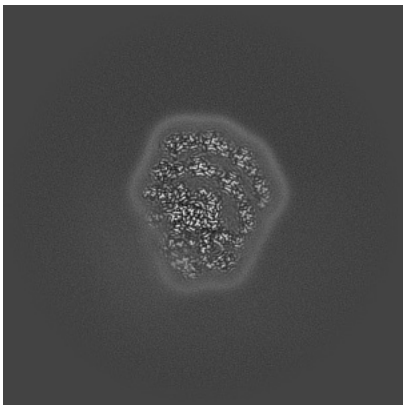


Z

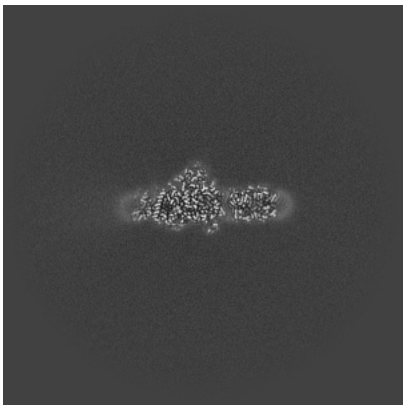
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

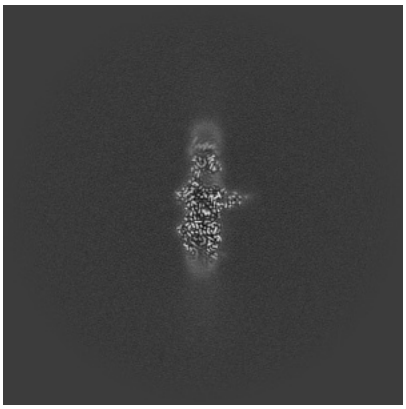
6.2.1 Primary map



X Index: 256

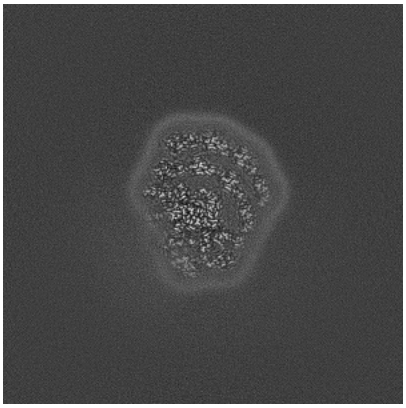


Y Index: 256

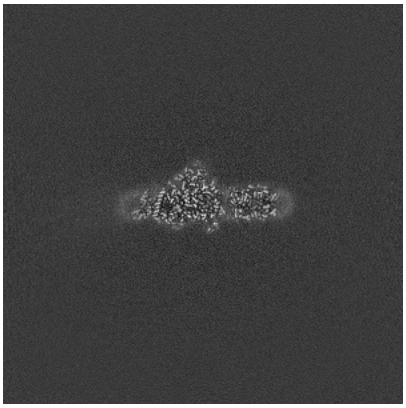


Z Index: 256

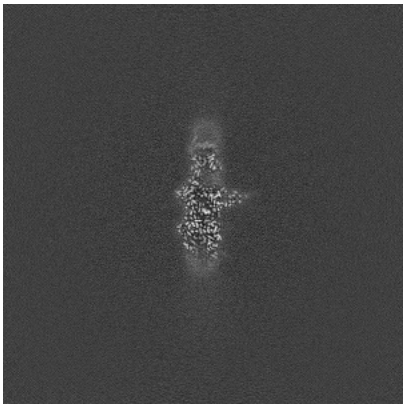
6.2.2 Raw map



X Index: 256



Y Index: 256

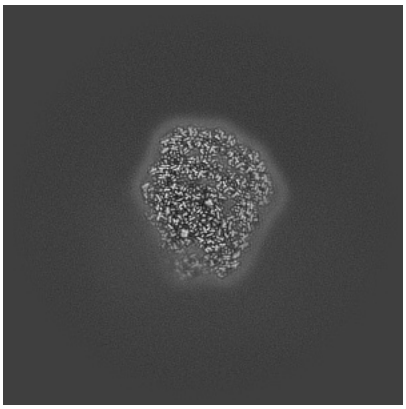


Z Index: 256

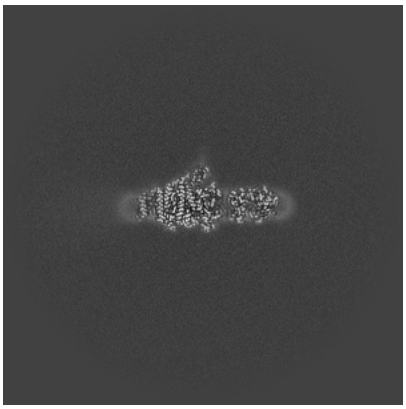
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

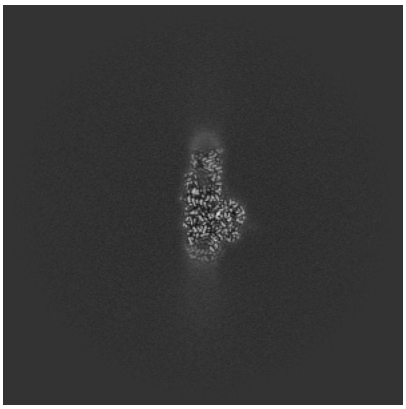
6.3.1 Primary map



X Index: 268

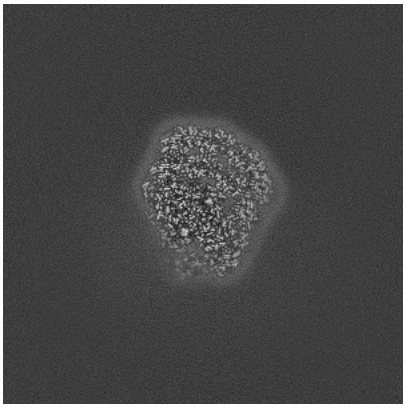


Y Index: 263

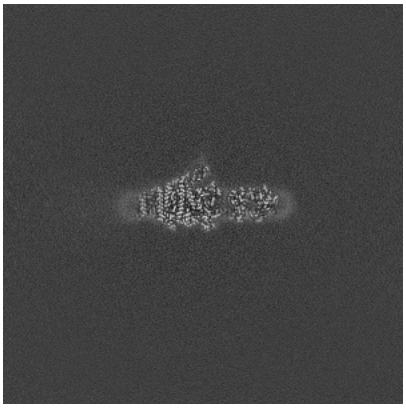


Z Index: 238

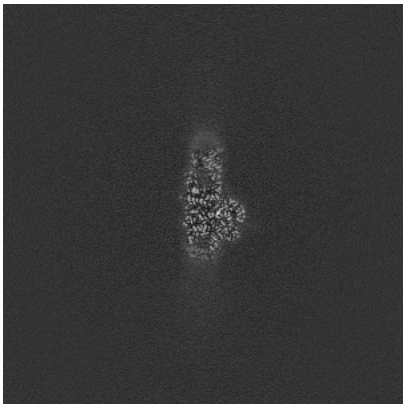
6.3.2 Raw map



X Index: 268



Y Index: 263

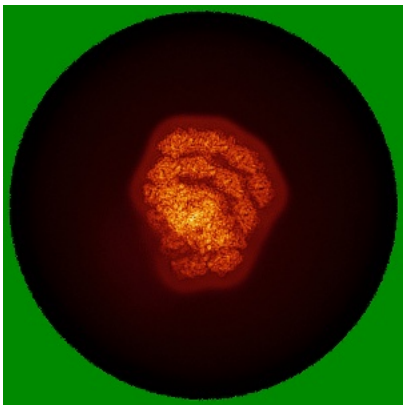


Z Index: 238

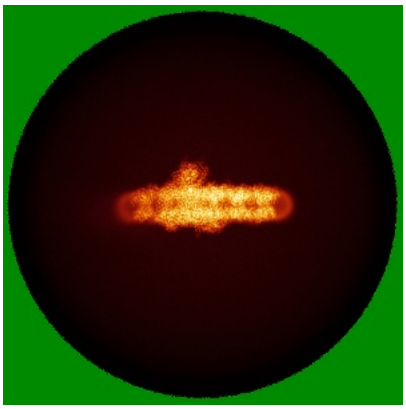
The images above show the largest variance slices of the map in three orthogonal directions.

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

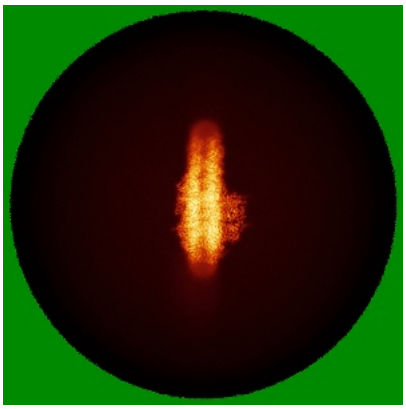
6.4.1 Primary map



X

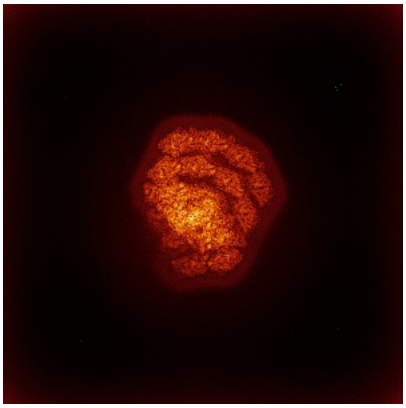


Y

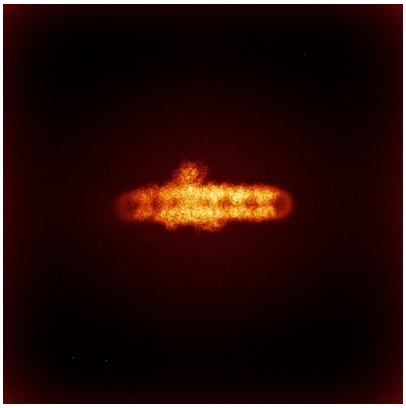


Z

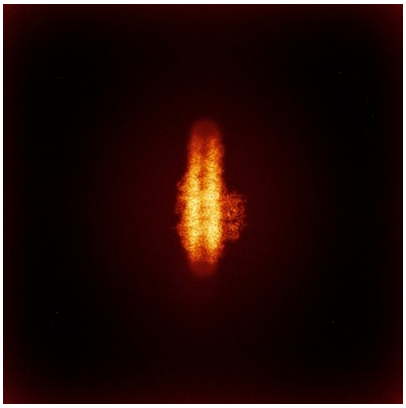
6.4.2 Raw map



X



Y

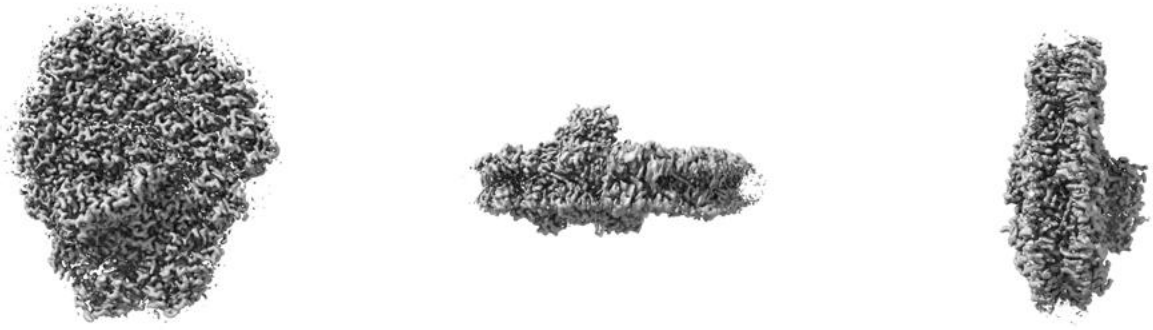


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

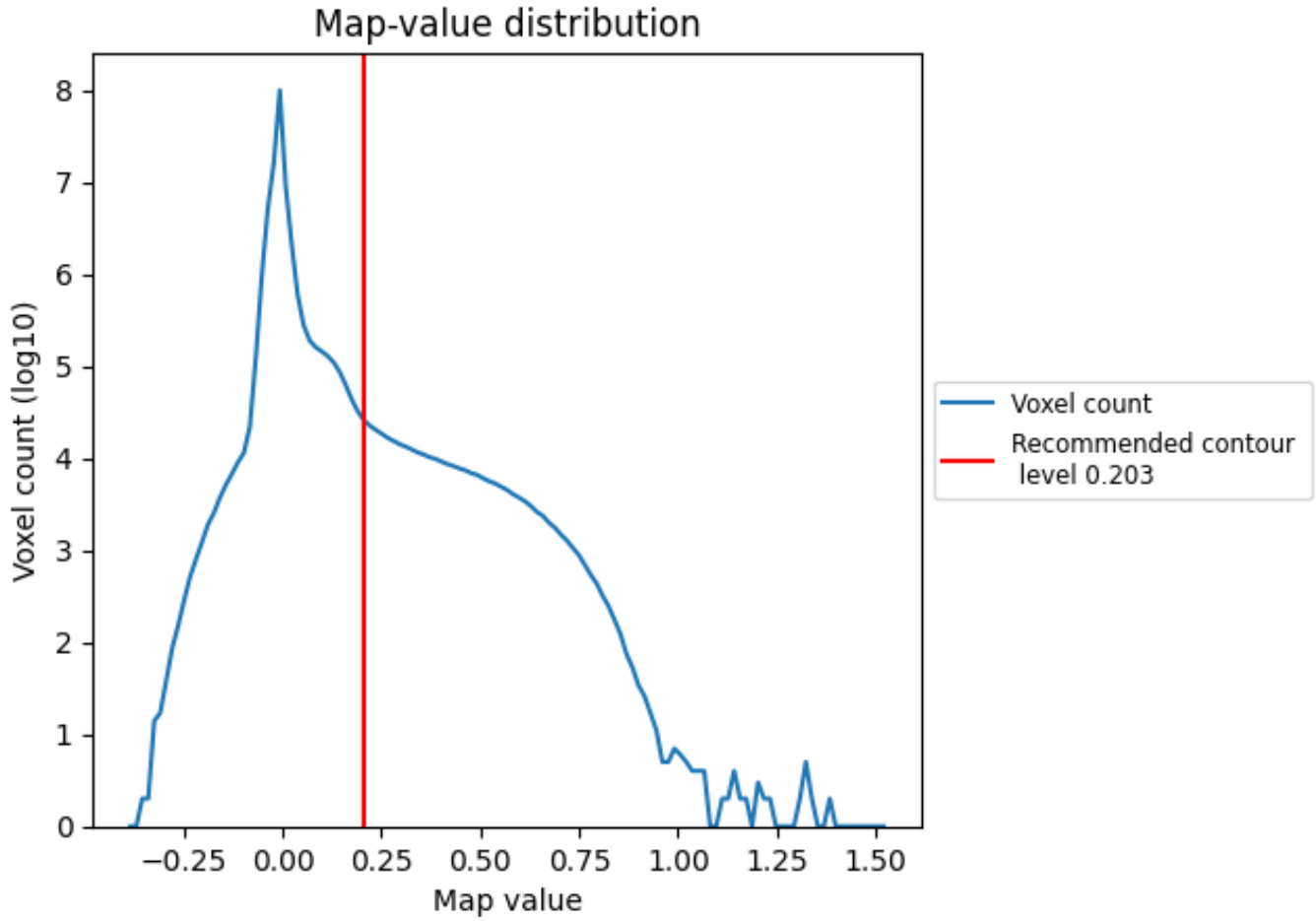
6.6 Mask visualisation (i)

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

7 Map analysis

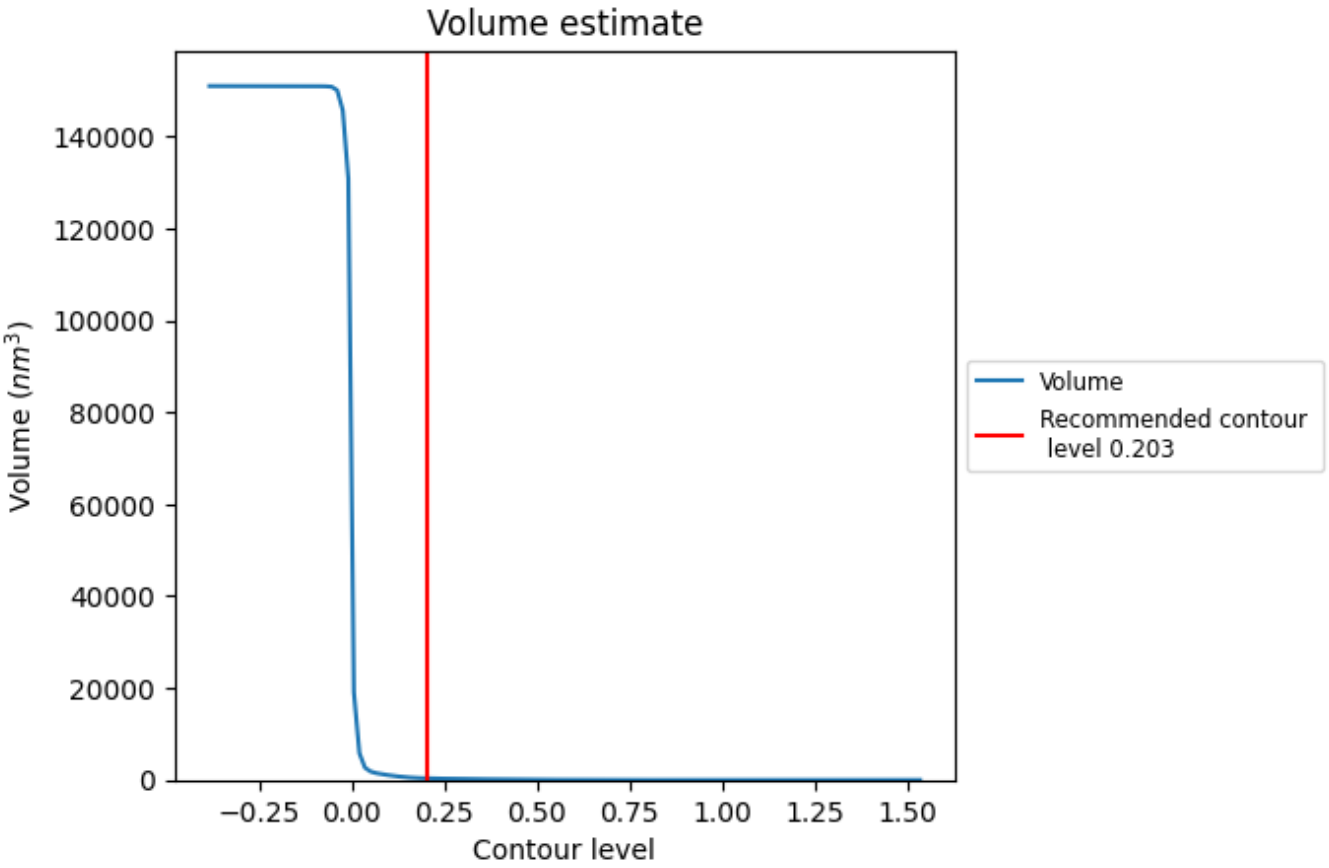
This section contains the results of statistical analysis of the map.

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.

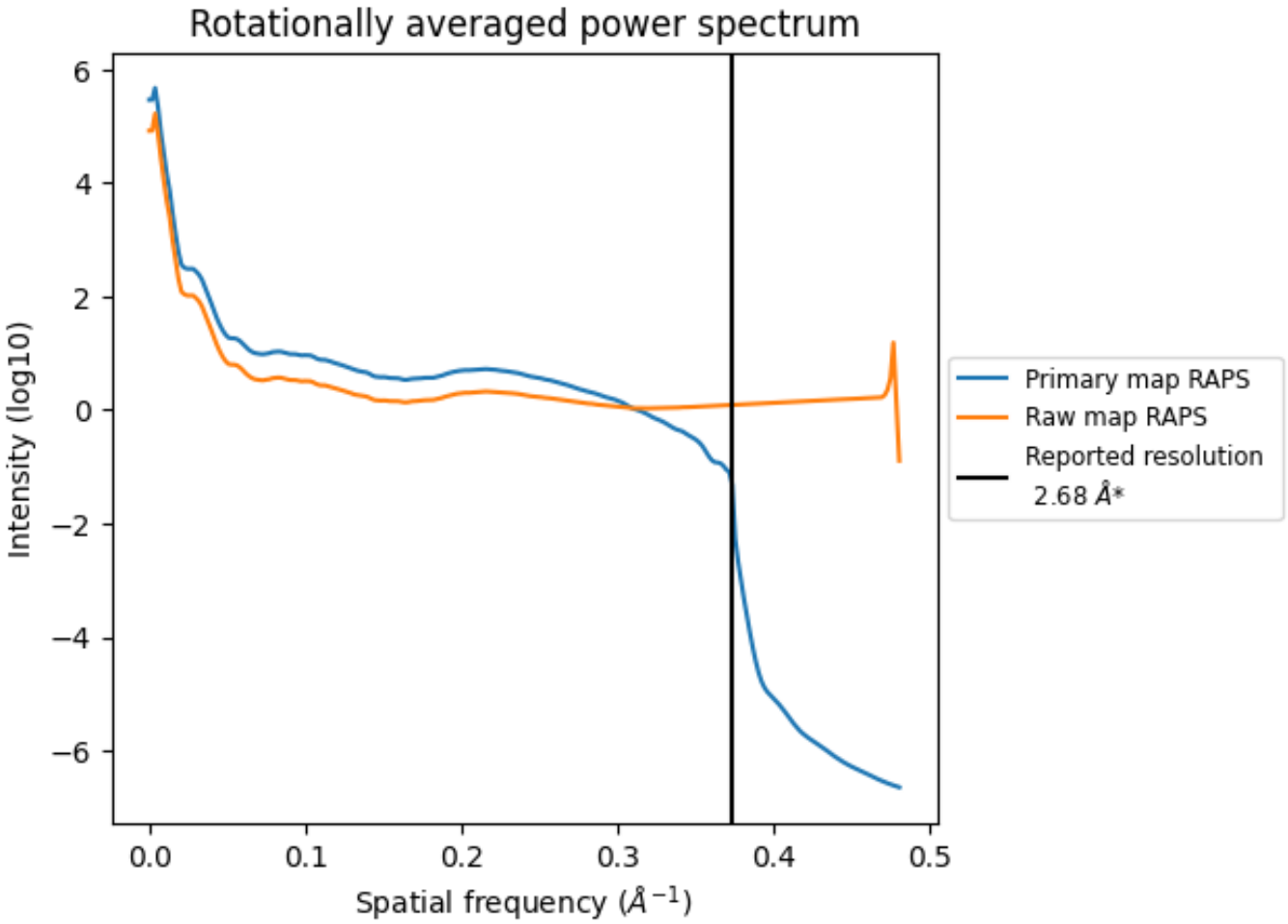
7.2 Volume estimate



The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 322 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)

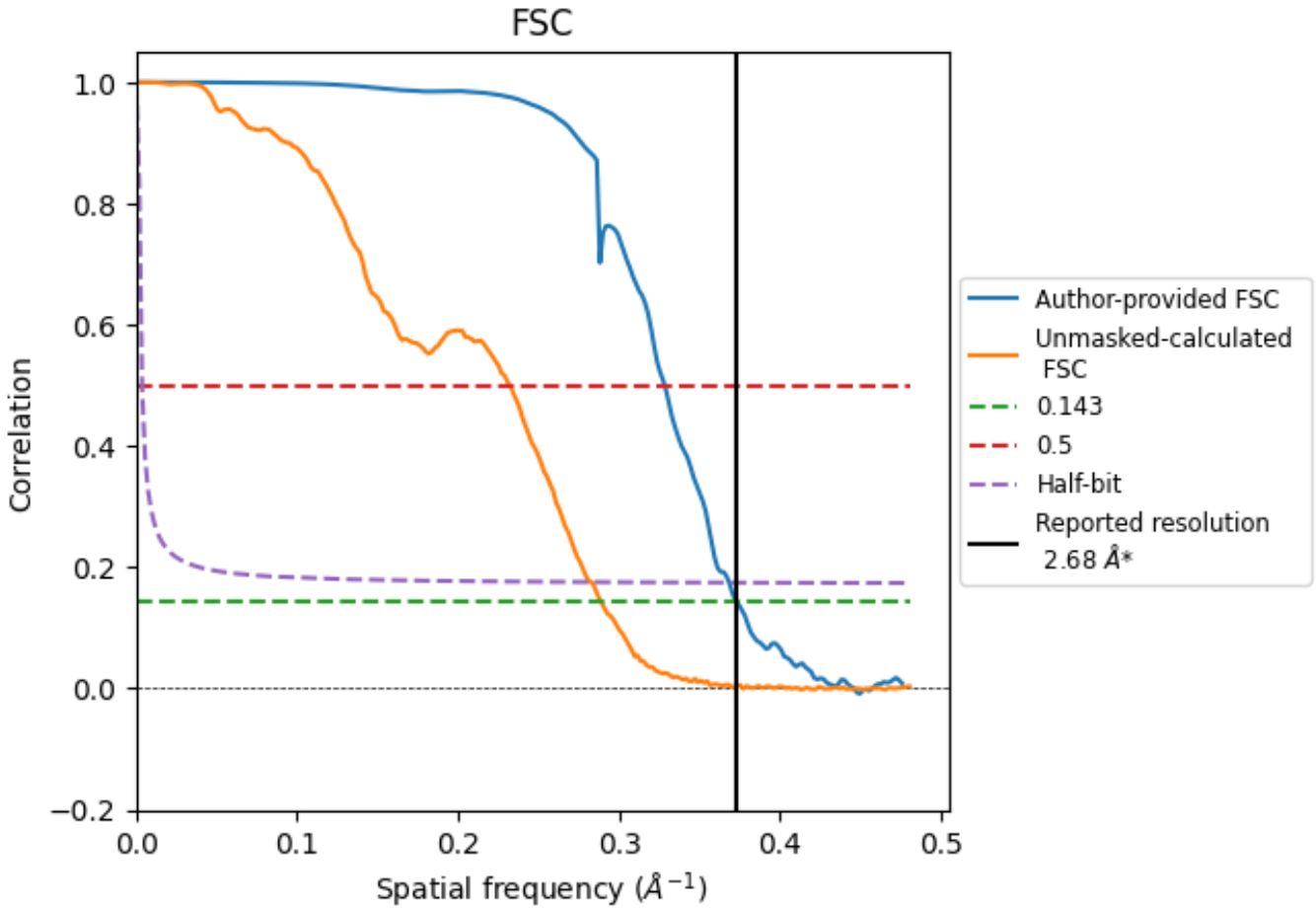


*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8.2 Resolution estimates (i)

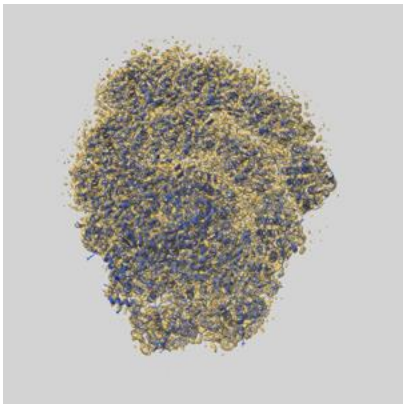
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.04	2.71
Unmasked-calculated*	3.46	4.30	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.68 by more than 10 %

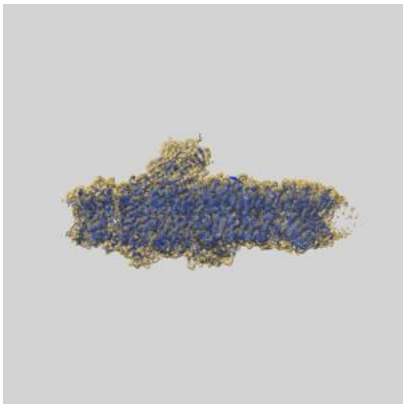
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61973 and PDB model 9K1E. Per-residue inclusion information can be found in section 3 on page 37.

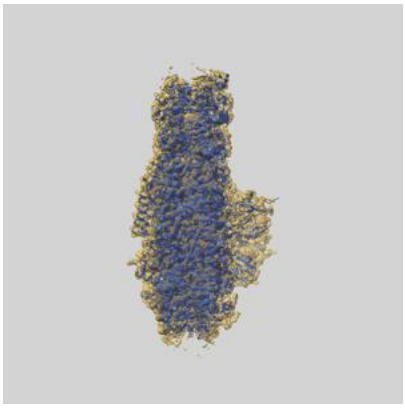
9.1 Map-model overlay



X



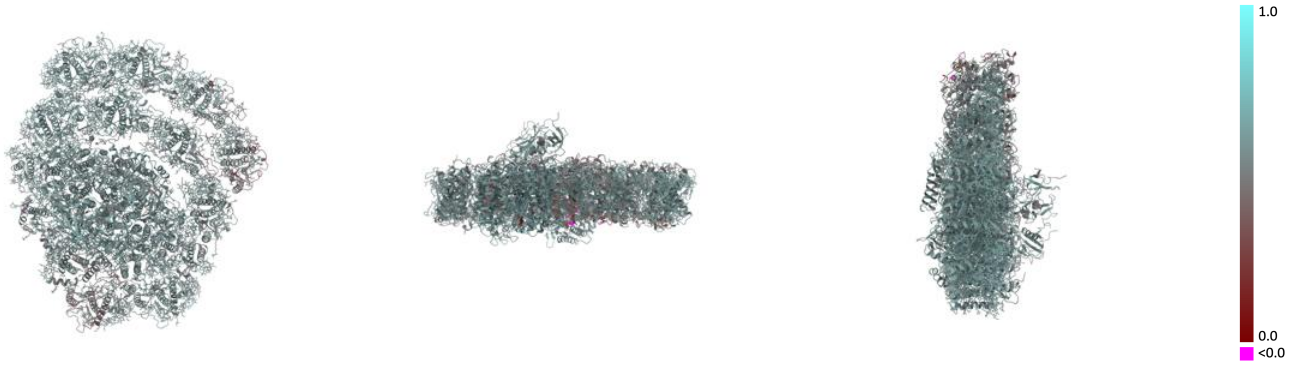
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

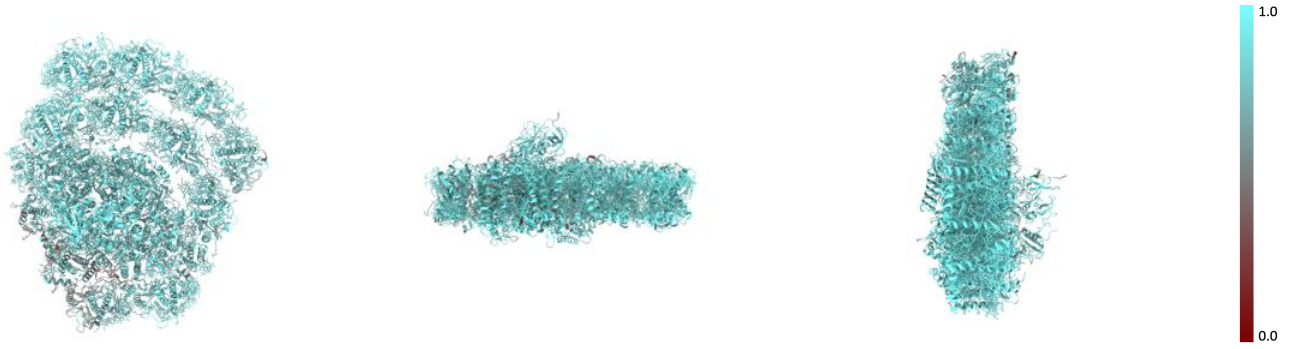
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

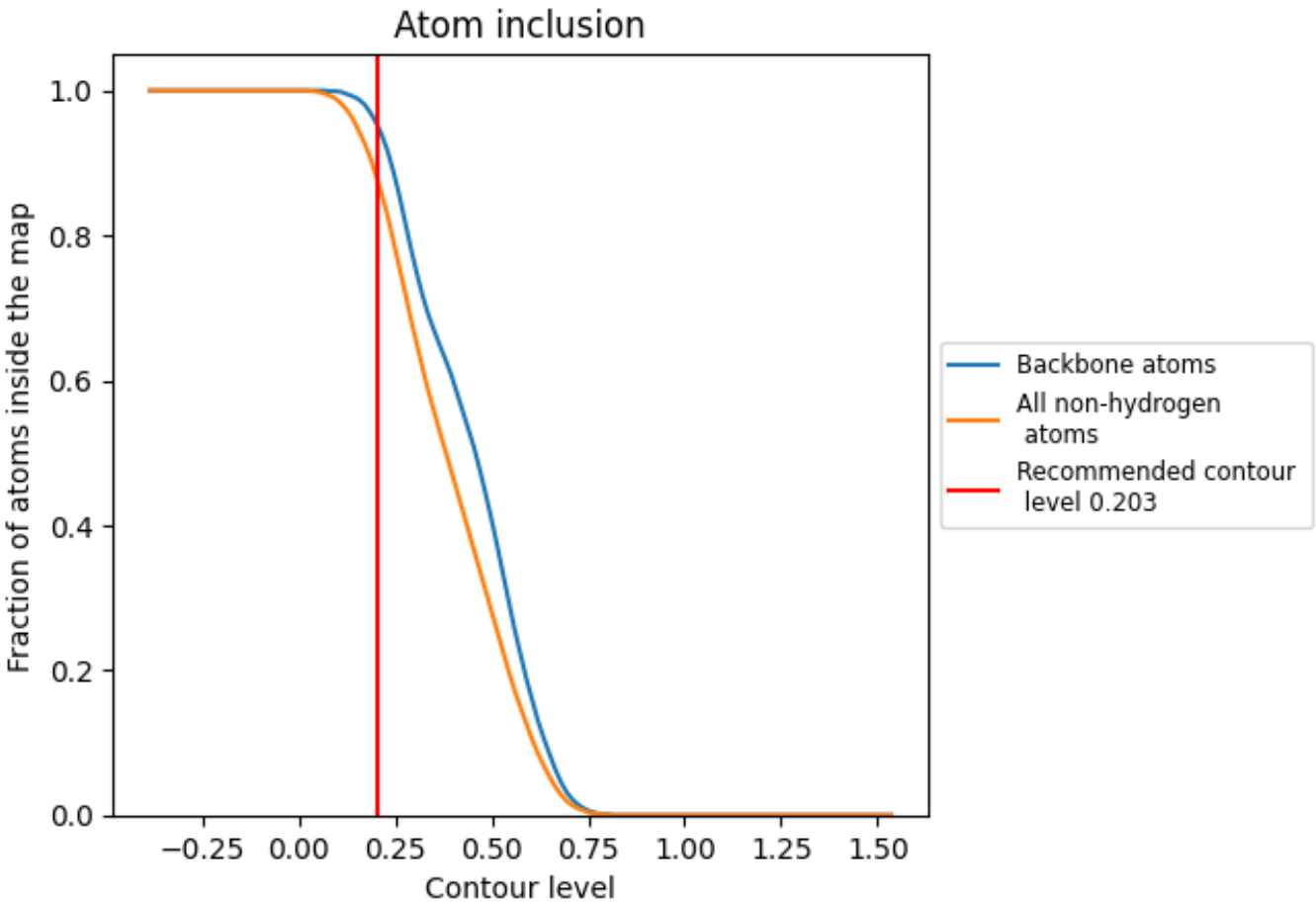
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.203).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5690
0	0.6840	0.4860
1	0.8580	0.5500
2	0.9240	0.5870
3	0.9240	0.5890
4	0.8710	0.5440
5	0.7850	0.4690
6	0.9090	0.5720
7	0.9070	0.5760
8	0.8660	0.5350
9	0.8650	0.5600
A	0.9370	0.6050
B	0.9420	0.6030
C	0.9600	0.5880
D	0.9110	0.5820
E	0.8580	0.5600
F	0.9030	0.5700
G	0.7840	0.5290
H	0.6250	0.5400
I	0.8210	0.5660
J	0.9140	0.5760
K	0.8720	0.5610
L	0.7190	0.5500
M	0.8900	0.5810
O	0.6960	0.5340